



Iterative methods for total variation based image reconstruction
by Mary Ellen Oman

A thesis submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in
Mathematics

Montana State University

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Abstract:

A class of efficient algorithms is presented for reconstructing an image from noisy, blurred data. This methodology is based on Tikhonov regularization with a regularization functional of total variation type. Use of total variation in image processing was pioneered by Rudin and Osher. Minimization yields a nonlinear integro-differential equation which, when discretized using cell-centered finite differences, yields a full matrix equation. A fixed point iteration is applied, and the intermediate linear equations are solved via a preconditioned conjugate gradient method. A multigrid preconditioner, due to Ewing and Shen, is applied to the differential operator, and a spectral preconditioner is applied to the integral operator. A multi-level quadrature technique, due to Brandt and Lubrecht is employed to find the action of the integral operator on a function. Application to laser confocal microscopy is discussed, and a numerical reconstruction of two-dimensional data from a laser confocal scanning microscope is presented. In addition, reconstructions of synthetic data and a numerical study of convergence rates are given.

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BASED IMAGE RECONSTRUCTION

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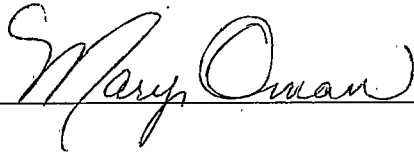
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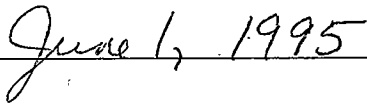
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ABSTRACT

A class of efficient algorithms is presented for reconstructing an image from noisy, blurred data. This methodology is based on Tikhonov regularization with a regularization functional of total variation type. Use of total variation in image processing was pioneered by Rudin and Osher. Minimization yields a nonlinear integro-differential equation which, when discretized using cell-centered finite differences, yields a full matrix equation. A fixed point iteration is applied, and the intermediate linear equations are solved via a preconditioned conjugate gradient method. A multigrid preconditioner, due to Ewing and Shen, is applied to the differential operator, and a spectral preconditioner is applied to the integral operator. A multi-level quadrature technique, due to Brandt and Lubrecht is employed to find the action of the integral operator on a function. Application to laser confocal microscopy is discussed, and a numerical reconstruction of two-dimensional data from a laser confocal scanning microscope is presented. In addition, reconstructions of synthetic data and a numerical study of convergence rates are given.

CHAPTER 1

Introduction

Throughout this work the problems under consideration are operator equations of the form

$$z = Ku + \epsilon, \quad (1.1)$$

where z is collected data, ϵ is noise, and u is to be recovered from the data z . Two cases will be considered. In the first case the operator K is a Fredholm first kind integral operator

$$Ku \stackrel{\text{def}}{=} \int k(x, y)u(y)dy. \quad (1.2)$$

Applications include seismology (see Bullen and Bolt [7]) and electric impedance tomography [1], which is also considered by Colton, Ewing, and Rundell in [8]. For other applications and references, see Groetsch [14].

Other important applications occur in image processing (see Jain [18]). In this context, k is of convolution type, $k(x, y) = k(x - y)$, and problem (1.1)-(1.2) is called *deblurring*. In the particular application of confocal microscopy, this problem has been described by Wilson and Sheppard [35], Hecht [16, pp. 392-515], and Bertero, Brianzi, and Pike [4].

A second model problem which arises in image processing and which will be considered in this thesis is the *denoising* problem

$$z = u + \epsilon. \quad (1.3)$$

Again ϵ is noise, and u is to be recovered from the observation z . Recall that the “delta function” satisfies

$$\int \delta(x - x_0)u(x)dx = u(x_0). \quad (1.4)$$

Although there is no explicit function δ , the right-hand side of (1.4) defines a functional on the space of smooth functions. There exist sequences of smooth functions $\delta_n(x)$ such that $\delta_n \rightarrow \delta$ in the sense that

$$\int \delta_n(x - x_0)u(x)dx \rightarrow u(x_0) \quad (1.5)$$

for smooth u . If the convolution kernel k is “delta-like,” i.e.,

$$\int k(x - x_0)u(x)dx \approx u(x_0), \quad (1.6)$$

for smooth u , then the model (1.1)-(1.2) is often replaced by (1.3). Data from a laser confocal scanning microscope (LCSM) will be considered in this context, and a denoised reconstruction of LCSM data will be presented in Chapter 7.

For typical applications modeled by (1.1)-(1.2), the operator K is compact, and the problem is ill-posed, i.e., a solution may not exist, or, if it does, small perturbations in z or K will produce wildly varying solutions u . Chapter 2 presents functional analytic preliminaries involved in studying such problems. These preliminaries include definitions of compact operators and ill-posedness as presented by Hutson and Pym [17], Kreyszig [20], and Nečas [24]. The proofs in Chapter 2 are standard and are provided for completeness.

To deal with ill-posedness, some type of regularization must be applied. This means to introduce a well-posed problem closely related to the ill-posed problem. The technique used here, Tikhonov regularization (see Tikhonov [29], [30]), is employed to obtain the related problem

$$\min T_\alpha(u) \quad (1.7)$$

where

$$T_\alpha(u) = \frac{1}{2}\|Ku - z\|^2 + \alpha J(u), \quad (1.8)$$

α is a positive parameter, J denotes the regularization functional, and $\|\cdot\|$ denotes the L^2 norm. Tikhonov regularization can be viewed as a penalty approach to the problem of minimizing $J(u)$ subject to the constraint

$$\|Ku - z\|^2 \leq c, \quad (1.9)$$

where c is a non-negative constant. Well-posedness for certain standard choices of J (for example, $J(u) = \int u^2 dx$ and $J(u) = \int |\nabla u|^2 dx$) is demonstrated in Chapter 2.

For many image processing applications, the regularization functional J should be chosen so that it damps spurious oscillations but, unlike standard regularization functionals, allows functions with sharp edges as possible solutions. The use of total variation in image processing was first introduced by Rudin, Osher, and Fatemi [26], who studied the denoising problem (1.3). Deblurring was later considered by Rudin, Osher, and Fu in [27]. In this work, a constrained least squares approach was taken. The problem considered was to minimize the functional

$$J_{TV}(u) = \int_{\Omega} |\nabla u| \quad (1.10)$$

under the constraint

$$\|Ku - z\|^2 \leq \sigma^2, \quad (1.11)$$

where the error level $\sigma = \|\epsilon\|$ is assumed to be known. The symbol on the right-hand side of (1.10) denotes the total variation of a function, regardless of whether or not u is differentiable. A rigorous definition of J_{TV} , applicable for nonsmooth u , will be presented in Chapter 3. The Euler-Lagrange equations yield a nonlinear partial differential equation on the constraint manifold which was solved using artificial time evolution. After discretization, an explicit time-marching scheme was used. This can

be viewed as a fixed step-size gradient descent method. The convergence of such a method can be extremely slow, particularly in the case when the matrix arising from the discretization of K is ill-conditioned.

The approach presented here is to use Tikhonov regularization (1.7)-(1.8) with a regularization functional of total variation type. Numerical difficulties associated with J_{TV} (e.g., non-differentiability of J_{TV}) motivate the modified total variation functional

$$J_\beta(u) = \int_\Omega \sqrt{|\nabla u|^2 + \beta^2}, \quad (1.12)$$

which is differentiable for $\beta > 0$. The resulting minimization problem is discretized with cell-centered finite differences. This discretization is particularly apt for image processing applications in that it makes no a priori smoothness assumptions on the image. A fixed point iteration is then developed for the resultant system obtained by minimizing T_α . This iteration is quasi-Newton in form and appears to display rapid global convergence. In two-dimensional deblurring applications, the linear system which arises for each fixed point iteration is non-sparse and very large (on the order of 10^6 unknowns). An efficient linear solver is presented which consists of nested preconditioned conjugate gradient iterations. A multi-level quadrature technique is applied to efficiently approximate the action of the integral operator on a function within the preconditioned conjugate gradient method.

The main contribution of this thesis is the assembly of known techniques—Tikhonov regularization, total variation regularization, cell-centered finite difference discretization, fixed point iteration, the preconditioned conjugate gradient method, multi-level quadrature—into an efficient algorithm for image reconstruction. This includes the development of effective preconditioners for the linear system solved at each fixed point iteration.

Chapter 3 is concerned with a rigorous variational definition of the total variation of a function and a discussion of the space of functions of bounded variation. The functional J_β (c.f. (1.12)), a modification of J_{TV} , is presented. This functional has certain advantages over the total variation functional, such as the differentiability of J_β when $\nabla u = 0$. The remainder of Chapter 3 is devoted to proving that the minimization problem

$$\min_u \left\{ \frac{1}{2} \|Ku - z\|^2 + \alpha J_\beta(u) \right\} \quad (1.13)$$

has a unique solution, using techniques developed by Giusti [12], Acar and Vogel [2], and others. The chapter ends with the derivation of the Euler-Lagrange equations for (1.13),

$$K^*Ku - \nabla \cdot \left(\frac{\nabla u}{\sqrt{\beta^2 + |\nabla u|^2}} \right) = K^*z. \quad (1.14)$$

Note that this is a nonlinear, elliptic, integro-differential equation.

In Chapter 4 the discretization of (1.13) is discussed. The standard Galerkin and finite difference discretization techniques are presented, as well as the cell-centered finite difference discretization scheme discussed by Ewing and Shen [11], Russell and Wheeler [28], and Weiser and Wheeler [34]. This latter discretization scheme is especially suited to image processing applications since there are no a priori differentiability conditions placed on the solution u .

Chapter 5 briefly reviews techniques for unconstrained minimization. Newton's method and a variation, the quasi-Newton method, are presented along with a discussion of standard convergence results. A fixed point iteration introduced by Vogel and Oman [32], is applied to the discretization of (1.13) to handle the nonlinearity. This iteration is shown to be quasi-Newton in form, and several properties of the iteration are given.

The linear system arising at each fixed point iteration is not only non-sparse, but also, for typical deblurring image processing applications, quite large (on the order of 10^6 unknowns). This means that direct methods are impractical. The approach taken here is to use the preconditioned conjugate gradient method (see, for example [13] or [3]), which is defined and discussed in Chapter 6. This technique is used to accelerate the convergence of the conjugate gradient method. The separate preconditioning techniques used for the denoising and deblurring operators are outlined in Chapter 6 as well (see also Oman [25]). A multigrid method (see Briggs [6] and McCormick [22], [23]) proves to be an effective preconditioner for the denoising operator. For the deblurring operator, a preconditioner based on the spectrum of the linear operator is presented.

Within the preconditioned conjugate gradient algorithm, it is necessary to apply the linear operator. As aforementioned, this operator, in the context of deblurring, is non-sparse. Traditionally, this type of calculation, which, for a system of n unknowns, involves applying an $n \times n$ full matrix to a vector, required $\mathcal{O}(n^2)$ operations. Multi-level quadrature, as presented by Brandt and Lubrecht in [5], will be used to approximately apply this operator. This approximation to the quadrature is significant in that it requires only $\mathcal{O}(n)$ floating point operations to calculate the action of the matrix operator on a grid function. A full presentation is included in Chapter 6.

In Chapter 7, one- and two-dimensional numerical results for the algorithm are presented. An actual LCSM scan is denoised, and deconvolution is done for artificial data. In addition, a numerical study of convergence results is presented for both the fixed point iteration and the various preconditioners.

CHAPTER 2

Mathematical Preliminaries

What follows is an introduction to the notation used in this thesis, followed by a brief discussion of ill-posed problems, compact operators, and a development of Tikhonov regularization with standard regularization operators. Although this material can be found in several sources (see, for example, [29], [30], [17], and [15]), it is included here to provide a basis for the subsequent work. Necessary terminology is introduced, and theorems useful to the development are presented. The purpose of this section is to demonstrate that the Tikhonov regularization problem defined below in (2.6) is well-posed for standard choices of the regularization functional J . Similar techniques will be used in Chapter 3 to show the existence of a solution to (2.6) when J is a functional of total variation type.

Notation

The following notation will be adhered to throughout this work except where explicitly stated. The symbol Ω denotes a bounded domain in $\mathbb{R}^d$ with a piecewise Lipschitz boundary $\partial\Omega$. In image processing applications, the domain is typically rectangular, and for the two-dimensional discretization discussion in Chapter 4, Ω will be assumed to be the unit square. The symbol $vol(\Omega)$ will refer to the volume of the domain (area, in two dimensions). The notation $L^2(\Omega)$ denotes the space of all square-integrable functions on Ω ; i.e., $u \in L^2(\Omega)$ if and only if $\int_{\Omega} |u|^2 dx < \infty$. The

space of all functions which are p times continuously differentiable on Ω and which vanish on $\partial\Omega$ is denoted $C_0^p(\Omega)$, and $C_0^\infty(\Omega)$ denotes infinitely differentiable functions which vanish on $\partial\Omega$.

The script letters $\mathcal{M}$, $\mathcal{B}$, and $\mathcal{H}$ denote metric, Banach, and Hilbert spaces, respectively. The notation $\langle \cdot, \cdot \rangle$ denotes the standard inner product in $L^2(\Omega)$, unless otherwise specified. All other inner products are distinguished by a subscript which denotes the Hilbert space considered; for example, $\langle \cdot, \cdot \rangle_{\mathcal{H}}$. The notation $\| \cdot \|$ refers to the L^2 norm, unless otherwise specified. All other norms are denoted $\| \cdot \|_{\mathcal{B}}$, where $\mathcal{B}$ is the space on which the norm applies. The symbol $| \cdot |$ will denote the Euclidean norm of a vector, $|\vec{x}| = (\sum x_i^2)^{1/2}$, and $| \cdot |_{TV}$ will denote the total variation of a function.

The symbol $H^1(\Omega)$ will denote the completion of $C^\infty(\Omega)$ under the norm $\|u\|_{H^1} \stackrel{\text{def}}{=} (\|u\|^2 + \int_{\Omega} |\nabla u|^2 dx)^{1/2}$ [17, p. 290]. For $1 \leq p \leq \infty$, the space $W^{1,p}(\Omega)$ will denote the completion of $C^\infty(\Omega)$ under the norm $\|u\|_{W^{1,p}} \stackrel{\text{def}}{=} (\|u\|_{L^p}^p + \int_{\Omega} |\nabla u|^p)^{1/p}$. Note that $H^1(\Omega) = W^{1,2}(\Omega)$. Both $H^1(\Omega)$ and $W^{1,p}$ are referred to as Sobolev spaces.

For a linear operator $A : \mathcal{M}_1 \rightarrow \mathcal{M}_2$, the range of A , a subset of $\mathcal{M}_2$, will be denoted $R(A)$. The null space of A , a subset of $\mathcal{M}_1$, will be denoted $N(A)$.

For any differentiable function u on $\mathbb{R}^d$, the gradient of u is the vector with components $\frac{\partial u}{\partial x_i}$, $i = 1, 2, \dots, d$, and will be denoted ∇u . For any vector-valued function $\vec{v}$ on $\mathbb{R}^d$, the divergence of $\vec{v}$ is denoted $\nabla \cdot \vec{v}$ and is given by

$$\nabla \cdot \vec{v} = \sum_{i=1}^d \frac{\partial v_i}{\partial x_i}. \quad (2.1)$$

The closure of a set S is denoted by $\bar{S}$. The orthogonal complement of a set S in a Banach space $\mathcal{B}$ is denoted $S^\perp$ and is defined to be

$$S^\perp = \{u^* \in \mathcal{B}^* : u^*(u) = 0, \text{ for all } u \in S\}, \quad (2.2)$$

where $\mathcal{B}^*$ is the dual, the set of all continuous linear functionals on $\mathcal{B}$. This notation is to be distinguished from the function decomposition $u = \bar{u} + u^\perp$ which will be defined in Chapter 3.

Ill-Posedness and Regularization

Definition 2.1 Let A be a mapping from $\mathcal{M}_1$ into $\mathcal{M}_2$. The problem $A(u) = z$ is *well-posed* in the sense of Hadamard [15] if and only if for each $z \in \mathcal{M}_2$ there exists a unique $u \in \mathcal{M}_1$ such that $A(u) = z$ and such that u depends continuously on z . If this problem is not well-posed, it is called *ill-posed*.

An important class of ill-posed problems are compact operator equations, in particular, Fredholm integral equations. Many applications, including image processing, use model equations of this type (see [14]).

Definition 2.2 Let $\mathcal{M}_1$ and $\mathcal{M}_2$ be metric spaces. A mapping K from $\mathcal{M}_1$ into $\mathcal{M}_2$ is *compact* if and only if the image $K(S)$ of every bounded set $S \subset \mathcal{M}_1$ is relatively compact in $\mathcal{M}_2$.

Let $\mathcal{B}_1(\Omega)$ and $\mathcal{B}_2(\Omega)$ be spaces of measurable functions on a domain $\Omega \subset \mathbb{R}^d$. Let K be an integral operator $K : \mathcal{B}_1(\Omega) \rightarrow \mathcal{B}_2(\Omega)$ defined by

$$Ku = \int_{\Omega} k(x, y)u(y)dy. \quad (2.3)$$

K is known as a *Fredholm integral operator of the first kind*. The kernel k of K is said to be *degenerate* if and only if

$$k(x, y) = \sum_{i=1}^n \phi_i(x)\psi_i(y) \quad (2.4)$$

for linearly independent sets $\{\phi_i\}_{i=1}^n, \{\psi_i\}_{i=1}^n$ and for a finite n . If k cannot be represented by such a finite sum, it is said to be *non-degenerate*. The corresponding operator K is also called degenerate or non-degenerate, accordingly.

It should be noted that a degenerate operator has finite-dimensional range, while a non-degenerate operator has infinite-dimensional range. Theorem 2.3 below is used to show that a nondegenerate operator can be uniformly approximated by degenerate operators. For a proof of Theorem 2.3, see [17, p. 180].

Theorem 2.3 Let $\{K_n\}$ be a sequence of compact operators mapping Banach spaces $\mathcal{B}_1$ to $\mathcal{B}_2$. If $K_n \rightarrow K$ uniformly, then K is a compact operator.

Example 2.4 Let K be a Fredholm first kind integral operator, $K : L^2(\Omega) \rightarrow L^2(\Omega)$, where the kernel k is measurable and $\int_{\Omega} \int_{\Omega} k(x, y)^2 dy dx < \infty$. What follows is a sketch of a proof that K is a compact operator; for details see [17]. The kernel k can be approximated in the $L^2(\Omega \times \Omega)$ norm by a sequence of degenerate kernels, k_n . The corresponding K_n are compact since the range of each is finite-dimensional, and $K_n \rightarrow K$ since $\|K_n - K\| \leq \|k_n - k\|_{L^2(\Omega \times \Omega)}$, where $\|K\|$ denotes the uniform operator norm of K . Hence, K is compact by Theorem 2.3.

Next it will be shown that nondegenerate compact operator equations are ill-posed. Theorem 2.6 contains this result, with Lemma 2.5 being a preliminary conclusion. Lemma 2.5 is also crucial to the discussion below of a pseudo-inverse for such an operator.

Lemma 2.5 Let $\mathcal{B}_1$ and $\mathcal{B}_2$ be Banach spaces and let K be a mapping from $\mathcal{B}_1$ into $\mathcal{B}_2$ such that K is compact and has infinite-dimensional range. Then $R(K)$ is not closed.

Proof: Assume that $R(K)$ is closed. Then $R(K)$ is a Banach space with respect to the norm on $\mathcal{B}_2$, and the Open Mapping Theorem [17, p. 78] implies that $K(S)$ is open in $R(K)$ where S is the open unit ball in $\mathcal{B}_1$. Hence, there exists a closed ball of non-zero radius in $K(S)$. Since K is compact, this ball is compact. But this implies that $R(K)$ is finite-dimensional [17, p. 140], a contradiction. Therefore, $R(K)$ is not closed. $\square$

Theorem 2.6 Let $\mathcal{B}_1, \mathcal{B}_2$ be Banach spaces, and let K be a compact operator $K : \mathcal{B}_1 \rightarrow \mathcal{B}_2$ with infinite-dimensional range. The problem, find $u \in \mathcal{B}_1$ such that $Ku = z$ for $z \in \mathcal{B}_2$, is ill-posed.

Proof: Since K has infinite-dimensional range, $R(K)$ is a proper subset of $\mathcal{B}_2$ by Lemma 2.5. So there exists $z \in \mathcal{B}_2$ which is not in the range of K . $\square$

Pseudo-inverse operators can sometimes be introduced to restore well-posedness [14]. However, it will be shown below that this approach will not work on a compact operator with infinite-dimensional range.

Let A be an operator from $\mathcal{H}_1$ into $\mathcal{H}_2$. A *least squares solution* to the problem $Au = z$ is a $u_{LS} \in \mathcal{H}_1$ such that $\|Au_{LS} - z\| \leq \|Au - z\|$ for all $u \in \mathcal{H}_1$. The *least squares minimum norm solution* is $u_{LSMN} \in \mathcal{H}_1$ such that $\|u_{LSMN}\| \leq \|u_{LS}\|$ for all least squares solutions, u_{LS} . The operator $A^\dagger$, a map from $\mathcal{H}_2$ into $\mathcal{H}_1$ such that $A^\dagger z = u_{LSMN}$, is called a Moore-Penrose *pseudo-inverse* operator.

Let K be a compact operator from $\mathcal{H}_1$ into $\mathcal{H}_2$, Define K_0 to be the restriction of K to $N(K)^\perp$; i.e., $K_0 u = Ku$ for $u \in N(K)^\perp$. Then K_0 is bijective, and $K^\dagger \stackrel{\text{def}}{=} K_0^{-1}P$, where P denotes the projection onto $\overline{R(K)}$, is such that $K^\dagger z = u_{LSMN}$. If

K is non-degenerate, $R(K_0) = R(K)$ is not closed in $\mathcal{H}_2$, which implies K_0^{-1} (and, hence, the pseudo-inverse $K^\dagger$) is unbounded.

