

Compact relaxations for polynomial programming problems

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- ☐ Focus on (nonconvex) polynomial programming problems
- ☐ Aim to solve with sBB
- □ Need a tight convex (linear) relaxation at each node
- □ Reformulate before relaxing

Exact reformulations



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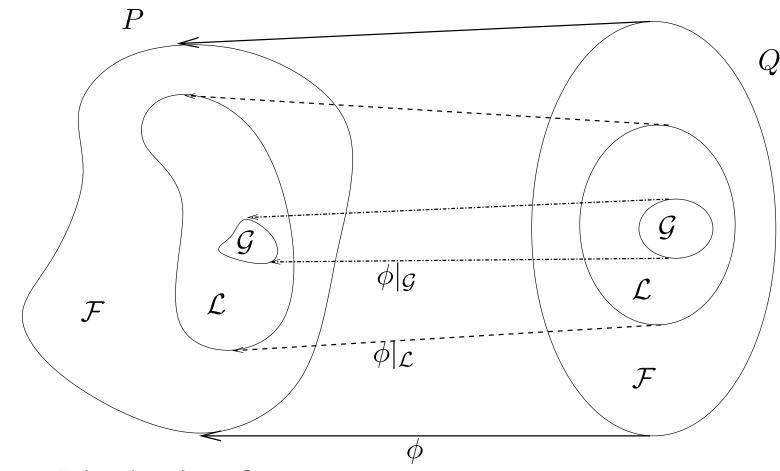
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- \square P harder than Q
- $\hfill\Box$ find optima in Q , map them back to P
- \square for each opt. in $P \exists$ corresponding opt. in Q



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Reformulation-Linearization Technique (RLT):

tightens the linear relaxation of mixed-integer (nonconvex) QCQPs

$$\begin{array}{cccc}
\min_{\mathbf{x} \in \mathbb{R}^{n_1} \times \mathbb{Z}^{n_2}} & \mathbf{c}_0 \mathbf{x} + \mathbf{x} Q_0 \mathbf{x} \\
\forall 1 \leq i \leq q & \mathbf{c}_i \mathbf{x} + \mathbf{x} Q_i \mathbf{x} \leq 0 \\
\forall 1 \leq i \leq m & \mathbf{a}_i \mathbf{x} \leq b_i \\
\mathbf{x} \in [\mathbf{x}^L, \mathbf{x}^U].
\end{array}\right\}$$

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 $\forall j, \ell \leq n = n_1 + n_2, i \leq m$, all factors non-negative \Rightarrow constraints are valid

$$(x_j - x_i^L)(x_\ell - x_\ell^L) \ge 0$$

$$(x_j - x_i^L)(x_\ell^U - x_\ell) \ge 0$$

$$(x_j^U - x_j)(x_\ell - x_\ell^L) \ge 0$$

$$(x_j^U - x_j)(x_\ell^U - x_\ell) \ge 0$$

$$(x_j - x_j^L)(b_i - \mathbf{a}_i \mathbf{x}) \ge 0$$

$$(x_j^U - x_j)(b_i - \mathbf{a}_i \mathbf{x}) \ge 0$$

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 $\forall j, \ell \leq n, i \leq m$, get:

$$x_{j}x_{\ell} - x_{\ell}^{L}x_{j} - x_{j}^{L}x_{\ell} + x_{j}^{L}x_{\ell}^{L} \geq 0$$

$$-x_{j}x_{\ell} + x_{\ell}^{U}x_{j} + x_{j}^{L}x_{\ell} - x_{j}^{L}x_{\ell}^{U} \geq 0$$

$$-x_{j}x_{\ell} + x_{\ell}^{L}x_{j} + x_{j}^{U}x_{\ell} - x_{j}^{U}x_{\ell}^{L} \geq 0$$

$$x_{j}x_{\ell} - x_{\ell}^{U}x_{j} - x_{j}^{U}x_{\ell} + x_{j}^{U}x_{\ell}^{U} \geq 0$$

$$-x_j \mathbf{a}_i \mathbf{x} + x_j^L \mathbf{a}_i \mathbf{x} + x_j b_i - x_j^L b_i \geq 0$$
$$x_j \mathbf{a}_i \mathbf{x} - x_j^U \mathbf{a}_i \mathbf{x} - x_j b_i + x_j^U b_i \geq 0$$

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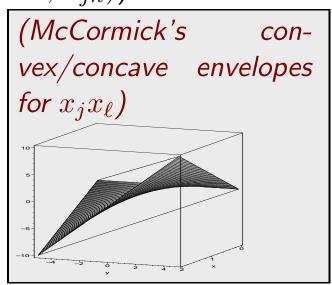
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Replace $x_j x_\ell$ by var. $w_{j\ell}$ ($\mathbf{w}_j = (w_{j1}, \dots, w_{jn})$):

$$\begin{array}{rcl} w_{j\ell} & \geq & x_{\ell}^{L}x_{j} + x_{j}^{L}x_{\ell} - x_{j}^{L}x_{\ell}^{L} \\ w_{j\ell} & \leq & x_{\ell}^{U}x_{j} + x_{j}^{L}x_{\ell} - x_{j}^{L}x_{\ell}^{U} \\ w_{j\ell} & \leq & x_{\ell}^{L}x_{j} + x_{j}^{U}x_{\ell} - x_{j}^{U}x_{\ell}^{L} \\ w_{j\ell} & \geq & x_{\ell}^{U}x_{j} + x_{j}^{U}x_{\ell} - x_{j}^{U}x_{\ell}^{U} \end{array}$$



$$\mathbf{a}_{i}\mathbf{w}_{j} \leq x_{j}^{L}\mathbf{a}_{i}\mathbf{x} + x_{j}b_{i} - x_{j}^{L}b_{i}$$
 $\mathbf{a}_{i}\mathbf{w}_{j} \geq x_{j}^{U}\mathbf{a}_{i}\mathbf{x} + x_{j}b_{i} - x_{j}^{U}b_{i}$. \mathbf{valid} linear relations between \mathbf{x} and \mathbf{w}

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 \Box $\forall i \leq q$, replace terms $x_i x_j$ in $\mathbf{x} Q_i \mathbf{x}$ with linearizing variables w_{ij}

$$\mathbf{w} = \left(egin{array}{ccc} w_{11} & \dots & w_{1n} \ dots & \ddots & dots \ w_{n1} & \dots & w_{nn} \end{array}
ight)$$

