A NONCONVEX MINLP OPTIMIZATION PROBLEM IN REACTOR DESIGN AND PRODUCTION ASSIGNMENT: ITS FORMULATION AND GLOBAL SOLUTION

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Abstract

In this work, we address the rigorous and efficient determination of the global solution of a nonconvex MINLP problem arising from product portfolio optimization introduced by Kallrath (2003). The goal of the optimization problem is to determine the optimal number and capacity of reactors satisfying the demand and leading to a minimal total cost. Based on the model developed by Kallrath (2003), an improved formulation is proposed, which consists of a concave objective function and linear constraints with binary and continuous variables. A variety of techniques are developed to tighten the model and accelerate the convergence to the optimal solution. A customized branch and bound approach that exploits the special mathematical structure is proposed to solve the model to global optimality. Computational results for two case studies are presented. In both case studies, the global solutions are obtained and proved optimal very efficiently in contrast to available commercial MINLP solvers.

Keywords

Global optimization, nonconvex MINLP, Portfolio optimization, Branch and bound.

Introduction

The modeling of decision making in many processes, such as the design of chemical plants, often leads to nonconvex mixed-integer nonlinear programming (MINLP) problems. The solution of this class of problems is very challenging due to the presence of both the integer variables and the nonconvexities. A number of approaches have been proposed for the solution of such problems within the branch and bound framework. For example, Adjiman et al. (2000) introduced a powerful theoretical and algorithmic framework based on the αBB global optimization approach for twice-differentiable nonlinear programming (NLP) problems (Adjiman et al., 1998). Adjiman et al. (2000) developed two broadly applicable algorithms for the solution of nonconvex MINLPs: a special structure mixed-integer αBB algorithm (SMIN-αBB) for problems with general nonconvexities in the continuous variables and restricted participation of the binary variables, and a general structure mixed-integer αBB algorithm (GMIN-αBB) for the broader class of problems whose continuous relaxations are twice-differentiable. Westerlund et al. (1998) proposed a new theoretical and algorithmic approach, the extended cutting plane algorithm, for addressing problems with pseudo-convex functions. Ryoo and Sahinidis (1996) developed a standard branch-and-reduce algorithm, in which they introduced domain reduction through feasibility and optimality tests. Smith and Pantelides (1999) introduced a reformulation/spatial branch-and-bound algorithm for mathematical models that feature factorable continuous functions and binary variables. For a comprehensive discussion of the theoretical, algorithmic, and application related issues for global optimization problems that include mixed-integer nonlinear optimization models, interested readers are referred to (Horst and Tuy, 1996) and (Floudas, 2000).

In this work, we address the global solution of a nonconvex mixed-integer nonlinear programming (MINLP) problem arising from product portfolio optimization. The problem and related data are taken from (Kallrath, 2003). This nonlinear nonconvex portfolio optimization problem contains a design problem (determining the number and sizes of chemical reactors) coupled with an assignment problem (assigning products to reactors). The solution defines the optimal production configuration, and, in a second step, will also help to perform product portfolio analysis. Kallrath (2003) developed a nonconvex MINLP model featuring concave terms in the objective function and trilinear products in the constraints. Kallrath (2003) addressed the problem using (i) a mixed-integer linear programming (MILP) representation with equivalent linear constraints

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and an approximate objective function; and (ii) some standard commercial solvers, such as SBB and BARON, which required a lot of computational time, especially for the large case study for which optimal solutions could not be found within many CPU hours (Kallrath, 2003). In this paper, we present a customized branch and bound approach based on the construction of a lower bounding problem by underestimating the concave objective function with piece-wise linear approximations aiming to solve the problem to global optimality efficiently.

Problem Description

Taken from (Kallrath, 2003), the portfolio optimization problem of interest is as follows. A business unit operating a number of batch reactors wants to analyze the dependence of investment and fixed costs on given demand spectra. In this paper we analyze two different scenarios: one includes a relatively large number of products (i.e., about 40 products) and the other involves a "*lean* assortment" with fewer products (i.e., about 20 products).

The analysis should determine cost minimal solutions. In addition to the costs, the following detailed results are expected: i) the number of reactors required and the number of batches per reactor; ii) the volumes of the reactors; iii)which batches are produced on a certain reactor; iv) the utilization rates of the reactors; and v) surplus production with respect to the demand.

