## Springer Series in Operations Research

Editors:

Peter Glynn Stephen M. Robinson

## Springer

New York Berlin Heidelberg Barcelona Hong Kong London Milan Paris Singapore Tokyo

### **Springer Series in Operations Research**

Altiok: Performance Analysis of Manufacturing Systems

Birge and Louveaux: Introduction to Stochastic Programming

Bonnans and Shapiro: Perturbation Analysis of Optimization Problems

Bramel and Simchi-Levi: The Logic of Logistics: Theory, Algorithms, and Applications for Logistics Management

Dantzig and Thapa: Linear Programming 1: Introduction

Drezner (Editor): Facility Location: A Survey of Applications and Methods

Fishman: Discrete-Event Simulation: Modeling, Programming, and Analysis

Fishman: Monte Carlo: Concepts, Algorithms, and Applications

Nocedal and Wright: Numerical Optimization Olson: Decision Aids for Selection Problems

Yao (Editor): Stochastic Modeling and Analysis of Manufacturing Systems

## Jorge Nocedal Stephen J. Wright

## Numerical Optimization

With 85 Illustrations



Jorge Nocedal ECE Department Northwestern University Evanston, IL 60208-3118 USA Stephen J. Wright Mathematics and Computer Science Division Argonne National Laboratory 9700 South Cass Avenue Argonne, IL 60439-4844 USA

Series Editors:
Peter Glynn
Department of Operations Research
Stanford University
Stanford, CA 94305
USA

Stephen M. Robinson Department of Industrial Engineering University of Wisconsin–Madison 1513 University Avenue Madison, WI 53706-1572 USA

Cover illustration is from *Pre-Hispanic Mexican Stamp Designs* by Frederick V. Field, courtesy of Dover Publications, Inc.

Library of Congress Cataloging-in-Publication Data Nocedal, Jorge.

Numerical optimization / Jorge Nocedal, Stephen J. Wright.

p. cm. — (Springer series in operations research)

Includes bibliographical references and index.

ISBN 0-387-98793-2 (hardcover)

1. Mathematical optimization. I. Wright, Stephen J., 1960- .

II. Title. III. Series. QA402.5.N62 1999 519.3—dc21

99-13263

#### © 1999 Springer-Verlag New York, Inc.

All rights reserved. This work may not be translated or copied in whole or in part without the written permission of the publisher (Springer-Verlag New York, Inc., 175 Fifth Avenue, New York, NY 10010, USA), except for brief excerpts in connection with reviews or scholarly analysis. Use in connection with any form of information storage and retrieval, electronic adaptation, computer software, or by similar or dissimilar methodology now known or hereafter developed is forbidden.

The use of general descriptive names, trade names, trademarks, etc., in this publication, even if the former are not especially identified, is not to be taken as a sign that such names, as understood by the Trade Marks and Merchandise Marks Act, may accordingly be used freely by anyone.

### To Our Parents:

Raúl and Concepción Peter and Berenice

## Preface

This is a book for people interested in solving optimization problems. Because of the wide (and growing) use of optimization in science, engineering, economics, and industry, it is essential for students and practitioners alike to develop an understanding of optimization algorithms. Knowledge of the capabilities and limitations of these algorithms leads to a better understanding of their impact on various applications, and points the way to future research on improving and extending optimization algorithms and software. Our goal in this book is to give a comprehensive description of the most powerful, state-of-the-art, techniques for solving continuous optimization problems. By presenting the motivating ideas for each algorithm, we try to stimulate the reader's intuition and make the technical details easier to follow. Formal mathematical requirements are kept to a minimum.

Because of our focus on continuous problems, we have omitted discussion of important optimization topics such as discrete and stochastic optimization. However, there are a great many applications that can be formulated as continuous optimization problems; for instance,

finding the optimal trajectory for an aircraft or a robot arm;

identifying the seismic properties of a piece of the earth's crust by fitting a model of the region under study to a set of readings from a network of recording stations; designing a portfolio of investments to maximize expected return while maintaining an acceptable level of risk;

controlling a chemical process or a mechanical device to optimize performance or meet standards of robustness:

computing the optimal shape of an automobile or aircraft component.