When the pseudo-inverse is unbounded, one must apply a regularization technique to restore well-posedness. A particular technique is Tikhonov regularization [29], [30], which is also known as penalized least squares. Again, let K from $\mathcal{H}_1$ into $\mathcal{H}_2$ be a compact linear operator. For a fixed $z \in \mathcal{H}_2$ and an $\alpha > 0$, define the functional T on $\mathcal{H}_1$ by

$$T(u) = \frac{1}{2} \|Ku - z\|_{\mathcal{H}_2}^2 + \frac{\alpha}{2} \|u\|_{\mathcal{H}_1}^2. \quad (2.5)$$

The problem

$$\text{find } \hat{u} \in \mathcal{H}_1 \text{ such that } T(\hat{u}) = \inf_{u \in \mathcal{H}_1} T(u) \quad (2.6)$$

is known as Tikhonov regularization with the identity operator.

The differentiability of the functional T will now be examined with a view to characterizing a minimum $\hat{u}$ of T . The terms defined below—the Gateaux derivative, adjoint operator, and self-adjoint operator—will be used throughout Chapters 2, 3, and 4, to characterize solutions to the Tikhonov regularization problem with various types of regularization operators.

Definition 2.7 Let A be a mapping from $\mathcal{B}_1$ into $\mathcal{B}_2$. For $u, v \in \mathcal{B}_1$, the *Gateaux derivative* of A at u with respect to v , denoted $dA(u; v)$, is defined to be

$$dA(u; v) \stackrel{\text{def}}{=} \lim_{\tau \rightarrow 0} \frac{A(u + \tau v) - A(u)}{\tau}, \quad (2.7)$$

if it exists.

Theorem 2.8 Let $\mathcal{B}$ be a Banach space, and let f be a functional on $\mathcal{B}$. If f has a minimum at $\hat{u} \in \mathcal{B}$ and $df(\hat{u}; v)$ exists for all $v \in \mathcal{B}$, then $df(\hat{u}; v) = 0$, for all $v \in \mathcal{B}$.

Proof: For $v \in \mathcal{B}$, define $\tilde{f} : \mathfrak{R} \rightarrow \mathfrak{R}$ by the following

$$\tilde{f}(\tau) = f(\hat{u} + \tau v). \quad (2.8)$$

Since $df(\hat{u}; v)$ exists, $\tilde{f}$ is differentiable on $\mathfrak{R}$. Hence

$$\tilde{f}(\tau) = f(\hat{u}) + \tau df(\hat{u}; v) + o(\tau^2). \quad (2.9)$$

Since f has a minimum at $\hat{u}$, $\tilde{f}$ has a minimum at $\tau = 0$, and hence, $\tilde{f}'(0) = df(\hat{u}; v) = 0$ for all $v \in \mathcal{B}$. □

Definition 2.9 Let $\mathcal{H}_1, \mathcal{H}_2$ be Hilbert spaces, and let A be a bounded linear operator from $\mathcal{H}_1$ into $\mathcal{H}_2$. The bounded linear operator A^* such that

$$\langle Au, v \rangle_{\mathcal{H}_2} = \langle u, A^*v \rangle_{\mathcal{H}_1} \quad (2.10)$$

for all $u \in \mathcal{H}_1$ and for all $v \in \mathcal{H}_2$ is called the *adjoint* of A .

Definition 2.10 Let A be a bounded linear operator on a Hilbert space $\mathcal{H}$. A is *self-adjoint* if and only if

$$\langle Au, v \rangle_{\mathcal{H}} = \langle u, Av \rangle_{\mathcal{H}} \quad (2.11)$$

for all $u, v \in \mathcal{H}$. In other words, $A^* = A$.

The following is an example of a self-adjoint operator. Let $\mathcal{H} = L^2(\Omega)$ and let K be a Fredholm first kind integral operator with square-integrable kernel k having the property, $k(x, y) = k(y, x)$. Then K is self-adjoint (see [17]).

Example 2.11 The functional T defined in equation (2.5) can be expressed

$$T(u) = \frac{1}{2} \langle Ku - z, Ku - z \rangle_{\mathcal{H}_2} + \frac{\alpha}{2} \langle u, u \rangle_{\mathcal{H}_1}. \quad (2.12)$$

Let

$$f(u) \stackrel{\text{def}}{=} \frac{1}{2} \|Ku - z\|_{\mathcal{H}_2}^2 \quad (2.13)$$

$$= \frac{1}{2} \langle Ku - z, Ku - z \rangle_{\mathcal{H}_2}. \quad (2.14)$$

Then for $v \in \mathcal{H}_1$,

$$df(u; v) = \lim_{\tau \rightarrow 0} \frac{1}{\tau} \{f(u + \tau v) - f(u)\} \quad (2.15)$$

$$= \lim_{\tau \rightarrow 0} \frac{1}{\tau} \left\{ \tau \langle Ku - z, Kv \rangle_{\mathcal{H}_2} + \frac{\tau^2}{2} \|Kv\|_{\mathcal{H}_2}^2 \right\} \quad (2.16)$$

$$= \langle Ku - z, Kv \rangle_{\mathcal{H}_2} \quad (2.17)$$

$$= \langle K^*(Ku - z), v \rangle_{\mathcal{H}_1}. \quad (2.18)$$

Similarly, for $J(u) = \frac{1}{2} \|u\|_{\mathcal{H}_1}^2$,

$$dJ(u; v) = \langle u, v \rangle_{\mathcal{H}_1}. \quad (2.19)$$

Consequently,

$$dT(u; v) = \langle K^*(Ku - z) + \alpha u, v \rangle_{\mathcal{H}_1}. \quad (2.20)$$

This implies that if T attains its infimum at $\hat{u}$, then

$$(K^*K + \alpha I)\hat{u} = K^*z. \quad (2.21)$$

The Hilbert-Schmidt Theorem, below, provides the spectral decomposition of the compact operator K^*K . The decomposition can be used to find a spectral representation for the solution $\hat{u}$ of the Tikhonov regularization problem. This representation also shows the effect of the regularization parameter α on the solution $\hat{u}$.

Definition 2.12 Let A be a bounded linear operator from $\mathcal{B}_1$ into $\mathcal{B}_2$. A complex number λ is an *eigenvalue* for A if and only if $(A - \lambda I)\phi = 0$ has a non-zero solution.

The set of eigenvalues is called the *point spectrum* of A , and the corresponding non-zero solutions are *eigenfunctions* for A . The set of complex values λ such that $(A - \lambda I)^{-1}$ is a bounded linear operator is the *resolvent set* of A . The complement of the resolvent set is the *spectrum* of A . If A is a finite-dimensional operator, the point spectrum and the spectrum are identical.

Theorem 2.13 (Hilbert-Schmidt Theorem [17, p. 191]) Let $\tilde{K}$ be a compact, self-adjoint operator on a Hilbert space $\mathcal{H}$. Then there exists a countable set of the eigenfunctions for $\tilde{K}$ which form an orthonormal basis for $\mathcal{H}$. Further, the eigenvalues of $\tilde{K}$ are real, and if $\{\lambda_i, \phi_i(x)\}_{i=1}^{\infty}$ are the eigenpairs for $\tilde{K}$, then for any $u \in \mathcal{H}$,

$$\tilde{K}u = \sum_{i=1}^{\infty} \lambda_i \langle u, \phi_i \rangle_{\mathcal{H}} \phi_i \quad (2.22)$$

Example 2.14 Let K be a compact linear operator from $\mathcal{H}_1$ into $\mathcal{H}_2$. Then $\tilde{K} = K^*K$ is a compact, linear, and self-adjoint operator on $\mathcal{H}_1$. Furthermore, $\langle \tilde{K}u, u \rangle_{\mathcal{H}_1} = \langle K^*Ku, u \rangle_{\mathcal{H}_1} = \|Ku\|_{\mathcal{H}_2}^2 \geq 0$, so the eigenvalues of $\tilde{K}$ are non-negative; i.e., $\tilde{K}$ is positive semi-definite. This implies that u and K^*z have Fourier series representations and that (2.21) can be expressed as

$$\sum_{i=1}^{\infty} [(\lambda_i + \alpha) \langle u, \phi_i \rangle_{\mathcal{H}_1} - \langle K^*z, \phi_i \rangle_{\mathcal{H}_1}] \phi_i = 0. \quad (2.23)$$

This leads to the following theorem.

Theorem 2.15 (Spectral representation for Tikhonov regularization) Let K be a compact operator from $\mathcal{H}_1$ into $\mathcal{H}_2$. Then the solution $\hat{u}$ of the Tikhonov regularization problem (2.6) has the form

$$\hat{u} = \sum_{i=1}^{\infty} \frac{1}{\lambda_i + \alpha} \langle K^*z, \phi_i \rangle_{\mathcal{H}_1} \phi_i. \quad (2.24)$$

The ensuing discussion establishes the well-posedness of the Tikhonov regularization problem with the identity operator. The main points necessary to the proof of well-posedness, coercivity and strict convexity of T , will also be necessary for the well-posedness of the Tikhonov problem with different types of regularization operators.

Definition 2.16 Let A be a linear operator on a Hilbert space $\mathcal{H}$. A is $\mathcal{H}$ -coercive if and only if there exists a $c > 0$ such that $\operatorname{Re}\langle Au, u \rangle_{\mathcal{H}} \geq c\|u\|_{\mathcal{H}}^2$ for all $u \in \mathcal{H}$. A functional f (not necessarily linear) on a Banach space $\mathcal{B}$, is said to be $\mathcal{B}$ -coercive if and only if $|f(u)| \rightarrow \infty$ whenever $\|u\|_{\mathcal{B}} \rightarrow \infty$.

Example 2.17 The functional T as defined in (2.5) is $\mathcal{H}_1$ -coercive, since

$$T(u) \geq \frac{\alpha}{2}\|u\|_{\mathcal{H}_1}^2. \quad (2.25)$$

Example 2.18 The operator, $K^*K + \alpha I$ as in (2.21) is $\mathcal{H}_1$ -coercive for $\alpha > 0$, since

$$\langle (K^*K + \alpha I)u, u \rangle_{\mathcal{H}_1} = \langle K^*Ku, u \rangle_{\mathcal{H}_1} + \alpha\|u\|_{\mathcal{H}_1}^2 \quad (2.26)$$

$$= \|Ku\|_{\mathcal{H}_2}^2 + \alpha\|u\|_{\mathcal{H}_1}^2 \quad (2.27)$$

$$\geq \alpha\|u\|_{\mathcal{H}_1}^2. \quad (2.28)$$

Theorem 2.19 If A is a bounded, linear, coercive mapping on $\mathcal{H}$, then $R(A)$ is closed in $\mathcal{H}$ and $A^{-1} : R(A) \rightarrow \mathcal{H}$ exists and is bounded.

Proof: Since $\langle Au, u \rangle_{\mathcal{H}} \geq \gamma\|u\|_{\mathcal{H}}^2$ for some $\gamma > 0$,

$$\|u\|_{\mathcal{H}}^2 \leq \frac{1}{\gamma}\langle Au, u \rangle_{\mathcal{H}} \leq \frac{1}{\gamma}\|Au\|_{\mathcal{H}}\|u\|_{\mathcal{H}}, \quad (2.29)$$

which implies

$$\|u\|_{\mathcal{H}} \leq \frac{1}{\gamma} \|Au\|_{\mathcal{H}}. \quad (2.30)$$

Hence, $Au = 0$ if and only if $u = 0$. Since A is linear, it is injective. Let $\{v_n\}$ be a sequence in $R(A)$ with $v_n \rightarrow v \in \mathcal{H}$. Then for each v_n , there exists a unique u_n such that $Au_n = v_n$. Since $\{v_n\}$ is Cauchy, so is $\{u_n\}$ by (2.30). Thus u_n converges to some u in $\mathcal{H}$. Because A is bounded,

$$Au = A(\lim_{n \rightarrow \infty} u_n) = \lim_{n \rightarrow \infty} Au_n = v. \quad (2.31)$$

Thus $v \in R(A)$ and $R(A)$ is closed in $\mathcal{H}$. This implies that $R(A)$ is a Hilbert space with respect to the $\mathcal{H}$ norm. The operator A^{-1} is bounded. Applying the Open Mapping Theorem [17],

$$\|A^{-1}v\| \leq \frac{1}{\gamma} \|v\|, \quad (2.32)$$

and hence, $\|A^{-1}\| \leq \frac{1}{\gamma}$. □

Definition 2.20 A functional f on a metric space $\mathcal{M}$ is *convex* if and only if for every $u, v \in \mathcal{M}$ and for each $\lambda \in [0, 1]$,

$$f(\lambda u + (1 - \lambda)v) \leq \lambda f(u) + (1 - \lambda)f(v). \quad (2.33)$$

f is *strictly convex* if and only if (2.33) holds with strict inequality whenever $u, v \in \mathcal{H}$, $u \neq v$, and $\lambda \in (0, 1)$.

Example 2.21 The norm on a Banach space $\mathcal{B}$ is convex. This can be shown by application of the triangle inequality and the property that $\|\gamma v\|_{\mathcal{B}} = |\gamma| \|v\|_{\mathcal{B}}$, for all $\gamma \in \mathbb{R}$ and for all $v \in \mathcal{B}$.

Example 2.22 Define the functional f on a Hilbert space $\mathcal{H}$ to be $f(u) = \|u\|_{\mathcal{H}}^2$. Let $\lambda \in (0, 1)$, and let $u, v \in \mathcal{H}$ such that $u \neq v$. It is shown in Kreyszig [20, p. 333] that a Hilbert space norm is strictly convex. The functional f can be written as $f(u) = g(h(u))$ where $g(x) = x^2$ and $h(u) = \|u\|_{\mathcal{H}}$. Since g is convex and strictly increasing on $[0, \infty)$ and h is strictly convex,

$$f(\lambda u + (1 - \lambda)v) = g(h(\lambda u + (1 - \lambda)v)) \quad (2.34)$$

$$< g(\lambda h(u) + (1 - \lambda)h(v)) \quad (2.35)$$

$$\leq \lambda g(h(u)) + (1 - \lambda)g(h(v)) \quad (2.36)$$

$$= \lambda f(u) + (1 - \lambda)f(v). \quad (2.37)$$

Hence, f is strictly convex.

From Example 2.22, it can be inferred that the functional T as defined in (2.5) is strictly convex, as it is the sum of two convex functionals, one of which is strictly convex.

Definition 2.23 A sequence $\{u_n\}$ in a Banach space $\mathcal{B}$ is *weakly convergent* if and only if there exists $u \in \mathcal{B}$ such that $\lim_{n \rightarrow \infty} f(u_n) = f(u)$ for all bounded linear functionals f on $\mathcal{B}$. In a Hilbert space, $\mathcal{H}$, the definition reduces to $\lim_{n \rightarrow \infty} \langle u_n, f \rangle_{\mathcal{H}} = \langle u, f \rangle_{\mathcal{H}}$ for all $f \in \mathcal{H}$. Weak convergence is denoted $u_n \rightharpoonup u$.

Definition 2.24 A functional f on a Banach space $\mathcal{B}$ is called *weakly lower semi-continuous* on $D(f) \subset \mathcal{B}$ if and only if for any weakly convergent sequence $\{u_n\} \subset D(f)$ such that $u_n \rightharpoonup u \in D(f)$, $f(u) \leq \liminf_{n \rightarrow \infty} f(u_n)$. Note that the domain $D(f)$ may be a proper subset of $\mathcal{B}$.

Lemma 2.25 Let $\mathcal{H}$ be a Hilbert space. Then for $u \in \mathcal{H}$,

$$\|u\|_{\mathcal{H}} = \sup_{\|v\|_{\mathcal{H}}=1} \langle u, v \rangle_{\mathcal{H}}. \quad (2.38)$$

The proof of Lemma 2.25 relies on the Hahn-Banach Theorem (see [20, p. 221]).

Example 2.26 Let A be a bounded linear operator on a Hilbert space $\mathcal{H}$. Then the functional $\|Au\|_{\mathcal{H}}$ is weakly lower semi-continuous. To see this, let $\{u_n\}$ be a sequence in $\mathcal{H}$ such that $u_n \rightharpoonup u \in \mathcal{H}$. Then for all $v \in \mathcal{H}$,

$$\langle Au, v \rangle_{\mathcal{H}} = \langle u, A^*v \rangle_{\mathcal{H}} \quad (2.39)$$

$$= \lim_{n \rightarrow \infty} \langle u_n, A^*v \rangle_{\mathcal{H}} \quad (2.40)$$

$$= \lim_{n \rightarrow \infty} \langle Au_n, v \rangle_{\mathcal{H}} \quad (2.41)$$

$$= \liminf_{n \rightarrow \infty} \langle Au_n, v \rangle_{\mathcal{H}} \quad (2.42)$$

$$\leq \liminf_{n \rightarrow \infty} \|Au_n\|_{\mathcal{H}} \|v\|_{\mathcal{H}}. \quad (2.43)$$

Using Lemma 2.25, take the supremum of both sides over all $v \in \mathcal{H}$ such that v has unit norm. Then

$$\|Au\|_{\mathcal{H}} = \sup_{\|v\|_{\mathcal{H}}=1} \langle Au, v \rangle_{\mathcal{H}} \quad (2.44)$$

$$\leq \liminf_{n \rightarrow \infty} \|Au_n\|_{\mathcal{H}}. \quad (2.45)$$

By setting $A = I$, Example 2.26 shows that a Hilbert space norm is weakly lower semi-continuous.

Example 2.27 The functional T as defined in (2.5) is weakly lower semi-continuous on $\mathcal{H}$. To see this, let $\{u_n\}$ be a sequence in $\mathcal{H}$ such that $u_n \rightharpoonup u$, and note that T

can be written

$$T(u) = \frac{1}{2} \|Ku\|_{\mathcal{H}_2}^2 - \langle Ku, z \rangle_{\mathcal{H}_2} + \frac{1}{2} \|z\|_{\mathcal{H}_2}^2 + \frac{\alpha}{2} \|u\|_{\mathcal{H}_1}^2. \quad (2.46)$$

In Example 2.26, it was shown that the first and fourth terms are weakly lower semi-continuous, and the third term is constant; it remains to show that the second term has this property as well.

$$\langle Ku, z \rangle_{\mathcal{H}_2} = \langle u, K^*z \rangle_{\mathcal{H}_1} \quad (2.47)$$

$$= \lim_{n \rightarrow \infty} \langle u_n, K^*z \rangle_{\mathcal{H}_1} \quad (2.48)$$

$$= \liminf_{n \rightarrow \infty} \langle u_n, K^*z \rangle_{\mathcal{H}_1} \quad (2.49)$$

$$= \liminf_{n \rightarrow \infty} \langle Ku_n, z \rangle_{\mathcal{H}_2}. \quad (2.50)$$

Hence,

$$T(u) \leq \liminf_{n \rightarrow \infty} T(u_n). \quad (2.51)$$

Theorem 2.28 The Tikhonov regularization problem (2.6) is well-posed.

Proof: Let $\{u_n\}_{n=1}^{\infty}$ be a minimizing sequence for T ; i.e., $T(u_n) \rightarrow \inf_u T(u) \stackrel{\text{def}}{=} \hat{T}$. Since T is coercive, the u_n 's are bounded. Hence, there exists a subsequence $\{u_{n_j}\}_{j=1}^{\infty}$ such that $u_{n_j} \rightharpoonup \hat{u}$ for some $\hat{u} \in \mathcal{H}_1$ (Banach-Alaoglu, [17, p. 158]). Since T is weakly lower semi-continuous,

$$T(u^*) \leq \liminf_{j \rightarrow \infty} T(u_{n_j}) \quad (2.52)$$

$$= \lim_{j \rightarrow \infty} T(u_{n_j}) = \hat{T}. \quad (2.53)$$

Therefore, a minimum, $\hat{u}$, exists. The functional T is strictly convex; hence, $\hat{u}$ is unique. To show continuous dependence on the data, observe that $dT(\hat{u}; v)$ exists for any $v \in \mathcal{H}_1$, and consider the characterization (2.21),

$$(K^*K + \alpha I)\hat{u} = K^*z. \quad (2.54)$$

The operator $K^*K + \alpha I$ is bounded, linear, and coercive, so by Theorem 2.19 it has a bounded inverse. Hence, the solution depends continuously on the data. $\square$

Tikhonov regularization can be applied with regularization operators other than the identity. For example, let $\mathcal{H}_1 = \mathcal{H}_2 = L^2(\Omega)$, where Ω is a bounded domain in $\mathbb{R}^d$. Let K be a Fredholm first kind integral operator such that $K(1) \neq 0$, and consider the functional T as follows:

$$T(u) = \frac{1}{2} \|Ku - z\|^2 + \frac{\alpha}{2} \int_{\Omega} |\nabla u|^2 dx. \quad (2.55)$$

The minimization of T is referred to as Tikhonov regularization with the first derivative.

Note that the domain of T in (2.55) is restricted to $u \in H^1(\Omega)$. Now consider the problem of finding $\hat{u} \in H^1(\Omega)$ such that $T(\hat{u})$ is a minimum.

First, define the functional J on $H^1(\Omega)$ to be the regularization functional of (2.55), i.e.,

$$J(u) \stackrel{\text{def}}{=} \frac{1}{2} \int_{\Omega} |\nabla u|^2 dx. \quad (2.56)$$

For any $u, v \in H^1(\Omega)$,

$$dJ(u; v) = \lim_{\tau \rightarrow 0} \frac{1}{2\tau} \left\{ \int_{\Omega} |\nabla(u + \tau v)|^2 dx - \int_{\Omega} |\nabla u|^2 dx \right\} \quad (2.57)$$

$$= \lim_{\tau \rightarrow 0} \frac{1}{2\tau} \int_{\Omega} [\nabla(u + \tau v) \cdot \nabla(u + \tau v) - \nabla u \cdot \nabla u] dx \quad (2.58)$$

$$= \lim_{\tau \rightarrow 0} \frac{1}{2\tau} \int_{\Omega} [2\tau \nabla u \cdot \nabla v + \tau^2 |\nabla v|^2] dx \quad (2.59)$$

$$= \int_{\Omega} \nabla u \cdot \nabla v dx \quad (2.60)$$

$$\stackrel{\text{def}}{=} \langle Lu, v \rangle. \quad (2.61)$$

This defines (in weak form) the linear differential operator L on $L^2(\Omega)$ with domain $H^1(\Omega)$.

