DETERMINISTIC GLOBAL OPTIMIZATION OF MIXED INTEGER BILEVEL PROGRAMMING PROBLEMS

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Abstract

Global optimization of mixed-integer nonlinear bilevel optimization problems is addressed using a novel technique. For problems where integer variables participate in both inner and outer problems, the outer level may involve general mixed-integer nonlinear functions. The inner level may involve functions that are mixed-integer nonlinear in outer variables, linear, polynomial, or multilinear in inner integer variables, and linear in inner continuous variables. The technique is based on reformulating the mixed-integer inner problem as continuous via its convex hull representation (Sherali and Adams 1990; 1994) and solving the resulting nonlinear bilevel problem by a novel deterministic global optimization framework. For problems where the integer variables are only in the outer problem, both the inner and outer problems may be nonlinear in both inner and outer variables. These are solved by a direct extension of the global optimization framework of Gümüş and Floudas (2001).

Keywords

Bilevel Programming, Bilevel Optimization, Mixed Integer Optimization, Global Optimization, Two-level Optimization, Mixed Integer Nonlinear Optimization

Introduction

Hierarchical decision making is of primary importance in many real world engineering problems. In chemical engineering design, often the main cost-based design objective is constrained by process property objectives. These can be modeled within a bilevel programming (BLP) framework where an (outer) optimization problem is constrained by another (inner) optimization problem. Applications of the BLP in chemical engineering are many and diverse, such as in design under uncertainty (Floudas et. al, 2001), design with chemical equilibrium (Gümüş and Ciric, 1997), and metabolic engineering (Burgard and Maranas, 2003) problems. If these problems involve discrete decisions in addition to continuous ones, the mixed-integer BLP problems arise.

The conventional solution method of the continuous BLP is to transform it into a single level problem by replacing the inner problem with the set of equations that define its Karush-Kuhn-Tucker (KKT) optimality conditions. However, the KKT optimality conditions use gradient information, so the conventional approach is not applicable when integer variables exist. Further, relaxing inner problem integer variables into continuous ones to obtain gradient information does not provide a valid BLP lower bound (unlike single-level mixed-integer problems). Thus, the conventional KKT-based methods inherently fail in locating the true optimal solution. However, it is extremely desirable to develop a technique that locates the global optimum of mixed-integer BLPs. Furthermore, it is worth noting that rigorous deterministic solution approaches do not exist in the open literature. Developments in this area will greatly expand the scope of problems that can be addressed via bilevel optimization.

The mixed-integer BLP inner problem is first transformed into mixed-binary and then reformulated as continuous by its convex hull representation. This reformulation eliminates the limitations that arise in the

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use of KKT transformation, as KKT optimality conditions of the reformulated inner problem are both necessary and sufficient. Epsilon global optimality in a finite number of iterations is theoretically guaranteed.

Problem Formulation

The general mixed-integer nonlinear BLP is of the form:

$$\begin{aligned}
\min_x \quad & F(\mathbf{x}, \mathbf{y}) \qquad (1)\\
\text{s.t.} \quad & \mathbf{G}(\mathbf{x}, \mathbf{y}) \le 0\\
& \mathbf{H}(\mathbf{x}, \mathbf{y}) = 0\\
& \min_y \quad f(\mathbf{x}, \mathbf{y})\\
& \text{s.t.} \quad \mathbf{g}(\mathbf{x}, \mathbf{y}) \le 0\\
& \qquad \mathbf{h}(\mathbf{x}, \mathbf{y}) = 0\\
& x_1, \ldots, x_i \in \Re,\ y_1, \ldots, y_j \in \Re\\
& x_{i+1}, \ldots, x_{n1} \in Z^+,\ y_{j+}1, \ldots, y_{n2} \in Y_{IN} \subseteq Z^+.
\end{aligned}$$

where **x** is a vector of outer problem variables, of which i are continuous and n_1-i are integer, y is a vector of inner problem variables, of which j are continuous and n_2-j are integer, F(**x**, **y**) and f(**x**, **y**) are outer and inner objective functions, **H**(**x**, **y**) and h(**x**, **y**) are outer and inner equality constraints and **G**(**x**, **y**) and g(**x**, **y**) are outer and inner inequality constraints.

The nonlinear mixed integer BLP can be classified into four categories depending on participation of integer and continuous variables: *(I)* Integer Upper, Continuous Lower; *(II)* Purely Integer; *(III)* Continuous Upper, Integer Lower; *(IV)* Mixed-Integer Upper and Lower.

The specific mathematical structure of mixed integer nonlinear BLP is of great importance in developing corresponding solution strategies. For problems of Type II, enumeration methods can be applied. However, BLPs of Type *III* and *IV* are very difficult to solve.

