

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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Contents

Optimization under Composite Monotonic Constraints and Constrained Optimization over the Efficient Set

<i>Hoang Tuy, N.T. Hoai-Phuong</i>	3
1 Introduction	3
2 Some basic concepts and results of monotonic optimization	5
3 Problems with composite monotonic constraints	7
4 Constrained optimization over the efficient set	11
5 Solution method for problem (Q)	15
6 Improvements for problems (OWE) and (OE)	19
7 Problems with a composite monotonic objective function	25
8 Illustrative examples and computational results	26
References	29

On a Local Search for Reverse Convex Problems

<i>Alexander Strekalovsky</i>	33
1 Introduction	33
2 Some features of RCP	34
3 Local search methods	36
4 Computational testing	40
5 Conclusion	42
References	42

Some Transformation Techniques in Global Optimization

<i>Tapio Westerlund</i>	45
1 Introduction	45
2 The MINLP Problem	46
3 The transformation approach	47
4 Examples of transformations	52
5 The GGPECP algorithm	55
6 Convergence to the globally optimal solution	57
7 A numerical example	59

8	Some aspects on the numerical solution approach	64
9	Conclusions	70
	References	71

Solving Nonlinear Mixed Integer Stochastic Problems: a Global Perspective

	<i>Maria Elena Bruni</i>	75
1	Introduction	76
2	Motivations	76
3	SMINLP: state of the art	77
4	Problem formulation	84
5	The two-phase solution approach	86
6	Illustrative application: the Stochastic Trim Loss Problem	98
7	Concluding Remarks	104
	References	106

Application of Quasi Monte Carlo Methods in Global Optimization

	<i>Sergei Kucherenko</i>	111
1	Introduction	111
2	Analysis of Quasirandom Search methods	114
3	Single linkage and multilevel single linkage methods	117
4	Computational experiments	120
5	Conclusion	131
	References	131

GLOB – A new VNS-based Software for Global Optimization

	<i>M. Dražić, V. Kovacević–Vujčić, M. Cangalović, N. Mladenović</i>	135
1	Introduction	135
2	VNS methodology	136
3	Software package GLOB	137
4	Numerical experiments	141
5	Conclusion	147
	References	148

Disciplined Convex Programming

	<i>Michael Grant, Stephen Boyd, Yinyu Ye</i>	155
1	Introduction	155
2	Motivation	156
3	Convex programming	162
4	Modeling frameworks	169
5	Disciplined convex programming	171
6	The convexity ruleset	172
7	The atom library	183
8	Verification	188
9	Creating disciplined convex programs	191

10 Implementing atoms 193
 11 Conclusion 199
 References 200

Writing Global Optimization Software

Leo Liberti 211
 1 Introduction 211
 2 Global Optimization algorithms 214
 3 Global Optimization software 223
 4 Optimization software framework design 232
 5 Symbolic manipulation of mathematical expressions 240
 6 Local solvers 247
 7 Global solvers 248
 8 Conclusion 257
 References 258

MathOptimizer Professional: Key Features and Illustrative Applications

János D. Pintér, Frank J. Kampas 263
 1 Introduction 263
 2 Global Optimization 266
 3 LGO Solver Suite 267
 4 MathOptimizer Professional 268
 5 Illustrative applications: solving sphere packing models 271
 6 Conclusions 276
 References 277

Variable Neighborhood Search for Extremal Graphs 14: The AutoGraphiX 2 System

M. Aouchiche, J.M. Bonnefoy, A. Fidahoussen, G. Caporossi, P. Hansen, L. Hiesse, J. Lacheré, A. Monhait 281
 1 Introduction 281
 2 AGX 2 Interactive functions 283
 3 Algebraic syntax used in AutoGraphiX 291
 4 Optimization using Variable Neighborhood Search 294
 5 AutoGraphiX Tasks 299
 6 Automated proofs 301
 7 Some examples 305
 8 Conclusion 308
 References 308

From Theory to Implementation: Applying Metaheuristics.

I.J. García del Amo, F. García López, M. García Torres,, B. Melián Batista, J.A. Moreno Pérez, J.M. Moreno Vega 311
 1 Introduction 311
 2 Class hierarchy 316

3	Implementation: The p -Median Problem	333
4	Conclusions	338
	References	339

***ooMILP* – A C++ Callable Object-oriented Library and the
Implementation of its Parallel Version using CORBA**

	<i>Panagiotis Tsiakis, Benjamin Keeping</i>	353
1	Introduction	353
2	<i>ooMILP</i> Overview	356
3	C++ objects and pre-CORBA serial implementation	357
4	Initial CORBA Version	361
5	Partially decomposable MILPs	366
6	Parallel solution software architecture	368
7	Conclusions	375
	References	375

**Global Order-Value Optimization by means of a Multistart
Harmonic Oscillator Tunneling Strategy**

	<i>R. Andreani, J.M. Martinez, M. Salvatierra, F. Yano</i>	379
1	Introduction	379
2	Local algorithm	381
3	Lissajous motions	382
4	Global algorithm	384
5	Hidden patterns	387
6	Numerical experiments	388
7	Conclusions	394
	References	397

**On generating Instances for the Molecular Distance Geometry
Problem**

	<i>Carlile Lavor</i>	405
1	Introduction	405
2	Moré-Wu instances	406
3	New instances	407
4	Conclusion	413
	References	414

	Index	415
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