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J. E. Dennis Jr.   Robert B. Schnabel

Numerical Methods for Unconstrained Optimization and Nonlinear Equations

无约束最优化与非线性方程的数值方法

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《国外数学名著系列》(影印版)序

要使我国的数学事业更好地发展起来，需要数学家淡泊名利并付出更艰苦地努力。另一方面，我们也要从客观上为数学家创造更有利的发展数学事业的外部环境，这主要是加强对数学事业的支持与投资力度，使数学家有较好的工作与生活条件，其中也包括改善与加强数学的出版工作。

从出版方面来讲，除了较好较快地出版我们自己的成果外，引进国外的先进出版物无疑也是十分重要与必不可少的。从数学来说，施普林格(Springer)出版社至今仍然是世界上最具权威的出版社。科学出版社影印一批他们出版的好的新书，使我国广大数学家能以较低的价格购买，特别是在边远地区工作的数学家能普遍见到这些书，无疑是对推动我国数学的科研与教学十分有益的事。

这次科学出版社购买了版权，一次影印了 23 本施普林格出版社出版的数学书，就是一件好事，也是值得继续做下去的事情。大体上分一下，这 23 本书中，包括基础数学书 5 本，应用数学书 6 本与计算数学书 12 本，其中有些书也具有交叉性质。 这些书都是很新的，2000 年以后出版的占绝大部分，共计 16 本，其余的也是 1990 年以后出版的。这些书可以使读者较快地了解数学某方面的前沿，例如基础数学中的数论、代数与拓扑三本，都是由该领域大数学家编著的“数学百科全书”的分册。对从事这方面研究的数学家了解该领域的前沿与全貌很有帮助。按照学科的特点，基础数学类的书以“经典”为主，应用和计算数学类的书以“前沿”为主。这些书的作者多数是国际知名的大数学家，例如《拓扑学》一书的作者诺维科夫是俄罗斯科学院的院士，曾获“菲尔兹奖”和“沃尔夫数学奖”。这些大数学家的著作无疑将会对我国的科研人员起到非常好的指导作用。

当然，23 本书只能涵盖数学的一部分，所以，这项工作还应该继续做下去。更进一步，有些读者面较广的好书还应该翻译成中文出版，使之有更大的读者群。

总之，我对科学出版社影印施普林格出版社的部分数学著作这一举措表示热烈的支持，并盼望这一工作取得更大的成绩。

王 元

2005 年 12 月 3 日

To Catherine, Heidi, and Cory

Preface to the Classics Edition

We are delighted that SIAM is republishing our original 1983 book after what many in the optimization field have regarded as "premature termination" by the previous publisher. At 12 years of age, the book may be a little young to be a "classic," but since its publication it has been well received in the numerical computation community. We are very glad that it will continue to be available for use in teaching, research, and applications.

We set out to write this book in the late 1970s because we felt that the basic techniques for solving small to medium-sized nonlinear equations and unconstrained optimization problems had matured and converged to the point where they would remain relatively stable. Fortunately, the intervening years have confirmed this belief. The material that constitutes most of this book—the discussion of Newton-based methods, globally convergent line search and trust region methods, and secant (quasi-Newton) methods for nonlinear equations, unconstrained optimization, and nonlinear least squares—continues to represent the basis for algorithms and analysis in this field. On the teaching side, a course centered around Chapters 4 to 9 forms a basic, in-depth introduction to the solution of nonlinear equations and unconstrained optimization problems. For researchers or users of optimization software, these chapters give the foundations of methods and software for solving small to medium-sized problems of these types.

We have not revised the 1983 book, aside from correcting all the typographical errors that we know of. (In this regard, we especially thank Dr. Oleg Burdakov who, in the process of translating the book for the Russian edition published by Mir in 1988, found numerous typographical errors.) A main reason for not revising the book at this time is that it would have delayed its republication substantially. A second reason is that there appear to be relatively few places where the book needs updating. But inevitably there are some. In our opinion, the main developments in the solution of small to medium-sized unconstrained optimization and nonlinear equations problems since the publication of this book, which a current treatment should include, are

1. improved algorithms and analysis for trust region methods for unconstrained optimization in the case when the Hessian matrix is indefinite [1, 2] and
2. improved global convergence analysis for secant (quasi-Newton) methods [3].

