LOGIC BASED OUTER APPROXIMATION FOR NONCONVEX SYNTHESIS OF PROCESS NETWORK PROBLEMS

Maria Lorena Bergamini and Pio A. Aguirre
INGAR – Instituto de Desarrollo y Diseño,
Santa Fe, Argentina

Ignacio E. Grossmann*
Carnegie Mellon University,
Pittsburgh, PA 15213, USA

Abstract

A new deterministic algorithm for the global optimization of process networks is presented in this work. A process network problem can be formulated as a Generalized Disjunctive Program, often involving nonconvex functions that may give rise to several local optima. However, flowsheet synthesis models have a special structure, which is exploited in this work. The proposed algorithm consists of an iterative procedure in which the problem is decomposed into continuous and discrete optimization subproblems. The continuous optimization subproblem requires the solution of reduced NLP subproblems to global optimality, while the discrete optimization subproblem is obtained through the solution of lower bounding problems. This subproblem is constructed replacing the nonconvex terms with piecewise estimators and its optimal solution is a lower bound of the solution of the GDP problem. Several examples were successfully solved with this algorithm.

Keywords

Outer Approximation, Global Optimization, Bilinear and Concave Functions, Piecewise Estimators.

Introduction

The synthesis of process networks can be formulated as Generalized Disjunctive Programming (GDP) problems (Raman and Grossmann, 1994). GDP problems can be solved as MINLP problems by replacing the disjunctions with its big-M or its convex hull reformulation (Lee and Grossmann, 2000). Major methods for MINLP problems include Branch-and-Cut, (Stubbs and Mehrotra, 1999) Generalized Benders Decomposition (GBD) (Geoffrion, 1972), Outer Approximation (OA) (Duran and Grossmann, 1986) and Extended Cutting Plane (ECP) method (Westerlund and Petterson, 1995).

Lee and Grossmann (2000) presented an optimization algorithm for solving general nonlinear GDP problems. This algorithm consists of a branch-and-bound search that branches on terms of the disjunctions and considers the convex hull relaxation of the remaining disjunctions. Turkay and Grossmann (1996) have proposed a Logic-Based Outer Approximation algorithm that solves nonlinear GDP problems for process networks involving two terms in the disjunction.

While the above mentioned algorithms assume convexity to guarantee convergence to the global optimal solution, rigorous global optimization algorithms have been proposed. For MINLP problems, it should be mentioned the works by Ryoo and Sahinidis (1995), Zamora and Grossmann (1999), Smith and Pantelides (1999) and Adjman et al (2000). Lee and Grossmann (2001) proposed a two-level branching scheme for solving nonconvex GDP problems to global optimality.

* To whom all correspondence should be addressed

Spatial branch-and-bound methods can be computationally expensive, since the tree may not be finite (except for ε-convergence). For the case of process networks there is the added complication that the NLP subproblems are usually difficult and expensive to solve. Thus, there is a strong motivation for developing a decomposition algorithm for this class of problems.

We propose a new algorithm for solving nonconvex GDP problems that arise in process synthesis. It exploits the particular structure of this kind of models, as in the case of the Logic Based OA algorithm by Turkay and Grossmann. The proposed modifications make the algorithm capable of handling nonconvexities, while guaranteeing globality of the solution of the optimal synthesis of process networks. This is accomplished by constructing a master problem that is a valid bounding representation of the original problem and by solving the NLP subproblems to global optimality.

GDP Model.

The GDP model for the synthesis of process networks is given as follows,

$$\begin{aligned}
&\min Z = \sum_j c_j + f(x) \\
&s.t. \quad g(x) \le 0 \\
&\begin{bmatrix} Y_j \\ h_j(x) \le 0 \\ c_j = \gamma_j \end{bmatrix} \vee \begin{bmatrix} \neg Y_j \\ B^j x = 0 \\ c_j = 0 \end{bmatrix} \quad j \in U \\
&\Omega(Y) = True \\
&x \ge 0, c \ge 0, Y_j \in \{True, False\}
\end{aligned} \tag{1}$$

The nonlinear model (1) has continuous variables x and c, and Boolean variables Y. The disjunctions in U apply for processing units. If unit j exists, a set of conditional constraints h_j is enforced and a fixed charge c_j is applied. Otherwise, a subset of continuous variables and the fixed charge are set to zero. There also are global constraints g in the continuous space and logical constraints Ω(Y).

Piecewise Underestimators.

The key point of the algorithm is the construction of a master problem that rigorously underestimates the objective and overestimates the original feasible region. To accomplish that, a convex GDP is derived, replacing the nonconvex terms in (1) by piecewise underestimators.

