

Final Report—Optimization Under Nonconvexity and Uncertainty: Algorithms and Software

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Jeff Linderoth, Principal Investigator

Department of Industrial and Systems Engineering

University of Wisconsin-Madison

3226 Mechanical Engineering Bldg

1513 University Avenue

Madison, WI 53706-157 USA

Phone: 608-890-1931

Fax: 608-262-8454

email: linderoth@wisc.edu

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DOE/Office of Science Technical Program Manager: Sandy Landsberg

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1 Overview

Numerical optimization is a pervasive tool for planning and controlling physical systems. A small sample of applications using optimization includes blending and process design, bioinformatics, environmental planning, national security, medical treatment planning, and financial asset and supply chain management. However, even with the advances made in optimization theory and algorithms, and with the increasing power and utility of large-scale computational platforms, there still exist areas in which the needs of users of optimization technology exceed the tools and solution capabilities of modern solvers. This continuation-transfer of an Early Career Principal Investigator Award primarily addressed solving optimization problems where nonconvexity in the problem arises from discrete choices for decision variable values.

Project Objectives: Develop new algorithmic techniques for solving large-scale numerical optimization problems, focusing on problems classes that have proven to be among the most challenging for practitioners: those involving uncertainty and those involving nonconvexity. This research advanced the state-of-the-art in solving mixed integer linear programs containing symmetry, mixed integer nonlinear programs, and stochastic optimization problems. The focus of the work done in the continuation was on Mixed Integer Nonlinear Programs (MINLP)s and Mixed Integer Linear Programs (MILP)s, especially those containing a great deal of symmetry.

2 Mixed Integer Nonlinear Programs

Many decision problems in scientific, engineering, and public sector applications involve both discrete decisions and nonlinear system dynamics that affect the quality of the final design or plan. Mixed-integer nonlinear programming (MINLP) problems combine the difficulty of optimizing over discrete variable sets with the challenges of handling nonlinear functions. MINLP is one of the most

flexible modeling paradigms available for optimization problems. Key applications that MINLP can accurately model include optimal power flow problems; network design and expansion; reactor reloading models; and energy storage system design problems. Unfortunately, the wealth of applications that can be accurately modeled using MINLP is not yet matched by the capability of even the best solvers for this important class of problems. Algorithms and software often cannot provide acceptable solutions to practically sized instances in reasonable computing time. Our work in this proposal was to make progress towards transform MINLP into a paradigm that can not only model wide varieties of important problems, but also deliver practical solutions to them.

Software: Our first fundamental contribution was the design and implementation of a software package FilMINT, an implementation of the LP/NLP-BB algorithm for convex MINLP. The software is among the most effective available solvers for convex instances [1]. Building on this work, we published a survey paper on algorithms and software for solving convex MINLPs [3].

Disjunctive Cutting Planes: We also did an extensive study with a Ph.D. student on disjunctive cutting planes in the context of MINLP, culminating with the Ph.D. thesis [9]. The paper [11] shows the relationship of disjunctive inequalities to strong branching, while in the work [10], we give a computationally viable mechanism for generating general disjunctive cutting planes for convex MINLPs. In [4], we surveyed these (and other) recent results on disjunctive cutting planes for convex MINLP.

Strong Relaxations: We studied MINLPs that are driven by a collection of indicator variables where each indicator variable controls a subset of the decision variables. We introduced the *perspective relaxation* in [7], and demonstrated its wide applicability in [8].

Multilinear Programming: In the recently-completed Ph.D. thesis [14], a student explored both theoretical and empirical issues in solving multilinear programs, a special case of a nonconvex MINLP. In [13], we are able to establish (to our knowledge) the first approximation-algorithm type results for the quality of specific relaxations for global optimization problems.

MINLP Probing: Bound tightening is an important component of algorithms for solving nonconvex MINLPs. In [15], we propose a variant of a strong bound-tightening algorithm known as *probing* where the consequences of tightening a bound is done by a truncated Branch-and-Bound algorithm. As this approach is computationally expensive, an interesting approach in this research was the use of machine learning techniques (a Support-Vector-Machine classifier) to infer whether or not the probing algorithm should be used.

Product Pooling: The pooling problem is a bilinear program that models linear blending in a network. Often, pooling problems contain binary variables that model network design issues. In [5], We study how to tighten relaxations of pooling problems with binary variables by studying the convex hull of simple sets associated with these problems.

Engineering Design: In [2], we applied MINLP techniques to the design of a thermal insulation system, and showed that useful solutions could be obtained without resorting to the use of “categorical” decision variables.

3 Mixed Integer Linear Programming

Orbital Branching: In [16], we introduce a novel branching methodology, called *orbital branching*, that may be used to effectively solve integer programs that contain a great deal of symmetry. The methodology has been adopted into state of the art MILP solvers such as Gurobi and CPLEX.

Steiner Triple Systems: A constraint-based variant of orbital branching, along with parallel enumeration of partial solution allowed us to answer some decades-old questions about the incidence-width of special Steiner Triple Systems [17, 18]

Football Pool Problem: The Football Pool Problem, which gets its name from a lottery-type game where participants predict the outcome of soccer matches, is to determine the smallest covering code of radius one of ternary words of length v . For $v = 6$, the optimal solution is not known, and is one of the most famous open problems in coding theory. In [12], using a combination of symmetry-enhanced branching, subcode enumeration, and linear-programming-based bounding, running on a high-throughput computational grid consisting of thousands of processors, we are able to improve the lower bound on the size of the optimal code from 65 to 71.

Lookahead Branching: In [6], we consider the effectiveness of a *lookahead* branching method for the selection of branching variable in branch-and-bound method for mixed integer programming. Specifically, we ask the following question: by taking into account the impact of the current branching decision on the bounds of the child nodes *two* levels deeper than the current node, can better branching decisions be made?

4 Conclusions

This report described the progress made on optimization algorithms and software for solving discrete optimization problems. Support from the Department of Energy under the earlier grant agreement DE-FG02-05ER25694 as well as the current agreement DE-FG02-09ER25869 is gratefully acknowledged. A complete list of publications supported at least in part by the grant DE-FG02-09ER25869 is given in the bibliography section.

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