- \Box Get $\mathbf{x}Q_i\mathbf{x} = Q_i\mathbf{w}$
- \square Use IA on $[\mathbf{x}^L,\mathbf{x}^U]$ to compute ranges $[\mathbf{w}^L,\mathbf{w}^U]$ for \mathbf{w}
- \square Adjoin commutativity constr. $\forall j \leq \ell \leq n \ w_{j\ell} = w_{\ell j}$
- \square Adjoin square constr. $\forall i \leq n$ s.t. x_i is binary $w_{ii} = x_i$

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Seminal paper

Adams & Sherali, Mgt. Sci. 1986:

$$\mathbf{x} \in \{0,1\}^n$$

MILP reformulation via Fortet's inequalities

$$w_{j\ell} \leq \min(x_j, x_\ell)$$

$$w_{j\ell} \geq \max(0, x_j + x_\ell - 1)$$

then continuous relaxation

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A TIGHT LINEARIZATION AND AN ALGORITHM FOR ZERO-ONE QUADRATIC PROGRAMMING PROBLEMS*

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This paper is concerned with the solution of linearly constrained zero-one quadratic programming problems. Problems of this kind arise in numerous economic, location decision, and strategic planning situations, including capital budgeting, facility location, quadratic assignment, media selection, and dynamic set covering. A new linearization technique is presented for this problem which is demonstrated to yield a tighter continuous or linear programming relaxation than is available through other methods. An implicit enumeration algorithm which uses Lagrangian relaxation, Benders' cutting planes, and local explorations is designed to exploit the strength of this linearization. Computational experience is provided to demonstrate the usefulness of the proposed linearization and algorithm.

(ZERO-ONE QUADRATIC PROGRAMMING; LINEARIZATION TECHNIQUES; IMPLICIT ENUMERATION; LAGRANGIAN RELAXATION; BENDERS' DECOMPOSITION)

1. Introduction

This paper is concerned with linearly-constrained zero-one quadratic programming problems (QP). Problems of this structure arise in numerous economic, facility location, and strategic planning situations. These include, for example, the media selection problem described by Zangwill (1965), the capital budgeting problem considered by Laughhunn (1970) and by Peterson and Laughhunn (1971), certain facility location problems given in Vaish (1974), a multitude of applications associated with quadratic assignment problems (see Sherali 1979), and dynamic facility relocation problems such as the dynamic set covering problem formulated in Chrissis et al. (1978).

Basically, the available solution procedures for Problem QP may be classified as attempting either to solve the problem directly or to transform Problem QP into an equivalent linear mixed-integer program, and then solve the latter problem. The direct methods involve partitioning techniques or implicit enumeration strategies. Lazimy (1982) considers a more general version of Problem QP, i.e., a mixed-integer quadratic programming problem, and demonstrates that one can transform this problem into an equivalent program without adding new variables or constraints. This renders the problem more amenable to Geoffrion's (1972) generalized Benders' technique, in that the cutting planes derived are linear in the integer variables. Balas (1969) suggests an alternative partitioning algorithm for the same class of problems, but requires the addition of an extra set of variables. Both these methods, however, are based on the use of a Dorn (1960) type of duality, and therefore require appropriate convexity assumptions in regard to the objective function. Another direct-search cutting plane algorithm is suggested by Kunzi and Oettli (1963) for all-integer quadratic programming problems.

The direct implicit enumeration procedures developed for Problem QP are more straightforward. These methods include the works of Cabot and Francis (1970), Hansen (1972), Mao and Wallingford (1968), and McBride and Yormark (1980). Recently, Carter (1984) has suggested methods for improving various direct-search schemes by

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0025-1909/86/3210/0000\$01.25 Conveight © 1966, The Institute of Management Sciences

^{*} Accepted by Alexander H. G. Rinnooy Kan; received July 1984. This paper was with the authors 4 months for 1 revision.

Mixed products





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Adams & Sherali, Op. Res. 1990:

 $\mathbf{x} \in \mathbb{R}^{n_1} \times \{0,1\}^{n_2}$ with products involving at least one binary variable

MII P reformulation

Theorem 1. Problems MIOPP and MILPR (and. hence, MILP) are equivalent in the following sense. Given any (x, y) feasible to MIQPP, there exists a(w, u) such that (x, y, w, u) is feasible to MILPR with the same objective value. Conversely, given any (x, y, w, u) feasible to MILPR, the solution (x, y) is feasible to MIQPP with the same objective value.

then continuous relaxation

LINEARIZATION STRATEGIES FOR A CLASS OF ZERO-ONE MIXED INTEGER PROGRAMMING PROBLEMS

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This paper is concerned with a new linearization strategy for a class of zero-one mixed integer programming problems that contains quadratic cross-product terms between continuous and binary variables, and between the binary variables themselves. This linearization scheme provides an equivalent mixed integer linear programming problem which yields a righter continuous relaxation than that obtainable via the alternative linearization techniques available in the literature. Moreover, the proposed technique provides a unifying framework in the sense that all the alternate methods lead to formulations that are accessible through appropriate surrogates of the constraints of the new linearized formulation. Extensions to various other types of mixed integer nonlinear programming problems are also discussed.

commonly used technique in the development A of solution procedures for nonlinear integer and mixed integer programming problems is that of linearization, that is, the construction of an equivalent linear (mixed) integer representation of the problem. Numerous authors, including Glover (1975), Glover and Woolsey (1973, 1974), Petersen (1971), Watters (1967) and Zangwill (1965) have suggested methods for obtaining linear reformulations of various classes of discrete nonlinear programming problems. The methods they propose appear to be seemingly unrelated, and the success obtained via these methods is highly dependent on the specific problem. Unfortunately, no central or unifying theory has beretofore been presented.

A crucial concern in the construction of a linear (mixed) integer representation of a nonlinear mixed integer programming problem is how well the linear formulation lends itself to existing solution strategies. As reported by many authors, for example, Bazaraa and Sherali (1980), Geoffrion and Graves (1974). Geoffrion and McBride (1979), Magnanti and Wong (1981), McDaniel and Devine (1977), Rardin and Unger (1976) and Williams (1974), an integer linear formulation whose continuous, or linear programming, relaxation closely approximates the convex hull of feasible integer solutions in the vicinity of the optimum is computationally advantageous. Hence, a linearization technique that provides a tight linear programming relaxation, while keeping the problem computationally tractable, is highly desirable.

The purpose of this paper is to present a new linearization technique for a general class of nonlinear mixed integer programming problems. This linearization technique possesses two principle advantages. First, it provides a type of unifying theory for the various existing linearization strategies. Second, the continuous relaxation of this linearization theoretically dominates those of other linearizations found in the literature. Moreover, in the types of problems we have solved thus far, the proposed linearization has demonstrated a significant computational advantage.