Type I: Integer Upper, Continuous Lower BLP

Solving BLPs of Type *I* is straightforward. The lower problem involves only continuous variables, so a KKT-based solution procedure is applicable. If the inner problem objective and constraints satisfy the convexity requirements of KKT optimality conditions, then the inner problem is replaced with its necessary and sufficient optimality conditions. Else, global optimization algorithm of Gümüş and Floudas (2001) is applied. This approach involves nonlinear problem relaxation prior to KKT transformation, and an iterative branch and bound scheme.

BLP with Inner Integer Variables

A natural first attempt to solve BLPs with integer inner variables is to transform the mixed-integer problem into an equivalent form in the continuous domain. This is performed in two steps: (i) transform integers into *(0-1)* binaries, (ii) transform the resulting problem that involves binary and continuous variables to a continuous problem.

Integer to Binary. Each integer variable, y, with lower and upper bounds $y^L \le y \le y^U$, is converted into a set of binary variables using the formula (Floudas, 1995):

$$y = y^L + z_1 + 2z_2 + 4z_3 + \ldots + 2^{(N-1)} z_N ; N = INT\left(\frac{\log(y^U - y^L)}{Log(2)}\right) \qquad (2)$$

where **z** is the vector of *(0-1)* variables, N is the minimum number of *(0-1)* variables needed, and *INT* truncates its real argument to an integer one.

Binary to Continuous. Binary variables can be transformed into continuous ones by adding $\mathbf{z}^T\mathbf{z} - \mathbf{z} = \mathbf{0}$, for $\mathbf{0} \le \mathbf{z} \le \mathbf{1}$. This constraint is nonconvex and within a global optimization procedure it will be underestimated into a continuous relaxation of **z**. However, note that (Bard and Moore, 1990):

Observation 1: R*elaxed BLP solution does not provide a valid lower bound on mixed-integer BLP solution.*

Thus, even if the relaxed problem solution is integral, an optimal solution of the continuous relaxation may not be a globally optimal solution of the original BLP. The integral relaxed BLP solution is globally optimal if and only if the following property is satisfied:

Property 1: *If inner problem constraint set, Y_{IN}, defines a vertex polyhedral convex hull, Y_{IN}, and all the vertices of the convex hull lie in Y_{IN}, then the optimal inner problem integer solution is equivalent to its linear programming relaxation. As a result, KKT conditions of relaxed inner linear problem are necessary and sufficient to define the optimal inner problem integer solution.*

The property is valid when outer variables also exist in the inner problem, such that the vertex polyhedral convex envelope is defined parametrically in the outer variables. Now that the integer problem solution lies at a vertex point, KKT optimality conditions locate the true optimal solution (Gümüş and Floudas, 2004).

Global Optimization of BLPs of Type *II*, *III* and *IV*

This procedure is based on a reformulation/ relinearization scheme combined with a global optimization framework. The key idea is that if the inner problem constraint set is represented as its vertex polyhedral convex envelope, then *Property 1* is satisfied, and the mixed-integer inner problem can be converted into an *equivalent* continuous problem. This convex hull representation is obtained for several classes of inner problems via the reformulation/ relinearization technique.

Reformulation/Relinearization

The mixed-binary inner constraint set is transformed into the continuous domain by converting it first into a polynomial problem and then relinearizing it into an extended linear problem by a method based on the work of Sherali and Adams (1990, 1994). First, a set of polynomial factors is introduced that multiply every constraint:

$$F_n(J_1,J_2) = \{(\prod_{j \in J_1} y_j)(\prod_{j \in J_2}(1-y_j)), J_1, J_2 \subseteq N \equiv 1,...,n,$$
$$J_1 \cap J_2 = 0, |J_1 \cup J_2| = n, 0 \leq y \leq 1\}, \quad (3)$$

Then, binary linear, multilinear and polynomial terms are relinearized by using the property $y^2 = y$ for quadratic terms, and by introducing new variables (z_{ii}) to transform multilinear terms into linear terms via successive substitution (e.g. bilinear to linear: $y_i y_j = z_{ij}$).

This technique is used for problems where inner problem is (i) purely integer linear or polynomial, or (ii) mixed-integer linear, multi-linear or polynomial in inner variables. Note that outer variables can be mixed-integer nonlinear without a restriction in form. The resulting linear set of equations defines a polyhedron with its extreme points the feasible *0-1* solutions of the inner problem, explicitly characterizing its convex hull.