A third, more recent development is the field of automatic (or computational) differentiation [4]. Although it is not yet fully mature, it is clear that this development is increasing the availability of analytic gradients and Jacobians and therefore reducing the cases where finite difference approximations to these derivatives are needed. A fourth, more minor but still significant development is a new, more stable modified Cholesky factorization method [5, 6]. Far more progress has been made in the solution of large nonlinear equations and unconstrained optimization problems. This includes the development or improvement of conjugate gradient, truncated-Newton, Krylov-subspace, and limited-memory methods. Treating these fully would go beyond the scope of this book even if it were revised, and fortunately some excellent new references are emerging, including [7]. Another important topic that is related to but not within the scope of this book is that of new derivative-free methods for unconstrained optimization [8].

The appendix of this book has had an impact on software in this field. The IMSL library created their unconstrained optimization code from this appendix, and the UNCMIN software [9] created in conjunction with this appendix has been and continues to be a widely used package for solving unconstrained optimization problems. This software also has been included in a number of software packages and other books. The UNCMIN software continues to be available from the second author (bobby@cs.colorado.edu).

Finally, one of the most important developments in our lives since 1983 has been the emergence of a new generation: a granddaughter for one of us, a daughter and son for the other. This new edition is dedicated to them in recognition of the immense joy they have brought to our lives and with all our hopes and wishes for the lives that lay ahead for them.

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Preface

This book offers a careful introduction, at a low level of mathematical and computational sophistication, to the numerical solution of problems in unconstrained optimization and systems of nonlinear equations. We have written it, beginning in 1977, because we feel that the algorithms and theory for small-to-medium-size problems in this field have reached a mature state, and that a comprehensive reference will be useful. The book is suitable for graduate or upper-level undergraduate courses, but also for self-study by scientists, engineers, and others who have a practical interest in such problems.

The minimal background required for this book would be calculus and linear algebra. The reader should have been at least exposed to multivariable calculus, but the necessary information is surveyed thoroughly in Chapter 4. Numerical linear algebra or an elementary numerical methods course would be helpful; the material we use is covered briefly in Section 1.3 and Chapter 3.

The algorithms covered here are all based on Newton's method. They are often called **Newton-like**, but we prefer the term **quasi-Newton**. Unfortunately, this term is used by specialists for the subclass of these methods covered in our Chapters 8 and 9. Because this subclass consists of sensible multidimensional generalizations of the secant method, we prefer to call them secant methods. Particular secant methods are usually known by the proper names of their discoverers, and we have included these servings of alphabet soup, but we have tried to suggest other descriptive names commensurate with their place in the overall scheme of our presentation.

The heart of the book is the material on computational methods for multidimensional unconstrained optimization and nonlinear equation problems covered in Chapters 5 through 9. Chapter 1 is introductory and will be more useful for students in pure mathematics and computer science than for readers with some experience in scientific applications. Chapter 2, which covers the one-dimensional version of our problems, is an overview of our approach to the subject and is essential motivation. Chapter 3 can be omitted by readers who have studied numerical linear algebra, and Chapter 4 can be omitted by those who have a good background in multivariable calculus. Chapter 10 gives a fairly complete treatment of algorithms for nonlinear least squares, an important type of unconstrained optimization problem that, owing to its special structure, is solved by special methods. It draws heavily on the chapters that precede it. Chapter 11 indicates some research directions in which the field is headed; portions of it are more difficult than the preceding material.

We have used the book for undergraduate and graduate courses. At the lower level, Chapters 1 through 9 make a solid, useful course; at the graduate level the whole book can be covered. With Chapters 1, 3, and 4 as remedial reading, the course takes about one quarter. The remainder of a semester is easily filled with these chapters or other material we omitted.

The most important omitted material consists of methods not related to Newton's method for solving unconstrained minimization and nonlinear equation problems. Most of them are important only in special cases. The Nelder-Meade simplex algorithm [see, e.g., Avriel (1976)], an effective algorithm for problems with less than five variables, can be covered in an hour. Conjugate direction methods [see, e.g., Gill, Murray, and Wright (1981)] properly belong in a numerical linear algebra course, but because of their low storage requirements they are useful for optimization problems with very large numbers of variables. They can be covered usefully in two hours and completely in two weeks.

