Deterministic Global Optimisation at CPSE: Models, Algorithms, and Software

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Abstract

Deterministic global optimisation is an active research area integrating: engineering applications; mathematical algorithms; computational software. This short article introduces global optimisation; we focus on advances made by researchers associated with the Centre for Process Systems Engineering. Our purposes are: (1) demonstrating global optimisation as an exciting research domain; (2) describing several industrially-relevant applications; (3) highlighting complementarity between disparate CPSE research groups; (4) offering a list of publications for further reading.

Keywords: Mixed-Integer Nonlinear Programming, MINLP, Deterministic Global optimisation, Branch & Bound

1. Introduction

Addressing the optimal design of multipurpose chemical plants, Grossmann and Sargent (1979) formulate a mathematical model as a mixed-integer nonlinear optimisation problem (MINLP) and write:

> This class of problem is very difficult to solve, and no general method of yet exists for its efficient solution.

Deterministic global optimisation of MINLP is NP-hard, so a general, efficient solution method will probably *never* exist. But MINLP has diverse application domains ranging from process networks to computational chemistry to finance. Focal points of research include: building effective mathematical models of

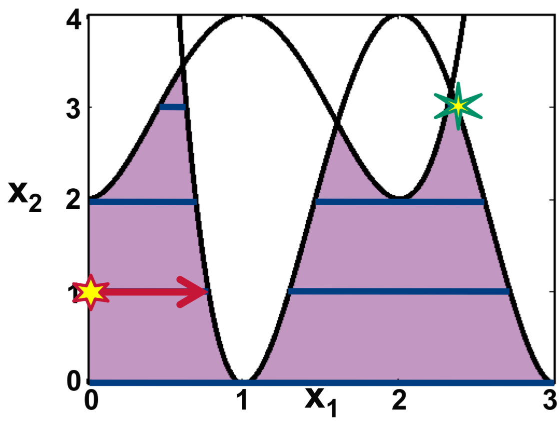

Figure 1: MINLP Example

industrially-relevant applications; designing algorithms which take advantage of special mathematical structure in optimisation problems; writing solver software integrating algorithms into a computational framework.

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Appendix A formally defines several classes (including MINLP) which can be addressed using deterministic global optimisation, but the simple example illustrated in Figure 1 can demonstrate the challenge of solving MINLP:

$$
\begin{aligned}
\max_{x_1,x_2} \quad & x_1 + x_2 \\
& 8 \cdot x_1^3 - 2 \cdot x_1^4 - 8 \cdot x_1^2 + x_2 \leq 2 \\
& 32 \cdot x_1^3 - 4 \cdot x_1^4 - 88 \cdot x_1^2 \\
& \qquad + 96 \cdot x_1 + x_2 \leq 36 \\
& x_1 \in [0,3] \\
& x_2 \in \{0, 1, 2, 3, 4\}
\end{aligned}
\tag{1}
$$

Example (1) is: *mixed-integer* because there are both continuous, $x_1 \in [0,3]$, and discrete, $x_2 \in \{0, 1, 2, 3, 4\}$, variables; *nonlinear* because of terms such as x_1^3; an *optimisation* problem because of the maximisation objective, $x_1 + x_2$. From Figure 1, it is obvious that the answer is the green star at $x_1 = 2.37$; $x_2 = 3$. But it is possible that a local solution method may initialise at a point such as the red star in the lower left of Figure 1; a local search staying within the feasible space would not reach the global solution.

Example (1) is a toy problem with only two variables; extensive research in the past 35 years has pushed the state-of-the-art to the point where ANTIGONE (Misener and Floudas, 2014a) can address several benchmarks up to $\mathcal{O}(10^4)$ variables and equations. Khor et al. (2014) use ANTIGONE to solve bilinear water network synthesis problems with up to 4657 continuous variables, 42 discrete variables, 5848 constraints, and 2704 nonconvex bilinear terms to deterministic global optimality; no other off-the-shelf optimisation software approached this efficacy.