Every year optimization algorithms are being called on to handle problems that are much larger and complex than in the past. Accordingly, the book emphasizes large-scale optimization techniques, such as interior-point methods, inexact Newton methods, limitedmemory methods, and the role of partially separable functions and automatic differentiation. It treats important topics such as trust-region methods and sequential quadratic programming more thoroughly than existing texts, and includes comprehensive discussion of such "core curriculum" topics as constrained optimization theory, Newton and quasi-Newton methods, nonlinear least squares and nonlinear equations, the simplex method, and penalty and barrier methods for nonlinear programming.

#### THE AUDIENCE

We intend that this book will be used in graduate-level courses in optimization, as offered in engineering, operations research, computer science, and mathematics departments. There is enough material here for a two-semester (or three-quarter) sequence of courses. We hope, too, that this book will be used by practitioners in engineering, basic science, and industry, and our presentation style is intended to facilitate self-study. Since the book treats a number of new algorithms and ideas that have not been described in earlier textbooks, we hope that this book will also be a useful reference for optimization researchers.

Prerequisites for this book include some knowledge of linear algebra (including numerical linear algebra) and the standard sequence of calculus courses. To make the book as self-contained as possible, we have summarized much of the relevant material from these areas in the Appendix. Our experience in teaching engineering students has shown us that the material is best assimilated when combined with computer programming projects in which the student gains a good feeling for the algorithms—their complexity, memory demands, and elegance—and for the applications. In most chapters we provide simple computer exercises that require only minimal programming proficiency.

#### EMPHASIS AND WRITING STYLE

We have used a conversational style to motivate the ideas and present the numerical algorithms. Rather than being as concise as possible, our aim is to make the discussion flow in a natural way. As a result, the book is comparatively long, but we believe that it can be read relatively rapidly. The instructor can assign substantial reading assignments from the text and focus in class only on the main ideas.

A typical chapter begins with a nonrigorous discussion of the topic at hand, including figures and diagrams and excluding technical details as far as possible. In subsequent sections, the algorithms are motivated and discussed, and then stated explicitly. The major theoretical results are stated, and in many cases proved, in a rigorous fashion. These proofs can be skipped by readers who wish to avoid technical details.

The practice of optimization depends not only on efficient and robust algorithms, but also on good modeling techniques, careful interpretation of results, and user-friendly software. In this book we discuss the various aspects of the optimization process—modeling, optimality conditions, algorithms, implementation, and interpretation of results—but not with equal weight. Examples throughout the book show how practical problems are formulated as optimization problems, but our treatment of modeling is light and serves mainly to set the stage for algorithmic developments. We refer the reader to Dantzig [63] and Fourer, Gay, and Kernighan [92] for more comprehensive discussion of this issue. Our treatment of optimality conditions is thorough but not exhaustive; some concepts are discussed more extensively in Mangasarian [154] and Clarke [42]. As mentioned above, we are quite comprehensive in discussing optimization algorithms.

#### **TOPICS NOT COVERED**

We omit some important topics, such as network optimization, integer programming, stochastic programming, nonsmooth optimization, and global optimization. Network and integer optimization are described in some excellent texts: for instance, Ahuja, Magnanti, and Orlin [1] in the case of network optimization and Nemhauser and Wolsey [179], Papadimitriou and Steiglitz [190], and Wolsey [249] in the case of integer programming. Books on stochastic optimization are only now appearing; we mention those of Kall and Wallace [139], Birge and Louveaux [11]. Nonsmooth optimization comes in many flavors. The relatively simple structures that arise in robust data fitting (which is sometimes based on the  $\ell_1$  norm) are treated by Osborne [187] and Fletcher [83]. The latter book also discusses algorithms for nonsmooth penalty functions that arise in constrained optimization; we discuss these briefly, too, in Chapter 18. A more analytical treatment of nonsmooth optimization is given by Hiriart-Urruty and Lemaréchal [137]. We omit detailed treatment of some important topics that are the focus of intense current research, including interior-point methods for nonlinear programming and algorithms for complementarity problems.

