NUMERICAL METHODS FOR LEAST SQUARES PROBLEMS

NUMERICAL METHODS FOR LEAST SQUARES PROBLEMS

ÅKE BJÖRCK

Linköping University
Linköping, Sweden

siam.

Society for Industrial and Applied Mathematics
Philadelphia

10 9 8 7 6 5

Library of Congress Cataloging-in-Publication Data

Björck, Åke, 1934-
Numerical methods for least squares problems / Åke Björck.
p.cm.
Includes bibliographical references (p. -)and index.
ISBN 978-0-898713-60-2 (pbk.)
1. Equations, Simultaneous–Numerical solutions. 2. Least squares. I. Title.
QA214.B56 1996
512.9'42—dc20
96-3908

Dedicated to

Germund Dahlquist

and

Gene H. Golub

Contents

Chapter 1

Preface

A basic problem in science is to fit a model to observations subject to errors. It is clear that the more observations that are available the more accurately will it be possible to calculate the parameters in the model. This gives rise to the problem of "solving" an overdetermined linear or nonlinear system of equations. It can be shown that the solution which minimizes a weighted sum of the squares of the residual is optimal in a certain sense. Gauss claims to have discovered the method of least squares in 1795 when he was 18 years old. Hence this book also marks the bicentennial of the use of the least squares principle.

The development of the basic modern numerical methods for solving linear least squares problems took place in the late sixties. The QR decomposition by Householder transformations was developed by Golub and published in 1965. The implicit QR algorithm for computing the singular value decomposition (SVD) was developed about the same time by Kahan, Golub, and Wilkinson, and the final algorithm was published in 1970. These matrix decompositions have since been developed and generalized to a high level of sophistication. Great progress has been made in the last decade in methods for generalized and modified least squares problems and in direct and iterative methods for large sparse problems. Methods for total least squares problems, which allow errors also in the system matrix, have been systematically developed.

Applications of least squares of crucial importance occur in many areas of applied and engineering research such as statistics, geodetics, photogrammetry, signal processing, and control. Because of the great increase in the capacity for automatic data capturing, least squares problems of large size are now routinely solved. Therefore, sparse direct methods as well as iterative methods play an increasingly important role. Applications in signal processing have created a great demand for stable and efficient methods for modifying least squares solutions when data are added or deleted. This has led to renewed interest in rank revealing QR decompositions, which lend themselves better to updating than the singular value decomposition. Generalized and weighted least squares problems and problems of Toeplitz and Kronecker structure are becoming increasingly important.

Chapter 1 gives the basic facts and the mathematical and statistical background of least squares methods. In Chapter 2 relevant matrix decompositions and basic numerical methods are covered in detail. Although most proofs are omitted, these two chapters are more elementary than the rest of the book and essentially self-contained. Chapter 3 treats modified least squares problems and includes many recent results. In Chapter 4 generalized QR and SVD decompositions are presented, and methods for generalized and weighted problems surveyed. Here also, robust methods and methods for total least squares are treated. Chapter 5 surveys methods for problems with linear and quadratic constraints. Direct and iterative methods for large sparse least squares problems are covered in Chapters 6 and 7. These methods are still subject to intensive research, and the presentation is more advanced. Chapter 8 is devoted to problems with special bases, including least squares fitting of polynomials and problems of Toeplitz and Kronecker structures. Finally, Chapter 9 contains a short survey of methods for nonlinear problems.

This book will be of interest to mathematicians working in numerical linear algebra, computational scientists and engineers, and statisticians, as well as electrical engineers. Although a solid understanding of numerical linear algebra is needed for the more advanced sections, I hope the book will be found useful in upper-level undergraduate and beginning graduate courses in scientific computing and applied sciences.

I have aimed to make the book and the bibliography as comprehensive and up-to-date as possible. Many recent research results are included, which were only available in the research literature before. Inevitably, however, the content reflects my own interests, and I apologize in advance to those whose work has not been mentioned. In particular, work on the least squares problem in the former Soviet Union is, to a large extent, not covered.

The history of this book dates back to at least 1981, when I wrote a survey entitled "Least Squares Methods in Physics and Engineering" for the Academic Training Programme at CERN in Geneva. In 1985 I was invited to contribute a chapter on "Least Squares Methods" in the *Handbook of Numerical Analysis*, edited by P. G. Ciarlet and J. L. Lions. This chapter [95] was finished in 1988 and appeared in Volume 1 of the *Handbook*, published by North-Holland in 1990. The present book is based on this contribution, although it has been extensively updated and made more complete.

The book has greatly benefited from the insight and knowledge kindly provided by many friends and colleagues. In particular, I have been greatly influenced by the work of Gene H. Golub, Nick Higham, and G. W. Stewart. Per-Åke Wedin gave valuable advice on the chapter on nonlinear problems. Part of the *Handbook* chapter was written while I had the benefit of visiting the Division of Mathematics and Statistics at CSIRO in Canberra and the Chr. Michelsen Institute in Bergen.

Thanks are due to Elsevier Science B.V. for the permission to use part of the material from the *Handbook* chapter. Finally, I thank Beth Gallagher and Vickie Kearn at SIAM for the cheerful and professional support they have given throughout the copy editing and production of the book.

Åke Björck
Linköping, February 1996