Convexification and Global Optimization in Continuous and Mixed-Integer Nonlinear Programming

Nonconvex Optimization and Its Applications

Volume 65

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Convexification and Global Optimization in Continuous and Mixed-Integer Nonlinear Programming

Theory, Algorithms, Software and Applications

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Preface

Interest in constrained optimization originated with the simple linear programming model since it was practical and perhaps the only computationally tractable model at the time. Constrained linear optimization models were soon adopted in numerous application areas and are perhaps the most widely used mathematical models in operations research and management science at the time of this writing. Modelers have, however, found the assumption of linearity to be overly restrictive in expressing the real-world phenomena and problems in economics, finance, business, communication, engineering design, computational biology, and other areas that frequently demand the use of nonlinear expressions and discrete variables in optimization models. Both of these extensions of the linear programming model are $\mathcal{NP}$-hard, thus representing very challenging problems. On the brighter side, recent advances in algorithmic and computing technology make it possible to revisit these problems with the hope of solving practically relevant problems in reasonable amounts of computational time.

Initial attempts at solving nonlinear programs concentrated on the development of local optimization methods guaranteeing globality under the assumption of convexity. On the other hand, the integer programming literature has concentrated on the development of methods that ensure global optima. The aim of this book is to marry the advancements in solving nonlinear and integer programming models and to develop new results in the more general framework of mixed-integer nonlinear programs (MINLPs) with the goal of devising practically efficient global optimization algorithms for MINLPs.

We embarked on the journey of developing an efficient global optimization algorithm for MINLPs in the early 1990s when we realized that there was no software that could even solve small-sized MINLPs to global optimality despite indications in the literature that such an algorithm could be easily constructed. Our initial attempts, however, found us struggling with many gaps in the literature in the specifications of such a global optimization algorithm. Therefore, about ten years ago, we decided to concentrate on special classes of mixed-integer nonlinear programs, including separable concave minimization problems and applications in capacity expansion of chemical processes. In the process, we developed the first branch-and-bound framework for MINLPs, the Branch-And-Reduce Optimization Navigator (BARON). Its initial purpose was to facilitate design and experimentation with global optimization algorithms. Drawing from this initial experience, in the last six years, we have concentrated on the automatic solution of a general class of MINLPs.

This book documents many of the theoretical advancements that have enabled us to develop BARON to the extent that it now makes it possible for the first time to solve many practically relevant problems in reasonable amounts of computational time in a completely automated manner. Theoretical and algorithmic developments that brought about this situation included:

- A constructive technique for characterizing convex envelopes of nonlinear functions (Chapter 2).

- Many strategies for reformulating mixed-integer nonlinear programs that enable efficient solution. For example, in Chapter 3, we show that "product disaggregation" (distributing the product over the sum) leads to tighter linear programming relaxations, much like variable disaggregation does in mixed-integer linear programming.

- Novel relaxations of nonlinear and mixed-integer nonlinear programs (Chapter 4) that are entirely linear and enable the use of robust and established linear programming techniques in solving MINLPs.

- A new theoretical framework for range reduction (Chapter 5) that helped us identify connections with Lagrangian outer-approximation and develop a unified treatment of existing and several new domain reduction techniques from the integer programming and constraint programming literatures.

- Techniques to traverse more efficiently the branch-and-bound tree, including:

    - the algorithm of Section 7.6.1 that finds all feasible solutions of systems of nonlinear equations as well as combinatorial optimization problems through enumeration of a single search tree;

- the postponement strategy of Section 7.6.3;
- the branching scheme of Section 7.6.4 that guarantees finite termination for classes of problems for which previous algorithms were either convergent only in limit (*i.e.*, infinite) or resorted to explicit enumeration.

We demonstrate through computational experience that our implementation of these techniques in BARON can now routinely solve problems previously not amenable to standard optimization techniques. In particular:

- In Section 3.6.2, we present a small but difficult instance of a nuclear reactor pattern design problem that was solved for the first time to global optimality using our algorithms.

- In Chapter 8, we completely characterize the feasible space of a refrigerant design problem proposed 15 years ago revealing all the 29 candidate refrigerants that meet the design specifications.

- In Chapters 3, 9, 10, and 11, we provide new solutions and/or improved computational results compared to earlier approaches on various benchmark problems in stochastic decision making, pooling and blending problems in the petrochemical industry, a restaurant location problem, engineering design problems, and a large set of benchmark nonlinear and mixed-integer nonlinear programs.

In writing this book we had three aims. First, to provide a very comprehensive account of material previously available only in journals. Second, to offer a unified and cohesive treatment of a wealth of ideas at the operations research and computer science interface. Third, to present (in over half of the book) new material, including new algorithms, a detailed description of the implementation, extensive computational results, and many geometric interpretations and illustrations of the concepts throughout the book.

We expect that the readership of this book will vary significantly due to the rich mathematical structure and significant potential for applications of mixed-integer nonlinear programming. Students and researchers who wish to focus on convex analysis and its applications in MINLP should find Chapters 2 through 5 and Chapter 9 of interest. Chapters 3, 6, 7, 10, and 11 will appeal to readers interested in implementation and computational issues. Finally, the material in Sections 3.6.2, 3.6.3, and 3.11.3 as well as Chapters 8, 9, 10, and 11 cover modeling and applications of mixed-integer nonlinear programming.

We hope that this book will be used in graduate level courses in nonlinear optimization, integer programming, global optimization, convex analysis, applied mathematics, and engineering design. We also hope that the book will kindle the interest of graduate students, researchers, and practitioners in global optimization algorithms for mixed-integer nonlinear programming and that in the coming years we will witness works that bring forth improvements and applications of the algorithms proposed herein. To facilitate developments in these directions, we plan to maintain detailed descriptions of many of the models used in this book as well as other related information at: `http://web.ics.purdue.edu/~mtawarma/minlpbook/`.

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