#### ADDITIONAL RESOURCE

The material in the book is complemented by an online resource called the NEOS Guide, which can be found on the World-Wide Web at

http://www.mcs.anl.gov/otc/Guide/

The Guide contains information about most areas of optimization, and presents a number of case studies that describe applications of various optimization algorithms to real-world problems such as portfolio optimization and optimal dieting. Some of this material is interactive in nature and has been used extensively for class exercises.

For the most part, we have omitted detailed discussions of specific software packages, and refer the reader to Moré and Wright [173] or to the Software Guide section of the NEOS Guide, which can be found at

http://www.mcs.anl.gov/otc/Guide/SoftwareGuide/

Users of optimization software refer in great numbers to this web site, which is being constantly updated to reflect new packages and changes to existing software.

#### **ACKNOWLEDGMENTS**

We are most grateful to the following colleagues for their input and feedback on various sections of this work: Chris Bischof, Richard Byrd, George Corliss, Bob Fourer, David Gay, Jean-Charles Gilbert, Phillip Gill, Jean-Pierre Goux, Don Goldfarb, Nick Gould, Andreas Griewank, Matthias Heinkenschloss, Marcelo Marazzi, Hans Mittelmann, Jorge Moré, Will Naylor, Michael Overton, Bob Plemmons, Hugo Scolnik, David Stewart, Philippe Toint, Luis Vicente, Andreas Waechter, and Ya-xiang Yuan. We thank Guanghui Liu, who provided help with many of the exercises, and Jill Lavelle who assisted us in preparing the figures. We also express our gratitude to our sponsors at the Department of Energy and the National Science Foundation, who have strongly supported our research efforts in optimization over the years.

One of us (JN) would like to express his deep gratitude to Richard Byrd, who has taught him so much about optimization and who has helped him in very many ways throughout the course of his career.

#### **FINAL REMARK**

In the preface to his 1987 book [83], Roger Fletcher described the field of optimization as a "fascinating blend of theory and computation, heuristics and rigor." The ever-growing realm of applications and the explosion in computing power is driving optimization research in new and exciting directions, and the ingredients identified by Fletcher will continue to play important roles for many years to come.

Jorge Nocedal Stephen J. Wright Evanston, IL Argonne, IL

# Contents

Pr	Preface				
1	Introduction	xxi			
	Mathematical Formulation	2			
	Example: A Transportation Problem	4			
	Continuous versus Discrete Optimization	4			
	Constrained and Unconstrained Optimization	6			
	Global and Local Optimization	6			
	Stochastic and Deterministic Optimization	7			
	Optimization Algorithms	7			
	Convexity	8			
	Notes and References	9			
2	Fundamentals of Unconstrained Optimization				
	2.1 What Is a Solution?	13			
	Recognizing a Local Minimum	15			
	Nonsmooth Problems	18			

	2.2	Overview of Algorithms	19
		Two Strategies: Line Search and Trust Region	19
		Search Directions for Line Search Methods	21
		Models for Trust-Region Methods	26
		Scaling	27
		Rates of Convergence	28
		R-Rates of Convergence	29
	Notes	s and References	30
	Exerc	ises	30
3	Line	Search Methods	34
	3.1	Step Length	36
		The Wolfe Conditions	37
		The Goldstein Conditions	41
		Sufficient Decrease and Backtracking	41
	3.2	Convergence of Line Search Methods	43
	3.3	Rate of Convergence	46
		Convergence Rate of Steepest Descent	47
		Quasi-Newton Methods	49
		Newton's Method	51
		Coordinate Descent Methods	53
	3.4	Step-Length Selection Algorithms	55
		Interpolation	56
		The Initial Step Length	58
		A Line Search Algorithm for the Wolfe Conditions	58
	Notes	s and References	61
	Exerc	ises	62
4	Trust	-Region Methods	64
		Outline of the Algorithm	67
	4.1	The Cauchy Point and Related Algorithms	69
		The Cauchy Point	69
		Improving on the Cauchy Point	70
		The Dogleg Method	71
		Two-Dimensional Subspace Minimization	74
		Steihaug's Approach	75
	4.2	Using Nearly Exact Solutions to the Subproblem	77
		Characterizing Exact Solutions	77
		Calculating Nearly Exact Solutions	78
		The Hard Case	82
		Proof of Theorem 4.3	84
	4.3	Global Convergence	87

