
RIGOROUS GLOBAL SEARCH: CONTINUOUS PROBLEMS

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CONTENTS

LIST OF FIGURES	vii
LIST OF TABLES	xi
PREFACE	xiii
1 PRELIMINARIES	1
1.1 Interval Arithmetic	3
1.2 Interval Linear Systems	18
1.3 Derivatives and Slopes	26
1.4 Automatic Differentiation and Code Lists	36
1.5 Interval Newton Methods and Interval Fixed Point Theory	50
1.6 The Topological Degree	66
2 SOFTWARE ENVIRONMENTS	71
2.1 INTLIB	71
2.2 Fortran 90 Interval and Code List Support	78
2.3 Other Software Environments	102
3 ON PRECONDITIONING	113
3.1 The Inverse Midpoint Preconditioner	115
3.2 Optimal Linear Programming Preconditioners	120
4 VERIFIED SOLUTION OF NONLINEAR SYSTEMS	145
4.1 An Overall Branch and Bound Algorithm	146
4.2 Approximate Roots and Epsilon-Inflation	150

4.3	Tessellation Schemes	154
4.4	Description of Provided Software	159
4.5	Alternate Algorithms and Improvements	167
5	OPTIMIZATION	169
5.1	Background and Historical Algorithms	170
5.2	Handling Constraints	177
5.3	Description of Provided Software	199
6	NON-DIFFERENTIABLE PROBLEMS	209
6.1	Extensions of Non-Smooth Functions	210
6.2	Use in Interval Newton Methods	218
7	USE OF INTERMEDIATE QUANTITIES IN THE EXPRESSION VALUES	227
7.1	The Basic Approach	227
7.2	An Alternate Viewpoint – Constraint Propagation	230
7.3	Application to Global Optimization	230
7.4	Efficiency and Practicality	232
7.5	Provided Software	233
7.6	Exercises	234
	REFERENCES	235
	INDEX	255

LIST OF FIGURES

Chapter 1

1.1	The united solution set $\Sigma(\mathbf{A}, \mathbf{B})$ for the system (1.19)	20
1.2	$\Sigma(\mathbf{A}, \mathbf{B}) \cap \mathbf{X}$ can still be bounded when $AX = B$ is underdetermined.	23
1.3	The difference between the interval slope $\mathbf{S}^\sharp(f, \mathbf{x}, \tilde{x})$ and the derivative range f'_u for $\mathbf{x} = [0, 2]$, $\tilde{x} = 1$ and $f(x) = x^2$	28
1.4	Two ways of computing the change in ϕ between $(\tilde{x}_1, \tilde{x}_2)$ and (x_1, x_2)	31
1.5	Sample program to compute a floating point function value from a code list	49
1.6	Non-uniqueness with slopes with $f(x) = (x^2 - 1)(x + 2)$, $\mathbf{x} = [-2, 3]$ and $\tilde{x} = 3$	64

Chapter 2

2.1	A FORTRAN-77 program using INTLIB	77
2.2	Illustration of use of the interval data type	79
2.3	A univariate interval Newton method program, used to generate the data in Table 1.3	82
2.4	Program that generates a code list for $f(x) = x^4 + x^3 + x$	85
2.5	Operation lines of the code list produced by the program of Figure 2.4	85
2.6	Sample OVERLOAD.CFG file	85
2.7	Accumulating a product for a dependent variable	86
2.8	Reassignment of a dependent variable	87
2.9	The code list operation lines for the program in Figure 2.8	87
2.10	(a) Function USR for Example 2.1	90
2.10	(b) Function USRD for Example 2.1	90
2.11	A program to generate a code list for $f_1(x) = f(x) - 2$, where $f(x)$ is as in Example 2.1	91

