Discrete Inverse Problems

Fundamentals of Algorithms

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Insight and Algorithms

Society for Industrial and Applied Mathematics
Philadelphia

10 9 8 7 6 5 4 3 2 1

Library of Congress Cataloging-in-Publication Data:

Hansen, Per Christian.
Discrete inverse problems : insight and algorithms / Per Christian Hansen.
p. cm. -- (Fundamentals of algorithms series)
Includes bibliographical references and index.
ISBN 978-0-898716-96-2
1. Inverse problems (Differential equations) I. Title.
QA371.H365 2010
515'.357--dc22
2009047057

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Preface

Inverse problems are mathematical problems that arise when our goal is to recover "interior" or "hidden" information from "outside"—or otherwise available—noisy data. For example, an inverse problem arises when we reconstruct a two-dimensional (2D) or three-dimensional (3D) medical image from tomography data, or when we reconstruct a sharper image from a blurred one. When we solve an inverse problem, we compute the source that gives rise to some observed data, using a mathematical model for the relation between the source and the data.

Inverse problems arise in many technical and scientific areas, such as medical and geophysical imaging, electromagnetic scattering, and nondestructive testing. Image deblurring arises, e.g., in astronomy or in biometric applications that involve fingerprint or iris recognition. The underlying mathematics is rich and well developed, and there are many books devoted to the subject of inverse (and ill-posed) problems.

So why yet another book? My experience from teaching this subject to engineering graduate students is that there is a need for a textbook that covers the basic subjects and also focuses on the computational aspects. Moreover, I believe that practical computational experience is important for understanding applied mathematics, and therefore the textbook should include a number of tutorial exercises to give the reader hands-on experience with the difficulties and challenges associated with the treatment of inverse problems.

The title of the book reflects this point of view: our *insight* about inverse problems must go hand-in-hand with our *algorithms* for solving these problems. Solving an inverse problem is rarely a matter of just picking an algorithm from a textbook, a research paper, or a software package. My experience is that each new inverse problem has its own features and peculiarities, which must be understood before one can decide on an algorithm (or, sometimes, develop a new one).

The present book is intended as a quite gentle introduction to a field characterized by advanced mathematics and sophisticated numerical methods. The book does not pretend to tell the whole story, to give all the details, or to survey all the important methods and techniques. The aim is to provide the reader with enough background in mathematics and numerical methods to understand the basic difficulties associated with linear inverse problems, to analyze the influence of measurement and approximation errors, and to design practical algorithms for computing regularized/stabilized solutions to these problems. Provided with this insight, the reader will be able to start reading the more advanced literature on the subject; indeed, anyone who wants to work in the area of linear inverse problems is advised to also consult some of the many well-written books on the subject, such as [3], [8], [14], [23], [24], [32], [64], [74], [76].

The focus of the book is on linear inverse problems in the form of Fredholm integral equations of the first kind. The presentation starts with a summary of the most important properties of linear inverse problems in the continuous setting. Then we briefly discuss discretization methods and describe how many of the properties of the integral equation directly carry over to the discretized system—in the form of a linear (perhaps overdetermined) system of equations. The next chapter is devoted to simple regularization methods for computing regularized solutions in the form of filtered spectral expansions; this is an important class of methods which clearly illustrates the basic ideas of regularization. Since no regularization algorithm is complete without a method for choosing the regularization parameter, we also include a discussion of some state-of-the-art parameter choice methods. We conclude with a chapter on iterative methods for large-scale problems, a chapter with a some real-world problems, and a chapter on a more general class of regularization methods. Sections and exercises marked with a * denote more advanced material that can be skipped in a basic course.

At the end of each section we give a number of exercises, most of them involving numerical experiments with the MATLAB package *Regularization Tools* [31], [33], which further illustrate the concepts and methods discussed in the corresponding section. The package is available from Netlib at http://www.netlib.org/numeralgo and from the MATLAB Central File Exchange at http://www.mathworks.com/matlabcentral/fileexchange/loadFile.do?objectId=52. It must be emphasized that the package is mainly intended for teaching and experimenting with small-scale inverse problems, and therefore the package is not designed to be efficient for large problems.