The omission we struggled most with is that of the Brown-Brent methods. These methods are conceptually elegant and startlingly effective for partly linear problems with good starting points. In their current form they are not competitive for general-purpose use, but unlike the simplex or conjugate-direction algorithms, they would not be covered elsewhere. This omission can be remedied in one or two lectures, if proofs are left out [see, e.g., Dennis (1977)]. The final important omission is that of the continuation or homotopy-based methods, which enjoyed a revival during the seventies. These elegant ideas can be effective as a last resort for the very hardest problems but are not yet competitive for most problems. The excellent survey by Allgower and Georg (1980) requires at least two weeks.

We have provided many exercises; many of them further develop ideas that are alluded to briefly in the text. The large appendix (by Schnabel) is intended to provide both a mechanism for class projects and an important reference for readers who wish to understand the details of the algorithms and perhaps to develop their own versions. The reader is encouraged to read the preface to the appendix at an early stage.

Several problems of terminology and notation were particularly troublesome. We have already mentioned the confusion over the terms "quasi-Newton" and "secant methods." In addition, we use the term "unconstrained optimization" in the title but "unconstrained minimization" in the text, since technically we consider only minimization. For maximization, turn the problems upside-down. The important term "global" has several interpretations, and we try to explain ours clearly in Section 1.1. Finally, a major notational problem was how to differentiate between the ith component of an n-vector x, a *scalar* usually denoted by x_i, and the ith iteration in a sequence of such x's, a *vector* also usually denoted x_i. After several false starts, we decided to allow this conflicting notation, since the intended meaning is always clear from the context; in fact, the notation is rarely used in both ways in any single section of the text.

We wanted to keep this book as short and inexpensive as possible without slighting the exposition. Thus, we have edited some proofs and topics in a merciless fashion. We have tried to use a notion of rigor consistent with good taste but subservient to insight, and to include proofs that give insight while omitting those that merely substantiate results. We expect more criticism for omissions than for inclusions, but as every teacher knows, the most difficult but important part in planning a course is deciding what to leave out.

We sincerely thank Idalia Cuellar, Arlene Hunter, and Dolores Pendel for typing the numerous drafts, and our students for their specific identification of unclear passages. David Gay, Virginia Klema, Homer Walker, Pete Stewart, and Layne Watson used drafts of the book in courses at MIT, Lawrence Livermore Laboratory, University of Houston, University of New Mexico, University of Maryland, and VPI, and made helpful suggestions. Trond Steihaug and Mike Todd read and commented helpfully on portions of the text.

Rice University — *J. E. Dennis, Jr.*

University of Colorado at Boulder — *Robert B. Schnabel*

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Before we begin, a program note

The first four chapters of this book contain the background material and motivation for the study of multivariable nonlinear problems. In Chapter 1 we introduce the problems we will be considering. Chapter 2 then develops some algorithms for nonlinear problems in just one variable. By developing these algorithms in a way that introduces the basic philosophy of all the nonlinear algorithms to be considered in this book, we hope to provide an accessible and solid foundation for the study of multivariable nonlinear problems. Chapters 3 and 4 contain the background material in numerical linear algebra and multivariable calculus required to extend our consideration to problems in more than one variable.

1

Introduction

This book discusses the methods, algorithms, and analysis involved in the computational solution of three important nonlinear problems: solving systems of nonlinear equations, unconstrained minimization of a nonlinear functional, and parameter selection by nonlinear least squares. Section 1.1 introduces these problems and the assumptions we will make about them. Section 1.2 gives some examples of nonlinear problems and discusses some typical characteristics of problems encountered in practice; the reader already familiar with the problem area may wish to skip it. Section 1.3 summarizes the features of finite-precision computer arithmetic that the reader will need to know in order to understand the computer-dependent considerations of the algorithms in the text.

1.1 PROBLEMS TO BE CONSIDERED

This book discusses three nonlinear problems in real variables that arise often in practice. They are mathematically equivalent under fairly reasonable hypotheses, but we will not treat them all with the same algorithm. Instead we will show how the best current algorithms seek to exploit the structure of each problem.

The simultaneous nonlinear equations problem (henceforth called "nonlinear equations") is the most basic of the three and has the least exploitable