2.12	Generation of a derivative code list corresponding to the code list in file <code>EX1.CDL</code>	92
2.13	Operation lines of the code list for the derivative of $f(x) = x^4 + x^3 + x$	92
2.14	Algebraic interpretation of the code list in Figure 2.13	92
2.15	A code list for the function in Example 2.2	93
2.16	The derivative code list corresponding to Figure 2.15	93
2.17	A program to generate a code list for $\phi(x_1, x_2) = x_1^2 + x_2^2$, subject to $x_1 + x_2 - 1 = 0$	100
2.18	Evaluation of the constraints in Example 2.3	100
Chapter 3		
3.1	Action of a C-preconditioner	125
3.2	Action of an E-preconditioner	125
3.3	Appropriate situation for a left-optimal preconditioner	126
3.4	Action of a magnitude-optimal C-preconditioner: $\max\{a, b\}$ is minimized.	127
3.5	Action of a magnitude-optimal E-preconditioner: $\min\{a, b\}$ is maximized.	128
Chapter 4		
4.1	Complementation of a box in a box	154
4.2	Complementation of a box in a list of boxes	156
4.3	Bisection of the second coordinate according to maximum smear, for Example 4.1	158
4.4	Program to produce a code list for a counterexample to a method of Branin	161
4.5	Box data file <code>BRANIN.DT1</code>	162
4.6	<code>RUN_ROOTS_DELETE</code> for <code>BRANIN.CDL</code> and <code>BRANIN.DT1</code>	162
4.7	Sample output to <code>RUN_ROOTS_DELETE</code>	163
4.8	Box data file <code>BRANIN.DT2</code>	163
4.9	Use of <code>RUN_ROOTS_DELETE</code> for uniqueness verification	164
Chapter 5		
5.1	“Peeling ” a box to produce lower-dimensional boundary elements	181

5.2	“Peeling” the box into lower-dimensional boundary elements	183
5.3	Proving that there exists a feasible point of an underdetermined constraint system	186
5.4	Proving existence in a reduced space when the approximate feasible point satisfies bound constraints	186
5.5	A common degenerate case, when \check{X} must be perturbed	187
5.6	Geometry of a feasibility proof with LP preconditioners	190
5.7	Box data file GOULD.DT1	202

Chapter 6

6.1	Program that generates a code list for $f(x) = x^2$ if $x < 1$, $f(x) = 2x - 1$ if $x \geq 1$	211
6.2	Operation lines of the code list produced by the program of Figure 6.1	212
6.3	Computation of slope bounds of a discontinuous function	214

LIST OF TABLES

Chapter 1

1.1	Some example operations and corresponding numerical codes	44
1.2	Tabular representation of the output to the program (1.36)	48
1.3	Illustration of quadratic convergence of the univariate interval Newton method for $f(x) = x^2 - 4$	54
1.4	Illustration of quadratic convergence of the Krawczyk method for F as in Example 1.5	58

Chapter 2

2.1	Elementary arithmetic routines in INTLIB	74
2.2	Standard function routines in INTLIB	75
2.3	Utility functions in INTLIB	75
2.4	Special interval functions in module INTERVAL_ARITHMETIC	80
2.5	Logical and interval operators in module INTERVAL_ARITHMETIC	81
2.6	Operations in module OVERLOAD and program MAKE_GRADIENT	84
2.7	Additional operations supported in module OVERLOAD	85
2.8	Operational complexity – generic routines	98
2.9	Ratio of interval to floating point CPU times CPURAT for ACRITH-XSC on an IBM 3090	105
2.10	Ratio of interval to floating point CPU times CPURAT for INTERVAL_ARITHMETIC on a Sun SPARC 20 model 51	105

Chapter 5

5.1	Summary attributes of various global optimization algorithms	177
5.2	Summary of handling of constraints in various global optimization algorithms	178

5.3	Summary of 3 methods of handling constraints for Example 5.2	198
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Chapter 6

6.1	Iterates of the interval Newton method for $f(x) = x^2 - x - 2x + 2$	225
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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@us1.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.

1

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*

$$\mathbf{X} = \{(x_1, x_2, \dots, x_n)^T \in \mathbb{R}^n \mid \underline{x}_i \leq x_i \leq \bar{x}_i, 1 \leq i \leq n\}, \quad (1.1)$$

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

Given $F : \mathbf{X} \rightarrow \mathbb{R}^n$, *rigorously* enclose *all* solutions $X^* \in \mathbf{X}$. That is, for each

$$X^* = (x_1^*, \dots, x_n^*)^T \in \mathbf{X}$$

with $F(X^*) = 0$, find bounds $a_i \leq x_i^* \leq b_i$ such that

- $b_i - a_i$ is small, $1 \leq i \leq n$, and
- it is mathematically but automatically proven that there is a unique root of F within each

$$\tilde{\mathbf{X}} = \{X = (x_1, \dots, x_n) \mid a_i \leq x_i \leq b_i, 1 \leq i \leq n\}.$$

(1.2)