

Solving Large Nonconvex Models with a Deterministic Global Optimization Solver

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1. Introduction

There are a variety of problems in production planning, process design and synthesis, supply chain management, resource allocation and elsewhere where a guaranteed global optimum, rather than just a local optimum, is desired. There is a wide array of nonlinear solvers available to solve such complex problems. However, traditional solvers are not able to cope with the challenge of finding the truly best solutions with a certainty. Probabilistic approaches, based on various ideas such as using random multiple start points with the algorithms, have been useful. It would be satisfying, however, to have a guarantee of finding truly best solutions to nonlinear/nonconvex models. We describe a deterministic global solver that is based on several ideas: a) constructing a convex linear relaxation of a nonlinear model, b) using a combination of interval analysis, constraint propagation and algebraic reformulation, and c) a branch-and-bound technique to exhaustively search over the subproblem partitions of the original model. A distinctive feature of the implementation is the wide range of mathematical functions recognized, including smooth, nonsmooth, and discontinuous functions, logical and operational operators, and probability distributions.

2. Algorithm Enhancements

Since its early development [1], this global solver has been used by various industries and applied to a wide array of real world nonlinear optimization problems. Not every modeler is an expert in setting up good models. Many of the models that we see are not concisely formulated, or contain expressions that are not suitable for building a tight relaxation. We have implemented a series of enhancements to cope with challenges raised from industrial applications and solve many previously intractable models. Those algorithms are general purpose and selectively invoked with a minimum overhead. Two examples of enhancements are in:

- 1) Preprocessing by extended interval analysis/constraint propagation schemes in bound range reduction, variable type induction, infeasible constraint/inconsistent expression detection, and numerical precision enhancement.

2) Automatic reformulation in the model parser to reformulate nonlinear models to be numerically friendly to the nonlinear solver and/or suitable to generate re-structured subproblems that result in a tight convex relaxation.

3. Applications and Performance

In this paper, we describe our experience in solving practical nonlinear/nonconvex/nonsmooth/integer constraint models to proven global optimum, based on new methods to reduce the convex relaxation gap and locate good solutions fast. Experience solving large spreadsheet nonconvex models demonstrates the ability to solve up to 10,000 variable problems.

1) Chemical Process Design: Flowsheets in Spreadsheets

The spreadsheet provides a convenient tool to model process/network related problems. One particular problem we encountered is to design an offshore process that splits oil into gas and condensate. The entire chemical process model is built within spreadsheet, which contains a data bank of all chemical component properties, and a flowsheet of numerical cells that depict pipeline network and separators. The main process has two input flows of crude oils with different compositions. The outflows are separated lines of fuel, gas, condensate, reinjection, and waste. The adjustable cells and design required constraints are specified explicitly in the spreadsheet. The objective cell is to maximize the ratio of condensate over gas. The underlying mathematical model contains 4,446 constraints, and 4,506 variables with 731 of them nonlinear. Modeling the behavior of chemicals in the separator results in nonlinear functions that have products, ratios, powers and logarithms of variables. The global solver finds the best solution at the root node and then takes 1 iteration and 15 seconds to prove global optimality on a 1.4GHz computer.

2) Energy Production Scheduling

The energy industry frequently needs to determine the optimal schedule to operate a group of turbine drivers for a series of pumps. The goal of modeling is to provide the maximum power generation with the online turbine drivers connected from a high steam header pressure to a lower steam pressure. Typically, the modeling of steam turbine output from fuel consumption involves the use of a high order (e.g., up to 6) univariate polynomial. For more complicated estimation, different polynomial curves apply for different ranges of fuel consumption. This results in a nonsmooth nonlinear segmental function, which represents a very challenging curve for the global solver to generate a tight convex relaxation. The characteristics of disjunction, nonlinearity and nonconvexity cause a serious overestimation to the function range estimation, which subsequently spreads out over the entire model, resulting in poor bounds for most of the variables and results in a very time consuming global search. The algorithm enhancement discussed in Section 2 overcomes these difficulties and makes previously unsolvable problems solveable in reasonable time. Of particular interest is a real world model that involves hourly scheduling of electric supply for 15 days. The objective is to minimize the ratio of

incremental capital cost over savings. The model includes 11,804 constraints and 14,688 variables with 1,083 of them nonlinear. The global solver finds the best solution at the root node and then takes 4 iteration and 3245 seconds to prove global optimality on a 1.4GHz machine.

3) Global supply chain management of chemicals

Global supply chain management has become a crucial consideration for international chemical companies, especially when multiple plants need to manufacture various chemicals to meet wide demand spread out around the world. If we expand the supply chain decisions to include every aspect of operations, the model gets more complicated (e.g., nonlinear, nonconvex and nonsmooth) to solve, not to mention solving for the best solution. For a particular global supply chain model from a renowned chemical company, the procedure is to plan ahead for several months the production schedule of a key chemical and make up delivery itinerary to multiple sites in three regions, Europe, US, and Asia. The objective is to minimize the total cost of production, logistics, resourcing, purchasing, and inventory holding. The model involves two types of nonlinear functions: algebraic and logic/disjunctive. The general algebraic functions are used to estimate production yields and manufacturing costs. They include the functions of multiplication, division, power, logarithm, and exponential. On the other hand, the logic/disjunctive functions are used to select costs/prices from a piecewise cost/price schedule, or select the minimum demand or maximum production ratio that needs to meet. The model includes 1635 constraints and 1895 variables with 481 of them as nonlinear. The global solver finds the best solution at the root node and then takes 1 iteration and 580 seconds to prove global optimality on a 1.4GHz machine.

4. Conclusion

We have outlined the features and techniques used in an enhanced global solver, which is capable of solving large nonconvex optimization problem for the global optimum in reasonable time. As demonstrated by real world applications, the challenge of solving nonlinear models to global optimality stems not only from the model size but also from the wide range of function types that arise in various applications. Continuing improvements will make this deterministic global optimization approach more attractive to and widely used by industry.

[1] C.-Y. Gau and L. E. Schrage, "Implementation and Testing of a Branch-and-Bound Based Method for Deterministic Global Optimization: Operations Research Applications," in *Frontiers in Global Optimization* (ed. C. A. Floudas and P. M. Pardalos), Kluwer Academic Publishers, pp. 145-165 (2003)