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A fast branch-and-bound algorithm for non-convex quadratic integer optimization subject to linear constraints using ellipsoidal relaxations

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ABSTRACT

We propose two exact approaches for non-convex quadratic integer minimization subject to linear constraints where lower bounds are computed by considering ellipsoidal relaxations of the feasible set. In the first approach, we intersect the ellipsoids with the feasible linear subspace. In the second approach we penalize exactly the linear constraints. We investigate the connection between both approaches theoretically. Experimental results show that the penalty approach significantly outperforms CPLEX on problems with small or medium size variable domains.

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1. Introduction

We address quadratic integer optimization problems with box constraints and linear equality constraints,

$$\begin{aligned} \min\ & q(x) = x^\top Qx + c^\top x \\ \text{s.t.}\ & Ax = b \\ & l \le x \le u \\ & x \in \mathbb{Z}^n, \end{aligned} \tag{1}$$

where $Q \in \mathbb{R}^{n\times n}$ is assumed to be symmetric but not necessarily positive semidefinite, $c \in \mathbb{R}^n$, and w.l.o.g. $A \in \mathbb{Z}^{m\times n}$ and $b \in \mathbb{Z}^m$. Moreover, we may assume $l < u$ and $l, u \in \mathbb{Z}^n$. Problems of this type arise, e.g., in quadratic min cost flow problems, where the linear equations model flow conservation, $l = 0$ and u represents edge capacities. Note that we can also handle linear inequalities in (1) by simply introducing slack variables.

Problems of type (1) are very hard to solve in theory and in practice. In general, the problem is NP-hard both due to the integrality constraints and due to the non-convexity of the objective function. Few exact algorithms have been proposed in the literature so far, most of them based on either linearization or convexification [1,9] or on SDP-relaxations [3].

For the variant of (1) containing only box constraints, but no other linear constraints, Buchheim et al. [2] recently proposed a branch-and-bound algorithm based on ellipsoidal relaxations of the feasible box. More precisely, a suitable ellipsoid E containing $[l, u]$ is determined and $q(x)$ is minimized over $x \in E$.

The latter problem is known as the trust region subproblem [4,6,8] and can be solved efficiently, thus yielding a lower bound in our context. Besides many other improvements, this branch-and-bound algorithm mostly relies on an intelligent preprocessing technique that allows to solve the dual of a trust region problem in each node of the enumeration tree in a very short time, making it possible to enumerate millions of nodes in less than a minute.

Our aim is to adapt this method to the presence of linear equations $Ax = b$. For this, we propose two different, but related approaches. In the first approach (see Section 2), we intersect the ellipsoid E with the subspace given by $Ax = b$. This leads, by considering an appropriate projection, to a trust region type problem that, in principle, can still be solved efficiently. In the second approach (see Section 3), we instead lift the constraints into the objective function by adding a penalty term $M\|Ax - b\|^2$ drawing inspiration from the augmented Lagrangians theory [7]. A finite and computable real value $\bar{M} > 0$ exists such that the resulting quadratic problem with only the simple constraints $[l, u] \cap \mathbb{Z}^n$ is equivalent to (1). Thus the branch-and-bound algorithm defined in [2] which uses an ellipsoidal relaxation E of the feasible set can be used in a straightforward way.

In Section 4, we show that the bound obtained from the penalty approach converges to the bound obtained in the projection approach when $M \to \infty$. We finally present the results of an

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experimental comparison of the penalty approach with CPLEX, see Section 5.

2. Projection approach

The first approach we propose for the computation of lower bounds for Problem (1) is based on the familiar partitioning of x into basic and non-basic variables x_B and x_N. Without loss of generality we assume that $\operatorname{rank}(A) = m$. Let B be a basis of A, then the equality constraint can be written as $Bx_B + Nx_N = b$; a similar idea is used, e.g., in [10]. This leads to a k-dimensional trust region type problem, where $k = n - m$ is the dimension of the kernel of the matrix A.

Let H be a positive definite matrix that, together with the center point x^0, defines an ellipsoid

$$E(H) = \{x \in \mathbb{R}^n \mid (x - x^0)^\top H(x - x^0) \le 1\}$$

such that $[l, u] \subseteq E(H)$. Consider the following relaxation of our original problem (1)

$$\begin{aligned} \min\ & q(x) = x^\top Qx + c^\top x \\ \text{s.t.}\ & Ax = b \\ & x^\top Hx \le 1 \end{aligned} \tag{2}$$

where w.l.o.g. we assumed $x^0 = 0$. We show that Problem (2) can be transformed into a trust-region type problem so that the branch-and-bound algorithm defined in [2] can be applied. Let us write vectors and matrices accordingly to the partition induced by B and N. Thus, the x_B variables can be eliminated via substituting