This paper is organized as follows. Section 1 presents and justifies the proposed linearization scheme. Section 2 compares this linearization strategy with those of Glover (1975); Glover and Woolsey (1973, 1974), Petersen (1971), Watters (1967) and Zangwill (1965) demonstrating that these alternate schemes are all obtainable through appropriate surrogates of constraints of the proposed linearized problem. Hence, not only does the new linearization provide a tighter linear programming relaxation, but it also provides a unifying framework which ties together all these alternate schemes. An example is then given to demonstrate that the proposed linearization strictly dominates the other available linearizations with respect to the continuous relaxation. The final section extends these ideas to some other, more general, types

Subject classifications: Programming: linear reformulations of nonlinear integer programming, nanger, nonlinear, mixed inleger programming,

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Relaxation of bilinear terms





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Sherali & Alameddine, JOGO 1992:

 $\mathbf{x} \in \mathbb{R}^n$ with bilinear products

LP relaxation

under special condition, LP is reformulation

A New Reformulation-Linearization Technique for Bilinear Programming Problems*

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(Received: 14 December 1990; accepted: 7 November 1991)

Abstract. This paper is concerned with the development of an algorithm for general bilinear programming problems. Such problems find numerous applications in economics and game theory, location theory, nonlinear multi-commodity network flows, dynamic assignment and production, and various risk management problems. The proposed approach develops a new Reformulation-Linearization Technique (RLT) for this problem, and imbeds it within a provably convergent branch-andbound algorithm. The method first reformulates the problem by constructing a set of nonnegative variable factors using the problem constraints, and suitably multiplies combinations of these factors with the original problem constraints to generate additional valid nonlinear constraints. The resulting nonlinear program is subsequently linearized by defining a new set of variables, one for each nonlinear term. This "RLT" process yields a linear programming problem whose optimal value provides a tight lower bound on the optimal value to the hilinear programming problem. Various implementation schemes and constraint generation procedures are investigated for the purpose of further (ightening the resulting linearization. The lower bound thus produced theoretically dominates, and practically is for tighter, than that obtained by using convex envelopes over hyper-rectangles. In fact, for some special cases, this process is shown to yield an exact linear programming representation. For the associated branch-and-bound algorithm, various admissible branching schemes are discussed, including one in which branching is performed by partitioning the intervals for only one set of variables x or y, whichever are fewer in number. Computational experience is provided to demonstrate the viability of the algorithm. For a large number of test problems from the literature, the initial bounding linear program itself solves the underlying bilinear programming problem.

Key words. Bilinear programming, nonconvex programming, global optimization, branch-and-bound, reformulation-linearization technique.

1. Introduction

This paper is concerned with the solution of bilinear programming problems of the form

BLP Minimize
$$\Phi(x, y) = c'x + d'y + x'Gy$$
 (1.1)

subject to
$$(x, y) \in Z = \begin{cases} (x, y); & A_1x + D_1y \leq b_1 \\ A_2x + D_2y = b_2 \end{cases}$$
 (1.2a)

$$(x, y) \in \Omega \equiv \{(x, y): 0 \le t \le x \le u < \infty, 0 \le L \le y \le U < \infty\},$$
 (1.3)

Journal of Global Optimization 2: 379-410, 1992.

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[&]quot;This paper was presented at the II. IIASA Workshop on Global Optimization, Sopron (Hungary), December 9-14, 1990.

Mixed products again





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Adams & Sherali, Math. Prog. 1993:

 $\mathbf{x} \in \mathbb{R}^{n_1} \times \{0,1\}^{n_2}$ specialized to bilinear products involving one continuous and one binary variable

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Mathematical Programming 59 (1993) 279-305 North-Holland 279

Mixed-integer bilinear programming problems

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Received 22 June 1987 Revised manuscript received 5 March 1992

This paper addresses a class of problems called mixed-integer bilinear programming problems. These problems are identical to the well known bilinear programming problems with the exception that one set of variables is restricted to be binary valued, and they arise in various production, location-allocation, and distribution application contexts. We first identify some special cases of this problem which are relatively more readily solvable, even though their continuous relaxations are still nonconvex. For the more general case, we employ a linearization technique and design a composite Lagrangian relaxation-implicit enumeration-cutting plane algorithm. Extensive computational experience is provided to test the efficacy of various algorithmic strategies and the effects of problem data on the computational effort of the proposed algorithm.

Key words: Bilinear program, linearization, cutting planes, Lagrangian relaxation.

1. Introduction

In this paper we study a class of mathematical programs referred to as mixed-integer bilinear programming problems (MIBLP). These problems may be stated as follows:

MIBLP:
$$minimize\{c^tx + d^ty + x^tCy: x \in X, y \in Y, y \text{ binary}\}$$
 (1.1)

where X and Y are nonempty, bounded polyhedral sets given respectively as

$$X = \left\{ x \in \mathbb{R}^m : \sum_{i=1}^m a_{ki} x_i = b_k \text{ for } k = 1, ..., K, x \ge 0 \right\}$$

and

$$Y = Y_1 \cap Y_2 \cap Y_3$$

with

$$Y_1 = \left\{ y \in \mathbb{R}^n : \sum_{j=1}^n G_{ij} y_j \ge g_i \text{ for } i = 1, ..., L \right\},$$

 $Y_2 = \left\{ y \in \mathbb{R}^n : \sum_{j=1}^n H_{ij} y_j = h_i \text{ for } p = 1, ..., P \right\},$

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Relaxation hierarchy





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Sherali & Adams, DAM 1994:

$$\mathbf{x} \in \mathbb{R}^{n_1} \times \{0,1\}^{n_2}$$

Convex hull of MILP feasible region obtained through hierarchy of RLT constraints

Level d RLT: let $J_1, J_2 \subseteq \{1, \dots, n_2\}$ with $|J_1 \cup J_2| = d$ and

$$F_d(J_1, J_2) = \prod_{j \in J_1} x_j \prod_{j \in J_2} (1 - x_j);$$

multiply RLT-(d-1) constraints by all $F_d(J_1,J_2)$ the linearize to obtain RLT-d



DISCRETE APPLIED MATHEMATICS

Discrete Applied Mathematics 52 (1994) 83-106

A hierarchy of relaxations and convex hull characterizations for mixed-integer zero-one programming problems

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(Received 21 October 1991, revised 18 August 1992)

Abstract

This paper is concerned with the generation of tight equivalent representations for mixedinteger zero-one programming problems. For the linear case, we propose a technique which first converts the problem into a nonlinear, polynomial mixed-integer zero-one problem by multiplying the constraints with some suitable d-degree polynomial factors involving the n-binary variables, for any given $d \in \{0, ..., n\}$, and subsequently linearizes the resulting problem through appropriate variable transformations. As d-varies from zero to n, we obtain a hierarchy of relaxations spanning from the ordinary linear programming relaxation to the convex hull of feasible solutions. The facets of the convex hull of feasible solutions in terms of the original problem variables are available through a standard projection operation. We also suggest an alternate scheme for applying this technique which gives a similar hierarchy of relaxations, but involving fewer "complicating" constraints. Techniques for tightening intermediate level relaxations, and insights and interpretations within a disjunctive programming framework are also presented. The methodology readily extends to multilinear mixed-integer zero-one polynomial programming problems in which the continuous variables appear linearly in the problem.