If $u \in C^2(\overline{\Omega}) \subset H^1(\Omega)$, then integration by parts, or Green's Theorem, can be applied to obtain

$$dJ(u; v) = - \int_{\Omega} v \nabla \cdot \nabla u dx + \int_{\partial\Omega} (\nabla u \cdot \vec{\eta}) v ds, \quad (2.62)$$

where $\vec{\eta}$ denotes the outward unit normal vector. Hence, the strong form of the operator L is

$$Lu = -\nabla^2 u, \quad x \in \Omega, \quad (2.63)$$

where $\nabla^2 = \nabla \cdot \nabla$ is the Laplacian operator. The associated boundary conditions are

$$\nabla u \cdot \vec{\eta} = 0, \quad x \in \partial\Omega. \quad (2.64)$$

Returning to the functional T in (2.55), it is seen that for any $v \in H^1(\Omega)$,

$$dT(u; v) = \langle K^*(Ku - z), v \rangle + \alpha dJ(u; v) \quad (2.65)$$

$$= \langle K^*(Ku - z) + \alpha Lu, v \rangle. \quad (2.66)$$

At a minimum, $\hat{u}$, $dT(\hat{u}; v) = 0$, or

$$\langle (K^*K + \alpha L)\hat{u}, v \rangle = \langle K^*z, v \rangle \quad (2.67)$$

for all $v \in H^1(\Omega)$. Written in strong form,

$$(K^*K - \alpha \nabla^2)\hat{u} = K^*z, \quad x \in \Omega \quad (2.68)$$

$$\nabla \hat{u} \cdot \vec{\eta} = 0, \quad x \in \partial\Omega, \quad (2.69)$$

a characterization of $\hat{u}$ analogous to that obtained from Tikhonov regularization with the identity (2.21).

By mimicking the steps taken to show that the Tikhonov problem with the identity operator is well-posed, it will now be shown that minimizing (2.55) over $H^1(\Omega)$ is also well-posed.

Lemma 2.29 (Poincaré's Inequality [24, p. 32]) Let $1 \leq p < \infty$, and let $u \in W^{1,p}(\Omega)$ with $\int_{\Omega} u = 0$. Then there exists $\gamma > 0$ dependent only on Ω such that

$$\int_{\Omega} |\nabla u|^p dx \geq \gamma \int_{\Omega} u^p dx. \quad (2.70)$$

Definition 2.30 Let A be a linear operator on a Hilbert space $\mathcal{H}$, and let $\{u_n\}$ be a sequence in $\mathcal{H}$ such that $u_n \in D(A)$ for all n , $\{u_n\}$ is convergent with limit u , and $\{Au_n\}$ is convergent. A is a *closed operator* if and only if for all such sequences $\{u_n\}$, $u \in D(A)$ and $\lim_{n \rightarrow \infty} Au_n = Au$.

Lemma 2.31 Let K be as in (2.55), and define

$$|||u||| = \left(\|Ku\|^2 + \alpha \int_{\Omega} |\nabla u|^2 dx \right)^{\frac{1}{2}}. \quad (2.71)$$

Then $|||\cdot|||$ is a norm on $H^1(\Omega)$ and is equivalent to $\|\cdot\|_{H^1}$. Furthermore, $K^*K + \alpha L$ is injective and closed on $L^2(\Omega)$.

Proof: It is easily shown that $|||\cdot|||$ possesses the non-negativity and symmetry properties of a norm. It is also clear that $|||cu||| = |c| |||u|||$ for any $c \in \mathfrak{R}$ and that the triangle inequality holds. Also,

$$|||u|||^2 = \|Ku\|^2 + \alpha \int_{\Omega} |\nabla u|^2 dx \quad (2.72)$$

$$\leq \|K\|^2 \|u\|^2 + \alpha \int_{\Omega} |\nabla u|^2 dx \quad (2.73)$$

$$\leq \max(\|K\|^2, \alpha) \|u\|_{H^1}^2, \quad (2.74)$$

where $\|K\|$ denotes the operator norm of K . Since K is compact, it is bounded, and $\max(\|K\|^2, \alpha) < \infty$.

To see that there exists a $\gamma > 0$ such that $|||u||| \geq \gamma \|u\|_{H^1}^2$, it suffices to show

$$\inf_{\|u\|_{H^1}=1} \left\{ \|Ku\|^2 + \frac{\alpha}{2} \int_{\Omega} |\nabla u|^2 dx \right\} \geq \gamma. \quad (2.75)$$

If this is not the case, then there is a sequence $\{v_n\} \subset H^1(\Omega)$ such that $\|v_n\|_{H^1} = 1$ for all n , and $\|Kv_n\|^2 + \frac{\alpha}{2} \int_{\Omega} |\nabla v_n|^2 dx \rightarrow 0$ as $n \rightarrow \infty$. Since both terms are positive, this implies $\|Kv_n\|^2 \rightarrow 0$ and $\int_{\Omega} |\nabla v_n|^2 dx \rightarrow 0$. This latter fact implies that there exists a subsequence $\{v_{n_j}\}$ such that $v_{n_j} \rightarrow v \in L^2(\Omega)$ (L^2 convergence), since the injection map from $H^1(\Omega)$ to $L^2(\Omega)$ is compact (see [24, p. 28]). Since $\int_{\Omega} |\nabla v_{n_j}|^2 dx \rightarrow 0$, $v_{n_j} \rightarrow v$ in the H^1 norm as well, and $v \in H^1(\Omega)$ with $\|v\|_{H^1} = 1$.

Any function $w \in H^1(\Omega)$ can be expressed as $w = \bar{w} + w^\perp$, where $\bar{w} = \frac{1}{\text{vol}(\Omega)} \int_{\Omega} w dx$ is the mean value of w on Ω and $w^\perp \in H^1(\Omega)$ is such that $\int_{\Omega} w^\perp dx = 0$. Using this decomposition, $\nabla v_{n_j} = \nabla v_{n_j}^\perp$. Hence, $\int_{\Omega} |\nabla v_{n_j}|^2 dx = \int_{\Omega} |\nabla v_{n_j}^\perp|^2 dx \rightarrow 0$ as $j \rightarrow \infty$. This implies that $v^\perp$ is a constant function whose mean value is 0, or $v^\perp \equiv 0$ on Ω . As $j \rightarrow \infty$,

$$\|Kv_{n_j}\|^2 + \frac{\alpha}{2} \int_{\Omega} |\nabla v_{n_j}|^2 dx \rightarrow \|Kv\|^2 + \frac{\alpha}{2} \int_{\Omega} |\nabla v|^2 dx \quad (2.76)$$

$$= \|K\bar{v} + Kv^\perp\|^2 + \int_{\Omega} |\nabla v^\perp|^2 dx \quad (2.77)$$

$$= \|K\bar{v}\|^2 \quad (2.78)$$

The limit was claimed to be 0, but since K does not annihilate constants and $\|v\|_{H^1} = 1$, this cannot be the case, a contradiction. Hence, the constant $\gamma > 0$ exists.

The above discussion implies that the norms $\|\cdot\|_{H^1}$ and $|||\cdot|||$ are equivalent. Also, note that $|||u|||^2 = \langle (K^*K + \alpha L)u, u \rangle$; hence $K^*K + \alpha L$ is injective. To see that $K^*K + \alpha L$ is a closed operator, let $\{u_m\}$ be a sequence converging to u in $H^1(\Omega)$ which satisfies the conditions of Definition 2.30. By the assumptions on the sequence $\{u_m\}$, $u_m \rightarrow u$ with respect to the H^1 norm which is equivalent to convergence in the $|||\cdot|||$ norm. Hence, $K^*K + \alpha L$ is a closed operator on H^1 . $\square$

Lemma 2.32 The functional T in (2.55) is H^1 -coercive and weakly lower semi-

continuous on $H^1(\Omega)$.

Proof: The H^1 -coercivity of T will be shown first. Note

$$T(u) = \frac{1}{2}\|Ku\|^2 - \langle Ku, z \rangle + \frac{1}{2}\|z\|^2 + \frac{\alpha}{2} \int_{\Omega} |\nabla u|^2 dx \quad (2.79)$$

$$= \frac{1}{2}|||u|||^2 - \langle Ku, z \rangle + \frac{1}{2}\|z\|^2 \quad (2.80)$$

$$\geq \frac{1}{2}|||u|||^2 - \|K\| \|u\| \|z\| + \frac{1}{2}\|z\|^2 \quad (2.81)$$

$$\geq \frac{1}{2}\gamma \|u\|_{H^1}^2 - \|K\| \|u\|_{H^1} \|z\| + \frac{1}{2}\|z\|^2 \quad (2.82)$$

$$\geq \frac{1}{2}\|u\|_{H^1} (\gamma \|u\|_{H^1} - \|K\| \|z\|) + \frac{1}{2}\|z\|^2, \quad (2.83)$$

for some $\gamma > 0$, since $|||\cdot|||$ and $\|\cdot\|_{H^1}$ are equivalent norms. As $\|u\|_{H^1} \rightarrow \infty$, so does $T(u)$.

Weak lower semi-continuity has been shown for the first and fourth terms of (2.79), and the third term is constant; it remains to show the weak lower semi-continuity of the second term. Let $\{u_n\}$ be a sequence in $H^1(\Omega)$ such that $u_n \rightharpoonup u$. This implies that $u_n \rightarrow u$ in $L^2(\Omega)$ (strong convergence). Hence, $\langle Ku, z \rangle$ is weakly lower semi-continuous. $\square$

Theorem 2.33 The Tikhonov regularization problem (2.6) with functional T defined in (2.55) is well-posed.

Proof: Proof of the existence and uniqueness of a minimizer, $\hat{u}$, is as in the proof of Theorem 2.28. To show continuous dependence on the data, note that $K^*K + \alpha L$ is injective and is a closed operator (Lemma 2.31) on $H^1(\Omega)$. Apply a corollary of the Closed Graph Theorem [17, p. 101] to show that $(K^*K + \alpha L)^{-1}$ is bounded. $\square$

CHAPTER 3

Total Variation

This chapter defines the total variation of a function and the space of functions of bounded variation. A modification of the total variation functional, J_β as in (3.7), is defined below and used as the regularization functional in Tikhonov regularization. The functional J_β has certain advantages over the total variation functional, such as the differentiability of J_β when $\nabla u = 0$. The subsequent discussion parallels the development in Chapter 2 with this new regularization functional. The highlight of this section is a proof of the existence of a solution to the Tikhonov problem with the regularization functional J_β . The section concludes with the derivation of the Euler-Lagrange equations for the minimization problem (2.6) with T_α as defined in (3.23). The material here has been gathered from several sources including Giusti [12], and Acar and Vogel [2]. It is presented here to pave the way for the discretization discussion in Chapter 4.

The presentation begins with the definition of the total variation of a function, the space $BV(\Omega)$, and the properties of each. Although the total variation of a function reduces to (3.3) for functions in $C^1(\Omega)$, it must be emphasized that functions of bounded variation are not necessarily continuous.

Definition 3.1 Let u be a real-valued function on a domain $\Omega \subset \mathbb{R}^d$. The *total variation* of u is defined by Giusti [12] to be

$$\sup_{\vec{w} \in \mathcal{W}} \int_{\Omega} -u \nabla \cdot \vec{w} dx \tag{3.1}$$

where

$$\mathcal{W} = \left\{ \vec{w} \in C_0^1(\Omega; \mathbb{R}^d) : |\vec{w}(x)| \leq 1, \text{ for all } x \in \Omega \right\}. \quad (3.2)$$

The total variation of u will be denoted $|u|_{TV}$.

For $u \in C^1(\Omega)$, the total variation of u may be expressed (via integration by parts) as

$$|u|_{TV} = \sup_{\vec{w} \in \mathcal{W}} \int_{\Omega} \vec{w} \cdot \nabla u dx. \quad (3.3)$$

If, in addition, $|\nabla u| \neq 0$, the supremum occurs for $\vec{w} = \nabla u / |\nabla u|$, and

$$|u|_{TV} = \int_{\Omega} |\nabla u| dx. \quad (3.4)$$

Definition 3.2 The set

$$\left\{ u \in L^1(\Omega) : |u|_{TV} < \infty \right\} \quad (3.5)$$

is known as the space of functions of *bounded variation* on Ω and will be denoted $BV(\Omega)$.

Definition 3.3 Define a functional on $BV(\Omega)$ as follows:

$$\|u\|_{BV} \stackrel{\text{def}}{=} \|u\|_{L^1} + |u|_{TV}. \quad (3.6)$$

Then $\|\cdot\|_{BV}$ is a norm on $BV(\Omega)$. The space $BV(\Omega)$ is a Banach space under $\|\cdot\|_{BV}$ (see [12]). The total variation functional $|\cdot|_{TV}$ is a semi-norm on $BV(\Omega)$ (a semi-norm since it does not distinguish between constants).

Theorem 3.4 (See [12].) For $1 \leq p \leq \frac{d}{d-1}$ and $\Omega \subset \mathbb{R}^d$, $BV(\Omega) \subset L^p(\Omega)$. The injection map from $BV(\Omega)$ into $L^p(\Omega)$ is compact for $1 \leq p < \frac{d}{d-1}$ and weakly compact for $p = \frac{d}{d-1}$.

A modification of the total variation functional, J_β , will now be considered. It will be shown that J_β has the same domain as $|\cdot|_{TV}$. The weak lower semi-continuity and convexity of J_β will also be shown.

Definition 3.5 For $\beta \geq 0$, define

$$J_\beta(u) \stackrel{\text{def}}{=} \sup_{\vec{w} \in \mathcal{W}} \left\{ \int_{\Omega} \left[-u \nabla \cdot \vec{w} + \beta \sqrt{1 - |\vec{w}(x)|^2} \right] dx \right\}. \quad (3.7)$$

The functional J_β agrees with $|\cdot|_{TV}$ for $\beta = 0$, and for $u \in C^1(\Omega)$, the supremum in (3.7) is attained for $\vec{w} = \nabla u / (\sqrt{|\nabla u|^2 + \beta^2})$, and hence,

$$J_\beta(u) = \int_{\Omega} \sqrt{\beta^2 + |\nabla u|^2} dx. \quad (3.8)$$

Lemma 3.6 The functional J_β satisfies $J_\beta(u) < \infty$ if and only if $|u|_{TV} < \infty$; hence, the domain of J_β is $BV(\Omega)$ for any $\beta \geq 0$. Also, $J_\beta(u) \rightarrow |u|_{TV}$ as $\beta \rightarrow 0$.

Proof: For $\vec{w} \in \mathcal{W}$,

$$\int_{\Omega} -u \nabla \cdot \vec{w} dx \leq \int_{\Omega} \left(-u \nabla \cdot \vec{w} + \beta \sqrt{1 - |\vec{w}|^2} \right) dx \quad (3.9)$$

$$= \int_{\Omega} -u \nabla \cdot \vec{w} dx + \beta \int_{\Omega} \sqrt{1 - |\vec{w}|^2} dx \quad (3.10)$$

$$\leq \int_{\Omega} -u \nabla \cdot \vec{w} dx + \beta \text{vol}(\Omega). \quad (3.11)$$

Taking the supremum of both sides over $\mathcal{W}$, one obtains

$$|u|_{TV} \leq J_\beta(u) \leq |u|_{TV} + \beta \text{vol}(\Omega). \quad (3.12)$$

Hence, $J_\beta(u) < \infty$ if and only if $|u|_{TV} < \infty$, and as $\beta \rightarrow 0$, $J_\beta(u) \rightarrow |u|_{TV}$. $\square$

Theorem 3.7 The functional J_β is weakly lower semi-continuous on $L^p(\Omega)$, for $1 \leq p < \infty$.

Proof: Let $\{u_n\} \subset L^p(\Omega)$ be such that $u_n \rightharpoonup u$ (weak L^p convergence). Then for any $\vec{w} \in \mathcal{W}$, by representation of bounded linear functionals on $L^p(\Omega)$ [17, p. 151],

$$\int_{\Omega} \left(-u \nabla \cdot \vec{w} + \beta \sqrt{1 - |\vec{w}|^2} \right) dx \quad (3.13)$$

$$= \lim_{n \rightarrow \infty} \int_{\Omega} \left(-u_n \nabla \cdot \vec{w} + \beta \sqrt{1 - |\vec{w}|^2} \right) dx \quad (3.14)$$

$$= \liminf_{n \rightarrow \infty} \int_{\Omega} \left(-u_n \nabla \cdot \vec{w} + \beta \sqrt{1 - |\vec{w}|^2} \right) dx \quad (3.15)$$

$$\leq \liminf_{n \rightarrow \infty} J_{\beta}(u_n). \quad (3.16)$$

Taking the supremum over $\mathcal{W}$ yields

$$J_{\beta}(u) \leq \liminf_{n \rightarrow \infty} J_{\beta}(u_n). \quad (3.17)$$

□

Lemma 3.8 The functional J_{β} is convex.

Proof: Let $u, v \in BV(\Omega)$ and $\lambda \in [0, 1]$. Then for any $\vec{w} \in \mathcal{W}$,

$$\int_{\Omega} \left\{ -[\lambda u + (1 - \lambda)v] \nabla \cdot \vec{w} + \beta \sqrt{1 - |\vec{w}|^2} \right\} dx \quad (3.18)$$

$$= \int_{\Omega} \left[\lambda \left(-u \nabla \cdot \vec{w} + \beta \sqrt{1 - |\vec{w}|^2} \right) + \right. \quad (3.19)$$

$$\left. (1 - \lambda) \left(-v \nabla \cdot \vec{w} + \beta \sqrt{1 - |\vec{w}|^2} \right) \right] dx \quad (3.20)$$

$$\leq \lambda J_{\beta}(u) + (1 - \lambda) J_{\beta}(v). \quad (3.21)$$

Taking the supremum over $\mathcal{W}$ implies

$$J_{\beta}(\lambda u + (1 - \lambda)v) \leq \lambda J_{\beta}(u) + (1 - \lambda) J_{\beta}(v). \quad (3.22)$$

□

Now employ J_{β} as the regularization functional in Tikhonov regularization.

As in Chapter 2, let K be a non-degenerate compact operator such that $K(1) \neq$

0. Tikhonov regularization can be applied with J_β as the regularization functional. Define the functional T_α as follows:

$$T_\alpha(u) = \frac{1}{2} \|Ku - z\|^2 + \frac{\alpha}{2} J_\beta(u), \quad (3.23)$$

and consider the problem to find $\hat{u} \in BV(\Omega)$ such that $T_\alpha(\hat{u})$ is a minimum.

Lemma 3.8 and Example 2.22 show that the functional T_α is convex. Strict convexity holds under some additional conditions, for example, when K has the trivial null space. Additional properties of T_α will now be established, including weak lower semi-continuity and BV -coercivity.

Lemma 3.9 Define

$$|||u||| \stackrel{\text{def}}{=} |\bar{u}| + |u|_{TV} \quad (3.24)$$

$$= |\bar{u}| + \sup_{\vec{w} \in \mathcal{W}} \left\{ \int_{\Omega} -u \nabla \cdot \vec{w} dx \right\}, \quad (3.25)$$

where $\bar{u}$ denotes the mean value of u on Ω , as in the proof of Lemma 2.31. Then $||| \cdot |||$ is a norm on $BV(\Omega)$ and is equivalent to $\| \cdot \|_{BV}$.

Proof: It is easily shown that $||| \cdot |||$ has the properties of a norm. To show equivalence, note that

$$|||u||| = \left| \frac{1}{\text{vol}(\Omega)} \int_{\Omega} u dx \right| + |u|_{TV} \quad (3.26)$$

$$\leq \frac{1}{\text{vol}(\Omega)} \int_{\Omega} |u| dx + |u|_{TV} \quad (3.27)$$

$$\leq \max \left(\frac{1}{\text{vol}(\Omega)}, 1 \right) \|u\|_{BV}. \quad (3.28)$$

To show that there exists a $\gamma > 0$ such that $|||u||| \geq \gamma \|u\|_{BV}$, it suffices to show that

$$|||u||| = |\bar{u}| + |u|_{TV} \geq \gamma, \quad (3.29)$$

whenever $\|u\|_{BV} = 1$. If the above statement does not hold, then there is a sequence $\{u_n\} \in BV(\Omega)$ such that $\|u_n\|_{BV} = 1$ and $|\bar{u}_n| + |u_n|_{TV} \rightarrow 0$ as $n \rightarrow \infty$. This implies that $|\bar{u}_n| \rightarrow 0$ and $|u_n|_{TV} \rightarrow 0$. This latter limit together with Theorem 3.4 imply that there is a subsequence $\{u_{n_j}\}$ such that $u_{n_j} \rightarrow u \in L^1(\Omega)$ (L^1 convergence). Since $|u_{n_j}|_{TV} \rightarrow 0$, $u_{n_j} \rightarrow u$ with respect to the BV norm as well and $\|u\|_{BV} = \|u\|_{L^1} = 1$.

Any $v \in BV(\Omega)$ can be written as $v = \bar{v} + v^\perp$, where $v^\perp \in BV(\Omega)$ satisfies $\int_\Omega v^\perp dx = 0$. Since $\bar{v}$ is constant, $|v|_{TV} = |v^\perp|_{TV}$. Since $|u_{n_j}|_{TV} \rightarrow 0$, $|u|_{TV} = |u^\perp|_{TV} = 0$. This together with the fact that $\int_\Omega u^\perp dx = 0$ implies that $u^\perp \equiv 0$ on Ω . Thus

$$|||u_{n_j}||| = |\bar{u}_{n_j}| + |u_{n_j}|_{TV} \quad (3.30)$$

$$\rightarrow |\bar{u}| + |u|_{TV}. \quad (3.31)$$

However,

$$1 = \|u\|_{L^1} \quad (3.32)$$

$$= \|\bar{u} + u^\perp\|_{L^1} \quad (3.33)$$

$$= \|\bar{u}\|_{L^1} \quad (3.34)$$

$$= |\bar{u}| \text{vol}(\Omega). \quad (3.35)$$

Hence, $|||u_{n_j}||| \rightarrow |\bar{u}| \neq 0$, contrary to the assumption. Therefore, the norms are equivalent. $\square$

Lemma 3.10 Let K be a bounded operator from L^p into L^2 . The functional T_α is weakly lower semi-continuous with respect to the L^p topology with $1 \leq p < \infty$.