The production configuration is subject to the following constraints. i) The demand for 20 and 40 products, specified per week and per product, needs to be satisfied. ii) All products are subject to shelflife limits. Actually, the products can be stored for about one week; if they are probably cooled they can survive a few more days. iii) All products are produced in batches of 6 hours. iv) The feasible volumes of the reactors are in the range between 20 and 250 m^3. v) The filling degree or utilization rate needs to be at least 40%.

For each reactor, the fixed cost and the investment cost are known. The investments cost is given by a nonlinear concave functions which relate the cost to the volume of the reactor. It is sufficient to consider investment costs which are qualitatively correct. The most important structural feature is that the investment–cost-versus-reactor–volume function is concave.

Mathematical Model

Based on the model in (Kallrath, 2003), an improved mathematical formulation is developed as follows.

Basic Formulation

First, we define the following notation.

Indices and sets:

$p \in P$ products; $r \in R$ reactors.

Parameters:

C_r^F [kEuro/week] fixed cost of reactor r.

C_r^I [kEuro] investment or depreciation cost per m^3 for reactor r per week.

C_r^T [hours] time capacity of reactor r.

T_p^P [hours] time required to produce one batch of product p.

D_p [m^3] demand for product p per week.

S surplus production allowed relative to the demand.

V_r^L, V_r^U [m^3] lower and upper limits on the reactor volume if reactor r is active.

$F(U_r^L)$ [m^3] lower limit on the utilization rates.

We introduce the following variables:

δ_r binary variable, selection of reactor r.

v_r [m^3] reactor volume of reactor r.

n_{rp} number of batches for product p in reactor r.

p_{rp} [m^3] production of product p in reactor r.

Based on this notation, the objective function and the constraints are formulated as follows:

Reactor volume bounds

$$V_r^L \cdot \delta_r \leq v_r \leq V_r^U \cdot \delta_r, \quad \forall r \in R \tag{1}$$

Production limits

$$n_{rp} \cdot v_r \cdot F \leq p_{rp} \leq n_{rp} \cdot v_r, \quad \forall r \in R, p \in P \tag{2}$$

Demand fulfillment

$$D_p \leq \sum_{r \in R} p_{rp} \leq (1+S) D_p, \quad \forall p \in P \tag{3}$$

Reactor time

$$\sum_p n_{rp} \cdot T_p^P \leq C_r^T \cdot \delta_r, \quad \forall r \in R \tag{4}$$

Objective function: minimization of all costs

$$Min \quad c^T := \sum_{r \in R} C_r^F \cdot \delta_r + \sum_{r \in R} \sqrt{C_r^I \cdot v_r} \tag{5}$$

The total cost consists of a fixed part and a variable part which depends nonlinearly on the volume of the reactors.

The following additional constraints proposed in (Kallrath, 2003) to improve the model are also included.

Breaking the symmetry of reactors

$$v_r \leq v_{r+1} \quad \forall r \in R, r \neq N^R \tag{6}$$

Total reactor volume requirement

$$28 \sum_{r \in R} v_r \geq \sum_{p \in P} D_p \tag{7}$$

Linear Transformation

Each integer variable n_{rp} can be represented by a set of binary variables as follows.

$$n_{rp} = \sum_{d \in D} n_{rpd}^B \cdot 2^d \tag{8}$$

where $d \in D$ is the d-th digit of a binary number and n_{rpd}^B is a binary variable that determines the value of the d-th digit of the binary representation of n_{rp}.

Constraints (2) consist of bilinear products between an integer variable and a continuous variable (i.e., $n_{rp} \cdot v_r$). The integer variables can be replaced by its binary representation (8), which leads to bilinear products between a binary variable and a continuous variable, $n_{rpd}^B \cdot v_r$. To transform the bilinear terms to a linear form, we introduce a set of auxiliary continuous variables, x_{rpd}, to replace the bilinear terms, and a set of additional linear constraints as follows (Floudas, 1995).

$$\begin{aligned} & v_r - v_r^U (1 - n_{rpd}^B) \leq x_{rpd} \leq v_r - v_r^L (1 - n_{rpd}^B) \\ & v_r^L \cdot n_{rpd}^B \leq x_{rpd} \leq v_r^U \cdot n_{rpd}^B \qquad \forall r \in R, p \in P \end{aligned} \tag{9}$$

Further Tightening of the Model

It is found that restricting the number of batches for each product in all of the reactors and/or in each reactor in a reasonably tight range, as represented by the following constraints, can tighten the model significantly.

$$N_p^L \leq \sum_{r\in R}\sum_{d\in D} n_{rpd}^B \cdot 2^d \leq N_p^U, \ \ \forall p \in P \tag{10}$$

$$N_{rp}^L \leq \sum_{d\in D} n_{rpd}^B \cdot 2^d \leq N_{rp}^U, \ \ p \in P, r \in R \tag{11}$$

where N_p^L, N_p^U, N_{rp}^L, and N_{rp}^U are the lower and upper bounds on the number of batches for product p in all reactors and in reactor r, respectively.

