Automatic Reformulation of Bilinear MINLPs

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1 Introduction

We show how to derive tight convex relaxations of Mixed-Integer Nonlinear Programming problems (MINLPs) involving bilinear terms and linear equation constraints. This is crucial for the efficiency of Branch-and-Bound algorithms. Such MINLPs occur frequently in many application fields, ranging from engineering [1] to graph theory [2]. Our method identifies a subset of Reformulation-Linearization Technique (RLT) constraints [8] which are shown to reformulate the problem exactly.

2 Reduction constraints

We first linearize the original problem so that each nonlinear term $g(x)$ (where x is a vector of n variables) is substituted by a *linearizing variable* w, and a corresponding *defining constraint* $w = g(x)$ is added to the formulation [9]. Secondly, we consider multiplying the set of linear equality constraints $\sum_{j=1}^{n} a_{ij}x_j = b_i$ $(i \in I)$ by a subset of problem variables x_k $(k \in K)$. We choose I and K such that the products create the least possible number of new bilinear terms [6]. Next, we replace the terms $x_j x_k$ by their linearizing variables w_{jk}, obtaining a system of linear equality constraints $\forall i \in I, k \in K$ $\sum_{j=1}^{n} a_{ij}w_{jk} = b_i x_k$ called *reduction constraints*, also written as :

$$\forall k \in K \;\; Aw_k - x_k b = 0, \tag{1}$$

where $Ax = b$ is the set of linear equations indexed by I and $w_k = (w_{1k}, \dots, w_{nk})$. Replacing $b = Ax$ yields $\forall k \in K$ $A(w_k - x_k x) = 0$. If we now define $z_{jk} = w_{jk} - x_j x_k$ for $j \leq n$ and $z_k = (z_{1k}, \dots, z_{nk})$, we can see that (1) is equivalent to

$$\forall k \in K \;\; Az_k = 0. \tag{2}$$

Let B, N be sets of index pairs such that z_{jk} is basic for (2) if $(j, k) \in B$ nonbasic if $(j, k) \in N$. Since (2) is homogeneous, setting $z_{jk} = 0$ for all $(j, k) \in N$ yields necessarily $z_{jk} = 0$ for all $j \in I, k \in K$. By definition of z_{jk}, this means that if we impose the bilinear defining constraints $w_{jk} = x_j x_k$ for $(j, k) \in N$ and system (1), the defining constraints indexed by B are implied automatically. Thus, the problem can be reformulated exactly to a form with more linear constraints (1) and fewer bilinear defining constraints. Since the convex relaxation only affects the nonconvex terms, fewer terms are relaxed in the reformulated problem. Consequently, the relaxation is likely to be tighter.

3 Reducing the convexity gap

For most linear systems (2) the partition B, N in basics/nonbasics is not unique. Consider a function $f : X \subseteq \mathbb{R}^n \to \mathbb{R}$ with convex lower bounding function $\underline{f}(x)$ and concave upper bounding function $\bar{f}(x)$. Then the set $\bar{S} = \{(x,w) \mid x \in X \wedge \underline{f}(x) \leq w \leq \bar{f}(x)\}$ is a convex relaxation of the set $S = \{(x,w) \mid x \in X \wedge w = f(x)\}$. We define the *convexity gap* o be the volume $\int_{x \in X} (\bar{f}(x) - \underline{f}(x))dx$ of the set $\bar{S}$. Let V_{jk} be the convexity gap of $x_j x_k$. It is possible to show that V_{jk} is a monotonically increasing function of the variable range sizes $x_j^U - x_j^L, x_k^U - x_k^L$. By Sect. 2, only the terms indexed by N are actually relaxed. Thus, we want to choose B, N such that $\sum_{(j,k) \in N} V_{jk}$ is minimum, or equivalently such that $\sum_{\{j,k\} \in B} V_{jk}$ is maximum. This problem has a matroidal structure, since it reduces to finding sets of linearly independent weighted columns of B. Thus, its solution is achieved by a simple greedy algorithm.

4 Applications

We implemented a spatial Branch-and-Bound for nonconvex NLPs based on the above ideas, and applied it to Pooling and Blending problems (PBPs) [7] with considerable success. The method has also been used in an application to Quantum Chemistry [4]. Furthermore, the ideas in this paper gave rise to a compact formulation for bilinear 0-1 programs [5] as well as an application to a scheduling problem [3].

Références

1. N. Adhya, M. Tawarmalani, and N.V. Sahinidis. A lagrangian approach to the pooling problem. *Industrial and Engineering Chemistry Research*, 38 :1956–1972, 1999.
2. I. Bomze, M. Budinich, P.M. Pardalos, and M. Pelillo. The maximum clique problem. In D.-Z. Du and P.M. Pardalos, editors, *Handbook of Combinatorial Optimization, Supp. A*, volume supp. A, pages 1–74, Dordrecht, 1998. Kluwer Academic Publishers.
3. T. Davidović, L. Liberti, N. Maculan, and N. Mladenović. Mathematical programming-based approach to scheduling of communicating tasks. *Cahiers de GERAD*, G-2004-99, December 2004.
4. C. Lavor, L. Liberti, N. Maculan, and M.A. Chaer Nascimento. Solving a quantum chemistry problem with deterministic global optimization. `www.optimization-online.org`, 2005.
5. L. Liberti. Compact linearization for bilinear mixed-integer problems. `www.optimization-online.org`, May 2005.
6. L. Liberti. Linearity embedded in nonconvex programs. *Journal of Global Optimization*, 33(2) :157–196, 2005.
7. L. Liberti and C.C. Pantelides. An exact reformulation algorithm for large nonconvex NLPs involving bilinear terms. *Journal of Global Optimization*, (submitted).
8. H.D. Sherali and A. Alameddine. A new reformulation-linearization technique for bilinear programming problems. *Journal of Global Optimization*, 2 :379–410, 1992.
9. E.M.B. Smith and C.C. Pantelides. A symbolic reformulation/spatial branch-and-bound algorithm for the global optimisation of nonconvex MINLPs. *Computers & Chemical Engineering*, 23 :457–478, 1999.