Deterministic global optimisation for MINLP is computationally expensive, but it is highly relevant to application domains where there is high reward for fractional improvements and sufficient time to explore the search space. For very large problems beyond the limit of current deterministic algorithms, heuristics and stochastic methods may be most effective. CPSE researchers have extensive expertise developing *non-deterministic* algorithms (Gjerdrum et al., 2002; Zilinskas and Bogle, 2004; Akrotirianakis and Rustem, 2005; Parpas and Rustem, 2009; Parpas et al., 2009) with applications such as financial portfolio optimisation (Parpas and Rustem, 2006; Maringer and Parpas, 2009) and molecular dynamics (Ho and Parpas, 2014).

This short article mainly discusses applications, algorithms, and software for global optimisation of MINLP, but CPSE contributes to a range of deterministic global optimisation research domains including: multi-parametric programming (Dua et al., 2002; Wittmann-Hohlbein and Pistikopoulos, 2013; Oberdieck et al., 2014); dynamic global optimisation (Papamichail and Adjiman, 2002, 2005; Chachuat and Latifi, 2004; Chachuat et al., 2006); bi-level optimisation (Faísca et al., 2007; Mitsos et al., 2009b; Kleniati and Adjiman, 2014a,b); guaranteed parameter estimation (Michalik et al., 2009; Paulen et al., 2013).

2. Engineering Applications

The most established application domain for deterministic global optimisation of MINLP is in the area of process networks; here the applications include: blending feed stocks with intermediate storage (Misener and Floudas, 2009); crude oil scheduling (Li et al., 2012); process synthesis (Baliban et al., 2012). Emerging opportunities are in areas such as: biological and biomedical engineering (Misener et al., 2014a); computational chemistry (Pereira et al., 2010); project scheduling (Wiesemann et al., 2010).

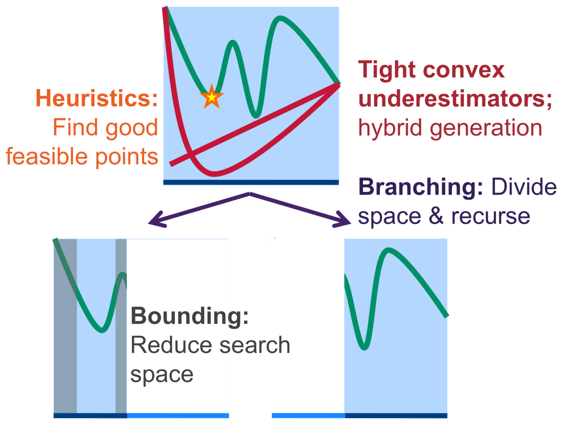

Figure 2: Branch & Bound Optimisation

We consider deterministic global optimisation of MINLP *through the lens of applications*; this is because researchers may be able to find and exploit *special mathematical structure* for particular problem classes. For example, Liberti and Pantelides (2006) use redundant constraints for process networks problems; Misener and Floudas (2013) automate an algorithmic variant in the software GloMIQO.

3. Mathematical Algorithms

The dominant solution method for deterministic global optimisation, shown in Figure 2, is *branch and bound*. Branch and bound is divide and conquer exhaustive search consisting of: (1) finding rigorous bounds on the global solution; (2) generating good feasible solutions using heuristics; (3) dividing the search space via domain branching; (4) reducing the search space via variable bounding.

As discussed in Section 4, CPSE is associated with three computational frameworks for solving general MINLP to global optimality. But CPSE is also responsible for many of the major research advances that make each of the four individual algorithmic components of branch and bound global optimisation effective. For example: Liberti and Pantelides (2003) develop a methodology for rigorously underestimating odd degree monomials; Mitsos et al. (2009a) design McCormick-based relaxations; Misener et al. (2014b) aggregate summations of bilinear terms. The heuristics in Section 1 are useful for deterministic global optimisation because the non-deterministic algorithms generate high-quality solutions quickly; this can be used to expedite the branch and bound process.

Bespoke methods may be useful for particular classes of problems. Kleniati et al. (2010a,b), Misener et al. (2010), and Wiesemann et al. (2010) design algorithms for solving polynomial optimisation, feedstock blending, and product scheduling problems, respectively.

4. Computational Software

CPSE is associated with two of the earliest deterministic global optimisation code bases and several of the latest contributions. Early software included αBB (Adjiman et al., 1998a,b) and a method on based factorable programming (Smith and Pantelides, 1997, 1999). These two pieces of software strongly influenced the development of GloMIQO (Misener and Floudas, 2012, 2013) and ANTIGONE (Misener and Floudas, 2014b,a); GloMIQO and ANTIGONE not only hybridise the algorithms of Adjiman et al. (1998a,b) and Smith and Pantelides (1997, 1999), but also incorporate a range of other cutting-edge algorithms.

