GLOBAL OPTIMIZATION METHODS IN GEOPHYSICAL INVERSION

SECOND EDITION

Making inferences about systems in the earth's subsurface from remotely sensed, sparse measurements is a challenging task. Geophysical inversion aims to find models that explain geophysical observations – a model-based inversion method attempts to infer model parameters by iteratively fitting observations with theoretical predictions from trial models. Global optimization often enables the solution of non-linear models, employing a global search approach to find the absolute minimum of an objective function so that predicted data best fit the observations.

This new edition provides an up-to-date overview of the most popular global optimization methods, including a detailed description of the theoretical development underlying each method, and a thorough explanation of the design, implementation, and limitations of algorithms.

A new chapter provides details of recently developed methods, such as the neighborhood algorithm and particle swarm optimization. An expanded chapter on uncertainty estimation includes a succinct description on how to use optimization methods for model space exploration to characterize uncertainty and now discusses other new methods such as hybrid Monte Carlo and multi-chain MCMC methods. Other chapters include new examples of applications, from uncertainty in climate modeling to whole-earth studies. Several different examples of geophysical inversion, including joint inversion of disparate geophysical datasets, are provided to help readers design algorithms for their own applications.

This is an authoritative and valuable text for researchers and graduate students in geophysics, inverse theory, and exploration geoscience, and an important resource for professionals working in engineering and petroleum exploration.

MRINAL K. SEN is a Jackson Chair Professor in Applied Seismology at the University of Texas, Austin, and in January 2012, while on leave, became Director of the National Geophysical Research Institute at Hyderabad, India. His research areas include seismic wave propagation, inverse problems, seismic imaging, reservoir characterization, and computational geophysics, and he is an expert on seismic wave propagation, including anisotropy and fractures, developing analytic and numerical techniques for forward and inverse modeling. Professor Sen is the principal author of two books on geophysical inversion and co-author of over 130 papers in peer-reviewed journals and has been an instructor for several industry short courses. He serves on several national and international committees and is an associate editor of leading journals such as *Geophysics*, and *Journal of Seismic Exploration*.

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Preface to the first edition (1995)

One of the major goals of geophysical inversion is to find earth models that explain geophysical observations. Thus the branch of mathematics known as *optimization* has found significant use in many geophysical applications. Geophysical inversion in this context involves finding an optimal value of a function of several variables. The function that we want to minimize (or maximize) is a misfit (or fitness) function that characterizes the differences (or similarities) between observed and synthetic data calculated by using an assumed earth model. The earth model is described by physical parameters that characterize the properties of rock layers, such as the compressional-wave velocity, shear-wave velocity, resistivity, etc.

Both *local* and *global* optimization methods are used in the estimation of material properties from geophysical data. As the title of this book suggests, our goal is to describe the application of several recently developed global optimization methods to geophysical problems. Although we emphasize the application aspects of these algorithms, we describe several parts of the theory in sufficient detail for readers to understand the underlying fundamental principles on which these algorithms are based. At this stage we take the opportunity to define some commonly used terms.

For many geophysical applications, the misfit surface as a function of the model parameters that are described by the mismatch between the predicted and observed geophysical data may be highly complicated and characterized by multiple hills and valleys. Thus such a function will have several minima and maxima; the minimum of all the minima is called the *global minimum*, and all other minima are called *local minima*. Note that the global minimum is one of the local minima, but the converse is not true, and it is also possible to have several minima of nearly the same depth. Local optimization or search algorithms such as gradient-descent methods typically attempt to find a local minimum in the close neighborhood of the starting solution. Almost all the local search methods are deterministic algorithms.

They use local properties of the misfit function to calculate an update to the current answer and search in the downhill direction. Thus these algorithms will miss the global minimum if the starting solution is nearer to one of the local minima than the global minimum. The local minimum syndrome has plagued geophysicists for over a decade now.

Recently (owing to the advent of powerful and relatively inexpensive computers), global optimization methods have been applied to several geophysical problems. Unlike local optimization methods, these methods attempt to find the global minimum of the misfit function. Most of the global optimization algorithms are stochastic in nature and use more global information about the misfit surface to update their current position. The convergence of these methods to the globally optimal solution is not guaranteed for all the algorithms. Only for some of the *simulated annealing* algorithms under certain conditions is convergence to the globally optimal solution statistically guaranteed. Also, with real observational data it is never possible to know whether the derived solution corresponds to the global minimum or not. However, our experience indicates that we are able to find many good solutions starting with only poor initial models using global optimization methods.