Let $f : R^m \to R$ be a nonconvex function and let D be the domain of interest. Let $f_D^u : R^m \to R$ be an underestimator of f constructed over D. Consider a partition of the domain D: $\{D_k\}_{k \in I}$. The piecewise underestimator over the partition is formulated as follows,

$$\bigvee_{k \in I} \begin{bmatrix} w_k \\ f^u(x) = f_{D_k}^u(x) \\ x \in D_k \end{bmatrix} \tag{2}$$

If f_D^u is such that has zero approximation gap in the boundary of D, the estimator f^u matches f in the boundary of the active subregion D_k.

These underestimators are included in the problem through its big-M or its convex hull reformulation. Thus, new binary variables w are added, representing the active subdomain D_k.

Lower Bounding Problems.

Assume the function f, g and h are the sum of convex, concave and bilinear terms. This is not a very restrictive assumption since Smith and Pantelides (1999) have shown that a suitable reformulation may transform any problem in an equivalent one with convex, concave univariate and bilinear terms.

Given a gridpoint set K, a new GDP problem is obtained by replacing the nonconvex terms by the piecewise underestimator constructed over the grid K.

$$\begin{aligned}
&\min \quad Z^L = \sum_j c_j + \alpha \\
&\alpha \ge f^o(x) + \sum_i f_{i,K}^u(x,w,t) \\
&g^o(x) + \sum_i g_{i,K}^u(x,w,t) \le 0 \\
&\begin{bmatrix} Y_j \\ h_j{}^o(x) + \sum_{i \in H} z_{ji}^h \le 0 \\ h_{ji,K}^u(x,w,t) \le z_{ji}^h \\ c_j = \gamma_j \end{bmatrix} \vee \begin{bmatrix} \neg Y_j \\ B^j \begin{pmatrix} x \\ w \\ t \end{pmatrix} = 0 \\ c_j = 0 \end{bmatrix} \\
&\Omega(Y) = True \\
&\alpha \in R;\ x, c \ge 0;\ Y \in \{True, False\}^m \\
&w \in \{0,1\}^{k \times s}, t \in R^{p \times q}
\end{aligned} \tag{3}$$

f^o, g^o and $h_j{}^o$ are the convex terms in f, g and h_j respectively. $f_{i,K}^u$, $g_{i,K}^u$, and $h_{ji,K}^u$ are piecewise underestimators of the nonconvex terms. They are expressed in terms of the original variables x, the new 0-1 variables w and the continuous variables t that are needed for defining the approximation in the grid. The subindex K means that these estimators are constructed using the gridpoint set K. The problem (3) is a relaxation of (1), and therefore the optimal solution of (3) is a lower bound to the solution of (1). If the optimal solution of (3) is a grid point, this is the global optimal of (1), since the underestimators have zero gap at the grid points. Also note that, if the original problem (1) has only concave, bilinear and linear fractional term, problem (3) is linear.

Reduced NLP and Local Bounding Problem.

Fixing the structure of the process network in (1) (Y=Y^k) yields an NLP problem, where only the variables and constraints related to the existing units are involved.

$$\begin{aligned} &\min \quad Z = \sum_j c_j + f(x) \\ &s.t. \quad g(x) \le 0 \\ &\left.\begin{aligned} h_j(x) \le 0 \\ c_j = \gamma_j \end{aligned}\right\} for \quad Y_j^k = True \\ &\left.\begin{aligned} B^j x = 0 \\ c_j = 0 \end{aligned}\right\} for \quad Y_j^k = False \\ &x, c \ge 0 \end{aligned} \tag{4}$$

Problem (4) is nonconvex and therefore it may not have a unique optimal solution. In order to obtain the global optimal solution a local bounding problem is constructed, replacing the nonconvex terms in (4) by the corresponding piecewise underestimators. The following convex MINLP is obtained,

$$\begin{aligned} &\min \quad Z = \sum_j c_j + \alpha \\ &s.t. \quad \alpha \ge f^o(x) + \sum_{i \in F} f_{i,K}^u(x,w,t) \\ &g^o(x) + \sum_{i \in G} g_{i,K}^u(x,w,t) \le 0 \\ &\left.\begin{aligned} h_j^o(x) + \sum_{i \in G} h_{i,K}^u(x,w,t) \le 0 \\ c_j = \gamma_j \end{aligned}\right\} for \quad Y_j^k = True \\ &\left.\begin{aligned} B^j x = 0 \\ c_j = 0 \end{aligned}\right\} for \quad Y_j^k = False \\ &x, c \ge 0, w \in \{0,1\}^{k \times s}, t \in R^{p \times q}, \alpha \in R \end{aligned} \tag{5}$$

Bound Contraction.

Having a fixed network structure allows to fix some variables to zero and contract the bounds for other variables. Tight variable bounds reduce the search space in the global optimization of the NLP problem, and reduce the approximation gap of the underestimators.

Bound contraction is performed in the variables involved in nonconvex terms, following the procedure proposed by Zamora and Grossmann (1999).

$$\begin{aligned} &\min/\max \; x_i \\ &s.t. \quad Z \le GUB \\ &\text{constraints in (5)} \end{aligned} \tag{6}$$

Problem (6) is a convex MINLP since it involves binary variables related to the piecewise estimators. However, if the domains for nonconvex terms are partitioned in only one region, it can be solved as a NLP problem.

