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Book Review

C.A. Floudas, *Deterministic Global Optimization: Theory, Algorithms and Applications*. Kluwer Academic Publishers, 2000, 760 pp., 315 US$, hardbound, ISBN 0-7923-6041-1 (Nonconvex Optimization and Its Applications, Vol. 37).

During the last decade, the field of deterministic global optimization has witnessed an explosive growth in theoretical advances, algorithmic developments, and applications across all disciplines of science and engineering. The book of C.A. Floudas, a leading authority in the field, provides a unified and insightful treatment of deterministic global optimization. It combines novel theoretical and algorithmic advances with the now ubiquitous domain of applications ranging from process design to process synthesis to process control to process operations to phase equilibrium to design under uncertainty to parameter estimation to azeotrope prediction to structure prediction in protein folding and peptide docking. As such it bridges the gap between theory, algorithms and applications and it represents a monumental milestone.

This textbook introduces theoretical and algorithmic advances that address the computation of global minima and maxima, determine lower and upper bounds on the global optima, and enclose all solutions of nonlinear constrained systems of equations.

Chapter 1 motivates the reader for studying global optimization, introduces the major classes of mathematical models studied, presents several important application areas, discusses the basics of complexity analysis, and outlines the contributions from the chemical engineering field.

Chapter 2 introduces, in a comprehensive way, the fundamentals of deterministic global optimization that include convex sets; convex, concave and nonconvex functions; quasiconvex and quasiconcave functions; pseudoconvex and pseudoconcave functions; convex envelopes; different types of underestimating functions; local and global minima; and difference of convex (d.c.) functions. This chapter provides an excellent exposition to the basics of convex analysis and the key principles of deterministic global optimization.

The remaining twenty-two chapters are divided into five major parts: Part I, covering *Biconvex and Bilinear Problems*, Part II, addressing *Signomial Problems*, Part III, discussing *General Twice Differentiable NLP Problems*, Part IV, dealing with *Nonlinear and Mixed Integer Optimization MINLP Problems*, and Part V, presenting the *Enclosure of All Solutions of Nonlinear Constrained Systems of Equations*.

Part I focuses on the global optimization of biconvex and bilinear mathematical models. Chapter 3 introduces the theory of the GOP primal relaxed dual decomposition algorithm and its application to quadratic programming problems, quadratically constrained problems and polynomial problems. In addition, it presents a branch and bound framework, discusses a reformulation of the relaxed dual as a single MILP and introduces a linear branching scheme. Chapter 4 describes the implementation and presents a variety of computational studies. Chapter 5 extends the theory to bilevel linear and quadratic optimization problems. Chapter 6 introduces the phase and chemical equilibrium problem and the application of the GOP to the minimization of the Gibbs free energy and the tangent plane stability criterion problems. Chapter 7 discusses the distributed implementation and its application to large scale pooling problems and indefinite quadratic programming problems.

Part II addresses the global optimization of generalized geometric programming problems. Chapter 8 introduces the theoretical analysis for signomial problems that includes the exponential transformation, the convex lower bounding approach, the updates of the bounds, the monotonicity analysis, and the branch and bound framework. Chapter 9 presents computational studies on chemical engineering design and robust stability analysis problems with real parametric uncertainty.

Part III, consisting of ten chapters, deals with general twice continuously differentiable nonlinear optimization NLP problems. Chapter 10 introduces the key theoretical developments that set the basis for the transition from biconvex and bilinear problems to general twice differentiable NLPs. Chapter 11 presents the theory of the αBB global optimization approach for box constrained twice differentiable NLPs. Chapter 12 introduces the theory of the αBB global optimization approach for general constrained NLPs and presents several rigorous methods for the calculation of the parameters α. Chapter 13 discusses the implementation of the αBB and presents a variety of computational studies. Chapters 14–19 present studies of several important application areas. Chapter 14 introduces the structure prediction of clusters. Chapter 15 focuses on the structure prediction of small acyclic molecules. Chapter 16 introduces the protein folding problem and discusses a novel framework for the structure prediction of unsolvated and solvated peptides. Chapter 17 introduces the peptide docking problem and presents a decomposition and global optimization approach for the interactions of pocket 1 of the HLA-DRB1 protein with small virus peptides. Chapter 18 deals with the batch design under uncertainty of multiproduct and multipurpose plants. Chapter 19 introduces a global optimization method for the parameter estimation problem of nonlinear algebraic models via the error in variables approach.

Part IV addresses mixed integer nonlinear optimization MINLP problems. Chapter 20 introduces the MINLPs and overviews the local MINLP approaches and the global MINLP methods. Chapter 21 presents the theory and computational studies of the SMIN-αBB global optimization approach which is applicable to special structure MINLP problems, while Chapter 22 introduces the theory and applications of the GMIN-αBB approach which can be applied to general MINLPs.

Part V addresses the enclosure of all solutions of nonlinear constrained systems of equations. Chapter 23 discusses the theory and algorithmic aspects of a deterministic global optimization approach. Chapter 24 deals with the problem of locating all azeotropes and presents a deterministic global optimization approach to the enclosure of all homogeneous azeotropes.

The organization and content of the material in each part results in a self-contained book, while appropriate links to other related works are maintained throughout the book as evidenced via the remarkable list of more than 600 references. Each chapter contains several illustrations and geometrical interpretations of the theoretical results presented, while the analysis of the presented applications illustrates clearly the power of the global optimization methods. The material is presented in a combination of an in-depth analysis of the theory, detailed but remarkably transparent algorithmic description, as well as elegant and insightful connection of the analysis and algorithms to several important areas of applications. The phenomenal clarity of presentation of the fundamental theoretical and algorithmic advances coupled with applications of utmost importance establish this textbook as a cornerstone in global optimization.

In summary, this book provides a unique exposition to the fascinating field of deterministic global optimization. Its impressive treatment of the subjects in depth, and the coverage of widespread applications make it accessible to students and researchers in a variety of disciplines including applied mathematics, chemical engineering, computational chemistry, computer science, molecular biology, operations research and economics. It is destined to take its place on the bookshelf of every researcher interested in global optimization, and will undoubtedly become a classic reference – an outstanding book which I recommend enthusiastically.

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