Key words. Mixed-integer zero-one problems, Tight relaxations, Convex hull representations, Facetial inequalities, Disjunctive programming

1. Introduction

Recently, Sherali and Adams [7] have proposed a new technique for generating a hierarchy of relaxations for linear and polynomial zero-one programming problems, spanning the spectrum from the continuous relaxation to the convex hull representation. The present paper provides an extension of this approach to the

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⁰¹⁶⁶⁻²¹⁸X/94/507.00 © 1994—Elsevier Science B.V. All rights reserved SSDI 0166-218X(92)00190-W

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extensions (polynomial and signomial programming, SDP, convex MINLP, disjunctive cuts) and applications



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Consider mixed-integer QCQP subject to linear equality constraints $A\mathbf{x} = \mathbf{b}$ (A has full rank)

$$\min_{\mathbf{x} \in \mathbb{R}^{n_1} \times \mathbb{Z}^{n_2}} \mathbf{c}_0 \mathbf{x} + \mathbf{x} Q_0 \mathbf{x} \\
\forall 1 \leq i \leq q \quad \mathbf{c}_i \mathbf{x} + \mathbf{x} Q_i \mathbf{x} \leq 0 \\
A \mathbf{x} = \mathbf{b} \\
\mathbf{x} \in \mathscr{X} \cap [\mathbf{x}^L, \mathbf{x}^U].$$

 ${\mathscr X}$ is a polyhedron

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 \Box Generate RLT constraints from $A\mathbf{x} = \mathbf{b}$

$$A\mathbf{x} = \mathbf{b} \Rightarrow$$

$$\forall \ell \leq n \quad x_{\ell}A\mathbf{x} = x_{\ell}\mathbf{b} \Rightarrow$$

$$\forall \ell \leq n \quad A\mathbf{w}_{\ell} = x_{\ell}\mathbf{b}$$

 \square Consider homogeneous system $\forall \ell \leq n \ (A\mathbf{w}_{\ell} = \mathbf{0})$ and a set N of nonbasic variable index pairs (j, ℓ) ; let:

$$C = \{(\mathbf{x}, \mathbf{w}) \mid A\mathbf{x} = \mathbf{b} \land \forall j, \ell \leq n \ (w_{j\ell} = x_j x_\ell)\}$$

$$R_N = \{(\mathbf{x}, \mathbf{w}) \mid A\mathbf{x} = \mathbf{b} \land \forall \ell \leq n \ (A\mathbf{w}_\ell = \mathbf{b} x_\ell) \land \forall (j, \ell) \in N \ (w_{j\ell} = x_j x_\ell)\}$$

Main result



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 $\mathsf{Thm}.$

Let
$$[n] = \{1, \ldots, n\}$$
; $\exists N \subseteq [n] \times [n] \ C = R_N$

Proof

(RRLT system)
$$\forall \ell \leq n \ A\mathbf{w}_{\ell} - x_{\ell}b = 0 \Rightarrow$$

(replace
$$b$$
 by Ax) $\forall \ell \leq n \ A\mathbf{w}_{\ell} - x_{\ell}A\mathbf{x} = 0 \Rightarrow$

$$(\mathbf{z} = \mathbf{w}_{\ell} - x_{\ell}\mathbf{x} \text{ are vars. of hom. sys.}) \quad \forall \ell \leq n \ A(\mathbf{w}_{\ell} - x_{\ell}\mathbf{x}) = 0.(1)$$

$$\left[\begin{array}{l} \text{(1) is homogeneous} \\ N \subseteq [n] \times [n] \text{: nonbasic of (1)} \\ \forall (j,\ell) \in N \ w_{j\ell} = x_j x_\ell \end{array} \right] \Rightarrow \left\{ \begin{array}{l} \text{get square nonsing. subsyst.} \\ A' \mathbf{z} = 0 \text{ of (1)} \\ \text{corresponding to basic cols.} \\ B = [n] \times [n] \setminus N \end{array} \right.$$

by basic linear algebra, $A'\mathbf{z} = 0$ implies $\forall (j, \ell) \in B \ (w_{j\ell} = x_j x_\ell)$.

Cor.

RRLT constraints \Rightarrow exact ref. with fewer quadratic terms

Proof

Only need quadratic terms indexed by N, RRLT implies those in B

Geometric interpretation



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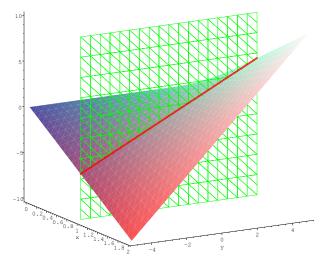
The quadratic case RRLT-1 constraints Main result Geometric interpretation

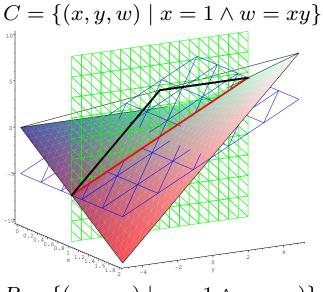
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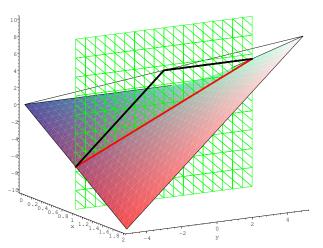
Why bother?