Furthermore, we eliminate the solution degeneracy resulted from products with the same demand amount. Assume that products p and p' have the same amount of demand and p precedes p' in set P, and there are three reactors, then the following constraints are introduced.

$$n_{r_1,p}28^2 + n_{r_2,p}28 + n_{r_3,p} \leq n_{r_1,p'}28^2 + n_{r_2,p'}28 + n_{r_3,p'} \tag{12}$$

Lower-Bounding Problem and Branch & Bound Framework

It should be pointed out that the mathematical formulation described above leads to a nonconvex MINLP problem with the following characteristics: i) the objective function consists of univariate concave terms and a constant term; and ii) all the constraints are linear.

A lower bounding problem can be constructed by underestimating the concave objective function with piecewise linear approximations (for details, see (Floudas, 1995)), which leads to a mixed integer linear programming (MILP) problem that can be solved efficiently. A branch and bound framework can then be used to solve for the global solution of the problem, which relies on the convergence between the lower bounds obtained by solving the lower bounding MILP problem and the upper bounds which are feasible solutions of the original MINLP problem (for more details of the branch and bound framework, see (Floudas, 2000)). Note that the constraints remain the same in the lower bounding problem and therefore any feasible solution obtained from the lower bounding problem is also a feasible solution of the original problem and the value of the objective function of the original problem, which can be obtained by simple function evaluation, provides a valid upper bound.

Computational Results of Specific Case Studies

Two different sets of demand data, taken from (Kallrath, 2003), are studied in this work, as shown in Table 1 and Table 2 respectively. The mathematical models in this work are formulated and solved with GAMS/CPLEX 7.0.

A Small Case Study

Two reactors are introduced and note that the bounds of the reactor volumes can be tightened based on the total demand and the time capacity. A total volume of 9860/28 = 352.14 m^3 is required, that is, $v_1 + v_2 \geq 352.14$. Because $v_2 \leq 250$, $v_1 \geq 102.14$; because $v_1 \leq v_2$, $v_2 \geq 176.07$. Based on the tightened ranges of reactor volumes and the product demands, lower and upper bounds on the number of batches for each product can be derived. The concave terms in the objective function are underestimated with 4-piece and 2-piece linear approximations. The branch and bound process requires only one iteration to solve the problem to global optimality with a 0.05% gap (i.e., the gap between the upper bound and the lower bound at the root node of the branch and bound tree is within the stopping criterion and hence the search procedure can be terminated right after solving the root node). The MILP lower bounding problem consists of 69 binary variables, 124 continuous variables and 489 equations. The solution requires 1721 CPU s on an HP J-2240 workstation. The optimal solution is provided in Table 1 and the corresponding minimal total cost is $c^T = 31.809$.

A Large Case Study

Three reactors are introduced and the bounds of the reactor volumes can be tightened to: $20 \leq v_1 \leq 50, 52.5 \leq v_2 \leq 250, 151.25 \leq v_3 \leq 250$. The range of the number of batches for each product can be derived based on the ordering of product demands. The concave terms in the objective function are underestimated with 1-piece, 4-piece and 2-piece linear approximations. The branch and bound process requires again only one iteration to solve the problem to global optimality with 0 gap. The MILP lower bounding problem consists of 124 binary variables, 263 continuous variables and 984 equations. The solution requires 741 CPU s on an HP J-2240 workstation. The optimal solution is presented in Table 2 and the corresponding minimal total cost is $c^T = 37.176$.

Conclusions

In this work, we address the global solution of a nonconvex MINLP problem arising from product portfolio optimization introduced by Kallrath (2003). The goal of the product portfolio analysis is to prove that complex portfolios lead to more costly scenarios caused by the requirement of more reactors. In order to do so we have formulated and solved optimization models to determine the optimal configurations of reactors with the minimal fixed and investment costs for two different scenarios of product demands. The model proposed by Kallrath (2003) is improved and the resulting mathematical formulation consists of a concave objective function and linear constraints with binary and continuous variables. A variety of techniques are developed to tighten the model and accelerate the convergence to the optimal solution. A customized branch and bound approach is proposed to solve the model to global optimality. Computational studies on the two scenarios are presented. In both cases, the global solutions are obtained and proved optimal very efficiently (i.e., essentially in one iteration), which demonstrate the effectiveness of the proposed approach. The reactor design problem in this work features concave cost functions and involves a relative small number of decision variables. Nevertheless, the important ideas and techniques underlying the modeling and solution approach we have presented here, such as the tightening of bounds and customization of the branch and bound procedure, can be extended to solve more complex real-world problems.