Proof: The functional T_α can be written

$$T_\alpha(u) = \frac{1}{2} \|Ku\|^2 - \langle Ku, z \rangle + \frac{1}{2} \|z\|^2 + \frac{\alpha}{2} J_\beta(u). \quad (3.36)$$

The weak lower semi-continuity of the first two terms was shown in Chapter 2, the third term is constant with respect to u , and Lemma 3.7 shows the property for the regularization functional J_β . Hence, T_α is weakly lower semi-continuous. $\square$

Theorem 3.11 The functional T_α is BV -coercive.

Proof: Let $\{u_n\} \subset BV(\Omega)$ such that $\|u_n\|_{BV} \rightarrow \infty$ as $n \rightarrow \infty$. By Lemma 3.9, $\|u_n\| \rightarrow \infty$ as well, and it suffices to show that T_α is coercive with respect to the $\|\cdot\|$ norm. There exists a subsequence $\{u_{n_j}\}$ such that $|\bar{u}_{n_j}| \rightarrow \infty$ or $|u_{n_j}|_{TV} \rightarrow \infty$. Since

$$T_\alpha(u_{n_j}) = \frac{1}{2} \|Ku_{n_j} - z\|^2 + \frac{\alpha}{2} J_\beta(u_{n_j}) \quad (3.37)$$

$$\geq \frac{\alpha}{2} J_\beta(u_{n_j}), \quad (3.38)$$

if $|u_{n_j}|_{TV} \rightarrow \infty$, so does $J_\beta(u_{n_j})$ by Lemma 3.6 and, hence, $T_\alpha(u_{n_j}) \rightarrow \infty$. For any $u \in BV(\Omega)$, u can be written as $u = \bar{u} + u^\perp$. This implies

$$T_\alpha(u_{n_j}) \geq \frac{1}{2} \|Ku_{n_j} - z\|^2 \quad (3.39)$$

$$= \frac{1}{2} \|K\bar{u}_{n_j} + Ku_{n_j}^\perp - z\|^2 \quad (3.40)$$

$$= \frac{1}{2} |\bar{u}_{n_j}|^2 \|K(1) + \frac{1}{\bar{u}_{n_j}} (Ku_{n_j}^\perp - z)\|^2. \quad (3.41)$$

If $|\bar{u}_{n_j}| \rightarrow \infty$, $T_\alpha(u_{n_j})$ does as well. $\square$

The following theorem establishes the existence of a solution to the Tikhonov problem with the regularization functional J_β . A condition for the uniqueness of a solution will also be provided. Stability with respect to perturbations in z , K , α , and β is quite technical and will be omitted here (see [2]).

Theorem 3.12 The Tikhonov regularization problem (2.6) with T_α as defined in (3.23) has a solution $\hat{u} \in L^p(\Omega)$ where $1 \leq p \leq \frac{d}{d-1}$. If T_α is strictly convex, this solution is unique.

Proof: Let $\{u_n\}_{n=1}^\infty \subset BV(\Omega)$ be a minimizing sequence for T_α , i.e., $T_\alpha(u_n) \rightarrow \inf_u T_\alpha(u) \stackrel{\text{def}}{=} \hat{T}_\alpha$. Since T_α is coercive, the u_n 's are bounded. By the weak compactness of $BV(\Omega)$ in $L^p(\Omega)$, $1 \leq p \leq \frac{d}{d-1}$ (Theorem 3.4) there exists a subsequence $\{u_{n_j}\}_{j=1}^\infty$ such that $u_{n_j} \rightharpoonup \hat{u} \in L^p(\Omega)$. Since T_α is weakly lower semi-continuous,

$$T_\alpha(\hat{u}) \leq \liminf_{j \rightarrow \infty} T_\alpha(u_{n_j}) \quad (3.42)$$

$$= \lim_{j \rightarrow \infty} T_\alpha(u_{n_j}) = \hat{T}_\alpha. \quad (3.43)$$

Therefore, a minimum, $\hat{u}$, exists. If T_α is strictly convex, $\hat{u}$ is unique. $\square$

Finally, the characterization of a minimizer of T_α is addressed. Both the weak and strong forms of the minimization problem are derived.

For $u, v \in H^1(\Omega)$,

$$dJ_\beta(u; v) = \lim_{\tau \rightarrow 0} \frac{J_\beta(u + \tau v) - J_\beta(u)}{\tau} \quad (3.44)$$

$$= \lim_{\tau \rightarrow 0} \frac{1}{\tau} \left\{ \int_\Omega \left(\sqrt{\beta^2 + |\nabla(u + \tau v)|^2} - \sqrt{\beta^2 + |\nabla u|^2} \right) dx \right\} \quad (3.45)$$

$$= \lim_{\tau \rightarrow 0} \frac{1}{\tau} \left\{ \int_\Omega \frac{2\tau \nabla u \cdot \nabla v + \tau^2 |\nabla v|^2}{\sqrt{\beta^2 + |\nabla(u + \tau v)|^2} + \sqrt{\beta^2 + |\nabla u|^2}} dx \right\} \quad (3.46)$$

$$= \int_\Omega \frac{\nabla u \cdot \nabla v}{\sqrt{\beta^2 + |\nabla u|^2}} dx \quad (3.47)$$

$$\stackrel{\text{def}}{=} \langle L_\beta(u)u, v \rangle. \quad (3.48)$$

This defines (in weak form) the nonlinear differential operator $L_\beta(u)$ on $H^1(\Omega)$. If $u \in C^2(\bar{\Omega})$ then integration by parts yields

$$dJ_\beta(u; v) = - \int_\Omega \nabla \cdot \left(\frac{\nabla u}{\sqrt{\beta^2 + |\nabla u|^2}} \right) v dx + \int_{\partial\Omega} \frac{\nabla u}{\sqrt{\beta^2 + |\nabla u|^2}} \cdot \vec{n} v ds. \quad (3.49)$$

where $\vec{\eta}$ denotes the outward normal vector. Hence, the strong form of the operator $L_\beta(u)$ is

$$L_\beta(u)v = -\nabla \cdot \left(\frac{1}{\sqrt{\beta^2 + |\nabla u|^2}} \nabla v \right) = 0, \quad x \in \Omega \quad (3.50)$$

with the associated boundary conditions

$$\nabla v \cdot \vec{\eta} = 0, \quad x \in \partial\Omega. \quad (3.51)$$

From Chapter 2 and (3.49),

$$dT_\alpha(u; v) = \langle K^*(Ku - z) + \alpha L_\beta(u)u, v \rangle \quad (3.52)$$

for $u, v \in H^1(\Omega)$. If $\hat{u}$ is a minimizer for T_α and $\hat{u} \in H^1(\Omega)$, then $dT_\alpha(\hat{u}; v) = 0$, or

$$\langle (K^*K + \alpha L_\beta(\hat{u})\hat{u}, v) = \langle K^*z, v \rangle \quad (3.53)$$

for all $v \in H^1(\Omega)$. If $\hat{u} \in C^2(\overline{\Omega})$, then it is a classical solution of

$$K^*Ku - \nabla \cdot \left(\frac{\nabla u}{\sqrt{\beta^2 + |\nabla u|^2}} \right) = K^*z, \quad x \in \Omega \quad (3.54)$$

$$\nabla u \cdot \vec{\eta} = 0, \quad x \in \partial\Omega. \quad (3.55)$$

CHAPTER 4

Discretization

In this chapter three methods of discretizing the minimization problem (2.6) with T_α as defined in (3.23) are presented. The standard methods of Galerkin and finite differences will be discussed first. The latter half of this chapter is devoted to a presentation of a cell-centered finite difference discretization for one- and two-dimensional domains. The systems which result from the three discretizations are of similar form; however, the cell-centered finite difference discretization has the advantage that it places no a priori smoothness condition on the solution.

Galerkin Discretization

Define the linear space $\mathcal{U}^h = \text{span} \{\phi_i\}_{i=1}^n$ where the $\phi_i \in H^1(\Omega)$ and are linearly independent. Typically, the ϕ_i are piecewise linear basis functions defined on a grid with mesh spacing h . Then for any $U \in \mathcal{U}^h$, $U = \sum_{i=1}^n u_i \phi_i$ for some set $\{u_i\}_{i=1}^n \subset \mathbb{R}$. Note that $H^1(\Omega) \subset BV(\Omega)$. Define the functional $J_\beta^h : \mathcal{U}^h \rightarrow \mathbb{R}$ as follows

$$J_\beta^h(U) = \int_{\Omega} \sqrt{|\nabla U|^2 + \beta^2} dx, \quad (4.1)$$

where $\nabla U = \sum_{i=1}^n u_i \nabla \phi_i$. From (3.44),

$$dJ_\beta^h(U; V) = \int_{\Omega} \frac{\nabla U \cdot \nabla V}{\sqrt{|\nabla U|^2 + \beta^2}} dx. \quad (4.2)$$

Let K be a Fredholm first kind integral operator and define $K_h : \mathcal{U}^h \rightarrow L^2(\Omega)$ by

$$K_h U = \sum_{i=1}^n u_i K \phi_i. \quad (4.3)$$

For any data z , approximate z by $Z \stackrel{\text{def}}{=} \sum_{i=1}^n z_i \phi_i$. Define the functional T_h on $\mathcal{U}^h$ to be

$$T_h(U) \stackrel{\text{def}}{=} \frac{1}{2} \|K_h U - Z\|^2 + \alpha J_\beta^h(U) \quad (4.4)$$

$$= \frac{1}{2} \|K_h U - Z\|^2 + \alpha \int_\Omega \sqrt{|\nabla U|^2 + \beta^2} dx. \quad (4.5)$$

For any $V \in \mathcal{U}^h$ the Gateaux derivative of T_h is

$$dT_h(U; V) = \langle K_h U - Z, K_h V \rangle + \alpha dJ_\beta^h(U; V) \quad (4.6)$$

$$= \langle K_h U - Z, K_h V \rangle + \alpha \int_\Omega \frac{\nabla U \cdot \nabla V}{\sqrt{|\nabla U|^2 + \beta^2}} dx. \quad (4.7)$$

At a minimum, $\hat{U}$, $dT_h(\hat{U}; V) = 0$ for all $V \in \mathcal{U}^h$, or equivalently, $dT_h(\hat{U}; \phi_j) = 0$ for $j = 1, 2, \dots, n$. This implies

$$\langle K_h \hat{U}, K_h \phi_j \rangle + \alpha \int_\Omega \frac{\nabla \hat{U} \cdot \nabla \phi_j}{\sqrt{|\nabla \hat{U}|^2 + \beta^2}} dx = \langle Z, K_h \phi_j \rangle, \quad (4.8)$$

for $j = 1, 2, \dots, n$. Hence, one obtains the finite dimensional system,

$$\sum_{i=1}^n \left[\langle K_h \phi_i, K_h \phi_j \rangle + \alpha \left\langle \frac{\nabla \phi_i}{\sqrt{|\nabla \hat{U}|^2 + \beta^2}}, \nabla \phi_j \right\rangle \right] u_i = \sum_{i=1}^n \langle \phi_i, K_h \phi_j \rangle z_i, \quad (4.9)$$

for $j = 1, 2, \dots, n$. To implement this, it is necessary to choose basis functions and a numerical quadrature scheme.

Finite Differences

For simplicity, let Ω be the interval $[0, 1]$ in $\mathbb{R}$ or the unit square in $\mathbb{R}^2$, and construct a mesh of $n_x + 1$ or $(n_x + 1) \times (n_y + 1)$ equally spaced grid points on Ω

with spacing $h = \frac{1}{n_x}$ where $n_x = n_y$ and $n = n_x$ or $n = n_x n_y$ is the total number of points. In $\mathfrak{R}$, denote these points x_i . In $\mathfrak{R}^2$, denote these points $x_I = (x_i, y_j)$, where $x_i = ih$ and $y_j = jh$. Let U denote a grid function approximation to u such that $[U]_I \approx u(x_I)$. Similarly, let $[Z]_I \approx z(x_I)$. For $\Omega \subset \mathfrak{R}$, I and i coincide. The finite difference approximation to the first derivative in one dimension is

$$[D_h V]_I = [D_h V]_i \stackrel{\text{def}}{=} \frac{[V]_{i+1} - [V]_i}{h}. \quad (4.10)$$

In two dimensions the finite difference approximation to the gradient is taken to be

$$[D_h V]_I = [D_h V]_{i,j} \stackrel{\text{def}}{=} \left(\frac{[V]_{i+1,j} - [V]_i}{h}, \frac{[V]_{i,j+1} - [V]_{i,j}}{h} \right). \quad (4.11)$$

Define a functional $J_\beta^h : \mathfrak{R}^n \rightarrow \mathfrak{R}$ by

$$J_\beta^h(U) = h^d \sum_I \sqrt{|[D_h U]_I|^2 + \beta^2}, \quad (4.12)$$

where d indicates dimension ($d = 1$ or 2), and

$$|[D_h U]_I|^2 = \begin{cases} \left(\frac{u_{i+1} - u_i}{h} \right)^2, & I = i \quad (d = 1) \\ \left(\frac{u_{i+1,j} - u_{i,j}}{h} \right)^2 + \left(\frac{u_{i,j+1} - u_{i,j}}{h} \right)^2, & I = (i, j) \quad (d = 2) \end{cases} \quad (4.13)$$

Let K be a Fredholm integral operator and let K_h denote a discretization of K such that

$$[K_h U]_I \approx (Ku)(x_I), \quad (4.14)$$

whenever U is a grid function approximation to u . Define the functional T_h on $\mathfrak{R}^n$ by

$$T_h(U) = \frac{h^d}{2} \|K_h U - Z\|_{\ell^2}^2 + \alpha J_\beta^h(U). \quad (4.15)$$

For any $V \in \mathfrak{R}^n$ the Gateaux derivative of T_h is

$$dT_h(U; V) = \langle K_h^*(K_h U - Z), V \rangle_{\ell^2} + \alpha \left\langle \frac{D_h U}{\sqrt{|D_h U|^2 + \beta^2}}, D_h V \right\rangle_{\ell^2} \quad (4.16)$$

$$= \langle K_h^*(K_h U - Z), V \rangle_{\ell^2} + \alpha \left\langle D_h^* \left(\frac{D_h U}{\sqrt{|D_h U|^2 + \beta^2}} \right), V \right\rangle_{\ell^2}. \quad (4.17)$$

Note that in one space dimension, from (4.10),

$$D_h^*(D_h U) = \frac{-U_{i+1} + 2U_i - U_{i-1}}{h^2}. \quad (4.18)$$

This is the finite difference approximation to the negative of the second derivative. Similarly, in two space dimensions, $D_h^* D_h$ gives the standard finite difference approximation to the negative Laplacian in two dimensions.

At a minimum, $\hat{U}$, $dT_h(\hat{U}; V) = 0$ for all V , and hence,

$$\left[K_h^* K_h + \alpha D_h^* \left(\frac{D_h}{\sqrt{|D_h \hat{U}|^2 + \beta^2}} \right) \right] \hat{U} = K_h^* Z. \quad (4.19)$$

The system in (4.19) is nearly identical to the system obtained via the Galerkin finite element discretization with piecewise linear basis functions and midpoint quadrature.

Cell-Centered Finite Differences

Let $\mathcal{W}$ be as in (3.2), and define the functional Q on $\mathcal{U} \times \mathcal{W}$ as follows:

$$Q(u, \vec{w}) \stackrel{\text{def}}{=} \int_{\Omega} \left(-u \nabla \cdot \vec{w} + \beta \sqrt{1 - |\vec{w}|^2} \right) dx. \quad (4.20)$$

Then the functional J_{β} in (3.5) can be written

$$J_{\beta}(u) = \sup_{\vec{w} \in \mathcal{W}} Q(u, \vec{w}). \quad (4.21)$$

Consider the specific one-dimensional case where $\Omega = (0, 1)$, and divide Ω into n cells in the following manner. Let $h = 1/n$, and let $x_i = (i - \frac{1}{2})h$, $i = 1, \dots, n$. Define $x_{i \pm \frac{1}{2}} = x_i \pm h/2$. The i^{th} cell, which has center x_i and is denoted c_i , is defined to be

$$c_i = \left\{ x : x_{i-\frac{1}{2}} < x < x_{i+\frac{1}{2}} \right\}. \quad (4.22)$$

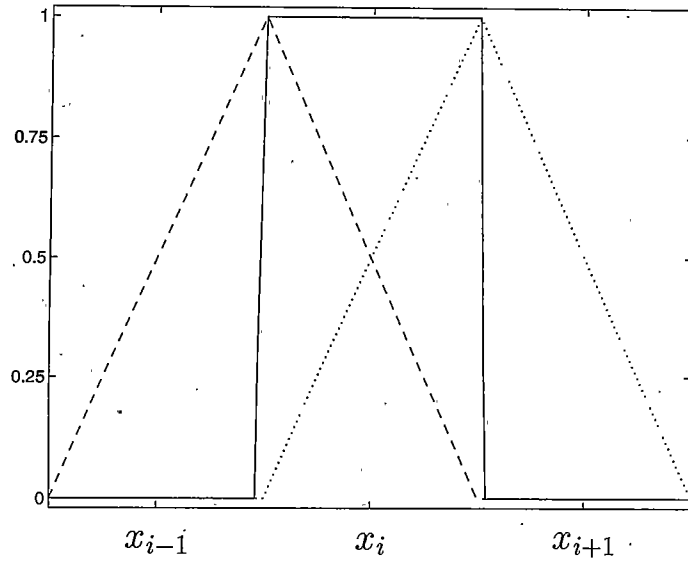


Figure 1: Diagram of χ_i (solid line), $\phi_{i-\frac{1}{2}}$ (dashed line), and $\phi_{i+\frac{1}{2}}$ (dotted line).

Let $\mathcal{U}^h$ denote the span of the piecewise constant functions χ_i , where

$$\chi_i(x) = \begin{cases} 1, & x \in c_i \\ 0, & x \notin c_i. \end{cases} \quad (4.23)$$

Approximate u by $U \in \mathcal{U}^h$, where

$$U(x) = \sum_{i=1}^n u_i \chi_i(x). \quad (4.24)$$

Consider the piecewise linear basis functions $\phi_{i+\frac{1}{2}}$ such that $\phi_{i+\frac{1}{2}}(x_{j+\frac{1}{2}}) = \delta_{ij}$, $i, j = 1, 2, \dots, n-1$. Let $\mathcal{W}^h$ consist of functions of the form

$$W(x) = \sum_{i=1}^{n-1} w_{i+\frac{1}{2}} \phi_{i+\frac{1}{2}}(x) \quad (4.25)$$

with the constraint $|W(x)| \leq 1$. This implies the constraints $|w_{i+\frac{1}{2}}| \leq 1$ on the coefficients. Graphs of the functions χ_i , $\phi_{i-\frac{1}{2}}$, and $\phi_{i+\frac{1}{2}}$ are shown in Figure 1.

Using the trapezoidal quadrature approximation and the fact that $W(0) = W(1) = 0$,

$$\int_0^1 \sqrt{1 - [W(x)]^2} dx \approx h \sum_{j=1}^{n-1} \sqrt{1 - [W(x_{j+\frac{1}{2}})]^2}, \quad (4.26)$$

define the functional Q^h on $\mathcal{U}^h \times \mathcal{W}^h$ by

$$Q^h(U, W) \stackrel{\text{def}}{=} - \sum_{j=1}^{n-1} \int_{\Omega} U w_{j+\frac{1}{2}} \phi'_{j+\frac{1}{2}} dx + \beta h \sum_{j=1}^{n-1} \sqrt{1 - (w_{j+\frac{1}{2}})^2} \quad (4.27)$$

$$= h \sum_{j=1}^{n-1} \frac{u_{j+1} - u_j}{h} w_{j+\frac{1}{2}} + \beta h \sum_{j=1}^{n-1} \sqrt{1 - (w_{j+\frac{1}{2}})^2} \quad (4.28)$$

$$= h \sum_{j=1}^{n-1} [D_h U]_j w_{j+\frac{1}{2}} + \beta h \sum_{j=1}^{n-1} \sqrt{1 - (w_{j+\frac{1}{2}})^2}. \quad (4.29)$$

Then for any fixed $U \in \mathcal{U}^h$,

$$\frac{\partial}{\partial w_{j+\frac{1}{2}}} Q^h(U, W) = - \int_{\Omega} U \phi'_{j+\frac{1}{2}} dx + \beta h \frac{w_{j+\frac{1}{2}}}{\sqrt{1 - (w_{j+\frac{1}{2}})^2}} \quad (4.30)$$

$$= -[D_h U]_j + \beta h \frac{w_{j+\frac{1}{2}}}{\sqrt{1 - (w_{j+\frac{1}{2}})^2}}. \quad (4.31)$$

For a fixed U , the maximum of $Q^h(U, W)$ over $\mathcal{W}^h$ occurs in the interior when $\frac{\partial}{\partial w_j} Q^h(U, W) = 0$ for all j . Then solving for $w_{j+\frac{1}{2}}$ in (4.31),

$$w_{j+\frac{1}{2}} = \frac{[D_h U]_j}{\sqrt{|[D_h U]_j|^2 + \beta^2}}. \quad (4.32)$$

For the remainder of the discussion, W_{max} will refer to the element of $\mathcal{W}^h$ with components $w_{j+\frac{1}{2}}$ as in (4.32). Define the functional J_{β}^h on $\mathcal{U}^h$ by

$$J_{\beta}^h(U) \stackrel{\text{def}}{=} Q^h(U, W_{max}) \quad (4.33)$$

$$= h \sum_{j=1}^{n-1} [D_h U]_j w_{j+\frac{1}{2}} + \beta h \sum_j \sqrt{1 - (w_{j+\frac{1}{2}})^2} \quad (4.34)$$

$$= h \sum_{j=1}^{n-1} \sqrt{[D_h U]_j^2 + \beta^2}. \quad (4.35)$$

Hence,

$$dJ_{\beta}^h(U; V) = h \sum_j \frac{[D_h V]_j [D_h U]_j}{\sqrt{|[D_h U]_j|^2 + \beta^2}} \quad (4.36)$$

$$\stackrel{\text{def}}{=} \langle L_{\beta}(U)U, V \rangle_{\ell^2}. \quad (4.37)$$

Note that $L_\beta(U)$ is an $n \times n$, symmetric, positive semi-definite tridiagonal matrix.