Thank you





$$R = \{(x,y,w) \mid x = 1 \land w = y)\}$$



McCormick's rel. of w=xy restricted to x=1

Notice C = R (straight red segment)

Equation w=y can be obtained via RRLT: multiply equation x=1 by y and linearize via w



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INTERNATIONAL TRANSACTIONS IN OPERATIONAL RESEARCH

Ind. Trans. in Op. Res. 11 (2004) 33-41

Reduction constraints for the global optimization of NLPs

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Received 3 July 2002; received in revised form 6 December 2002; accepted 13 January 2003

Abstract

Convergence of branch-and-bound algorithms for the solution of NLPs is obtained by finding ever-nearer

Keywords: global optimization; valid cut; NLP; branch-and-bound

lower and upper bounds to the objective function. The lower bound is calculated by constructing a convex relaxation of the NLP. Reduction constraints are new linear problem constraints which are (a) linearly independent from the existing constraints; (b) redundant with reference to the original NLP formulation; (c) not redundant with reference to its convex relaxation. Thus, they can be successfully employed to reduce the feasible region of the convex relaxation without cutting the feasible region of the original NLP.

1. Introduction

Global nonlinear optimization has witnessed a remarkable theoretical development in the last decade (Adjiman, Schweiger and Floudas, 1998; Floudas, 2001; Pardalos, Romeijin, 2000). A lot of new algorithms have been proposed, either geared towards a specific problem or class of problems (Hirafuji and Hagan, 2000; Hägglöf, Lindberg and Svensson, 1995), or more general (Adjiman et al., 1998; Adjiman, Androulakis and Floudas, 1998; Kesavan and Barton, 2000; Ryoo and Sahinidis 1995; Smith and Pantelides, 1999; Vaidyanathan and El-Halwagi, 1996). Software implementations of these algorithms, however, are scarce, not easily available, and more importantly, not really ready for practical use. One could draw a parallel with the development of LP solvers, where the straight implementation of an algorithm is usually not enough to give birth to a good piece of code; all sorts of 'implementation tricks' are necessary to this end. We feel that at the present state, global optimization solvers for NLPs are in their basic form, with the algorithm in place but devoid of other speeding-up devices which are crucial for practical usability.

In this article we describe the theory and implementation of one such speeding-up device, named 'method of reduction constraints', to be used in a branch-and-bound solution framework.

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L., ITOR 2004:

RRLT constraints are linearly independent

Preliminary results pooling problems

General theory





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L., JOGO 2005:

General theory of RRLT constraints

Reformulation proofs

Journal of Global Optimization (2005) 33: 157–196 DOI 10.1007/s10898-004-0864-2 © Springer 2005

Linearity Embedded in Nonconvex Programs

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(Received 4 May 2003; accepted in revised form 19 May 2004)

Abstract. Nonconvex programs involving bilinear terms and linear equality constraints often appear more nonlinear than they really are. By using an automatic symbolic reformulation we can substitute some of the bilinear terms with linear constraints. This has a dramatically improving effect on the tightness of any convex relaxation of the problem, which makes deterministic global optimization algorithms like spatial Branch-and-Bound much more efficient when applied to the problem.

Key words: Bilinear, Convex relaxation, Global optimization, MINLP, Reduction constraint, Reformulation, RLT

1. Introduction

This paper is concerned with programming problems of the form:

$$\min_{x} x^{T}Qx + c^{T}x + f(x),$$

$$Ax = b,$$

$$g(x) = 0,$$

$$h(x) \leq 0,$$

$$x \in X,$$

$$x^{L} \leq x \leq x^{U},$$
(1)

where $Q = (q_g)$ is an $n \times n$ matrix, $x, c, x^1, x^0 \in \mathbb{R}^n$, $A = (a_g)$ is an $m \times n$ matrix having rank $m, b \in \mathbb{R}^m$, $f : \mathbb{R}^n \to \mathbb{R}$, $g : \mathbb{R}^n \to \mathbb{R}^{m_1}$, $h : \mathbb{R}^n \to \mathbb{R}^{m_2}$ and X is an arbitrary subset of \mathbb{R}^n (which might express integrality constraints on the decision variables, for example). Notice f, g, h are completely arbitrary functions. Notice also that we assume $m \leq n$, otherwise the feasible region may be empty. Such a formulation is very general and encompasses many instances of problems arising from mathematical modelling of real life processes.

Because the theory developed herein will enable us to substitute some of the bilinear terms with linear constraints, we can restrict our attention to a more standard formulation (2) of the bilinear problem. This does not mean that the methods described only applies to problems in formulation (2),

Automatic reformulation





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L. & Pantelides, JOGO 2006:

Graph-based automatic reformulation algorithm

Full computational results on pooling and blending problems

Journal of Global Optimization (2006) 36: 161–189 DOI 10.1007/s10898-006-9005-4 © Springer 2006

An Exact Reformulation Algorithm for Large Nonconvex NLPs Involving Bilinear Terms

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(Received 2 February 2004; accepted in revised form 29 January 2006; Published online 22 April 2006)

Abstract. Many nonconvex nonlinear programming (NLP) problems of practical interest involve bilinear terms and linear constraints, as well as, potentially, other convex and nonconvex terms and constraints. In such cases, it may be possible to augment the formulation with additional linear constraints (a subset of Reformulation-Linearization Technique constraints) which do not affect the feasible region of the original NLP but tighten that of its convex relaxation to the extent that some bilinear terms may be dropped from the problem formulation. We present an efficient graph-theoretical algorithm for effecting such exact reformulations of large, sparse NLPs. The global solution of the reformulated problem using spatial Branch-and Bound algorithms is usually significantly faster than that of the original NLP. We illustrate this point by applying our algorithm to a set of pooling and blending global optimization problems.

Key words: Bilinear, Convex relaxation, Global optimization, NLP, Reformulationlinearization technique, RRLT constraints

1. Introduction

We consider the solution of nonlinear programs (NLPs) of the following standard form.

$$[P]: \min z_i$$
 (1)

$$z=b$$
 (2)

$$z_i = z_j z_k \quad \forall i, j, k \in B$$
 (3)

$$z_i = \frac{z_f}{z_i}$$
 $\forall i, j, k \in F$ (4)

$$z_i = f_i(z_j) \quad \forall i, j \in \mathbb{N}$$
 (5)

$$z^L \leq z \leq z^U$$
(6)

where $z = (z_1, \dots, z_p) \in \mathbb{R}^p$ are the problem variables, l is an index in the set $\{1, \dots, p\}$, $A = (a_{ij})$ is an $M \times p$ matrix of rank $M, b \in \mathbb{R}^M$, B, F are

Application to quantum chemistry





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L., Lavor, Maculan, Chaer Nascimento, DAM 2009:

Application of an RRLT-2 subset to solving Hartree-Fock systems



Reformulation in mathematical programming: An application to quantum chemistry

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MSC 90C20 90C26 90C11

Keywords: Harmee-Fock Clobal optimization Branch, and Bound ABSTRACT

This paper concerns the application of reformulation techniques in mathematical programming to a specific problem arising in quantum chemistry, namely the solution of Hartree-Fock systems of equations, which describe atomic and molecular electronic wave functions based on the minimization of afunctional of the energy. Their traditional solution method does not provide a guarantee of global optimality and its output depends on a provided initial starting point. We formulate this problem as a multi-extremal nonconvex polynomial programming problem, and solve it with a spatial Branch and Bound algorithm for global optimization. The lower bounds at each node are provided by reformulating the problem in such a way that its convex relaxation is tight. The validity of the proposed approach was established by successfully computing the ground-state of the helium and beryllium atoms.