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Table 1. Product demand and the optimal solution for the small case study

Product	Demand	Reactor 1: v_1 = 132.5 m^3			Reactor 2: v_2 = 250 m^3		
	m^3/week	production	batches	utilization rate	production	of batches	utilization rate
L1	2,600	100	1	0.76	2,500	10	1
L2	2,300	1050	8	0.99	1,250	5	1
L3	1,700	0	0	-	1,700	7	0.97
L4	530	530	4	1	0	0	-
L5	530	530	4	1	0	0	-
L6	280	53	1	0.40	250	1	1
L7	250	0	0	-	250	1	1
L8	230	0	0	-	230	1	0.92
L9	160	0	0	-	160	1	0.64
L10	90	90	1	0.68	0	0	-
L11	70	70	1	0.53	0	0	-
L12	390	390	3	0.98	0	0	-
L13	250	0	0	-	250	1	1
L14	160	0	0	-	160	1	0.64
L15	100	100	1	0.76	0	0	-
L16	70	70	1	0.53	0	0	-
L17	50	100	1	0.76	0	0	-
L18	50	100	1	0.76	0	0	-
L19	50	100	1	0.76	0	0	-
Total	9,860	3,283	28		6,750	28	
				Total production: 10,033			

Table 2. Product demand and the optimal solution for the large case study

Product	Demand	Reactor 1: v_1 = 20 m^3			Reactor 2: v_2 = 100 m^3			Reactor 3: v_3 = 250 m^3		
	m^3/week	production	batches	utilization rate	production	batches	utilization rate	production	batches	utilization rate
L1	2,600	0	0	-	100	1	1	2500	10	1
L2	2,300	0	0	-	50	1	0.50	2250	9	1
L3	450	0	0	-	200	2	1	250	1	1
L4	1,200	0	0	-	200	2	1	1000	4	1
L5	560	0	0	-	100	1	1	460	2	0.92
L6	530	0	0	-	300	3	1	230	1	0.92
L7	530	0	0	-	300	3	1	230	1	0.92
L8	140	0	0	-	140	2	0.70	0	0	-
L9	110	20	1	1	90	1	0.90	0	0	-
L10	110	20	1	1	90	1	0.90	0	0	-
L11	10	20	1	1	0	0	-	0	0	-
L12	110	20	1	1	90	1	0.90	0	0	-
L13	90	0	0	-	90	1	0.90	0	0	-
L14	90	0	0	-	90	1	0.90	0	0	-
L15	90	0	0	-	90	1	0.90	0	0	-
L16	70	0	0	-	70	1	0.70	0	0	-
L17	50	50	3	0.83	0	0	-	0	0	-
L18	30	30	2	0.75	0	0	-	0	0	-
L19	10	20	1	1	0	0	-	0	0	-
L20	10	20	1	1	0	0	-	0	0	-
L21	10	20	1	1	0	0	-	0	0	-
L22	190	0	0	-	190	2	0.95	0	0	-
L23	180	0	0	-	180	2	0.90	0	0	-
L24	70	0	0	-	70	1	0.70	0	0	-
L25	70	0	0	-	70	1	0.70	0	0	-
L26	40	40	2	1	0	0	-	0	0	-
L27	40	40	2	1	0	0	-	0	0	-
L28	40	40	2	1	0	0	-	0	0	-
L29	30	30	2	0.75	0	0	-	0	0	-
L30	20	20	1	1	0	0	-	0	0	-
L31	20	20	1	1	0	0	-	0	0	-
L32	20	20	1	1	0	0	-	0	0	-
L33	10	20	1	1	0	0	-	0	0	-
L34	10	20	1	1	0	0	-	0	0	-
L35	10	20	1	1	0	0	-	0	0	-
L36	10	20	1	1	0	0	-	0	0	-
L37	10	20	1	1	0	0	-	0	0	-
Total	9,870	530	28		2,510	28		6,920	28	
						Total production: 9,960				