Define the functional T_h on $\mathcal{U}^h$ by

$$T_h(U) = \frac{1}{2} \|K_h U - Z\|^2 + \alpha J_\beta^h(U), \quad (4.38)$$

where K_h denotes a discretization of the operator K , and $Z \approx z$ is a fixed element of $\mathcal{U}^h$. Then the problem to find $\hat{U} \in \mathcal{U}^h$ such that $T_h(\hat{U})$ is a minimum is equivalent to finding $U \in \mathbb{R}^n$ such that

$$K_h^*(K_h U - Z) + L_\beta(U)U = 0, \quad (4.39)$$

which can also be written

$$[K_h^* K_h + L_\beta(U)]U = K_h^* Z. \quad (4.40)$$

In two dimensions, consider the domain $\Omega = (0,1) \times (0,1)$. To discretize using cell-centered finite differences, construct a grid system. Let $n_x = n_y$ denote the number of cells in the x and y directions, respectively, and let $h = 1/n_x$ be the dimension of each cell. The total number of cells is given by $n = n_x n_y$. The cell centers are given by (x_i, y_j) and are defined to be

$$x_i = \left(i - \frac{1}{2}\right) h, \quad i = 1, \dots, n_x, \quad (4.41)$$

$$y_j = \left(j - \frac{1}{2}\right) h, \quad j = 1, \dots, n_y. \quad (4.42)$$

The cell edges are given by

$$x_{i \pm \frac{1}{2}} = x_i \pm \frac{h}{2}, \quad (4.43)$$

$$y_{j \pm \frac{1}{2}} = y_j \pm \frac{h}{2}. \quad (4.44)$$

The ij^{th} cell, denoted c_{ij} , which is centered at (x_i, y_j) is defined to be

$$c_{ij} = \left\{ (x, y) : x_{i-\frac{1}{2}} < x < x_{i+\frac{1}{2}}, y_{j-\frac{1}{2}} < y < y_{j+\frac{1}{2}} \right\} \quad (4.45)$$

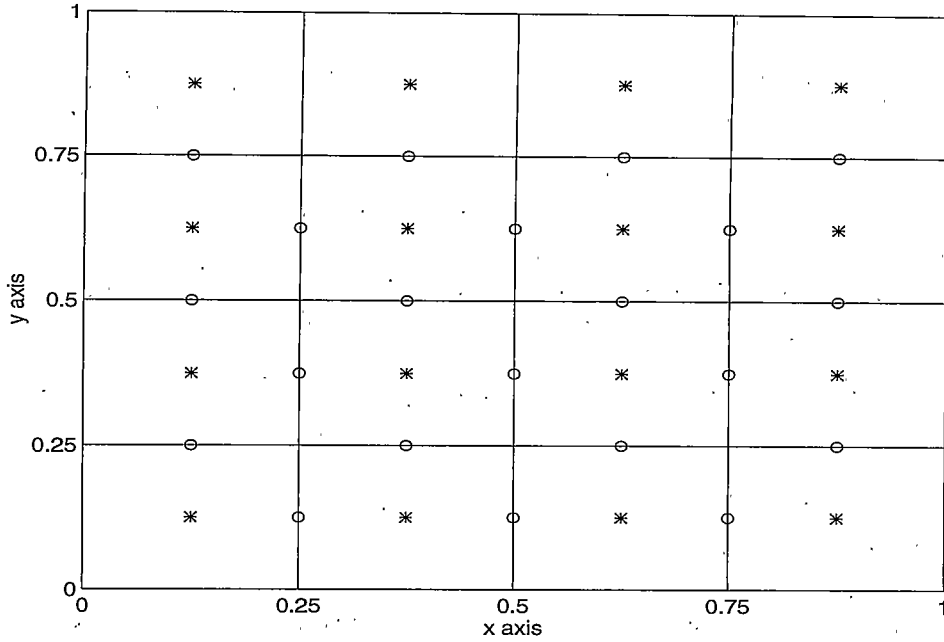


Figure 2: Diagram of a 4×4 cell-centered finite difference grid. Stars (*) indicate cell centers (x_i, y_j) . Circles (o) indicate interior x -edge midpoints $(x_{i\pm\frac{1}{2}}, y_j)$ and y -edge midpoints $(x_i, y_{j\pm\frac{1}{2}})$.

and has area

$$|c_{ij}| = h^2. \quad (4.46)$$

This cell-centered grid scheme is depicted in Figure 2.

Approximate u by

$$u(x, y) \approx U(x, y) \stackrel{\text{def}}{=} \sum_{i=1}^{n_x} \sum_{j=1}^{n_y} u_{ij} \chi_i(x) \chi_j(y) \quad (4.47)$$

where $\chi_i(x)$ and $\chi_j(y)$ denote the characteristic functions on the intervals $(x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}})$ and $(y_{j-\frac{1}{2}}, y_{j+\frac{1}{2}})$, respectively. Approximate the components w^x and w^y of $\vec{w}$ by

$$w^x(x, y) \approx W^x(x, y) \stackrel{\text{def}}{=} \sum_{i=1}^{n_x-1} \sum_{j=1}^{n_y} w_{ij} \phi_{i+\frac{1}{2}}(x) \chi_j(y) \quad (4.48)$$

$$w^y(x, y) \approx W^y(x, y) \stackrel{\text{def}}{=} \sum_{i=1}^{n_x} \sum_{j=1}^{n_y-1} w_{ij} \chi_i(x) \phi_{j+\frac{1}{2}}(y) \quad (4.49)$$

where $\phi_{i+\frac{1}{2}}$ are the continuous, piecewise linear functions that have been defined above.

The rest follows as for the one-dimensional case by using the product quadrature approximation

$$\int_0^1 \int_0^1 f(x, y) dy dx \approx \begin{cases} h^2 \sum_{i=1}^{n_x-1} \sum_{j=1}^{n_y} f(x_{i+\frac{1}{2}}, y_j) \\ h^2 \sum_{i=1}^{n_x} \sum_{j=1}^{n_y-1} f(x_i, y_{j+\frac{1}{2}}) \end{cases}, \quad (4.50)$$

corresponding to (4.48)-(4.49) in equations (4.27) - (4.29), and by replacing the single summations by double summations in equations (4.34) - (4.36) (see also [31] and [33]).

The resulting system has the same form as the system (4.39). With lexicographical ordering of unknowns, the matrix $L_\beta(U)$ is a symmetric, positive semi-definite, block tridiagonal matrix.

CHAPTER 5

Nonlinear Unconstrained Optimization Methods

The minimization problem (2.6) with T_α as defined in (3.23) is nonlinear. Standard techniques for unconstrained minimization include Newton and quasi-Newton methods, and are presented by Dennis and Schnabel [9]. Newton's method is favored for its quadratic convergence rate, but the quasi-Newton methods, which use an approximation to the Hessian, are usually easier to implement. In spite of the fact that convergence is slower than for Newton's method, the Quasi-Newton methods may also be more efficient because an approximate Hessian can often be updated more quickly than the true Hessian. The Newton and quasi-Newton methods will be briefly described below. Globalization techniques, such as line searches and trust regions (see [9, pp. 120-25], are often used to ensure global convergence, i.e., to ensure that the method will converge to a minimum for *any* initial guess. A fixed point iteration is presented for finding a solution to the discrete problems obtained in Chapter 4. This iteration is shown to be a quasi-Newton method for the minimization of $f(U) = \frac{1}{2}\|K_h U - Z\|_{\ell^2}^2 + \alpha J_\beta^h(U)$. Several properties of this fixed point iteration are described.

Let F be a map from a set D into itself. Then $u \in D$ is a *fixed point* for F if and only if $F(u) = u$. An iteration of the form $u^{q+1} = F(u^q)$ is known as a fixed point iteration. Two particular fixed point iterations are Newton's method and the quasi-Newton method as defined in [9] and other sources.

In the following discussion, $f : \mathfrak{R}^n \rightarrow \mathfrak{R}$ is assumed to be twice continuously differentiable, and $u^0 \in \mathfrak{R}^n$ is an initial guess. The gradient of f at u which will be denoted $g(u)$, is the vector with components $\left[\frac{\partial f}{\partial u_i}\right]$. The Hessian matrix of f at u will be denoted $H(u)$ and is the matrix with components $\left[\frac{\partial^2 f}{\partial u_i \partial u_j}\right]$. Note that the Hessian is symmetric.

Algorithm 5.1 *Newton's Method* to find a minimum of f is as follows. For $q = 0, 1, \dots$,

- (i) Solve $H(u^q)s^q = -g(u^q)$ for s^q .
- (ii) Update the approximate solution $u^{q+1} = u^q + s^q$.

Equivalently, it can be expressed in the fixed point form,

$$u^{q+1} = u^q - [H(u^q)]^{-1} g(u^q) \quad (5.1)$$

$$\stackrel{\text{def}}{=} F_{\text{Newton}}(u^q). \quad (5.2)$$

If u^* is a minimizer of f , then the sequence $\{u^q\}$ generated by Newton's Method will converge to u^* provided u^0 is sufficiently close to u^* and $H(u^*)$ is positive definite. This is proved in [9, p. 90]. If u^0 is not sufficiently close to guarantee convergence, one may implement a line search [9, pp. 126-9]. Replace step (ii) in Algorithm 5.1 by

$$u^{q+1} = u^q + \lambda s^q, \quad (5.3)$$

where $\lambda \in (0, 1)$ minimizes $f(u^q + \lambda s^q)$.

Algorithm 5.2 The *quasi-Newton Method* has the same form as Newton's Method except that an approximate Hessian, H_q , is used in place of $H(u^q)$. See [9] for standard

Hessian approximations. This method can also be expressed in fixed point form as

$$u^{q+1} = u^q - (H_q)^{-1} g(u^q) \quad (5.4)$$

$$\stackrel{\text{def}}{=} F_Q(u^q). \quad (5.5)$$

Under certain conditions on H_q , it can be shown that $u^q \rightarrow u^*$ where $\{u^q\}$ is generated by the quasi-Newton iteration, (see [9, pp. 118-125]).

A fixed point iteration for the non-linear system obtained for any of the discretizations of Chapter 4, is given by

$$\text{For } q = 0, 1, 2, \dots \quad (5.6)$$

$$(K_h^* K_h + \alpha L_\beta(U^q)) U^{q+1} = K_h^* Z, \quad (5.7)$$

where $U^0 \in \mathbb{R}^n$. This can also be expressed

$$U^{q+1} = (K_h^* K_h + \alpha L_\beta(U^q))^{-1} K_h^* Z \quad (5.8)$$

$$= U^q - U^q + (K_h^* K_h + \alpha L_\beta(U^q))^{-1} K_h^* Z \quad (5.9)$$

$$= U^q - (K_h^* K_h + \alpha L_\beta(U^q))^{-1} (K_h^* (K_h U^q - Z) + \alpha L_\beta(U^q)), \quad (5.10)$$

which is a quasi-Newton method to minimize

$$f(U) = \frac{1}{2} \|K_h U - Z\|_{\ell^2}^2 + \alpha J_\beta^h(U). \quad (5.11)$$

Note that the gradient of f is

$$g(U) = K_h^* (K_h U^q - Z) + \alpha L_\beta(U^q), \quad (5.12)$$

and

$$H_q = K_h^* K_h + \alpha L_\beta(U^q) \quad (5.13)$$

is an approximation to the true Hessian

$$H(U) = K_h^* K_h + \alpha L_\beta(U^q) + \alpha L'_\beta(U^q) U^q. \quad (5.14)$$

In the denoising case when Ku is replaced by u in (1.1) of Chapter 1, the fixed point iteration is as follows.

$$[I + \alpha L_\beta(U^q)] U^{q+1} = Z. \quad (5.15)$$

The following theorem gives two properties which hold for this fixed point iteration.

Theorem 5.3 For the fixed point iteration in (5.15), for iterations $q = 1, 2, \dots$,

1. $\|U^q\|_{\ell^2} \leq \|Z\|_{\ell^2}$
2. The iteration is mean preserving, i.e.,

$$\frac{1}{n} \sum_I [U^q]_I = \frac{1}{n} \sum_I [Z]_I. \quad (5.16)$$

Proof: The first property follows from noting that $\alpha L_\beta(U^q)$ is a symmetric, positive semi-definite matrix; hence, the norm of $[I + \alpha L_\beta(U^q)]$ is bounded below by one.

Thus

$$\|U^q\|_{\ell^2} = \|[I + \alpha L_\beta(U^{q-1})]^{-1} Z\|_{\ell^2}. \quad (5.17)$$

$$\leq \|[I + \alpha L_\beta(U^{q-1})]^{-1}\| \|Z\|_{\ell^2} \quad (5.18)$$

$$\leq \|Z\|_{\ell^2}. \quad (5.19)$$

To show the second property, take the inner product of both sides of (5.15) with 1, where 1 denotes the grid function which is identically 1, using the finite difference discretization in (4.19). Note that $D_h(1) = 0$. Then

$$\left\langle \left[I + \alpha D_h^* \left(\frac{D_h}{\sqrt{|D_h U^{q-1}|^2 + \beta^2}} \right) \right] U^q, 1 \right\rangle_{\ell^2} = \langle Z, 1 \rangle_{\ell^2}, \quad (5.20)$$

which implies

$$\langle U^q, 1 \rangle_{\ell^2} + \alpha \left\langle D_h^* \left(\frac{D_h}{\sqrt{|D_h U^{q-1}|^2 + \beta^2}} \right) U^q, 1 \right\rangle_{\ell^2} = \langle Z, 1 \rangle_{\ell^2}. \quad (5.21)$$

The second term of the left hand side can be expressed

$$= \alpha \left\langle D_h^* \left(\frac{D_h}{\sqrt{|D_h U^{q-1}|^2 + \beta^2}} \right) U^q, 1 \right\rangle_{\ell^2} \quad (5.22)$$

$$= \alpha \left\langle \frac{D_h}{\sqrt{|D_h U^{q-1}|^2 + \beta^2}}, D_h(1) \right\rangle_{\ell^2} \quad (5.23)$$

$$= 0. \quad (5.24)$$

Thus

$$\langle U^q, 1 \rangle_{\ell^2} = \langle Z, 1 \rangle_{\ell^2}, \quad (5.25)$$

which implies the result. Similar techniques can be used to show this property for the other discretizations of Chapter 4 as well. $\square$

Recently, Dobson and Vogel [10] have proved local convergence of the fixed point iteration for denoising as given in (5.15). In all numerical experiments, both for the denoising (5.15) and the deconvolution (5.7), *global* convergence has been observed. Thus, there appears to be no need for any type of globalization technique, such as a line search or trust region.

CHAPTER 6

Methods for Discrete Linear Systems

Herein are presented efficient techniques for solving the linear systems $AU^q = \tilde{Z}$, where

$$A = I + \alpha L_\beta(U^q), \quad (6.1)$$

and

$$A = K_h^* K_h + \alpha L_\beta(U^q), \quad (6.2)$$

and $\tilde{Z}$ is the appropriate right-hand side, either Z or $K_h^* Z$. These systems arise at each fixed point iteration in (5.7) of Chapter 5. First, the conjugate gradient method will be discussed along with the idea of preconditioning. Then suitable preconditioners for both (6.1) and (6.2) will be presented. A cell-centered finite difference multigrid preconditioner will be used for the former, while a preconditioning matrix of the form $bI + \alpha L_\beta(U^q)$ will be applied to the latter. This chapter also includes a presentation of Brandt and Lubrecht's multi-level quadrature method [5] for fast approximate evaluation of $K_h^* K_h U$, a calculation essential to the conjugate gradient method. This chapter together with Chapters 4 and 5 contains all the tools for efficient approximation of a solution to the minimization problem (2.6) with T_α as defined in (3.23). The complete algorithm will be given in Chapter 7.

Preconditioned Conjugate Gradient Method

The basic conjugate gradient method will be stated first with a discussion of its convergence properties. Throughout this section the Hilbert space under consideration will be $\mathfrak{R}^n$ with the standard Euclidean, or ℓ^2 , inner product and norm denoted $\langle \cdot, \cdot \rangle$ and $\| \cdot \|$, respectively.

For a fixed $b \in \mathfrak{R}^n$ define a functional f on $\mathfrak{R}^n$ by

$$f(u) \stackrel{\text{def}}{=} \frac{1}{2} \langle u, Au \rangle - \langle u, b \rangle, \quad (6.3)$$

where A is an $n \times n$ symmetric, positive definite matrix. For any $v \in \mathfrak{R}^n$, the Gateaux derivative of f is

$$df(u; v) = \langle v, Au - b \rangle, \quad (6.4)$$

so at a minimum, $\hat{u}$, $df(\hat{u}; v) = 0$ for all $v \in \mathfrak{R}^n$, or

$$A\hat{u} = b. \quad (6.5)$$

Algorithm 6.1 The *conjugate gradient method* can be employed to find the minimizer, $\hat{u} = A^{-1}b$, of the functional f where A is a symmetric, positive definite matrix. First, define the energy inner product

$$\langle u, v \rangle_A \stackrel{\text{def}}{=} \langle u, Av \rangle. \quad (6.6)$$

Choose u_0 . Then the conjugate gradient algorithm is as follows:

$$r_0 = Au_0 - b \quad (6.7)$$

$$d_0 = -r_0 \quad (6.8)$$

$$(6.9)$$

For $k = 0, 1, \dots$

$$a_k = -\frac{\langle r_k, d_k \rangle}{\langle d_k, d_k \rangle_A} \quad (6.10)$$

$$u_{k+1} = u_k + a_k d_k \quad (6.11)$$

$$r_{k+1} = Au_{k+1} - b \quad (6.12)$$

$$c_k = \frac{\langle r_{k+1}, d_k \rangle_A}{\langle d_k, d_k \rangle_A} \quad (6.13)$$

$$d_{k+1} = -r_{k+1} + c_k d_k \quad (6.14)$$

The d_k 's denote successive search directions beginning with the negative gradient. The r_k denotes the residual at each step which is also the gradient of f at u_k .

Lemma 6.2 ([19, p. 132]) Let r_i and d_i be as in Definition 6.1. Then

$$\text{span} \{d_0, d_1, \dots, d_m\} = \text{span} \{r_0, r_1, \dots, r_m\} = \text{span} \{r_0, Ar_0, \dots, A^m r_0\}. \quad (6.15)$$

The nested subspaces, $\text{span} \{r_0\} \subset \text{span} \{r_0, Ar_0\} \subset \dots \subset \text{span} \{r_0, Ar_0, \dots, A^m r_0\}$ are called Krylov subspaces.

Lemma 6.3 ([19, p. 132]) The search directions, d_i , are pairwise A -conjugate; i.e., $\langle d_i, d_j \rangle_A = 0$ if $i \neq j$. Furthermore, the gradients, r_i , are pairwise orthogonal.

Theorem 6.4 (Expanding Subspace Theorem [21, p. 171]) Let $\{d_i\}_{i=0}^{n-1}$ be a sequence of non-zero, pairwise A -conjugate vectors in $\mathbb{R}^n$. Then for any $u_0 \in \mathbb{R}^n$, the sequence $\{u_k\}$ generated by the conjugate gradient method has the property that u_k minimizes f on the line $u = u_{k-1} + ad_{k-1}$ for $a \in \mathbb{R}$, as well as on the affine space $u_0 + \text{span} \{d_i\}_{i=0}^{k-1}$.

Lemma 6.5 If the sequence $\{u_k\}$ is obtained by the conjugate gradient method with u_0 any vector in $\mathbb{R}^n$, then

$$\|u_{k+1} - \hat{u}\|_A^2 \leq \max_{\lambda_i} [1 + \lambda_i \mathcal{P}_k(\lambda_i)]^2 \|u_0 - \hat{u}\|_A^2, \quad (6.16)$$

where $\mathcal{P}_k$ is any k^{th} degree polynomial.

Proof: Let $q_1, q_2, \dots, q_n$ be the mutually orthogonal, normalized eigenvectors of A . Then for some $\xi_1, \xi_2, \dots, \xi_n$,

$$A(u_0 - \hat{u}) = \sum_{i=1}^n \lambda_i \xi_i q_i. \quad (6.17)$$

Hence,

$$\|u_0 - \hat{u}\|_A^2 \stackrel{\text{def}}{=} \langle u_0 - \hat{u}, u_0 - \hat{u} \rangle_A \quad (6.18)$$

$$= \sum_{i=1}^n \lambda_i \xi_i^2. \quad (6.19)$$

By Theorem 6.4, $u_{k+1} = u_0 + \mathcal{Q}_k(A)r_0$ where $\mathcal{Q}_k$ is a polynomial of degree k such that $\|u_{k+1} - \hat{u}\|_A$ is a minimum on $\text{span}\{A^i r_0\}_{i=0}^k$. This implies that

$$u_{k+1} - \hat{u} = [I + A\mathcal{Q}_k(A)](u_0 - \hat{u}). \quad (6.20)$$

Then

$$\|u_{k+1} - \hat{u}\|_A^2 = (u_0 - \hat{u})^T A [I + A\mathcal{Q}_k(A)]^2 (u_0 - \hat{u}) \quad (6.21)$$

$$= \sum_{i=1}^n [1 + \lambda_i \mathcal{Q}_k(\lambda_i)]^2 \lambda_i \xi_i^2 \quad (6.22)$$

$$= \sum_{i=1}^n [1 + \lambda_i \mathcal{Q}_k(\lambda_i)]^2 \|u_0 - \hat{u}\|_A^2 \quad (6.23)$$

$$\leq \max_{\lambda_i} [1 + \lambda_i \mathcal{P}_k(\lambda_i)]^2 \|u_0 - \hat{u}\|_A^2, \quad (6.24)$$

where $\mathcal{P}_k$ is any polynomial of degree k . □

The next theorem shows the effect of eigenvalue clustering on the convergence of the conjugate gradient method.