Inner Problem KKT Conditions and Complementarity

After reformulation/relinearization, inner problem is replaced by the set of equations that define its necessary and sufficient KKT optimality conditions at constant **x**:

$$\frac{\partial f^r}{\partial y^*} + \sum_{j=1}^{J} \lambda_j^* \frac{\partial g_j^r}{\partial y^*} + \sum_{i=1}^{I} \mu_i^* \frac{\partial h_i^r}{\partial x^*} = 0,$$
$$\mathbf{h}^r(\mathbf{x}, \mathbf{y}^*) = \mathbf{0}; \qquad \mathbf{g}^r(\mathbf{x}, \mathbf{y}^*) + \mathbf{s}^* = \mathbf{0},$$
$$\boldsymbol{\lambda}^* \mathbf{s}^* = \mathbf{0} \ (\text{cs}); \qquad \boldsymbol{\lambda}^*, \mathbf{s}^* \geq \mathbf{0}, \quad (4)$$

where f^r, $\mathbf{h}^r$ and $\mathbf{g}^r$ are the reformulated inner objective, equality and inequality constraints, $\boldsymbol{\lambda}$ and $\boldsymbol{\mu}$ are Lagrange multipliers of inner inequality and equality constraints, and **s** are slack variables associated with complementarity.

Active Set Strategy

The complementarity condition constraints (cs) involve binary decisions on the inner problem active constraint set, imposing a major difficulty in solution of the transformed problem. To overcome this difficulty, Active Set Strategy (Grossmann and Floudas, 1987) is employed, that involves the reformulation of the complementarity constraints:

$$\boldsymbol{\lambda} - U\mathbf{Y} \leq \mathbf{0}; \quad \mathbf{s} - \mathrm{U}(\mathbf{1} - \mathbf{Y}) \leq \mathbf{0}; \quad \boldsymbol{\lambda}, \mathbf{s} \geq \mathbf{0}; \quad \mathbf{Y} \in \{0,1\} \quad (5)$$

where U is an upper bound on slack variables **s** and **Y** are additional binary variables due to complementarity. If inequality constraint j is active, $Y_j=1$, and if inactive, $Y_j=0$. Note that now the integer variable set includes binary variables **Y** *in addition to* outer problem integer variables.

BLP Underestimation

After the above steps, resulting single level problem may contain nonlinear terms due to complementarity and stationarity conditions. Further, nonlinear terms may exist due to outer problem variables in either the inner or outer problem constraints. Thus, the resulting is a mixed integer (nonlinear) optimization problem, and should be solved by a global optimization procedure such as SMIN-αBB or GMIN-αBB (Adjiman et. al, 2000; Floudas, 2000). The steps of the proposed framework are summarized below.

Global Optimization Algorithm

Step 1 Establish variable bounds by solving the problems:

$$\mathbf{y}^L, \ \mathbf{y}^U = \min \ \mathbf{y}, -\mathbf{y}$$
$$\text{s.t. inner problem constraint set}$$

to obtain simple lower and upper bounds on **y**, $\mathbf{y}^L \leq \mathbf{y} \leq \mathbf{y}^U$.

Step 2 If inner integer variables are not binary convert into a set of binaries using Eq. (2).

Step 3 Obtain the vertex polyhedral convex envelope of the inner problem feasible region via reformulation/ linearization (Sherali and Adams, 1990). Inner problem is now linear in both inner binary and continuous variables and parametric in outer problem variables, **x.**

Step 4 Replace the inner problem with the set of equations that define its necessary and sufficient KKT optimality conditions. The resulting problem is single level.

Step 5 Solve to global optimality. Inner integer variables are all separable, linear and binary at the beginning of this step. If the final problem is a Mixed Integer Linear Problem (MILP), then use CPLEX. Notice that the problem is an MILP only for simplest cases. If there are continuous nonlinear variables, but integer variables are all binary, linear and separable, use SMIN-αBB. If there are nonlinear integer terms, then use GMIN-αBB (Adjiman et. al, 2000; Floudas, 2000).

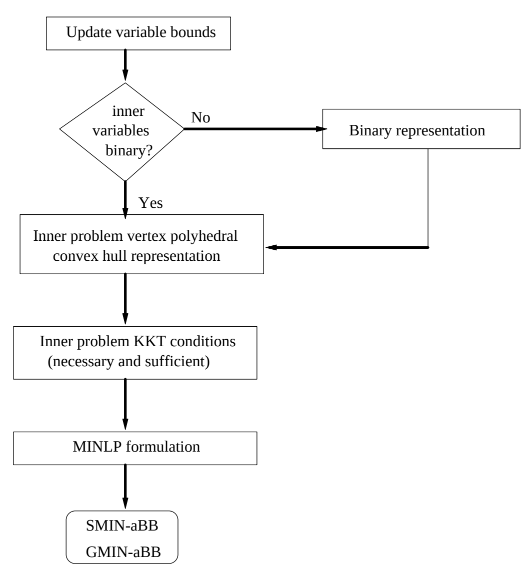

Figure 1. Algorithm Flowsheet for Type II, III, IV BLP.

