RIGOROUS GLOBAL SEARCH: CONTINUOUS PROBLEMS

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PREFACE

This work grew out of several years of research, graduate seminars and talks on the subject. It was motivated by a desire to make the technology accessible to those who most needed it or could most use it. It is meant to be a self-contained introduction, a reference for the techniques, and a guide to the literature for the underlying theory. It contains pointers to fertile areas for future research. It also serves as introductory documentation for a Fortran 90 software package for nonlinear systems and global optimization.

The subject of the monograph is deterministic, *automatically verified* or *rigorous* methods. In such methods, directed rounding and computational fixed-point theory are combined with exhaustive search (branch and bound) techniques. Completion of such an algorithm with a list of solutions constitutes a *rigorous mathematical proof* that all of the solutions within the original search region are within the output list.

The monograph is appropriate as an introduction to research and technology in the area, as a desk reference, or as a graduate-level course reference. Knowledge of calculus, linear algebra, and elementary numerical analysis is assumed. Interval computations are presented from the beginning, although the more advanced material is mainly to support development of ideas in nonlinear systems and global optimization. The style is meant to balance the need to inform newcomers with the need to provide concise treatment for experts. The emphasis in the advanced topics is on the author's own contributions to the field. The book contains numerous references and cross-references, as well as an extensive index. A logical thread is provided for easy initial reading, with gateways for subsequent in-depth study.

Although the major goal of the book is to explain techniques and software for rigorous solution of nonlinear systems and rigorous, deterministic global optimization, the extensive introduction in Chapter 1 is suitable as a general introduction or reference for interval arithmetic. Thus, this introduction can also be useful in studying verified quadrature or verified solutions of differential equations, for example.

Similarly, the software described in Chapter 2 includes general-use interval arithmetic software. This software includes a Fortran-90 module for interval arithmetic and Fortran 90 modules for automatic differentiation (termed `INTLIB_90`), freely available from the author (email: `rbk@usl.edu`), and also includes more special-purpose nonlinear equations and global optimization codes (termed `INTOPT_90`). Chapter 2 also contains a review of alternate programming languages and packages for interval computations, with a discussion of the advantages and disadvantages of each.

In Chapter 3, previously unpublished material on optimal preconditioners for interval linear systems is presented. Illustrations and examples are meant to point the reader to the contexts in which such preconditioners can be advantageous, as well as to give necessary explanation for implementation. (The author's software contains routines for one type of optimal preconditioner.)

Chapter 4 contains an introduction to algorithmic constructs for global search methods for solutions to nonlinear systems of equations. These constructs include overall algorithm structure, as well as methods for subdividing the region and taking advantage of accurate approximate solutions. Some of these techniques and algorithmic constructs are shared by global optimization algorithms, described in the next chapter. Chapter 4 also contains a description of the author's software for nonlinear equations, in an overall package (termed `INTOPT_90`).

Chapter 5 deals with actual global optimization techniques and algorithms. Beginning with an overall view, historical algorithms and recent, more sophisticated algorithms are reviewed. This is followed by an extensive review of how inequality and equality constraints are handled, including some of the author's proposed techniques and experience. The chapter concludes with a description of the routines available in `INTOPT_90`.

Chapter 6 deals with special techniques for non-differentiable problems, such as l_1 and l_∞ optimization. In particular, formulas are listed for interval extensions of non-smooth and discontinuous functions, as well as representation of derivative information for non-smooth and discontinuous functions. Surprisingly, such interval extensions, even for discontinuous functions, can be effective in interval Newton methods; examples are given, and a convergence analysis is reviewed. Support for the techniques is available in the author's software, `INTLIB_90`.

Chapter 7 deals with using the interval values of *subexpressions*, obtained while evaluating objective functions and gradients. These techniques are tied to the preconditioner techniques of Chapter 3, and are also related to the established field of *constraint propagation*.

Throughout the book, techniques and software are presented not only to explain available work, but also to guide interested readers to future improvements or to ways of using individual techniques in different contexts.

Elements of the theory deemed most relevant are presented. However, theorems appear within the context of the meaning and practical impact of their results. Where proofs are presented, it is mainly for the purpose of giving additional insight. Where proofs are not presented, references to the original research are given.

Exercises after many sections amplify the preceding presentation.

The references are available electronically in BibTeX form, via anonymous FTP from

`interval.usl.edu`

in the directory

`pub/interval_math/bibliographies/optimization_book.bib`

I wish to thank my former student Dr. Xiaofa Shi, and my colleagues George Corliss, Panos Pardalos, Dietmar Ratz, and Siegfried Rump for the careful reading and suggestions that improved this book considerably. I also would like to thank Layne Watson for introducing me to TeX and for encouraging me, early on, to work hard.

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PRELIMINARIES

The main purpose of this book is to introduce techniques and software for the verified solution of nonlinear systems of equations and for rigorous, deterministic unconstrained and constrained global optimization. Specifically, global optima or solutions of nonlinear equations will be sought within the *box*

$$\boldsymbol{X} = \left\{(x_1, x_2, \ldots, x_n)^T \in \mathbb{R}^n \,\middle|\, \underline{x}_i \le x_i \le \overline{x}_i, 1 \le i \le n\right\}, \tag{1.1}$$

for some set of lower bounds $\{\underline{x}_i\}_{i=1}^n$ and upper bounds $\{\overline{x}_i\}_{i=1}^n$. The fundamental nonlinear equations problem is

(1.2)

> Given $F : \boldsymbol{X} \to \mathbb{R}^n$, *rigorously* enclose *all* solutions $X^* \in \boldsymbol{X}$. That is, for each
>
> $$X^* = (x_1^*, \ldots, x_n^*)^T \in \boldsymbol{X}$$
>
> with $F(X^*) = 0$, find bounds $a_i \le x_i^* \le b_i$ such that
>
> - $b_i - a_i$ is small, $1 \le i \le n$, and
> - it is mathematically but automatically proven that there is a unique root of F within each
>
> $$\check{\boldsymbol{X}} = \left\{X = (x_1, \ldots, x_n) \,\middle|\, a_i \le x_i \le b_i, 1 \le i \le n\right\}.$$