These global optimization methods are computationally intensive, but with the advent of vector computers, parallel computers, and powerful desktop workstations, use of these methods is becoming increasingly practical. While finding the optimal solution will always be a goal, and the global optimization methods described here are well suited for this purpose, they can also be used to obtain additional information about the nature of the solution. In particular, the description of a solution is not complete without assigning uncertainties to the derived answer. With noisy data it may not even be advisable to search for the so-called global minimum. In these situations, a statistical formulation of the inverse problem is often appealing. Consequently, we also describe how global optimization methods can be applied in a statistical framework to estimate the uncertainties in the derived result.

This is not a book on inverse theory per se; several excellent texts already exist (e.g., Menke 1984; Tarantola 1987). Our goal is to describe in sufficient detail the fundamentals of several optimization methods with application to geophysical inversion such that students, researchers, and practitioners will be able to design practical algorithms to solve their specific geophysical inversion problems. We attempted to make this book virtually self-contained so that there are no prerequisites, except for a fundamental mathematical background that includes a basic understanding of linear algebra and calculus. The material presented in this book can easily be covered in a one-semester graduate-level course on geophysical inversion. We believe that after reviewing the materials presented in this book, readers will be able to develop specific algorithms for their own applications. We will be happy to mail sample Fortran codes of prototype Metropolis simulated annealing (SA), heat bath SA, very fast simulated annealing (VFSA), and a basic genetic algorithm to those interested.

Much of our work on non-linear inversion has been supported by grants from the National Science Foundation, the Office of Naval Research, Cray Research, Inc., and the Texas Higher Education Coordinating Board. We acknowledge The University of Texas System Center for High Performance Computing for their support and computational resources. Adre Duijndam, Jacob Fokkema, Cliff Frohlich, John Goff, Lester Ingber, Tad Ulrych, and Lian-She Zhao reviewed the manuscript and offered valuable suggestions. Milton Porsani, who worked with us for one year as a visiting scientist, along with several of our graduate students, including Faruq Akbar, Carlos Calderon, Raghu Chunduru, Mike Jervis, Vik Sen, Mehmet Tanis, and Carlos Varela, participated in the research and reviewed the manuscript. Their contribution to this project has been extremely valuable. We thank Milo Backus for his many critical comments during the early stages of the work that helped tremendously in shaping our ideas on inverse theory in general. Charlene Palmer receives our thanks for painstakingly typesetting the manuscript. We also thank Gus Berkhout and Jacob Fokkema for inviting us to write the book for the series *Advances in Exploration Geophysics*.

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Mrinal K. Sen wishes to thank his wife, Alo, and children, Amrita and Ayon, for their sacrifice and encouragement. He also thanks Neil Frazer for his suggestion following the 1990 Society of Exploration Geophysicists Meeting to write a book on this subject.

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Preface to the second edition (2013)

The first edition of the book went out of print a few years ago. We received many requests for a copy of the book, and therefore, an invitation from Cambridge University Press to publish a revised version of this book was a welcome message. Since the publication of the first edition, a couple of review articles on Monte Carlo methods have been published in the geophysical literature. A large number of applications have also been reported. This book, however, still remains as the only publication providing a comprehensive overview of global optimization methods for geophysical applications. Global optimization methods, which were at the time of the first edition considered too slow to be of practical use, are now being used routinely in many applications. In this revised version, we have expanded several sections, including one on local optimization; we include recent global optimization methods such as the neighborhood algorithm (NA) and particle swarm optimization (PSO), and we add several new applications of global optimization methods, including the joint inversion of diverse data. Although no major new algorithmic developments of genetic algorithms (GAs) and simulated annealing (SA) have been reported, their application to solving complex problems has increased significantly since the first edition. We apologize for not being able to include all these successful applications in our reference list.

We remain indebted to our graduate students and postdoctoral fellows for collaboration. We thank our families for their unconditional support.

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