		Reduction Obtained by the Cauchy Point	87
		Convergence to Stationary Points	89
		Convergence of Algorithms Based on Nearly Exact Solutions	93
	4.4	Other Enhancements	94
		Scaling	94
		Non-Euclidean Trust Regions	96
	Note	s and References	97
		cises	97
5	Conj	ugate Gradient Methods	100
	5.1	The Linear Conjugate Gradient Method	102
		Conjugate Direction Methods	102
		Basic Properties of the Conjugate Gradient Method	107
		A Practical Form of the Conjugate Gradient Method	111
		Rate of Convergence	112
		Preconditioning	118
		Practical Preconditioners	119
	5.2	Nonlinear Conjugate Gradient Methods	120
		The Fletcher–Reeves Method	120
		The Polak–Ribière Method	121
		Quadratic Termination and Restarts	122
		Numerical Performance	124
		Behavior of the Fletcher–Reeves Method	124
		Global Convergence	127
	Note	s and References	131
	Exerc	cises	132
6	Prac	tical Newton Methods	134
	6.1	Inexact Newton Steps	136
	6.2	Line Search Newton Methods	139
		Line Search Newton–CG Method	139
		Modified Newton's Method	141
	6.3	Hessian Modifications	142
		Eigenvalue Modification	143
		Adding a Multiple of the Identity	144
		Modified Cholesky Factorization	145
		Gershgorin Modification	150
		Modified Symmetric Indefinite Factorization	151
	6.4	Trust-Region Newton Methods	154
		Newton–Dogleg and Subspace-Minimization Methods	154
		Accurate Solution of the Trust-Region Problem	155
		Trust-Region Newton-CG Method	156

		Preconditioning the Newton–CG Method
		Local Convergence of Trust-Region Newton Methods 159
	Note	s and References
	Exerc	ises
7	Calc	ılating Derivatives 164
	7.1	Finite-Difference Derivative Approximations
		Approximating the Gradient
		Approximating a Sparse Jacobian
		Approximating the Hessian
		Approximating a Sparse Hessian
	7.2	Automatic Differentiation
	,	An Example
		The Forward Mode
		The Reverse Mode
		Vector Functions and Partial Separability
		Calculating Jacobians of Vector Functions
		Calculating Hessians: Forward Mode
		· ·
	NT (	Current Limitations
		s and References
	Exerc	ises
8	01106	i-Newton Methods
O	8.1	The BFGS Method
	0.1	Properties of the BFGS Method
		Implementation
	8.2	
	0.2	
	0.2	Properties of SR1 Updating
	8.3	The Broyden Class
	0.4	Properties of the Broyden Class
	8.4	Convergence Analysis
		Global Convergence of the BFGS Method
		Superlinear Convergence of BFGS
		Convergence Analysis of the SR1 Method
	Note	s and References
	Exerc	ises
9	Large	e-Scale Quasi-Newton and Partially Separable Optimization 222
	9.1	Limited-Memory BFGS
	9.1	Relationship with Conjugate Gradient Methods
	0.2	
	9.2	General Limited-Memory Updating

		Compact Representation of BFGS Updating	230
		SR1 Matrices	232
		Unrolling the Update	232
	9.3	Sparse Quasi-Newton Updates	233
	9.4	Partially Separable Functions	235
		A Simple Example	236
		Internal Variables	237
	9.5	Invariant Subspaces and Partial Separability	240
		Sparsity vs. Partial Separability	242
		Group Partial Separability	243
	9.6	Algorithms for Partially Separable Functions	244
		Exploiting Partial Separability in Newton's Method	244
		Quasi-Newton Methods for Partially Separable Functions	245
	Notes	and References	247
	Exerci	ises	248
10	Nonli	inear Least-Squares Problems	250
	10.1	Background	253
		Modeling, Regression, Statistics	253
		Linear Least-Squares Problems	256
	10.2	Algorithms for Nonlinear Least-Squares Problems	259
		The Gauss–Newton Method	259
		The Levenberg–Marquardt Method	262
		Implementation of the Levenberg–Marquardt Method	264
		Large-Residual Problems	266
		Large-Scale Problems	269
	10.3	Orthogonal Distance Regression	271
	Notes	and References	273
		ises	274
11	Nonli	inear Equations	276
	11.1	Local Algorithms	281
		Newton's Method for Nonlinear Equations	281
		Inexact Newton Methods	284
		Broyden's Method	286
		Tensor Methods	290
	11.2	Practical Methods	292
		Merit Functions	292
		Line Search Methods	294
		Trust-Region Methods	298
	11.3	Continuation/Homotopy Methods	304
		Madination	204