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1. Introduction

The quantum behavior of atoms and molecules, in the absence of relativistic effects and any external time-dependent perturbations, is determined by the time-independent Schrödinger equation:

where H, the Hamiltonian operator of the system, represents the total energy (kinetic + potential) of all the particles of the system.

Analytical solutions for this equation are only possible for very simple systems. Hence, for the majority of problems of interest, one has to rely on some approximate model. In the Hartree-Fock (HF) model, the electrons in atoms and molecules move independently of each other, the motion of each one of the electrons being determined by the attractive electrostate potential of the nuclei and by a repulsive average field due to all the other electrons of the system. In this model, the approximate solutions Φ_0 of Eq. (1) are anti-symmetrized products of one-electron wave functions [Φ_0] (also called orbitals), which are solutions of the HF equations for the system under study. This model gives rise to a set of coupled integro-differential equations which can only be solved numerically. Alternatively, each orbital Ψ_0 , can be expanded in a complete basis set $\{\chi_1\}_{n=1}^\infty$. In order to transform the HF equations into a less cumbersome algebraic problem, we only

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Feasible region of QCQP: use R_N instead of C



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Why bother?

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- \square Feasible region of QCQP: use R_N instead of C
- \square R_N relies on quadratic constraints $\forall (j,\ell) \in N \ (w_{j\ell} = x_j x_\ell)$



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Why bother?

Thank you

- Feasible region of QCQP: use R_N instead of C
- R_N relies on quadratic constraints $\forall (j,\ell) \in N \ (w_{j\ell} = x_j x_\ell)$
- **Degree of freedom**: choice of basic/nonbasic partition $B, N \text{ of } [n] \times [n]$



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Thank you

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- □ **Degree of freedom**: choice of basic/nonbasic partition

 $B, N \text{ of } [n] \times [n]$

 \Box $(j,\ell) \leftrightarrow \text{volume } V_{i\ell} \text{ of conv. env. of } x_i x_\ell$



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$$B,N \text{ of } [n] \times [n]$$

- \Box $(j,\ell) \leftrightarrow \text{volume } V_{j\ell} \text{ of conv. env. of } x_j x_\ell$
- \square Convexity gap: $\mathcal{V}(N) = \sum\limits_{(j,\ell) \in N} V_{j\ell}$



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Thank you

- Feasible region of QCQP: use R_N instead of C
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$$B, N \text{ of } [n] \times [n]$$

- $(j,\ell) \leftrightarrow \text{volume } V_{i\ell} \text{ of conv. env. of } x_i x_\ell$
- Convexity gap: $\mathcal{V}(N) = \sum V_{j\ell}$ $(j,\ell) \in N$
- Let $N^* = \arg\min_N \mathcal{V}(N)$

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- $(j,\ell) \leftrightarrow \text{volume } V_{i\ell} \text{ of conv. env. of } x_j x_\ell$
- Convexity gap: $\mathcal{V}(N) = \sum_{i\ell} V_{i\ell}$ $(j,\ell) \in N$
- Let $N^* = \arg\min_N \mathcal{V}(N)$

Smaller gap ⇒ tight bound more likely

Optimal RRLT



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- \square Feasible region of QCQP: use R_N instead of C
- \square R_N relies on quadratic constraints $\forall (j,\ell) \in N \ (w_{j\ell} = x_j x_\ell)$
- □ **Degree of freedom**: choice of basic/nonbasic partition

$$B, N ext{ of } [n] imes [n]$$

- \Box $(j,\ell) \leftrightarrow \text{volume } V_{j\ell} \text{ of conv. env. of } x_j x_\ell$
- \square Convexity gap: $\mathcal{V}(N) = \sum_{(j,\ell) \in N} V_{j\ell}$
- \square Let $N^* = \arg\min_N \mathcal{V}(N)$

Smaller gap ⇒ tight bound more likely

 $\square \quad B, N \text{ partition } [n] \times [n] \Rightarrow N^* = [n] \times [n] \setminus \arg \max_B \mathcal{V}(B)$

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- Feasible region of QCQP: use R_N instead of C
- R_N relies on quadratic constraints $\forall (j,\ell) \in N \ (w_{i\ell} = x_i x_\ell)$
- **Degree of freedom**: choice of basic/nonbasic partition

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- $(j,\ell) \leftrightarrow \text{volume } V_{i\ell} \text{ of conv. env. of } x_j x_\ell$
- Convexity gap: $\mathcal{V}(N) = \sum_{i\ell} V_{i\ell}$ $(j,\ell) \in N$
- Let $N^* = \arg\min_{N} \mathcal{V}(N)$

Smaller gap ⇒ tight bound more likely

- [B,N] partition $[n] \times [n] \Rightarrow N^* = [n] \times [n] \setminus \arg\max_B \mathcal{V}(B)$
- Reduces to finding a max-weight basis of a linear system

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- $\ \square$ Feasible region of QCQP: use R_N instead of C
- \square R_N relies on quadratic constraints $\forall (j,\ell) \in N \ (w_{j\ell} = x_j x_\ell)$
- □ **Degree of freedom**: choice of basic/nonbasic partition

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- \Box $(j,\ell) \leftrightarrow \text{volume } V_{j\ell} \text{ of conv. env. of } x_j x_\ell$
- \square Convexity gap: $\mathcal{V}(N) = \sum_{(j,\ell) \in N} V_{j\ell}$
- \Box Let $N^* = \arg\min_N \mathcal{V}(N)$

Smaller gap ⇒ tight bound more likely

- $\square \quad B, N \text{ partition } [n] \times [n] \Rightarrow N^* = [n] \times [n] \setminus \arg \max_B \mathcal{V}(B)$
- ☐ Reduces to finding a max-weight basis of a linear system
- ☐ Greedy algorithm solves problem optimally



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Consider general polynomial programming MINLP

general polynomial programming MINLP
$$\min_{\substack{x \in \mathbb{R}^{n_1} \times \mathbb{Z}^{n_2} \\ \forall i \leq q \quad g_i(x) \leq 0 \\ A\mathbf{x} = \mathbf{b} \\ \mathbf{x} \in \mathscr{X} \cap [\mathbf{x}^L, \mathbf{x}^U]} \right\}$$
 E $\mathbb{Q}[\mathbf{x}]$ for all $i \in \{0, \dots, q\}$

where $g_i \in \mathbb{Q}[\mathbf{x}]$ for all $i \in \{0, \dots, q\}$



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 \square **Reformulation**: for all $J \subseteq [n-1]$ multiply $A\mathbf{x} = \mathbf{b}$ by

$$\prod_{j \in J} x_j$$



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Why bother?