Theorem 6.6 If A has m distinct eigenvalues, then the conjugate gradient method converges to the solution vector, $\hat{u} = A^{-1}b$, in at most m iterations [19].

Proof: If there are m distinct eigenvalues, choose the polynomial $\mathcal{P}_{m-1}$ of Lemma 6.5 such that its zeros occur at the eigenvalues λ_i . Then $\|u_m - \hat{u}\|_A^2 = 0$. $\square$

Corollary 6.7 The conjugate gradient method converges to the solution, $\hat{u} = A^{-1}b$, in at most n iterations [19].

Proof: The matrix A has at most n eigenvalues. Apply Theorem 6.6. $\square$

The condition number of a matrix will now be defined, followed by a discussion of the effect of the condition number of A on the convergence of the conjugate gradient method.

Definition 6.8 The *condition number* of a nonsingular square matrix A is

$$\text{cond}(A) = \|A\|_2 / \|A^{-1}\|_2, \quad (6.25)$$

where $\|\cdot\|_2$ denotes the matrix 2-norm,

$$\|A\|_2 = \max_{\|u\|_{\ell^2}=1} \|Au\|_{\ell^2}. \quad (6.26)$$

If A is singular, then $\text{cond}(A) = \infty$. The matrix A is said to be *well-conditioned* if $\text{cond}(A) \approx 1$. If A is an $n \times n$ symmetric, positive definite matrix, then $\text{cond}(A) = \lambda_1 / \lambda_n$, where λ_1 and λ_n denote the largest and smallest eigenvalues of A , respectively.

Theorem 6.9 The rate of convergence of the conjugate gradient method depends on the condition number of the matrix [3] as follows:

$$\|u_j - \hat{u}\|_A \leq 2\|u_0 - \hat{u}\|_A \left(\frac{\sqrt{\text{cond}(A)} - 1}{\sqrt{\text{cond}(A)} + 1} \right)^j. \quad (6.27)$$

Proof: Select the polynomial $\mathcal{P}_{k-1}(\lambda)$ in Lemma 6.5 to be such that

$$1 + \lambda \mathcal{P}_{k-1}(\lambda) = T_k \left(\frac{\lambda_1 + \lambda_n - 2\lambda}{\lambda_1 - \lambda_n} \right) / T_k \left(\frac{\lambda_1 + \lambda_n}{\lambda_1 - \lambda_n} \right), \quad (6.28)$$

where T_k denotes the k^{th} degree Chebyshev polynomial, and λ_1 and λ_n denote the largest and smallest eigenvalues of A , respectively. The k^{th} degree Chebyshev polynomial can be expressed (see [3, p. 423]) as

$$T_k(x) \stackrel{\text{def}}{=} \frac{1}{2} \left[(x + \sqrt{x^2 - 1})^k + (x - \sqrt{x^2 - 1})^k \right]. \quad (6.29)$$

Then

$$\|u_k - \hat{u}\|_A^2 \leq [1 + \lambda_1 \mathcal{P}_{k-1}(\lambda_1)]^2 \|u_0 - \hat{u}\|_A^2 \quad (6.30)$$

$$= \left[\frac{T_k(-1)}{T_k \left(\frac{\lambda_1 + \lambda_n}{\lambda_1 - \lambda_n} \right)} \right]^2 \|u_0 - \hat{u}\|_A^2 \quad (6.31)$$

$$= \left[T_k \left(\frac{\text{cond}(A) + 1}{\text{cond}(A) - 1} \right) \right]^{-2} \|u_0 - \hat{u}\|_A^2 \quad (6.32)$$

$$= 4 \left[\left(\frac{\sqrt{\text{cond}(A)} + 1}{\sqrt{\text{cond}(A)} - 1} \right)^k + \left(\frac{\sqrt{\text{cond}(A)} - 1}{\sqrt{\text{cond}(A)} + 1} \right)^k \right]^{-2} \|u_0 - \hat{u}\|_A^2 \quad (6.33)$$

$$\leq 4 \left(\frac{\sqrt{\text{cond}(A)} + 1}{\sqrt{\text{cond}(A)} - 1} \right)^{-2k} \|u_0 - \hat{u}\|_A^2, \quad (6.34)$$

which proves the result. $\square$

Theorems 6.6 and 6.9 lead to the observation that if A is a well-conditioned $n \times n$ matrix, and/or A has $m \ll n$ distinct eigenvalues, the conjugate gradient

method will exhibit rapid convergence. However, the matrices in question, (6.1) and (6.2) are not well-conditioned. To effectively use the conjugate gradient method in such a case, it is expedient to implement a preconditioner to improve performance. This is done by choosing a preconditioning matrix, C , such that $\text{cond}(CA) \ll \text{cond}(A)$ and/or CA has far fewer distinct eigenvalues than A , and $Cy = w$ is easy to solve for y . The first two requirements will ensure faster convergence, while the third condition is necessary for rapid calculation inside the method itself.

Algorithm 6.10 The *preconditioned conjugate gradient method* is defined by the following algorithm.

Choose $u_0 \in \mathbb{R}^n$. Then

$$r_0 = Au_0 - b. \quad (6.35)$$

$$h_0 = C^{-1}r_0 \quad (6.36)$$

$$d_0 = -h_0 \quad (6.37)$$

$$(6.38)$$

For $k = 0, 1, \dots$,

$$a_k = \frac{\langle r_k, h_k \rangle}{\langle d_k, d_k \rangle_A} \quad (6.39)$$

$$u_{k+1} = u_k + a_k d_k \quad (6.40)$$

$$r_{k+1} = Au_{k+1} - b \quad (6.41)$$

$$h_{k+1} = C^{-1}r_{k+1} \quad (6.42)$$

$$c_k = \frac{\langle r_{k+1}, h_{k+1} \rangle}{\langle r_k, h_k \rangle} \quad (6.43)$$

$$d_{k+1} = -h_{k+1} + c_k d_k. \quad (6.44)$$

Note that for a symmetric, positive definite C , this algorithm is equivalent to performing the conjugate gradient method of Definition 6.1 to minimize the functional

$$\tilde{f}(v) \stackrel{\text{def}}{=} \frac{1}{2} \langle \tilde{u}, \tilde{A}v \rangle - \langle \tilde{u}, \tilde{b} \rangle, \quad (6.45)$$

where $\tilde{A} = C^{-1/2}AC^{-1/2}$, $\tilde{b} = C^{-1/2}b$, and $\tilde{u} = C^{1/2}u$. To see this, assume Algorithm 6.1 is applied to minimize $\tilde{f}$, and let

$$\bar{u}_{k+1} = C^{-1/2}\tilde{u}_{k+1} \quad (6.46)$$

and

$$\bar{r}_{k+1} = C^{-1/2}\tilde{r}_{k+1} \quad (6.47)$$

$$= C^{-1/2}(\tilde{A}\tilde{u}_{k+1} - \tilde{b}). \quad (6.48)$$

Note that $\bar{u}_{k+1}$ is not the same as u_{k+1} unless $C = I$. Then equation (6.12) of Algorithm 6.1 can be rewritten as

$$\tilde{r}_{k+1} = \tilde{A}\tilde{u}_{k+1} - \tilde{b} \quad (6.49)$$

$$= C^{-1/2}(A\bar{u}_{k+1} - b) \quad (6.50)$$

or

$$\bar{r}_{k+1} = A\bar{u}_{k+1} - b. \quad (6.51)$$

This is equation (6.41) of Algorithm 6.10. Similarly, the other steps of the two algorithms can be shown to be equivalent.

The explicit implementation of the preconditioned conjugate gradient method for operators (6.1) and (6.2) arising in the fixed point iteration will now be discussed. It should be noted that the discretization U is used in place of u in the preconditioned conjugate gradient algorithm.

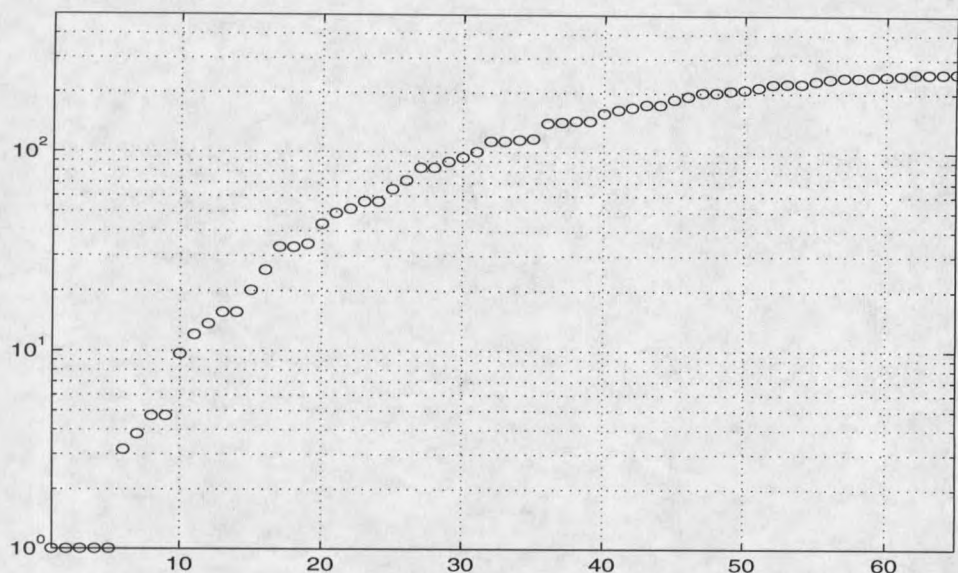


Figure 3: Eigenvalues of the matrix $I + \alpha L_\beta(U)$ where $\alpha = 10^{-2}$ and $\beta = 10^{-4}$. The vertical axis represents magnitude.

Multigrid preconditioner for the differential operator L

To begin the task of finding a suitable preconditioner for (6.2), consider the simplified operator (6.1). In applications, this corresponds to the “denoising” problem mentioned in the introduction.

Figure 3 displays the spectrum of the discrete operator for a discontinuous u with $\alpha = 10^{-2}$ and $\beta = 10^{-4}$. Notice that $\text{cond}(I + \alpha L_\beta(U)) \approx 10^3$, which implies that the convergence of the conjugate gradient method may be slow. Figure 4 shows this possibility to be fact by depicting the convergence rate of the conjugate gradient method applied to the system with A as in (6.1) without any preconditioning.

The multigrid method is known to work well on elliptic problems with diffusivity bounded away from 0 (see [23]). For the problem described here, the diffusivity,

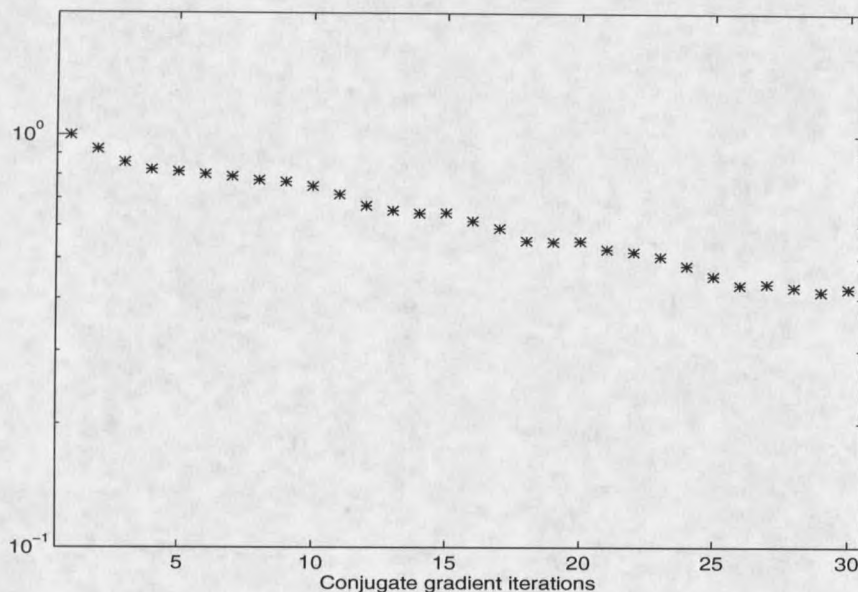


Figure 4: Relative residual norms of successive iterates of the conjugate gradient method to solve $(I + \alpha L_\beta(U^q))U^{q+1} = Z$ for a fixed q (no preconditioning), $\alpha = 10^{-2}$.

$1/\sqrt{|D_h U|^2 + \beta^2}$, is not bounded away from zero uniformly in h , hence, multigrid may not perform well. However, multigrid can be used effectively as a preconditioner for the conjugate gradient method. In this case, the preconditioning matrix C of Definition 6.10 is not explicitly given. Instead, steps (6.36) and (6.42) are completed by performing one multigrid iteration on the system $Ah = r$.

For simplicity, a two-grid scheme is presented here. A complete description of basic multigrid techniques and algorithms, is contained in [6] or [23]. For a bounded $\Omega \in \mathbb{R}^d$, $\Omega^h \subset \Omega$ will be defined to be a discrete set of n uniform grid points, where a uniform grid is understood to be a grid with mesh points which are equi-spaced in d directions with spacing h . To facilitate nested grids, h is taken to be $1/2^k$ where k is the number of nested grids, or levels, in the multigrid scheme. The lower-case symbols, h and n will be used to indicate, respectively, the mesh spacing and number

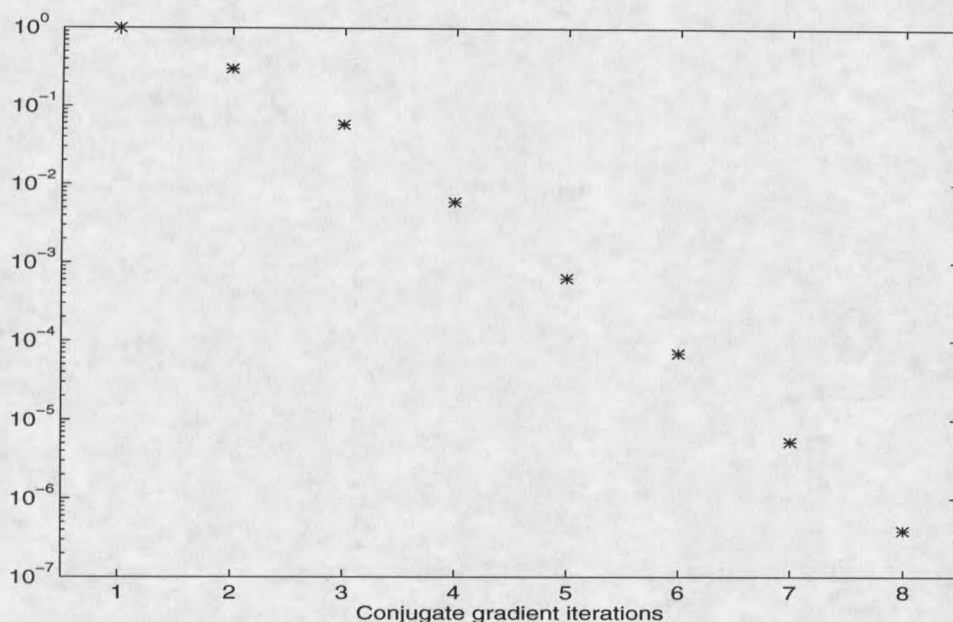


Figure 5: Relative residual norms of successive iterates of the conjugate gradient method with a multigrid preconditioner to solve $(I + \alpha L_\beta(U^q))U^{q+1} = Z$ for a fixed q , $\alpha = 10^{-2}$.

of nodes on the fine grid, and similarly the upper-case symbols, H and N define the coarse grid with $N \ll n$. For ease of reference, define A as in (6.1). Operators and grid functions will have the h or H superscript, dependent on the grid to which they belong. The operators Π_H^h and Π_h^H are coarse-to-fine (interpolation) and fine-to-coarse (projection) inter-grid transfer operators, respectively. The term “smoother” will henceforth be used to indicate a stationary linear solver, e.g., a Jacobi or Gauss-Seidel iteration.

Algorithm 6.11 A basic *multigrid cycle* on a two-grid system is outlined in the following manner:

- (i) Apply ν_1 iterations of the smoother to the system $A^h U^h = Z^h$ on Ω^h with initial guess V^h .

- (ii) Compute the residual, $r^H = \Pi_h^H(Z^h - A^h V^h)$.
- (iii) Solve $A^H e^H = r^H$ for the error on Ω^H .
- (iv) Correct the current V^h by setting $V^h = V^h + \Pi_H^h e^H$.
- (v) Apply ν_2 iterations of the smoother to the system $A^h U^h = Z^h$ on Ω^h with new initial guess, V^h .

On the coarsest grid, $A^H e^H = r^H$ is solved exactly if possible. To extend this to a multiple grid system, simply replace step 3 above by a recursive restart of the algorithm on the system $A^H e^H = r^H$ with initial guess $V^H = 0$. In practice, it is usually sufficient to set ν_1 and ν_2 small, such as 1 or 2.

For the system at hand, it has already been noted in Chapter 4 that A is a block tridiagonal matrix. Thus, a Gauss-Seidel iteration is easy to implement with grid operations; in other words, the actual matrix A does not need to be stored for any grid level. In the numerical experiments presented here, a red-black Gauss-Seidel iteration was used as the smoother [33]. This iteration is based on a checker-board layout of the grid which decouples the “red” and “black” grid nodes. The Gauss-Seidel iteration can then be implemented on the red and black nodes independently, making the iteration extremely computationally efficient. The intergrid transfer operators employed are those developed explicitly for the cell-centered finite difference discretization by Ewing and Shen [11]. These transfers can also be computed very efficiently since they involve only constant coefficients grid operators.

Figures 4 and 5 demonstrate the effectiveness of this preconditioning. Figure 4 depicts the relative residual norms of successive iterates of the conjugate gradient

method applied to the system $(I + \alpha L_\beta(U^q))U^{q+1} = Z$ for a fixed q . No preconditioning has been done, and it is easily seen that the convergence is quite slow. In Figure 5 the multigrid preconditioner described above has been applied to the same system, and the relative residual norms of successive iterates have again been plotted. Note the drastic improvement in the rate of convergence.

Preconditioning for the integro-differential operator

The case when K is the integral operator as in (1.2) will now be considered. This implies that the linear system to be solved at the q^{th} fixed point iteration is

$$AU^{q+1} = K_h^* Z, \quad (6.52)$$

where A is as in (6.2).

For insight into the choice of a preconditioner, consider the one-dimensional case on $0 \leq x \leq 1$ with $L_\beta(U)$ replaced by the negative Laplacian and periodic boundary conditions, where K is the convolution operator, $Ku = \int_0^1 k(x-y)u(y)dy$, with Gaussian convolution kernel, $k(x) = \sqrt{\frac{2}{\pi}}e^{-x^2/\sigma^2}$. Then L has eigenvalues $\lambda_j \stackrel{\text{def}}{=} j^2\pi^2$ which tend to infinity, K^*K has eigenvalues $\mu_j \stackrel{\text{def}}{=} \frac{2}{\pi}e^{-\sigma^2 j^2/2}$ which tend to zero, and L commutes with K . Figure 6 shows the first 64 eigenvalues of $K^*K + \alpha L$ where $\sigma = .075$ and $\alpha = 10^{-2}$. Notice that $\text{cond}(K^*K + \alpha L) \approx 10^3$.

This eigenvalue structure suggests a preconditioner of the form $C = bI + \alpha L$. This choice for C has eigenvalues $b + \alpha\lambda_j$; hence, as j gets larger, the eigenvalues of L dominate as they do for the matrix $K^*K + \alpha L$. For a proper choice of b , the matrix C^{-1} should be a rough approximation to $(K^*K + \alpha L)^{-1}$. With C in this form, the iteration matrix $C^{-1/2}(K^*K + \alpha L)C^{-1/2} = C^{-1}(K^*K + \alpha L)$ (since L and

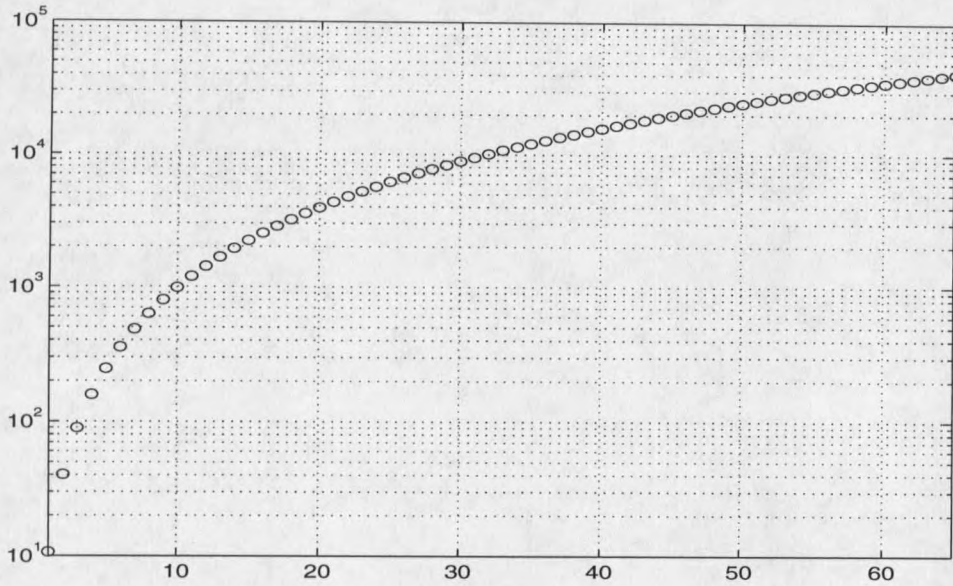


Figure 6: First 64 eigenvalues (in ascending order) of the operator $K^*K + \alpha L$ where $L = -\nabla^2$ and K is a convolution operator with kernel $k(x) = \left(\frac{2}{\pi}\right) e^{-x^2/\sigma^2}$, $\alpha = 10^{-2}$, $\sigma = .075$. The vertical axis represents magnitude.