		Practical Continuation Methods	306
	Notes	and References	310
	Exerc	ises	311
12	Theo	ry of Constrained Optimization	314
		Local and Global Solutions	316
		Smoothness	317
	12.1	Examples	319
		A Single Equality Constraint	319
		A Single Inequality Constraint	321
		Two Inequality Constraints	324
	12.2	First-Order Optimality Conditions	327
		Statement of First-Order Necessary Conditions	327
		Sensitivity	330
	12.3	Derivation of the First-Order Conditions	331
		Feasible Sequences	331
		Characterizing Limiting Directions: Constraint Qualifications	336
		Introducing Lagrange Multipliers	339
		Proof of Theorem 12.1	341
	12.4	Second-Order Conditions	342
		Second-Order Conditions and Projected Hessians	348
		Convex Programs	349
	12.5	Other Constraint Qualifications	350
	12.6	A Geometric Viewpoint	353
	Notes	and References	356
		ises	357
13	Linea	r Programming: The Simplex Method	360
13	Linea	Linear Programming	362
	13.1	Optimality and Duality	364
	13.1	Optimality Conditions	364
		The Dual Problem	365
	13.2	Geometry of the Feasible Set	368
	13.2	Basic Feasible Points	368
		Vertices of the Feasible Polytope	
	13.3	The Simplex Method	370
	13.3	Outline of the Method	372
		Finite Termination of the Simplex Method	374
		A Single Step of the Method	374
	12 4	Linear Algebra in the Simplex Method	
	13.4		377
	13.5	Other (Important) Details	381
		Pricing and Selection of the Entering Index	381

		Starting the Simplex Method	384
		Degenerate Steps and Cycling	387
	13.6	Where Does the Simplex Method Fit?	389
	Notes	and References	390
		ses	391
14	Linear	r Programming: Interior-Point Methods	392
	14.1	Primal–Dual Methods	394
		Outline	394
		The Central Path	397
		A Primal–Dual Framework	399
		Path-Following Methods	400
	14.2	A Practical Primal–Dual Algorithm	402
		Solving the Linear Systems	406
	14.3	Other Primal–Dual Algorithms and Extensions	407
		Other Path-Following Methods	407
		Potential-Reduction Methods	407
		Extensions	408
	14.4	Analysis of Algorithm 14.2	409
	Notes	and References	414
		ses	415
15	Funda	amentals of Algorithms for Nonlinear Constrained Optimization	418
		Initial Study of a Problem	420
	15.1	Categorizing Optimization Algorithms	422
	15.2	Elimination of Variables	424
		Simple Elimination for Linear Constraints	426
		General Reduction Strategies for Linear Constraints	429
		The Effect of Inequality Constraints	431
	15.3	Measuring Progress: Merit Functions	432
	Notes	and References	436
	Exerci	ses	436
1.	0 1	d' B	420
10	-	ratic Programming	438
		An Example: Portfolio Optimization	440
	16.1	Equality-Constrained Quadratic Programs	441
	16.2	Properties of Equality-Constrained QPs	442
	16.2	Solving the KKT System	445
		Direct Solution of the KKT System	446
		Range-Space Method	447
		Null-Space Method	448
		A Method Based on Conjugacy	450