Illustrative Example

The following problem (Sahin and Ciric, 1998) can not be solved to global optimality using current deterministic approaches in the literature for integer BLPs.

$$\min_x \left(\frac{2}{5}x_1^2x_2 - 4x_2^2\right)y_1y_2 + \left(x_2^3 - 3x_1^2x_2\right)(1-y_1)y_2 - (2x_2^2 - x_1)(1-y_2)$$
$$\text{s.t.} \quad \min_y -\left(x_1^2x_2^2 + 8x_2^3 - 14x_1^2 - 5x_1\right)y_1y_2$$
$$-\left(-x_1x_2^2 + 5x_1x_2 + 4x_2\right)(1-y_1)y_2 - (8x_1y_1)(1-y_2)$$
$$\text{s.t.} \quad y_1 + y_2 \geq 1, \quad y_1, y_2 \in \{0,1\}^2$$
$$0 \leq x_1 \leq 10, \quad 0 \leq x_2 \leq 10, \quad x \in \Re. \tag{6}$$

Here, variable bounds are given, with $0 \leq \mathbf{x} \leq 10$, and the inner variables y_1 and y_2 already defined as binaries.

Step 3: Inner problem has $N_y=2$ binary variables. Hence, multiply the inner constraint $y_1 + y_2 \geq 1$ with factors of degree $N_y=2$: y_1y_2, $y_1(1-y_2)$, $(1-y_1)y_2$, $(1-y_1)(1-y_2)$. Eliminate redundant constraints. Inner constraint set becomes:

$$y_1y_2 \geq 0, \quad y_1 + y_2 - y_1y_2 - 1 \geq 0, \tag{7}$$

Assign a new variable, z_{12}, where $z_{12}=y_1y_2$, and introduce:

$$z_{12} \geq 0, \quad y_1 - z_{12} \geq 0, \quad y_2 - z_{12} \geq 0, \quad -y_1 - y_2 + z_{12} \geq -1, \tag{8}$$

Note that from Eq. (7) and Eq. (8), z_{12} is eliminated via direct substitution. Thus, Eq. (7) is reformulated as:

$$y_1 + y_2 - 1 \geq 0, \quad 1 - y_1 \geq 0, \quad 1 - y_2 \geq 0. \tag{9}$$

The inner problem is now continuous and linear in inner variables **y**, and parametric in outer variables **x**.

Step 4: Replace inner problem with the set of equations that define its necessary *and* sufficient KKT conditions:

$$-x_1x_2^2 + 5x_1x_2 + 4x_2 - 8x_1 + \lambda_2 - \lambda_2 = 0;$$
$$-\lambda_1 - x_1^2x_2^2 - 8x_2^3 + 14x_1^2 + 13x_1 + \lambda_3 = 0;$$
$$-y_1 - y_2 + 1 + s_1 = 0; \quad y_1 + s_2 = 0; \quad y_2 + s_3 = 0;$$
$$\boldsymbol{\lambda} - U\mathbf{Y} \leq 0; \quad \mathbf{s} + U\mathbf{Y} \leq U,$$
$$\mathbf{Y} \in \{0,1\}; \quad \mathbf{s}, \boldsymbol{\lambda} > \mathbf{0}; \quad \mathbf{0} \leq \mathbf{y} \leq \mathbf{1} \tag{10}$$

where for every constraint j, λ_j are Lagrange multipliers, s_j are slack variables and Y_j are complementarity binaries.

Step 5: Resulting single level problem contains nonlinear terms, but integer variables are all binary, linear and separable. Solve to global optimality using SMIN-αBB (Adjiman et. al., 2000; Floudas, 2000). Global optimal solution is at *($\mathbf{x}^*$, $\mathbf{y}^*$) = (6.038, 2.957, 0, 1).*

Example

Consider an Integer Linear Fractional BLP:

$$F = \min_x -\frac{2y+3x}{y+4x+6}$$
$$\text{s.t.} \quad x + y \leq 5$$
$$x + 3y \leq 10$$
$$\min_y -\frac{3y+4x}{6y+4x+3} \quad \text{s.t.} \quad y \geq 0, \quad x, y \in Z^+ \tag{11}$$

(Thirwani and Arora, 1997). The novel framework locates the global optimum solution at *(F^*, x^*, y^*) = (-0.667, 0, 3).*

Conclusions

A novel global optimization framework that solves several classes of mixed-integer nonlinear bilevel optimization problems is presented. If inner problem is nonlinear and outer problem is linear, then the BLP is solved using the method of Gümüş and Floudas (2001). Else, a novel method is introduced that is based on reformulation of the mixed-integer inner problem feasible space to generate its convex hull, with vertices corresponding to binary solutions. This allows the equivalence of the inner optimization problem to the set of equations that define its KKT optimality conditions, with which it is replaced. The resulting single level problem is solved to global optimality. This is arguably the first deterministic technique that can solve several classes of mixed-integer nonlinear BLPs to global optimality.

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