Algorithm.

Initialization: Initialize global lower and upper bounds GLB and GUB, and local lower and upper bounds LLB and LUB. Set local and global convergence tolerances ε and η.

Outer Optimization: Set the global variables bounds and the initial gridpoint set K. Solve (3) and denote Z^{L*} the optimal solution and Y^* the values of the boolean variables. Update GLB = Z^{L*} and LLB = Z^{L*}. Fix Y = Y^*. Check global convergence: if GUB – GLB ≤ η stop. Otherwise, go to Bound contraction step.

Bound Contraction: solve (6) for the variables involved in nonconvex terms, and update the bound for those variables.

Inner Optimization: Find the global solution of (4), using a NLP global optimizer or through the following procedure:

Upper Bounding: solve (4) with a local optimizer and denote Z^{U*} the solution. Update GUB = min{GUB, Z^{U*}} and LUB = min{LUB, Z^{U*}}. Check global and local convergence: if GUB – GLB ≤ η stop. If LUB – LLB ≤ ε, go to New structure. Otherwise go to Local bounding step

Local Bounding: Update the grid adding the solution of the previously solved bounding problem. Solve (5) and denote Z^{l*} the solution. Update LLB = Z^{l*}. Check global and local convergence: if GUB – GLB ≤ η stop. If LUB – LLB ≤ ε, go to New structure. Otherwise go to Upper bounding step.

New Structure: Add an integer cut to become infeasible the structure defined by Y^*. Unfix the Boolean variables. Go to Outer Optimization Step.

Numerical Example.

The performance of the proposed algorithm has been tested on a number of test problems in the full length version of this paper. Here we illustrate it with a heat exchanger network problem with two hot stream and two cold streams. The mathematical model uses the staged superstructure proposed by Yee and Grossmann (1990). A superstructure with three stages is proposed. The global constraints define heat balances and inlet and outlet temperatures. Disjunctions are considered for each one of the 16 potential exchangers. If the exchanger exists, the exchanged heat, required area and cost is defined. If the exchanger does not exist, the exchanged heat, area and cost are set to zero. The corresponding GDP problem in (1) has 16 boolean variables, 82 continuous variables and a total of 112 constraints.

The arithmetic mean driving force temperature difference was used to calculate the areas, and the area cost were modeled as a nonlinear concave function to reflect the economies of scale. Moreover, no stream splitting was assumed. Thus, the nonconvexities in the model are due to the area calculation and the area costs. The disjunctive model (1) has 16 bilinear terms (involving area, heat load and temperature difference variables) and 16 concave terms. When these terms are replaced by piecewise estimators constructed over the partition for the area domains (3) remains linear. In this example, the initial grid for the outer optimization steps is constituted by a unique interval. Problem (3) has 16 boolean variables, 82 continuous variables and 254 equations. There are also 16 binary variables *w* related to the piecewise estimators. Data for this problem were taken from example 4 in Zamora and Grossmann (1998). However, while they used linear costs for the areas, the exponent considered here is 0.8 for exchangers and 0.7 for coolers and heaters.

The algorithm was implemented in GAMS (Brooke et al, 1997) on a 1.5 GHz Pentium 4 PC. CONOPT3 was used as an NLP solver and XPRESS solved the bounding MILP problems. The algorithm found the optimal solution in a total time of 57 CPU sec. The global solution has a cost of $52265.19, involving 6 units (4 exchangers and 2 cooler). The optimal structure was found in the first outer iteration, and 5 inner iterations were needed to reach local convergence. Inner optimization took 4.07 CPU sec (2.25 CPU sec for solving the NLP problems (4) and 1.82 CPU sec for solving the bounding MILP problems (5)). However, 12 outer iterations were required to obtain convergence to the global optimum. In the subsequent iterations, the bound reduction procedure determined that the selected structures are suboptimal and the algorithm did not solve the NLP subproblems.

This problem was also solved with BARON (Sahinidis, 1996) as an MINLP solver. It found the global solution at iteration 5104, but the lower bound could not converge in less than 1000 CPU sec. The lower bound was 35% lower than the global solution.

Conclusions.

A new deterministic algorithm for the global optimization of synthesis of processes network problems has been presented, as well as a new methodology for constructing underestimators of nonconvex functions based on partitions of the entire domain. In this work, the derivation of this class of estimators for univariate concave terms and bilinear terms has been developed.

The proposed algorithm relies on an outer approximation methodology. The global solution of the problem is achieved by solving problems that are relaxations of the original one. As iterations proceed, the bounding problem approximates the original problem with more accuracy.

The computational experience suggests that this algorithm presents some advantages with respect to typical branch and bound algorithms.

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