	16.3	Inequality-Constrained Problems	451
		Optimality Conditions for Inequality-Constrained Problems	452
		Degeneracy	453
	16.4	Active-Set Methods for Convex QP	455
		Specification of the Active-Set Method for Convex QP	460
		An Example	461
		Further Remarks on the Active-Set Method	463
		Finite Termination of the Convex QP Algorithm	464
		Updating Factorizations	465
	16.5	Active-Set Methods for Indefinite QP	468
	10.0	Illustration	470
		Choice of Starting Point	472
		Failure of the Active-Set Method	473
		Detecting Indefiniteness Using the $LBL^T$ Factorization	473
	16.6		
	16.6	The Gradient–Projection Method	474
		Cauchy Point Computation	475
		Subspace Minimization	478
	16.7	Interior-Point Methods	479
		Extensions and Comparison with Active-Set Methods	482
	16.8	Duality	482
	Notes	and References	483
	Exerci	ises	484
17	Penal	ty, Barrier, and Augmented Lagrangian Methods	488
	17.1	The Quadratic Penalty Method	490
		Motivation	490
		Algorithmic Framework	492
		Convergence of the Quadratic Penalty Function	493
	17.2	The Logarithmic Barrier Method	498
	1,12	Properties of Logarithmic Barrier Functions	498
		Algorithms Based on the Log-Barrier Function	503
		Properties of the Log-Barrier Function and Framework 17.2	505
		Handling Equality Constraints	507
		Relationship to Primal–Dual Methods	508
	17.3		
		Exact Penalty Functions	510
	17.4	Augmented Lagrangian Method	511
		Motivation and Algorithm Framework	512
		Extension to Inequality Constraints	514
		Properties of the Augmented Lagrangian	517
		Practical Implementation	520
	17.5	Sequential Linearly Constrained Methods	522
	Notes	and References	523

	Exerci	ises	524
18	Seque	ential Quadratic Programming	526
	18.1	Local SQP Method	528
		SQP Framework	529
		Inequality Constraints	531
		IQP vs. EQP	531
	18.2	Preview of Practical SQP Methods	532
	18.3	Step Computation	534
		Equality Constraints	534
		Inequality Constraints	536
	18.4	The Hessian of the Quadratic Model	537
		Full Quasi-Newton Approximations	538
		Hessian of Augmented Lagrangian	539
		Reduced-Hessian Approximations	540
	18.5	Merit Functions and Descent	542
	18.6	A Line Search SQP Method	545
	18.7	Reduced-Hessian SQP Methods	546
		Some Properties of Reduced-Hessian Methods	547
		Update Criteria for Reduced-Hessian Updating	548
		Changes of Bases	549
		A Practical Reduced-Hessian Method	550
	18.8	Trust-Region SQP Methods	551
		Approach I: Shifting the Constraints	553
		Approach II: Two Elliptical Constraints	554
		Approach III: $S\ell_1QP$ (Sequential $\ell_1$ Quadratic Programming)	555
	18.9	A Practical Trust-Region SQP Algorithm	558
	18.10	Rate of Convergence	561
		Convergence Rate of Reduced-Hessian Methods	563
	18.11	The Maratos Effect	565
		Second-Order Correction	568
		Watchdog (Nonmonotone) Strategy	569
	Notes	and References	571
	Exerci	ises	572
A	Backg	ground Material	574
	A.1	Elements of Analysis, Geometry, Topology	575
		Topology of the Euclidean Space $\mathbb{R}^n$	575
		Continuity and Limits	578
		Derivatives	579
		Directional Derivatives	581
		Mean Value Theorem	582

#### **xx** Contents

	Implicit Function Theorem	583
	Geometry of Feasible Sets	584
	Order Notation	589
	Root-Finding for Scalar Equations	590
A.2	Elements of Linear Algebra	591
	Vectors and Matrices	591
	Norms	592
	Subspaces	595
	Eigenvalues, Eigenvectors, and the Singular-Value Decomposition	596
	Determinant and Trace	597
	Matrix Factorizations: Cholesky, LU, QR	598
	Sherman–Morrison–Woodbury Formula	603
	Interlacing Eigenvalue Theorem	603
	Error Analysis and Floating-Point Arithmetic	604
	Conditioning and Stability	606
Reference	es	609
Index		623