- Reformulation: for all $J \subseteq [n-1]$ multiply $A\mathbf{x} = \mathbf{b}$ by $\prod_{j \in J} x_j$
- Linearization: replace each term $\prod_{j \in J} x_j$ by the added variable w_J (for all $J \subseteq [n]$)



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Why bother?

Thank you

 \square **Reformulation**: for all $J \subseteq [n-1]$ multiply $A\mathbf{x} = \mathbf{b}$ by

$$\prod_{j \in J} x_j$$

 \square Linearization: replace each term $\prod_{i \in J} x_i$ by the added

variable w_J (for all $J \subseteq [n]$)

 \square Adjoin defining constraints $w_J = \prod_{i \in J} x_i$



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Thank you

- Reformulation: for all $J \subseteq [n-1]$ multiply $A\mathbf{x} = \mathbf{b}$ by $\prod_{i \in J} x_i$
- \square **Linearization**: replace each term $\prod_{j \in J} x_j$ by the added

variable w_J (for all $J \subseteq [n]$)

- \square Adjoin defining constraints $w_J = \prod_{i \in J} x_i$
- \square Define natural extensions of C, R_N :

$$C = \{(\mathbf{x}, \mathbf{w}) \mid A\mathbf{x} = \mathbf{b} \land \forall J \subseteq [n-1] \ (w_J = \prod_{j \in J} x_j\}$$

$$R_N = \{(\mathbf{x}, \mathbf{w}) \mid A\mathbf{x} = \mathbf{b} \land \forall J \subseteq [n-1] \ (A\mathbf{w}_J = \mathbf{b}w_J) \land \forall J \in N \ (w_J = \prod_{j \in J} x_j)\}$$

where
$$\mathbf{w}_{J} = (w_{(J,1)}, \dots, w_{(J,n)})$$



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Why bother?

Thank you

- Reformulation: for all $J \subseteq [n-1]$ multiply $A\mathbf{x} = \mathbf{b}$ by $\prod_{i \in J} x_i$
- \square Linearization: replace each term $\prod_{j \in J} x_j$ by the added

variable w_J (for all $J \subseteq [n]$)

- \square Adjoin defining constraints $w_J = \prod_{i \in J} x_i$
- \square Define natural extensions of C, R_N :

$$C = \{(\mathbf{x}, \mathbf{w}) \mid A\mathbf{x} = \mathbf{b} \land \forall J \subseteq [n-1] \ (w_J = \prod_{j \in J} x_j\}$$

$$R_N = \{(\mathbf{x}, \mathbf{w}) \mid A\mathbf{x} = \mathbf{b} \land \forall J \subseteq [n-1] \ (A\mathbf{w}_J = \mathbf{b}w_J) \land \forall J \in N \ (w_J = \prod_{j \in J} x_j)\}$$

where
$$\mathbf{w}_{J} = (w_{(J,1)}, \dots, w_{(J,n)})$$

Main result $C = R_N$ still holds



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Why bother?

Thank you

 \square Choice of optimal N extends from quadratic case, but:



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Why bother?

- \sqsupset Choice of optimal N extends from quadratic case, but:
- ☐ Added complication:



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Why bother?

- \square Choice of optimal N extends from quadratic case, but:
- ☐ Added complication:
 - V_{ij} and V_{ijk} are expressed in different units of measure



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Why bother?

- \square Choice of optimal N extends from quadratic case, but:
- ☐ Added complication:
 - V_{ij} and V_{ijk} are expressed in different units of measure
 - Summing up V_J for J's of different sizes may not make much sense



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Why bother?

- \square Choice of optimal N extends from quadratic case, but:
- □ Added complication:
 - V_{ij} and V_{ijk} are expressed in different units of measure
 - Summing up V_J for J's of different sizes may not make much sense
- \square Multi-objective problem: $\forall p \in [n] \quad \max_{|J|=p} V_J$



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Thank you

- \square Choice of optimal N extends from quadratic case, but:
- □ Added complication:
 - V_{ij} and V_{ijk} are expressed in different units of measure
 - Summing up V_J for J's of different sizes may not make much sense
- \square Multi-objective problem: $\forall p \in [n] \quad \max_{|J|=p} V_J$

 $\mathsf{Thm}.$

Efficient solution is an optimum of $\max \sum_{J\subseteq [n]} V_J$



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Why bother?

Thank you

- \square Choice of optimal N extends from quadratic case, but:
- ☐ Added complication:
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- \square Multi-objective problem: $\forall p \in [n] \quad \max_{|J|=p} V_J$

 $\mathsf{Thm}.$

Efficient solution is an optimum of $\max \sum_{J\subseteq [n]} V_J$

☐ Greedy is still OK



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Why bother?

Thank you

- □ Polynomial programs are never dense in practice
- \square RRLT needs $B \cup N = \mathscr{P}([n])$
- □ Need to introduce exponentially many new monomials

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Why bother?

Thank you

 \Box β =set of multi-indices for monomials already in problem



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Why bother?

- $\beta=$ set of multi-indices for monomials already in problem
 - Every new monomial $J \not\in \beta$ yields a new variable w_J



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Why bother?

- β =set of multi-indices for monomials already in problem
- Every new monomial $J \not\in \beta$ yields a new variable w_J
- Sometimes $\exists J \not\in \beta$ s.t. w_J yields > 1 new RRLT constr.