ANTIGONE[1] and GloMIQO[2] are available as off-the-shelf codes from GAMS[3] and Princeton University; GAMS is a modelling platform

[1] helios.princeton.edu/ANTIGONE/
[2] helios.princeton.edu/GloMIQO/
[3] www.gams.com

used worldwide by optimisation practitioners and researchers. MC++[4], an open source developer's toolbox distributed by COIN-OR, is another code base available from CPSE. MC++ prototypes and tests novel algorithms in global and robust optimisation, including problems with differential equations (Sahlodin and Chachuat, 2011a,b).

5. Conclusions

This short manuscript has given a very brief introduction to deterministic global optimisation and some of the intellectual contributions made by the Centre for Process Systems Engineering. The references listed in the bibliography are a good place to explore this interesting research topic further; the bibliography offers a cross section of: mathematical models; algorithms; software.

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[4]https://projects.coin-or.org/MCpp

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Appendix A. Mathematical Definitions

MINLP is defined:

$$
\begin{aligned}
&\min_{\boldsymbol{x}} \quad f_0(\boldsymbol{x}) \\
&\text{s.t.} \\
&b_i^{\mathrm{LO}} \le f_i(\boldsymbol{x}) \le b_i^{\mathrm{UP}} && \forall\, i \in \mathscr{M} := \{1, \ldots, M\} \\
&x_j \in \left[x_j^{\mathrm{LO}}, x_j^{\mathrm{UP}}\right] && \forall\, j \in \mathscr{N} := \{1, \ldots, N\} \\
&x_j \in \mathbb{Z} && \forall\, j \in \mathscr{I} \subseteq \mathscr{N}
\end{aligned}
\tag{MINLP}
$$

where $\mathscr{M}$, $\mathscr{N}$, and $\mathscr{I}$ represent sets of constraints, variables, and discrete variables, respectively. The objective and constraints are functions $f_i : \mathbb{R}^N \mapsto \mathbb{R}\ \forall\, i \in \{0, \ldots, M\}$. Parameters $b_i^{\mathrm{LO}} \in \mathbb{R} \cup \{-\infty\}$ and $b_i^{\mathrm{UP}} \in \mathbb{R} \cup \{+\infty\}$ bound the set of constraints $\mathscr{M}$; parameters $x_j^{\mathrm{LO}} \in \mathbb{R} \cup \{-\infty\}$ and $x_j^{\mathrm{UP}} \in \mathbb{R} \cup \{+\infty\}$ bound the set of variables $\mathscr{N}$. We assume: (1) that it is possible to infer finite bounds on the variables participating in nonlinear terms; (2) that the image of f_i is finite on $\boldsymbol{x}$; (3) that a linear programming (LP) relaxation of MINLP is bounded. Typical expressions for $f_i(\boldsymbol{x})$ are:

$$
\begin{aligned}
f_i(\boldsymbol{x}) = & c_i + a_i^T \boldsymbol{x} + \boldsymbol{x}^T Q_i \boldsymbol{x} + \\
& \sum_{s=1}^{S_i} c_{s,i} \cdot \prod_{j \in \mathscr{N}} x_j^{p_{s,i,j}} + \sum_{j \in \mathscr{N}} c_{e,i,j}\, e^{x_j} + \\
& \sum_{j \in \mathscr{N}} c_{\ell,i,j} \log x_j
\end{aligned}
\tag{A.1}
$$

where the powers $p_{s,i,j}$ and coefficients $c_i, a_i, Q_i, c_{s,i}, c_{e,i,j}, c_{\ell,i,j}$ are constant reals; $s \in \{1, \ldots, S_i\}$ indexes the signomial terms.

Interesting special cases of MINLP include: nonlinear programming (when all variables are continuous, $\mathscr{I} = \varnothing$); mixed-integer quadratically-constrained quadratic programming (when all nonlinearities are quadratic); mixed-integer signomial optimisation (when there are no exponential or logarithmic terms); mixed-integer linear programming (when there are no nonlinearites).

Global optimisation may also be used in: bi-level optimisation; dynamic programming; multi-parametric programming. But these are not covered in this short article.