K commute) has eigenvalues

$$\gamma_j = \frac{\mu_j + \alpha\lambda_j}{b + \alpha\lambda_j}, j = 1, 2, \dots \quad (6.53)$$

The γ_j 's tend to one as j goes to infinity, independent of b . To ensure $\gamma_j \approx 1$ for small values of j , choose the largest eigenvalue of K^*K for b ,

$$b = \rho(K^*K) = \mu_1 = \frac{2}{\pi} e^{-\sigma^2/2} \quad (6.54)$$

where $\rho(K^*K)$ denotes the spectral radius of K^*K .

Figure 7 shows the eigenvalues of the iteration matrix $C^{-1}(K^*K + \alpha L)$, which result from this choice of b . Notice that the condition number of this matrix is approximately 1. This implies that the conjugate gradient method will converge very rapidly.

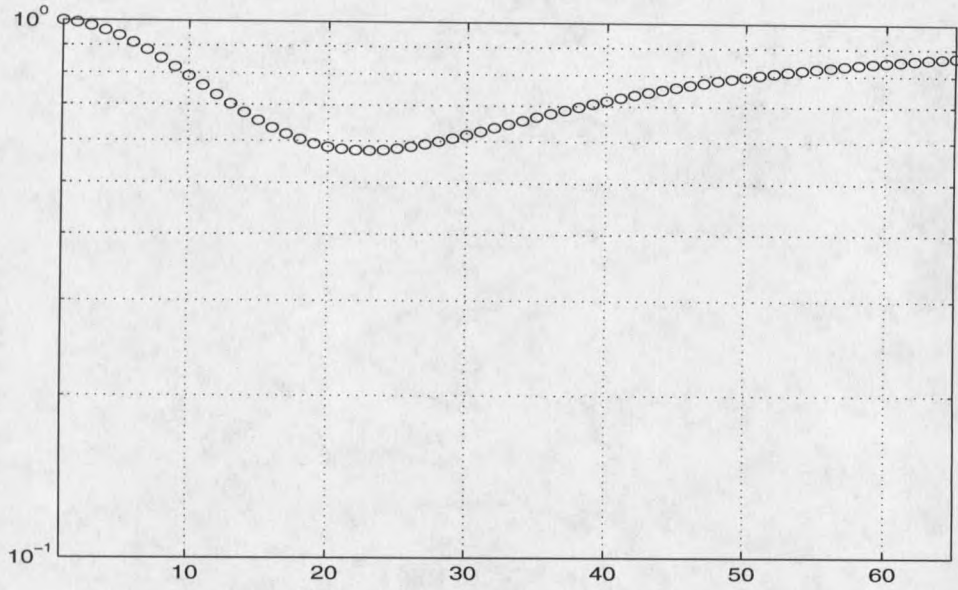


Figure 7: First 64 eigenvalues of the preconditioned operator $C^{-1}(K^*K + \alpha L)$ (indexed according to the eigenvalues of L in ascending order), where $C = bI + \alpha L$, $L = -\nabla^2$, $b = \rho(K^*K)$, $\alpha = 10^{-2}$, and $\beta = 10^{-4}$. The vertical axis represents magnitude.

With the more general operator defined in (6.2), this choice of b is still reasonable as shown in Figures 8 and 9. In Figure 8, the eigenvalues of the matrix A are given. In this case, $\text{cond}(A) \approx 10^4$. Figure 9 shows the eigenvalues of the preconditioned matrix, $C^{-1/2}AC^{-1/2}$, where $C = bI + \alpha L_\beta(U)$ and $b = \rho(K^*K)$. Although the eigenvalues are not all near one as in the constant diffusivity case, most are near one. The “stray” eigenvalues appear to correspond to jump discontinuities in U . Thus, $C = bI + \alpha L_\beta(U)$ is an effective preconditioner for the non-constant diffusivity case as well.

Multi-level Quadrature

Algorithm 6.10 requires the application of the operator $K_h^*K_h$. Commonly

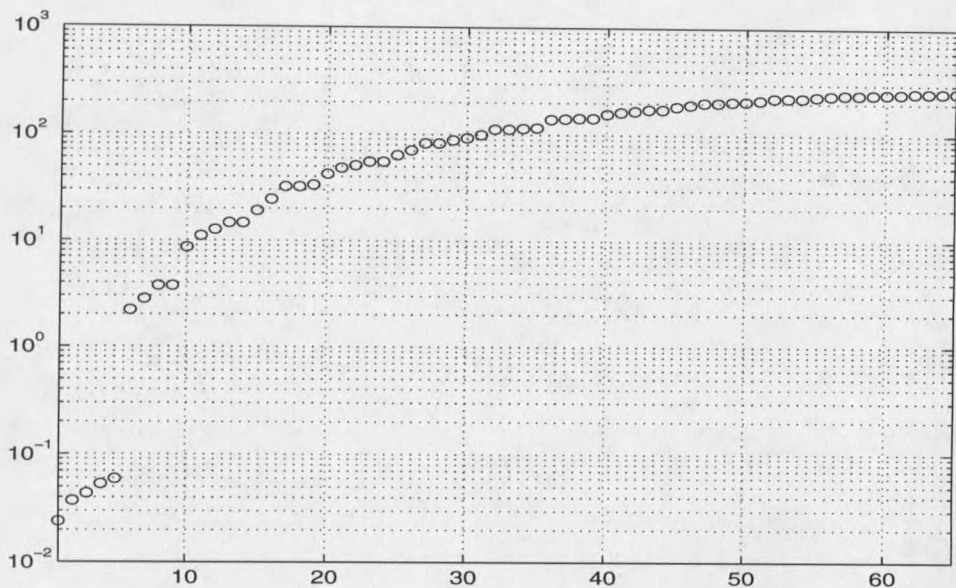


Figure 8: Eigenvalues of the matrix $A = K_h^* K_h + \alpha L_\beta(U)$, where $\alpha = 10^{-2}$, $\beta = 10^{-4}$, and $L_\beta(U)$ is a non-constant diffusion operator. The vertical axis represents magnitude.

used numerical techniques for evaluating discrete representations of integral operators applied to grid functions require $\mathcal{O}(n^2)$ floating point operations. In [5], Brandt and Lubrecht describe a method based on multigrid techniques for approximately evaluating an integral operator $\tilde{K} \stackrel{\text{def}}{=} K^* K$ applied to v which requires only $\mathcal{O}(n)$ operations. The following is a brief description of this technique.

The two-grid system in one dimension will be as defined previously for the multigrid preconditioner. The domain Ω^h will again be defined to be a set of n equispaced grid points, where $n = \text{vol}(\Omega)/h$, for Ω a connected domain in $\mathbb{R}$. And h will again be taken to be $1/2^k$ where k is the number of nested grids, or levels, in the multigrid scheme.

With $\tilde{K}^h$ denoting the discretization of the integral operator $\tilde{K}$ on the finest

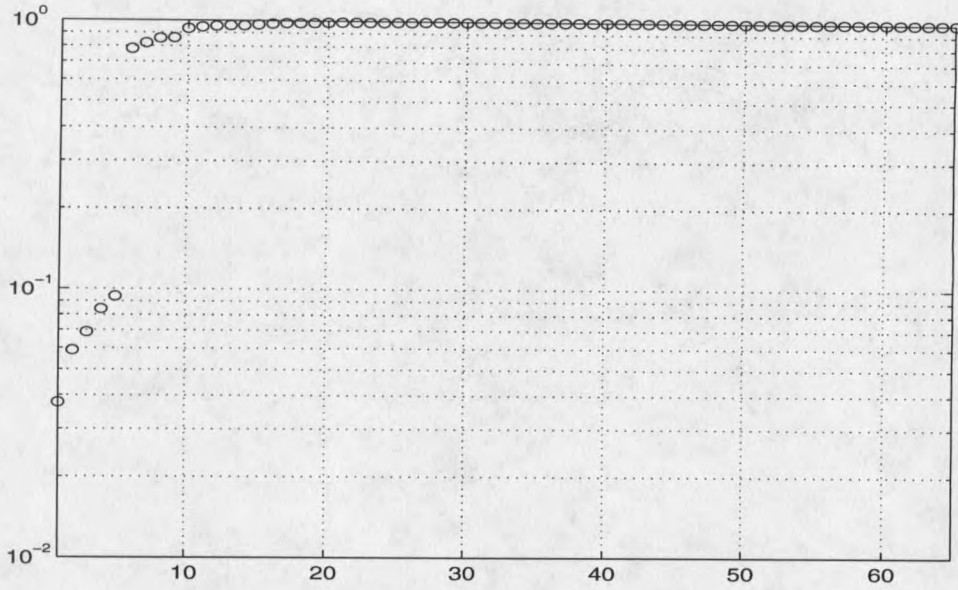


Figure 9: Eigenvalues of the preconditioned matrix $C^{-1/2}AC^{-1/2}$, where $C = bI + \alpha L_\beta(U)$ and $b = \rho(K^*K)$, $\alpha = 10^{-2}$, $\beta = 10^{-4}$. The vertical axis represents magnitude.

grid, the method of Brandt and Lubrecht [5] can be represented symbolically as

$$\tilde{K}v \approx \tilde{K}^h V^h \approx \Pi_H^h \tilde{K}^H (\Pi_h^H V^h). \quad (6.55)$$

As before, h and n indicate, respectively, the mesh spacing and number of nodes on the fine grid, and similarly, H and N define the coarse grid with $N \ll n$. The operators Π_H^h and Π_h^H are coarse-to-fine and fine-to-coarse inter-grid transfer operators, respectively. The lower case v denotes the continuous function, while the upper case V denotes the grid function. The superscripts h and H distinguish between the fine and coarse grid functions, and the subscripts i and I refer to the components of the fine and coarse grid functions, respectively. For example, V_i^h denotes the approximation to $v(x_i^h)$. This is in contrast to the multi-indexing with i and I which appears in Chapter 4.

To evaluate $\tilde{K}^h V^h$ cheaply, restrict V^h to the coarse grid, apply the coarse grid

operator $\tilde{K}^H$ at a cost of $\mathcal{O}(N^2)$ operations, and then interpolate $\tilde{K}^H V^H$ back to the fine grid. To see the details of this approximation, choose q^{th} order transfer operators: Π_H^h , a coarse-to-fine mesh transfer (interpolation), and Π_h^H , a fine-to-coarse mesh transfer (restriction). Using p^{th} order quadrature, the operation becomes

$$\begin{aligned}
 [\tilde{K}v](x_I^H) &= \int_0^1 \tilde{k}(x_I^H, y) v(y) dy, \quad I = 1, \dots, N \\
 &= h \sum_{j=1}^n \tilde{k}(x_I^H, x_j^h) V_j^h + \mathcal{O}(h^p) \\
 &= h \sum_{j=1}^n [\tilde{k}(x_I^H, x_j^H) \Pi_H^h]_j V_j^h + \mathcal{O}(h^p) + \mathcal{O}(H^q) \\
 &= h \sum_{J=1}^N \tilde{k}(x_I^H, x_J^H) [(\Pi_H^h)^T V^h]_J + \mathcal{O}(h^p) + \mathcal{O}(H^q)
 \end{aligned} \tag{6.56}$$

The coarse-grid function, $[\tilde{K}v](x_I^H)$, can then be interpolated to the fine grid by Π_H^h with $\mathcal{O}(H^q)$ accuracy. The entire application looks like

$$\tilde{K}^h V^h = \Pi_H^h \tilde{K}^H (\Pi_H^h)^T V^h + \mathcal{O}(h^p) + \mathcal{O}(H^q). \tag{6.57}$$

If $N^2 \approx n$ and $q = 2p$, then $H^q \approx h^p$, and this calculation requires only $\mathcal{O}(n)$ operations and maintains $\mathcal{O}(h^p)$ accuracy. To see this, let $n = 2^{\text{lev}}$ ($\text{lev} \in \mathbb{Z}^+$ is the number of levels, or nested grids), and let $n + 1$ be the number of points in the finest mesh with spacing $h = \frac{1}{n}$, and let the coarsest mesh have $N + 1$ points with spacing $H = \frac{1}{N}$ where $N = 2^{\text{lev}/2}$. With second order quadrature ($p = 2$), $K^H \Pi_h^H V^h$ can be calculated in $\mathcal{O}(N^2) = \mathcal{O}((2^{\text{lev}/2})^2) = \mathcal{O}(n)$ operations. Fourth order transfer operators ($q = 4$) ensure that the accuracy of $\Pi_H^h \tilde{K}^H \Pi_h^H V^h$ is $\mathcal{O}(h^2) + \mathcal{O}(H^4) = \mathcal{O}(h^2)$. Note that $\Pi_h^H = c(\Pi_H^h)^T$, with $c = H/h$; hence, the operator $\Pi_H^h \tilde{K}^H (\Pi_H^h)^T$ is symmetric when $\tilde{K}$ is a symmetric integral operator.

Algorithm for the Linear System

The algorithm used to solve the linear systems arising from the fixed point

iteration can now be presented.

Algorithm 6.12 The algorithm to solve $(K_h^* K_h + \alpha L_\beta(U^q)) U^{q+1} = K_h^* Z$ is as follows.

- (i) Apply the preconditioned conjugate gradient method to the system with preconditioner $C = bI + \alpha L_\beta(U^q)$ where $b = \rho(K^* K)$.
- (ii) Within this preconditioned conjugate gradient method, use multi-level quadrature to apply $K_h^* K_h$.
- (iii) Within each iteration of the preconditioned conjugate gradient method, solve equations of the form $Cv = (bI + \alpha L_\beta(U))v = f$ by the preconditioned conjugate gradient method with the multigrid preconditioner described.

It should be noted that the preconditioner $C = bI + \alpha L_\beta(u)$ is essentially the same as the operator in a fixed point iteration of the denoising problem (6.1); thus, solving $Cv = f$ for v utilizing the multigrid preconditioned conjugate gradient technique is of the same complexity as the linear solver for a fixed point iteration in the denoising problem. The multi-level integration is $\mathcal{O}(n)$ as shown in Chapter 6 and in [5]. Therefore, the preconditioned conjugate gradient method to solve $(K_h^* K_h + \alpha L_\beta(U^{(q)}))U^{(q+1)} = K_h^* Z$ is a very efficient operation.

CHAPTER 7

Numerical Implementation and Results

The numerical results of applying the methodology described previously are given here, both for denoising and deconvolution. The data sets for one-dimensional denoising and for two-dimensional deconvolution are synthetically created as will be described. In the case of two-dimensional denoising, actual LCSM data is used. Aside from displaying the reconstructed images, this chapter briefly explores the roles of the parameters α and β in the reconstruction process. The chapter concludes with demonstrations of convergence for the fixed point iteration and the preconditioned conjugate gradient method.

Denoising

First consider the one-dimensional test problem of denoising data. This corresponds to the case where $K = I$. Note that in this case the linear operator which arises in the fixed point iteration is a tridiagonal, symmetric positive definite matrix. For the discussion here, the exact (noise-free) solution is

$$u_{\text{exact}}(x) = \chi_{[1/6, 1/4]} + \frac{3}{2}\chi_{[1/3, 5/8]}, \quad (7.1)$$

where $\chi_{[a,b]}$ denotes the indicator function for the interval $a \leq x \leq b$. The data was generated by evaluating u_{exact} at $N = 128$ equi-spaced points in the interval

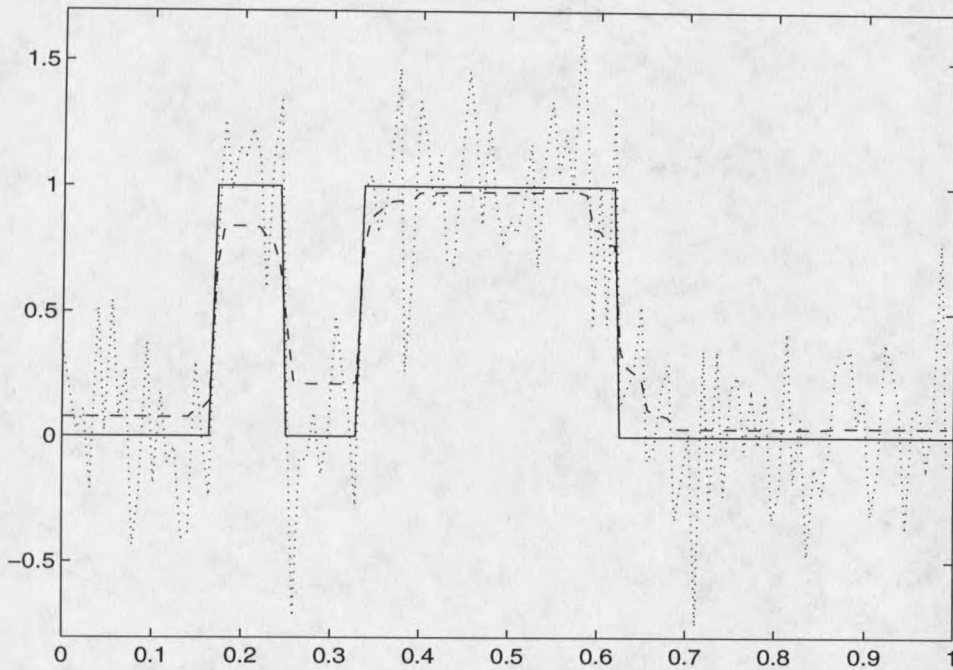


Figure 10: The true solution (solid line), noisy data (dotted line), and reconstruction (dashed line) on a 128-point mesh with a noise-to-signal ratio of .5 (denoising), $\alpha = 10^{-2}$, $\beta = 10^{-4}$.

$0 \leq x \leq 1$ and adding pseudo-random, uncorrelated error (so-called “discrete white noise”) $\{\epsilon_i\}_{i=1}^N$ having a Gaussian distribution with mean 0 and variance s^2 selected so the noise to signal ratio

$$\sqrt{\frac{E(\sum_{i=1}^N \epsilon_i^2)}{\sum_{i=1}^N u(x_i)^2}} = 0.5. \quad (7.2)$$

Figure 10 depicts the true solution, the noisy data, and the reconstruction utilizing the fixed point method. In this reconstruction $\alpha = 10^{-2}$ and $\beta = 10^{-4}$.

Figure 11 shows the recovered images for various α 's, $0 < \alpha_1 < \alpha_2 < \alpha_3$. As expected, a large α causes a loss of features in the solution, since the regularization functional is given so much weight in the minimization functional, that the first term, $\frac{1}{2}\|Ku - z\|^2$ is inconsequential. With a small value for α , very little regularization is done; hence, the reconstruction retains much of the noise of the data.

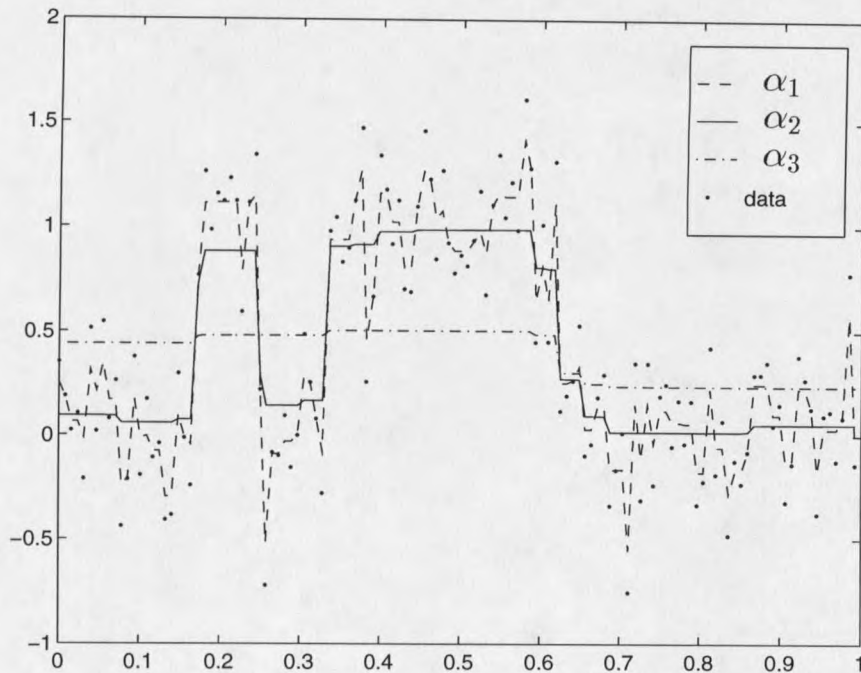


Figure 11: Recovery of u from noisy data (denoising) for various α values, $\alpha_1 = 10$, $\alpha_2 = 10^{-2}$, and $\alpha_3 = 10^{-4}$ on a 128-point mesh.