Acknowledgments. This tutorial grew out of a series of lectures given at the Fifth Winter School in Computational Mathematics in Geilo, Norway, in February of 2005. The atmosphere there was very positive, and I enjoyed the chance to teach one of my favorite subjects to a dedicated audience. The presentation is based on many years of experience from numerous collaborations, too many to mention here, and I thank everyone I worked with for inspiration and motivation. In particular, I thank Zdeněk Strakoš for insightful discussions about regularizing iterations, Maurizio Fedi for sharing his insight in potential field inversion, Søren Holdt Jensen for introducing me to all kinds of noise, Jim Nagy for showing me that structure is everything in image deblurring, and Bill Lionheart for all kinds of thoughts on inverse problems. I also thank Ann Manning Allen, Elizabeth Greenspan, Nancy Griscom, and Sara Murphy from SIAM for their competent handling of this book.

Per Christian Hansen
Lyngby, 2009

List of Symbols

Symbol	Quantity	Dimension
A	coefficient matrix	$m \times n$
A_k	TSVD matrix	$m \times n$
$A_k^\dagger$	pseudoinverse of A_k	$n \times m$
b	right-hand side	m
B_k	lower bidiagonal matrix	$(k+1) \times k$
c_λ	curvature of Tikhonov L-curve in lin-lin scale	scalar
$\hat{c}_\lambda$	ditto in log-log scale	scalar
e	noise component in right-hand side	m
E	error in quadrature or expansion method	scalar
f	solution function (integral equation)	
g	right-hand side function (integral equation)	
G	GCV function	
h	grid spacing	scalar
I	identity matrix	
k	truncation parameter (TSVD)	integer
k_η	transition index	integer
K	kernel function (integral equation)	
$\mathcal{K}_k$	Krylov subspace of dimension k	
ℓ_i	eigenvalue of kernel	scalar
L	regularization matrix	$p \times n$
L_1	discrete 1. order derivative	$(n-1) \times n$
L_2	discrete 2. order derivative	$(n-2) \times n$
m, n	matrix dimensions, $m \geq n$	scalars
s, t	independent variables (integral equation)	
u_i	left singular function or vector	m
U	left singular matrix	$m \times n$
v_i	right singular function or vector	n
V	right singular matrix	$n \times n$
w_k	basis vectors of projection method; also CGLS and Lanczos vectors	n
W_k	matrix of basis vectors	$n \times k$

Symbol	Quantity	Dimension
x	"naive" solution	n
x_k, x_λ	TSVD and Tikhonov solutions	n
$x^{[k]}$	Landweber, Cimmino, ART iteration vector	n
$x^{(k)}$	solution computed via projection; also CGLS solution	n
$x_\lambda^{(k)}$	regularized solution via projection	n
$y^{(k)}$	solution to projected problem	k
α	relative decay of SVD coefficients	scalar
α_k, β_k	from bidiagonalization algorithm	scalars
$\bar{\alpha}_k$, $\bar{\beta}_k$	from CGLS algorithm	scalars
γ, γ_k, $\hat{\gamma}_k$, γ_λ	constants in perturbation bounds	scalars
Γ	Gamma function	
δ	upper bound on solution norm also delta function	scalar
ΔA	matrix perturbation	$m \times n$
Δb	right-hand side perturbation	m
ε	upper bound on residual norm	scalar
ε_k, ε_λ	TSVD and Tikhonov regularization errors	scalars
ζ_j	expansion coefficient	scalar
η	standard deviation for noise	scalar
κ_k, κ_λ	TSVD and Tikhonov condition numbers	scalars
λ	regularization parameter (Tikhonov)	scalar
μ_i	singular value of kernel	scalar
μ	safety factor (in various methods)	scalar
ξ, $\hat{\xi}$	solution norm squared, log of ditto	scalars
ρ, $\hat{\rho}$	residual norm squared, log of ditto	scalars
σ_i	singular value of matrix	scalar
Σ	diagonal matrix with singular values	$n \times n$
τ	threshold in SSVD method	scalar
ϕ_i, ψ_i	basis functions	
φ_i	generic filter factor	scalar
$\varphi_i^{[k]}$	filter factor for an iterative method	scalar
$\varphi_i^{[\lambda]}$	Tikhonov filter factor	scalar
$\Phi^{[\cdot]}$	diagonal matrix of filter factors	$n \times n$
Ψ	matrix used to generate colored noise	$m \times m$
χ_i	"top hat" ⎍ function	
ω_j	quadrature weight	scalar
$\langle \cdot, \cdot \rangle$	inner product	
$\Vert \cdot \Vert_2$, $\Vert \cdot \Vert_F$	2-norm and Frobenius norm	
$\mathrm{cond}(\cdot)$	condition number	
$\mathrm{Cov}(\cdot)$	covariance matrix	
$\mathcal{E}(\cdot)$	expected value	
$\mathrm{span}\{\cdots\}$	subspace spanned by vectors	
$\widetilde{\square}$	perturbed version of $\square$	