

Global Optimization: from Theory to Implementation

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To Anne-Marie and Kja

Preface

The idea for this book was born on the coast of Serbia-Montenegro, in October 2003, when we were invited to the thirtieth Serbian Conference on Operations Research (SYM-OP-IS 2003). During those days we talked about many optimization problems, going from discussion to implementation in a matter of minutes, reaping good profits from the whole “hands-on” process, and having a lot of fun in the meanwhile. All the wrong ideas were weeded out almost immediately by failed computational experiments, so we wasted little time on those. Unfortunately, translating ideas into programs is not always fast and easy, and moreover the amount of literature about the implementation of global optimization algorithm is scarce.

The scope of this book is that of moving a few steps towards the systematization of the path that goes from the invention to the implementation and testing of a global optimization algorithm. The works contained in this book have been written by various researchers working at academic or industrial institutions; some very well known, some less famous but expert nonetheless in the discipline of *actually getting global optimization to work*.

The papers in this book underline two main developments in the implementation side of global optimization: firstly, the introduction of symbolic manipulation algorithms and automatic techniques for carrying out algebraic transformations; and secondly, the relatively wide availability of extremely efficient global optimization heuristics and metaheuristics that target large-scale nonconvex constrained optimization problems directly.

The book is divided in three parts. The first part is about new global optimization methods. The chapters in the first part are rather theoretical in nature, although a computational experiments section is always present. The second part is oriented towards the implementation, focusing on description of existing solvers and guidelines about building new global optimization software. This part follows two main trends: the first four chapters deal with continuous methods, the last three with combinatorial ones. The third (and last) part presents two applications of global optimization in Data Mining and Molecular Conformation.

More specifically, a lot of work has been carried out on the application of Variable Neighbourhood Search to global optimization (Chapters 6, 8, 10 and 11). A MultiStart-type algorithm based on low-discrepancy sequences generated deterministically has also been thoroughly explored (Chapters 5, 8). A full description of an API for interfacing to metaheuristic codes is given in Chapter 11. Deterministic algorithms can be found in Chapters 1 (Branch-and-Bound algorithms), 3 (a Cutting Plane algorithm), 4 (a Branch-and-Bound based method for stochastic mixed-integer nonlinear problems) and 8 (where the implementation of a spatial Branch-and-Bound algorithm is described).

Chapter 1 and 2 are more theoretical than most other chapters. Chapter 1 considers global optimization problems where the objective functions and constraints are difference of monotonic functions, and proposes some deterministic solution methods; Chapter 2 reports on a special local search method for reverse convex problems. In both chapters, a section on computational results is presented, discussing the efficiency of different solution approaches.

Chapter 4 describes one of the very few existing implementations of a deterministic global optimization software targeting robust nonconvex programming. In order to face the huge computational resources needed to solve multi-scenario nonconvex problems, the author proposes a Branch-and-Bound approach where the lower bounds are computed by solving a nonconvex Lagrangian relaxation through a standard global optimization algorithm. This multi-level solution method requires careful software design to obtain a working implementation.

As has been mentioned, a particularly important development is the introduction of symbolic manipulation algorithms in optimization. Chapter 7 describes a modelling language by which it is possible to keep track of the convexity property of the optimization problem being described. Although Chapter 7 is about convex programming, the role of convexity is so important in Branch-and-Bound based algorithms for global optimization that it was decided to include it in this book. In Chapter 8 the reader can find the description of some symbolic algorithms for differentiation, algebraic simplification and generation of convex relaxations. Chapter 3 introduces some effective convexity transformations for a large class of multilinear problems, as well as discussing some nonlinear cuts. Chapter 10 employs even more sophisticated symbolic techniques about automated theorem proving.

Chapters 9 and 12 describe working implementations of commercial-grade software. In particular, Chapter 9 is about the Lipschitz Global Optimization (LGO) solver suite, and its embedding within the Mathematica software framework; Chapter 12 describes a solver for Mixed-Integer Linear Programming problems (commercialized by Process Systems Enterprise, Ltd.): this software relies on CORBA techniques to automate the parallelization and distributed running of the solver.

As far as the applications are concerned, Chapter 13 describes an extremely interesting class of problems arising in Data Mining and Nonlinear

Classification. Chapter 14 describes a new way to generate instances for the Molecular Distance Geometry Problem, which is one of the hardest problems in Molecular Conformation.

Some of these papers have inter-relations and cross-references, due both to collaborations among the authors and to emergence of new trends in global optimization. Most of these inter-relations have been emphasized by means of footnotes, which have all been added by the editors.

We hope that the reader will find this book interesting and enlightening, and that it will serve as a source of ideas as well as a desktop companion for people who need to implement global optimization software.

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