As a two-dimensional example, consider Figures 12 and 13. Figure 12 depicts an actual LCSM scan of rod-shaped bacteria on a stainless steel surface. The vertical axis represents light intensity, while the horizontal axes represent scaled pixel locations on a 64×64 grid. Figure 13 is a total variation reconstruction obtained using 10 iterations of the fixed point algorithm with a multigrid preconditioned conjugate gradient method to solve the linear systems at each fixed point iteration. The linear operator which arises in the two-dimensional denoising case is a block tridiagonal, symmetric positive definite matrix. In this reconstruction, $\alpha = .05$, $\beta = 10^{-4}$, and there were 10 fixed point iterations done with a conjugate gradient tolerance of 10^{-5} . Figure 14 plots the norm of the gradient,

$$g(U^{q+1}) = (I + \alpha L_\beta(U^q))U^{q+1} - Z, \quad (7.3)$$

for successive fixed point iterations. The decrease in the gradient indicates conver-

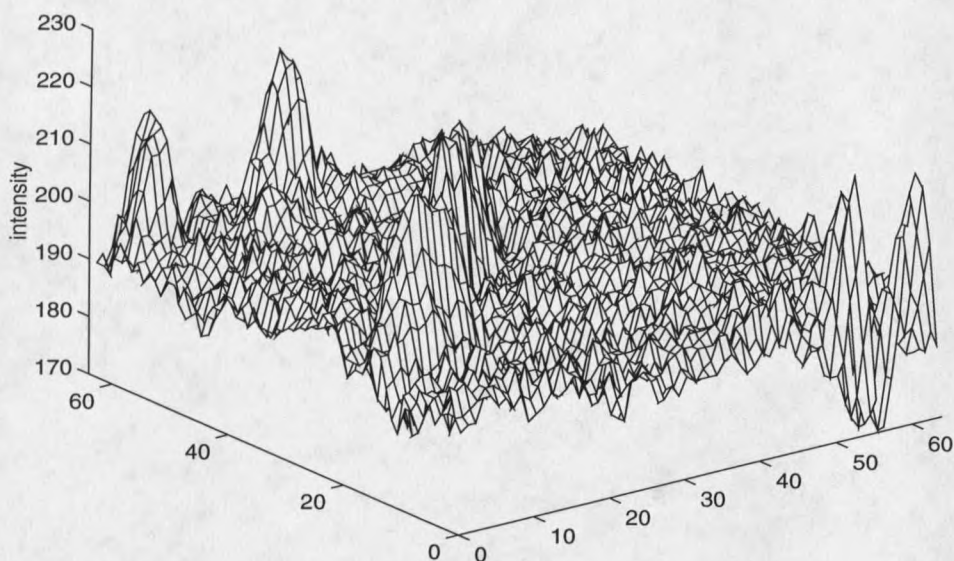


Figure 12: A scanning confocal microscope image of rod-shaped bacteria on a stainless steel surface.

gence of the iteration.

Deconvolution

Herein results for the two-dimensional deconvolution problem will be discussed. First, the reconstruction algorithm is outlined below with a special note on using the preconditioner $C = bI + \alpha L_\beta(u)$. Figures depicting the image reconstructions and numerical convergence studies follow.

Algorithm 7.1 An algorithm for the fast reconstruction of the image u from noisy, blurred data z via the minimization problem (1.8) of Chapter 1 with regularization functional J_β as defined in (3.7) of Chapter 3 and the subsequent discrete fixed point iteration (4.40) described in Chapter 4.

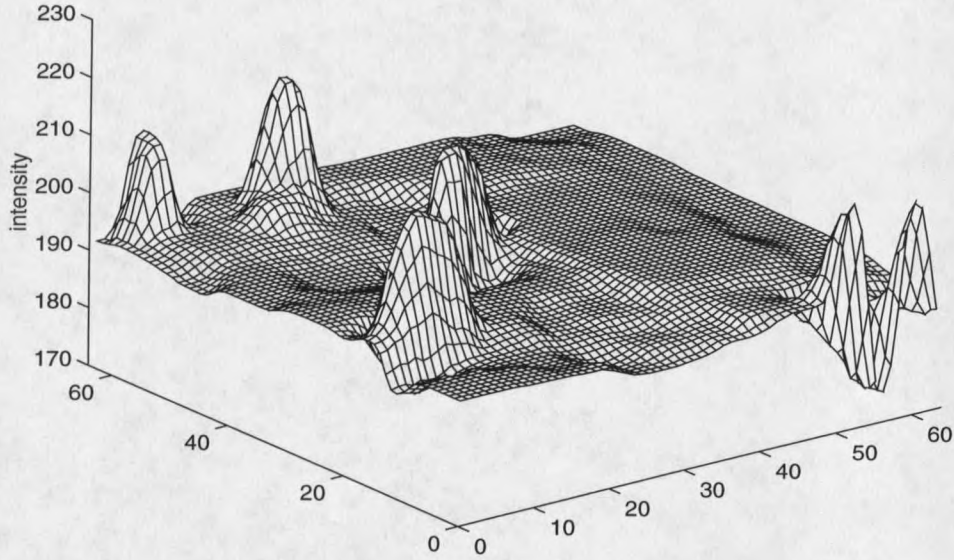


Figure 13: Reconstruction of LCSM data utilizing the fixed point algorithm and inner conjugate gradient method with a multigrid preconditioner, $\alpha = .05$, $\beta = 10^{-4}$.

(i) Apply fixed point iteration as in (4.40).

(ii) Solve linear system $(K_h^* K_h + \alpha L_\beta(U^q))U^{q+1} = K_h^* z$ by means of Algorithm 6.12 of Chapter 6.

It should be noted that the linear operator $K_h^* K_h + \alpha L_\beta(U^q)$ is a non-sparse, symmetric positive definite matrix.

In Figures 17 through 18, the operator K has been taken to be the integral operator

$$(Ku)(x_1, x_2) = \int_0^1 \int_0^1 k(y_1 - x_1, y_2 - x_2)u(y_1, y_2)dy_1 dy_2 \quad (7.4)$$

with Gaussian kernel,

$$k(x_1, x_2) = \left(\frac{2}{\pi}\right)^{1/2} e^{-(x_1^2 + x_2^2)/\sigma^2}. \quad (7.5)$$

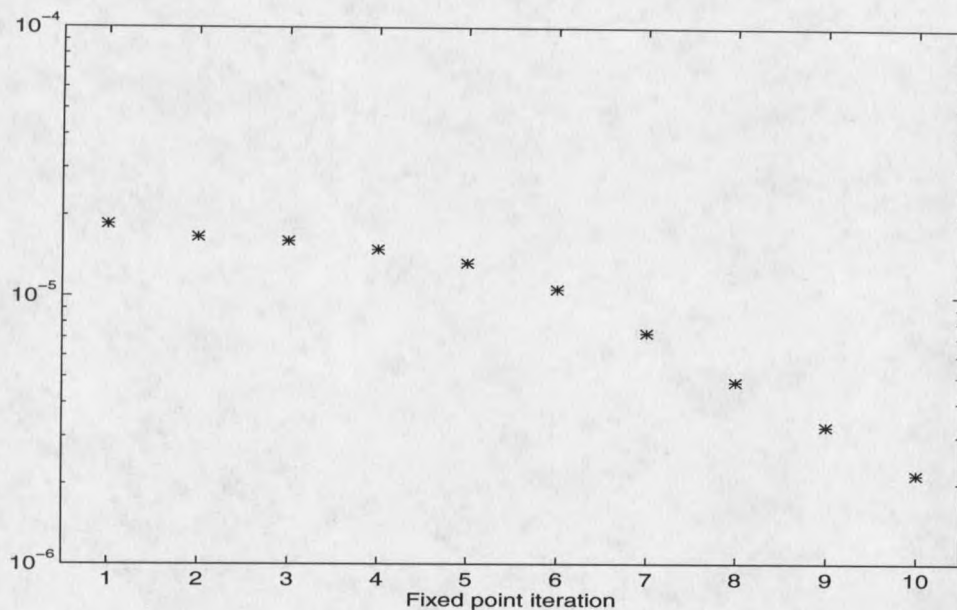


Figure 14: Norm of difference between successive fixed point iterates for two-dimensional denoising of an LCSM scan, measured in the L^1 norm.

Figures 15 through 17 show the noisy data, $z = Ku_{\text{exact}} + \epsilon$ (where ϵ is assumed to be Gaussian white noise as before), the exact solution, and the reconstruction obtained by the above algorithm for a two-dimensional example with noise-to-signal ratio = 1 and kernel-width parameter, $\sigma = .075$. Notice that in the data, the smaller feature is not discernible; however, this feature is detected by the reconstruction.

Figures 18, 19, and 20, present convergence results for this example. Figure 18 depicts the norms of the differences between successive iterates. This demonstrates the convergence of the fixed point iteration.

Figure 20 shows the norm of the gradient,

$$g(U) = K_h^*(K_h U^{q+1} - Z) + L_\beta(U^q)U^{q+1} \quad (7.6)$$

as in (4.39). Figures 18 and 20 indicate convergence. Figure 21 plots the preconditioned conjugate gradient convergence factor for each fixed point iteration where the

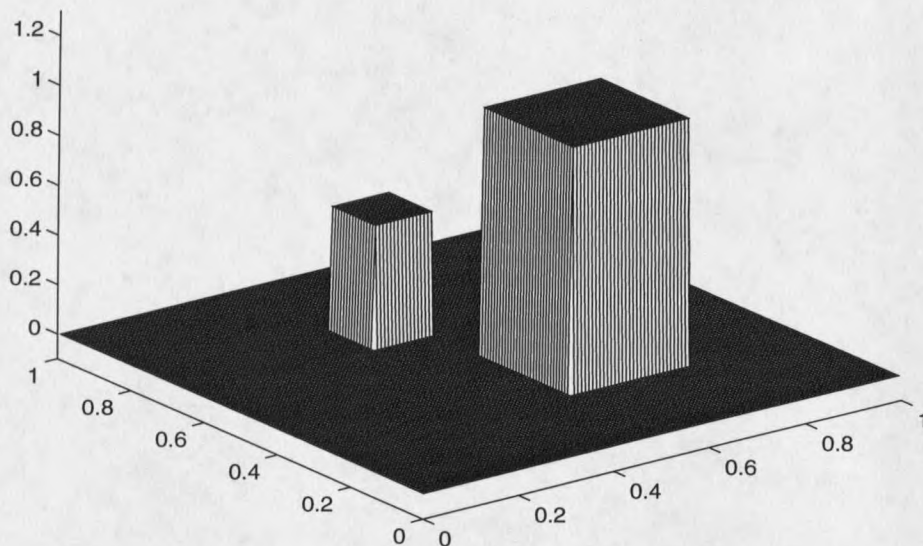


Figure 15: Exact 128×128 image. Vertical image represents light intensity.

geometric mean convergence factor is calculated by

$$\text{convergence factor} = \exp \left[\frac{1}{M} \sum_{m=1}^M \ln \left(\frac{res^{m+1}}{res^m} \right) \right] \quad (7.7)$$

where res^m is the residual calculated at the $(m-1)^{\text{st}}$ preconditioned conjugate gradient iterate. This demonstrates the robustness and effectiveness of the preconditioner, $C = bI + \alpha L_{\beta}(U^q)$.

Figure 19 records the norms of the residuals at each preconditioned conjugate gradient iteration for the tenth fixed point iteration. (This is preconditioning of the integral operator, $K_h^* K_h$.) Note the rapid residual decay obtained with the preconditioner $C = bI + \alpha L_{\beta}(U^q)$.

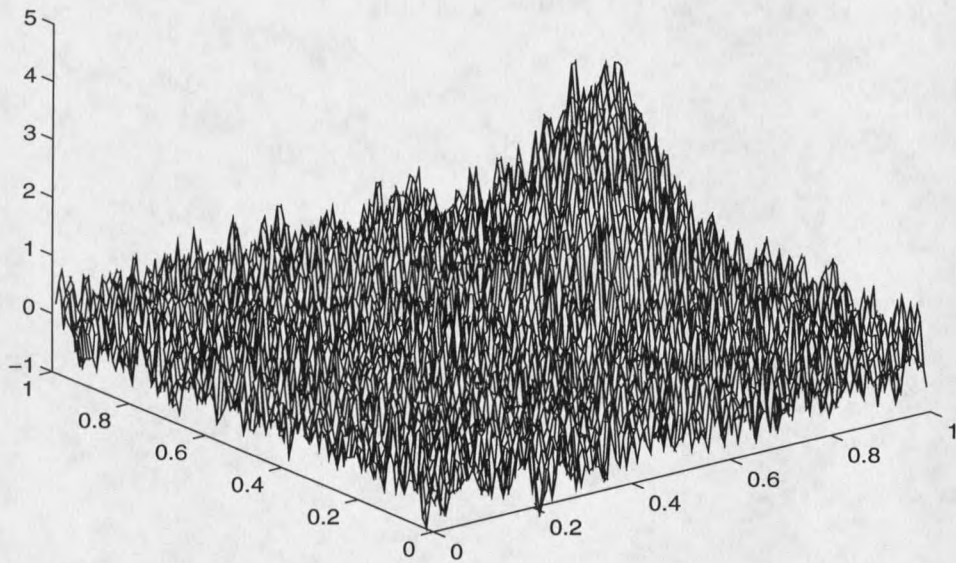


Figure 16: Data obtained by convolving the true image with the Gaussian kernel k (as indicated in text) with $\sigma = .075$, and adding noise with noise-to-signal ratio = 1. The vertical axis represents intensity.

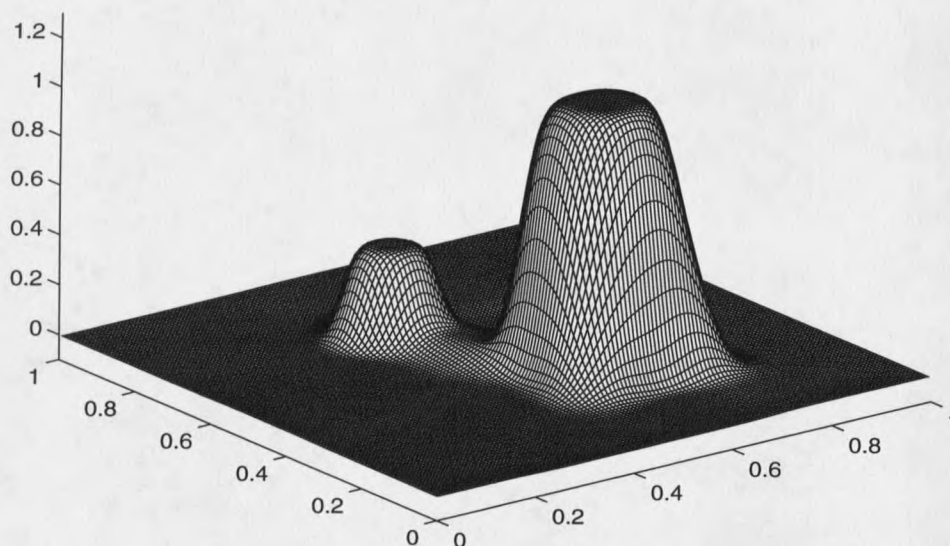


Figure 17: Reconstruction from blurred, noisy data using the fixed point algorithm with $\alpha = 10^{-2}$, $\beta = 10^{-4}$, and 10 fixed point iterations. The vertical axis represents light intensity.

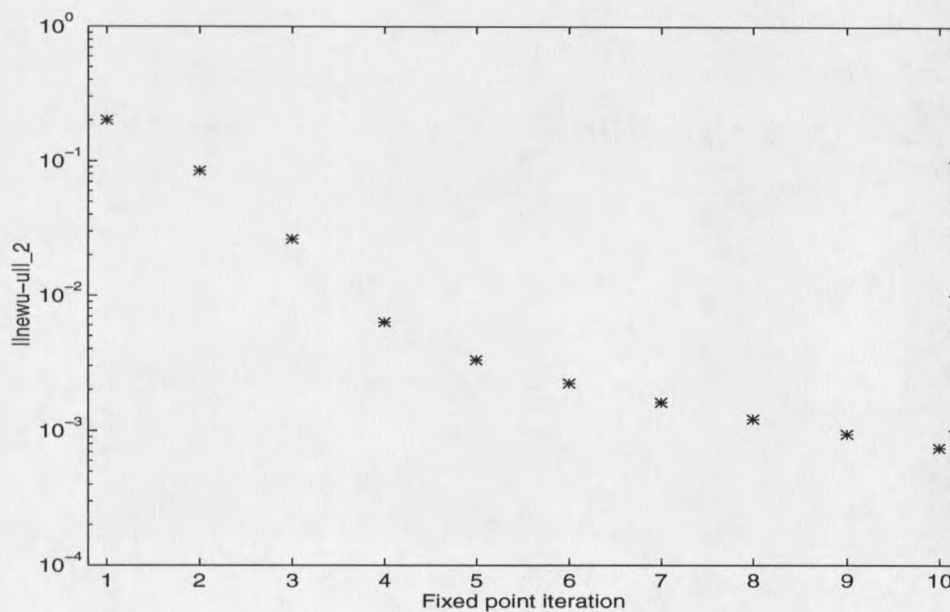


Figure 18: Differences between successive fixed point iterates, measured in the L^1 norm for deconvolution.

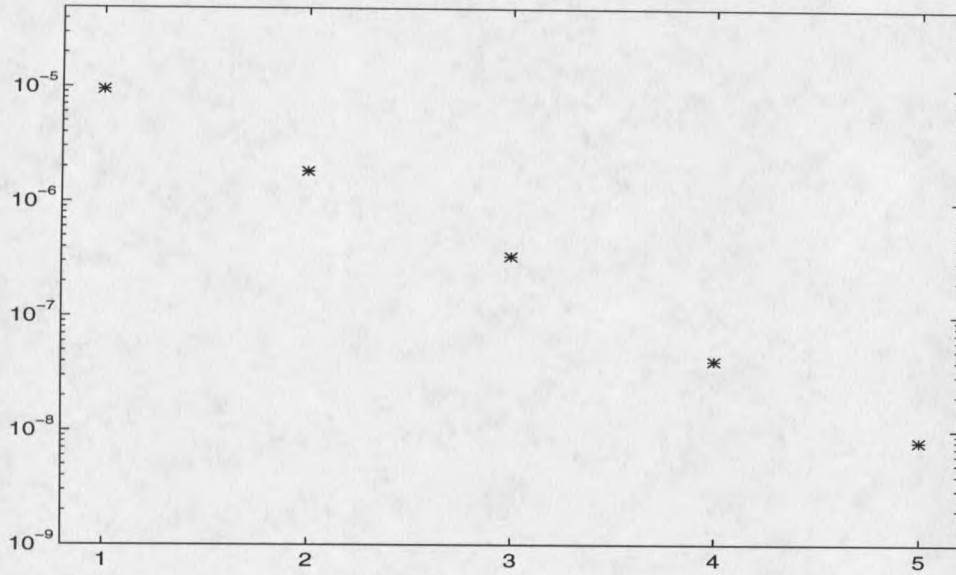


Figure 19: Norms (L^2) of successive residuals of five preconditioned conjugate gradient iterations at the tenth fixed point iteration. (The horizontal axis corresponds to the current conjugate gradient iteration.)

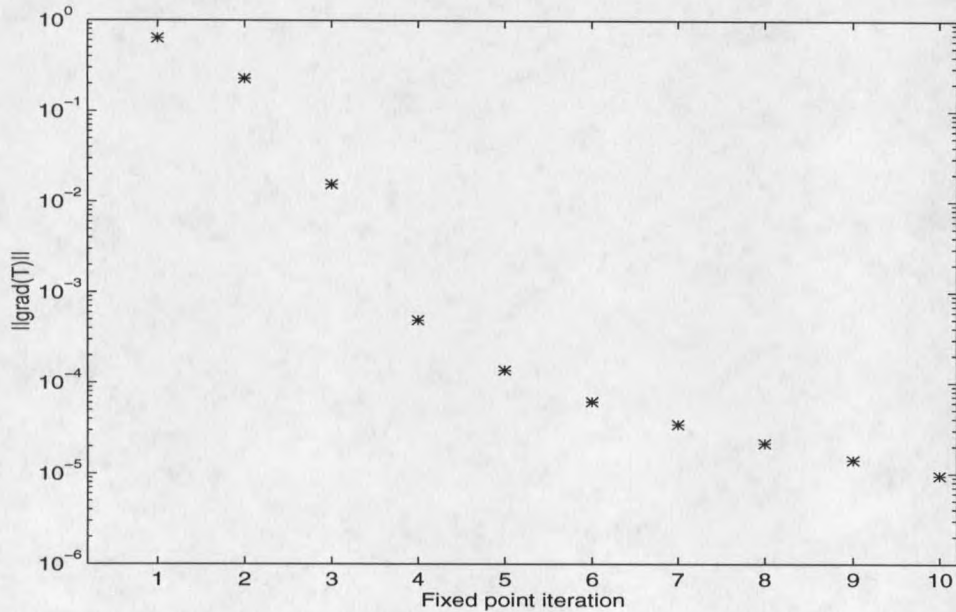


Figure 20: The L^2 norm of the gradient of T_α , at successive fixed point iterates for two-dimensional deconvolution.

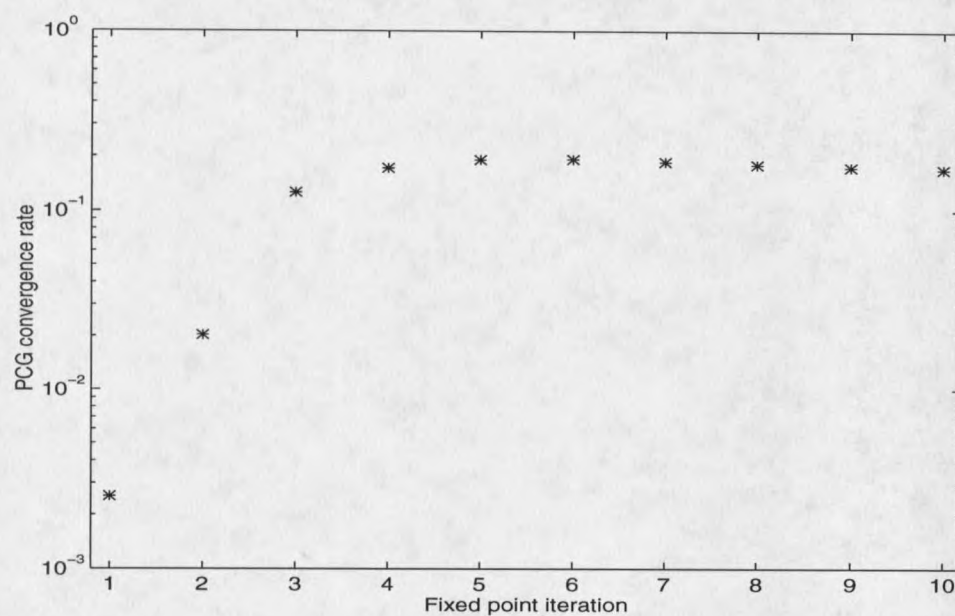


Figure 21: Geometric mean convergence factor for the preconditioned conjugate gradient at each fixed point iteration for deconvolution.

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