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Thank you

- \square β =set of multi-indices for monomials already in problem
- \square Every new monomial $J
 ot\in eta$ yields a new variable w_J
- \square Sometimes $\exists J \not\in \beta$ s.t. w_J yields > 1 new RRLT constr.
- □ E.g.:

$$x_1 + x_2 = 1 \land 2x_1 - x_2 = 3 \land \beta = \{(1,3)\}\$$

one new monomial $(x_2x_3) \Rightarrow$ **two** new RRLT constraints



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$$x_1 + x_2 = 1 \land 2x_1 - x_2 = 3 \land \beta = \{(1,3)\}\$$

one new monomial $(x_2x_3) \Rightarrow$ **two** new RRLT constraints

$$x_1 + x_2 = 1 \quad (\times x_3 =) \quad w_{13} + w_{23} = x_3$$

$$2x_1 - x_2 = 3 \quad (\times x_3 =) \quad 2w_{13} - w_{23} = 3x_3$$

□ **Principle**: one new equation, one fewer degrees of freedom



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- \square β =set of multi-indices for monomials already in problem
- \sqsupset Every new monomial $J
 ot\in eta$ yields a new variable w_J
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- □ E.g.:

$$x_1 + x_2 = 1 \land 2x_1 - x_2 = 3 \land \beta = \{(1,3)\}\$$

one new monomial $(x_2x_3) \Rightarrow$ **two** new RRLT constraints

$$x_1 + x_2 = 1$$
 $(\times x_3 =)$ $w_{13} + w_{23} = x_3$
 $2x_1 - x_2 = 3$ $(\times x_3 =)$ $2w_{13} - w_{23} = 3x_3$

□ Principle: one new equation, one fewer degrees of freedom

Create fewer J's than new RRLT constraints



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Thank you

Problem:

Look for subset ρ of rows of $A\mathbf{x} = \mathbf{b}$ to be multiplied by a subset σ of $\mathcal{P}([n-1])$ such that the number of new vars w_J is < number of new RRLT constraints



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Why bother?

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☐ Problem:

Look for subset ρ of rows of $A\mathbf{x} = \mathbf{b}$ to be multiplied by a subset σ of $\mathscr{P}([n-1])$ such that the number of new vars w_J is < number of new RRLT constraints

 \square Formalization: consider bipartite graph (U, V, E)

$$w_L \times (\mathbf{a}_1 \mathbf{x} = b_1)$$
 $w_H \times (\mathbf{a}_1 \mathbf{x} = b_1)$
 \bar{H}
 $w_L \times (\mathbf{a}_2 \mathbf{x} = b_2)$
 \bar{L}
 $w_J \times (\mathbf{a}_i \mathbf{x} = b_i)$

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 $w_L \times (\mathbf{a}_2 \mathbf{x} = b_2)$
 \bar{L}
 $w_J \times (\mathbf{a}_i \mathbf{x} = b_i)$

U=row i by var. w_J (indexed by (i,J))

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Look for subset ρ of rows of $A\mathbf{x} = \mathbf{b}$ to be multiplied by a subset σ of $\mathscr{P}([n-1])$ such that the number of new vars w_J is < number of new RRLT constraints

 \Box **Formalization**: consider bipartite graph (U, V, E)

$$w_L imes (\mathbf{a}_1 \mathbf{x} = b_1)$$
 $w_H imes (\mathbf{a}_1 \mathbf{x} = b_1)$
 \overline{B}
 $w_L imes (\mathbf{a}_2 \mathbf{x} = b_2)$
 \overline{L}
 $w_J imes (\mathbf{a}_i \mathbf{x} = b_i)$

- \square $U=\text{row } i \text{ by var. } w_J \text{ (indexed by } (i,J))$
- \square V=var. $w_{\bar{J}}$ with $\bar{J} \not\in \beta$ (indexed by \bar{J})

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Problem:

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 $w_H imes (\mathbf{a}_1 \mathbf{x} = b_1)$
 \overline{b}_1
 $w_L imes (\mathbf{a}_2 \mathbf{x} = b_2)$
 \overline{b}_2
 \overline{b}_3
 $w_J imes (\mathbf{a}_i \mathbf{x} = b_i)$

- \square U=row i by var. w_J (indexed by (i,J))
- \square V=var. $w_{\bar{J}}$ with $\bar{J} \not\in \beta$ (indexed by \bar{J})
- \square Edges: E=incidence of added vars in RRLT constrs

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Problem:

Look for subset ρ of rows of $A\mathbf{x} = \mathbf{b}$ to be multiplied by a subset σ of $\mathscr{P}([n-1])$ such that the number of new vars w_J is < number of new RRLT constraints

Formalization: consider bipartite graph (U, V, E)

$$w_L imes (\mathbf{a}_1 \mathbf{x} = b_1)$$
 $w_H imes (\mathbf{a}_1 \mathbf{x} = b_1)$
 \overline{H}
 $w_L imes (\mathbf{a}_2 \mathbf{x} = b_2)$
 \overline{L}
 $w_J imes (\mathbf{a}_i \mathbf{x} = b_i)$

- U=row i by var. w_J (indexed by (i,J))
- $V{=}$ var. $w_{ar{J}}$ with $J \not\in \beta$ (indexed by $ar{J}$)
- Edges: E=incidence of added vars in RRLT constrs

Aim: find induced subgraph (U', V', E') such that |U'| is maximum, |U'| > |V'|, and V' = neighb(U')



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Why bother?

Thank you

Mathematical Programming formulation:

$$\max \sum_{(i,J')\in U} u_{i,J'} \\ \sum_{(i,J')\in U} u_{i,J'} \geq \sum_{J\not\in\beta} v_J + 1 \\ \forall \{(i,J'),J\}\in E \qquad v_J \geq u_{i,J'} \\ u \in \{0,1\}^{|U|} \\ v \in \{0,1\}^{|\mathscr{P}([n])\setminus\beta|}.$$



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Why bother?

Thank you

Mathematical Programming formulation:

$$\max \sum_{(i,J')\in U} u_{i,J'} \\ \sum_{(i,J')\in U} u_{i,J'} \geq \sum_{J\not\in\beta} v_J + 1 \\ \forall \{(i,J'),J\}\in E \qquad v_J \geq u_{i,J'} \\ u \in \{0,1\}^{|U|} \\ v \in \{0,1\}^{|\mathscr{P}([n])\setminus\beta|}.$$

Thm.

This problem is in P

Proof

Use matching-based algorithm



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Use within sBB



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- Use within sBB
- Thank you

- ☐ CPU time in sBB: number of nodes, time to solve each node
- □ Need few, small convex relaxation LPs
- Usually concentrate on few (tight bound) but large (valid cuts)
- □ Different approach: slacken bound, aim to solve each LP faster

Use within sBB



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Thank you

- ☐ CPU time in sBB: number of nodes, time to solve each node
- □ Need few, small convex relaxation LPs
- Usually concentrate on few (tight bound) but large (valid cuts)
- Different approach: slacken bound, aim to solve each LP faster

Outcome:

- bound quality: 0.07% worse;
- CPU improvement: 40%
- □ *Future work*: embed in sBB



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