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# Reformulation and Convex Relaxation Techniques for Global Optimization

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**Abstract** We survey the main results obtained by the author in his PhD dissertation supervised by Prof. Costas Pantelides. It was defended at the Imperial College, London. The thesis is written in English and is available from `http://or.elet.polimi.it/people/Liberti/phdtesis.ps.gz`.

The most widely employed deterministic method for the global solution of nonconvex NLPs and MINLPs is the spatial Branch-and-Bound (sBB) algorithm, and one of its most crucial steps is the computation of the lower bound at each sBB node. We investigate different reformulations of the problem so that the resulting convex relaxation is tight. In particular, we suggest a novel technique for reformulating a wide class of bilinear problems so that some of the bilinear terms are replaced by linear constraints. Moreover, an in-depth analysis of a convex envelope for piecewise-convex and concave terms is performed. All the proposed algorithms were implemented in $oo\mathcal{OPS}$, an object-oriented callable library for constructing MINLPs in structured form and solving them using a variety of local and global solvers.

## 1 Introduction

Many engineering optimization problems can be formulated as nonconvex mixed-integer nonlinear programming problems (MINLPs) involving a nonlinear objective function subject to nonlinear constraints. Such problems may exhibit more than one locally optimal point. However, one is often solely or primarily interested in determining the globally optimal point. This thesis is concerned with techniques for establishing such global optima using spatial Branch-and-Bound (sBB) algorithms.

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A key issue in optimization is that of mathematical formulation, as there may be several different ways in which the same problem can be expressed mathematically. This is particularly important in the case of global optimization as the solution of different mathematically equivalent formulations may pose very different computational requirements. Based on the concept of *reduction constraints* (see section 3), we present a graph-theoretical algorithm which automatically reformulates large sparse nonconvex NLPs involving linear constraints and bilinear terms. It is shown that the resulting exact reformulations involve fewer bilinear terms and have tighter convex relaxations than the original NLPs. Numerical results illustrating the beneficial effects of applying such automatic reformulations to the well-known pooling and blending problem are presented.

All sBB algorithms rely on the construction of a convex relaxation of the original NLP problem. Relatively tight convex relaxations are known for many categories of algebraic expressions. One notable exception is that of monomials of odd degree, i.e. expressions of the form $x^{2n+1}$ where $n \geq 1$, when the range of the variable $x$ includes zero. These occur often (e.g. as cubic or quintic expressions) in practical applications. The thesis presents a novel method for constructing the convex envelope of such monomials, as well as a tight linear relaxation of this envelope.

Finally, the thesis discusses some of the software engineering issues involved in the design and implementation of codes for sBB, especially in view of the large amounts of both symbolic and numerical information required by these codes. A prototype object-oriented software library, $oo\mathcal{OPS}$, is described.

## 2 Thesis contents

In Chapter 1 we give the basic definitions related to nonlinear programming, we explain the goals of the research, we discuss the history of global optimization, and finally describe the theoretical framework of sBB algorithms and their convergence properties. Chapter 2 is an extensive literature review on reformulation techniques for NLPs in general form $\min\{f(x) | l \leq \mathbf{g}(x) \leq u, x^L \leq x \leq x^U\}$, where $f, \mathbf{g}$ may be nonconvex, $l, u \in \mathbb{R}^m$, $x, x^L, x^U \in \mathbb{R}^n$. Chapter 3 focuses on the most important contribution of this thesis, namely *reduction constraints*. These are used to replace bilinear terms with linear constraints in a wide class of NLPs. Reduction constraints can be generated very efficiently by using an algorithm based on bipartite matching. Computational experiments on blending and pooling problems show that reduction constraints can help reduce computational times by as many as 5 orders of magnitude. In Chapter 4 we discuss a novel convex envelope for monomials of odd degree, and some of its mathematical properties. Chapter 5 discusses the sBB algorithm with symbolic reformulation as described in Smith and

Pantelides (1999), introduces some improvements, and describes an implementation within the optimization software framework *oo$\mathcal{OPS}$* (whose reference manual is found in the Appendix). We give some concluding remarks in chapter 6. Unfortunately, the *oo$\mathcal{OPS}$* library cannot be freely distributed as the distributing rights belong to Imperial College (contact the author for further information).

## 3 Reduction constraints

For lack of space, we have to limit this discussion to just one of the key aspects of this thesis: namely, the theory of reduction constraints. These provide an exact reformulation for generalized bilinear problems where some of the bilinear terms are replaced by linear constraints (with the resulting convex relaxation being therefore much tighter).

Consider the *generalized bilinear problem*:

$$\min\{x^T Qx + f(x) \mid Ax = b, x \in X \subseteq \mathbb{R}^n\} \tag{3.1}$$

where $Q$ is $n \times n$ upper-triangular matrix, $f$ is a function $\mathbb{R}^n \to \mathbb{R}$, $A$ is an $m \times n$ matrix with full rank $m$, and $b \in \mathbb{R}^m$. By substituting each bilinear term $x_i x_j$ with a linearizing variable $w_i^j$ we obtain an exact reformulation:

$$\left.\begin{array}{rr} \displaystyle\min_{x\in X} & p^T w + f(x) \\ & Ax = b \\ \forall i \le j \le n & w_i^j = x_i x_j. \end{array}\right\} \tag{3.2}$$

for a suitable constant vector $p \in \mathbb{R}^{\frac{1}{2}n(n+1)}$. Multiply the system $Ax = b$ by each problem variable $x_k$ to obtain the following *reduction constraint system*:

$$\forall k \le n \ (Aw_k - bx_k = 0), \tag{3.3}$$

where $w_k = (w_k^1, \ldots, w_k^n)^T$. Substitute $b = Ax$ in (3.3) to obtain:

$$\forall k \le n \ (A(w_k - x_k x) = 0);$$

now substitute $z_i^j = w_i^j - x_i x_j$ for all $i \le j \le n$ to get the following *companion system*:

$$\forall k \le n \ (Az_k = 0), \tag{3.4}$$

where $z_k = (z_k^1, \ldots, z_k^n)^T$. System (3.4) can be written as $Mz = 0$ for a suitable matrix $M$ ($z$ is the vector of all $z_i^j$ for $i \le j \le n$). Partition $z$ in a set $B$ and $N$ of basic and nonbasic variables w.r.t. system $Mz = 0$. By setting all the nonbasic variables to zero, for $Mz = 0$ to hold, the basic variables must also be zero. Thus, by setting $w_i^j = x_i x_j$ for all $(i, j)$ such that $z_i^j \in N$, the reduction constraint system (3.3) implies that $w_i^j = x_i x_j$ for all

$(i, j)$ such that $z_i^j \in B$. In other words, the system (3.3) of linear equations replaces those bilinear constraints in (3.2) corresponding to basic variables of system (3.4). Thus, the following reformulation of (3.1), involving more linear constraints but less bilinear terms than the original problem, is exact:

$$\left.\begin{array}{rr} \min\limits_{x \in X} & p^T w + f(x) \\ & Ax = b \\ \forall k \leq n & Aw_k - bx_k = 0 \\ \forall (i,j) : z_i^j \in N & w_i^j = x_i x_j . \end{array}\right\} \tag{3.5}$$

Whilst the idea of multiplying linear constraints by problem variables is not new (Sherali and Alameddine, 1992), the analysis that shows the reduction in the number of bilinear terms is, to the best of our knowledge, completely original.

## References

H. Sherali and A. Alameddine (1992). A new reformulation-linearization technique for bilinear programming problems. *Journal of Global Optimization*, 2:379–410.

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