$$x_B = B^{-1}b - B^{-1}Nx_N$$

in (2). We obtain

$$\begin{aligned} \min\ & x_N^\top \widetilde{Q} x_N + \widehat{c}^\top x_N + d \\ \text{s.t.}\ & x_N^\top \widetilde{H} x_N + \widetilde{h}^\top x_N \le 1 - b^\top B^{-\top} H_{BB} B^{-1} b \\ & x_N \in \mathbb{R}^k, \end{aligned} \tag{3}$$

where

$$\begin{aligned} \widetilde{Q} &= Q_{NN} + N^\top B^{-\top} Q_{BB} B^{-1} N - Q_{BN}^\top B^{-1} N - N^\top B^{-\top} Q_{BN} \\ \widehat{c} &= 2(-N^\top B^{-\top} Q_{BB} B^{-1} + Q_{NB} B^{-1}) b - (B^{-1}N)^\top c_B + c_N \\ d &= b^\top B^{-\top} Q_{BB} B^{-1} b + c_B^\top B^{-1} b \\ \widetilde{H} &= H_{NN} + N^\top B^{-\top} H_{BB} B^{-1} N - H_{NB} B^{-1} N - N^\top B^{-\top} H_{BN} \\ \widetilde{h} &= 2\left(-N^\top B^{-\top} H_{BB} B^{-1} + H_{NB} B^{-1}\right) b. \end{aligned}$$

Let

$$x_N^0 = -\frac{1}{2}\widetilde{H}^{-1}\widetilde{h}$$

be the center of the ellipsoidal constraint in problem (3). Then we can rewrite Problem (3) as

$$\begin{aligned} \min\ & x_N^\top \widetilde{Q} x_N + \widehat{c}^\top x_N + d \\ \text{s.t.}\ & (x_N - x_N^0)^\top \widetilde{H} (x_N - x_N^0) \le \alpha \\ & x_N \in \mathbb{R}^k, \end{aligned}$$

where

$$\alpha = 1 - b^\top B^{-\top} H_{BB} B^{-1} b + \frac{1}{4}\widetilde{h}^\top \widetilde{H}^{-1}\widetilde{h}.$$

Next we consider the transformation $z = x_N - x_N^0$ and obtain the following problem which is exactly of the desired form

$$\begin{aligned} \min\ & z^\top \widetilde{Q} z + \widetilde{c}^\top z + \widetilde{d} \\ \text{s.t.}\ & z^\top \widetilde{H} z \le \alpha \\ & z \in \mathbb{R}^k, \end{aligned} \tag{4}$$

where

$$\begin{aligned} \widetilde{c} &= 2\widetilde{Q} x_N^0 + \widehat{c}, \\ \widetilde{d} &= \widehat{c}^\top x_N^0 + (x_N^0)^\top \widetilde{Q} x_N^0 + d. \end{aligned}$$

This approach can be embedded into the branch-and-bound procedure proposed in [2], where the enumeration strategy is depth-first and branching is done by fixing the value of the variables in a predetermined order. By the latter restriction, we ensure that the matrices $\widetilde{Q}$ and $\widetilde{H}$ only depend on the depth of the node in the branch-and-bound tree, i.e., on which variables have been fixed so far, but not on their values: first, a basis B^0 of A can be computed in the preprocessing phase. By always fixing non-basic variables, we get at each level $\ell = 0, \ldots, n-m$ that a basis of A^ℓ (the reduced matrix A indexed by only non-fixed variables) is $B^\ell = B^0$, whereas N^ℓ is obtained by simply removing columns from N^0. When all non-basic variables have been fixed to $\bar{x}_N$, then the corresponding node is a leaf and either $\bar{x}_B := (B^\ell)^{-1}b - B^{-1}N^\ell \bar{x}_N \in \mathbb{Z}^m$ or the node is infeasible.

Now the matrices $\widetilde{Q}$ and $\widetilde{H}$ in a given node of the branch-and-bound tree depend only on Q^ℓ, H^ℓ, B^ℓ, and N^ℓ, where Q^ℓ and H^ℓ denote the reduced matrices Q and H on level ℓ, which in turn depend only on the ordering of variables and not on the fixings of variables and hence they are shared by all the nodes at level ℓ. This implies that only n different matrices $\widetilde{Q}^\ell$ and $\widetilde{H}^\ell$ appear in the entire branch-and-bound tree, so that, similarly to [2], all time-consuming calculations concerning $\widetilde{Q}^\ell$ and $\widetilde{H}^\ell$ can be performed in a preprocessing phase.

On the other hand, the construction of problem (4) at every node of the branch-and-bound tree requires the computation of $\widetilde{c}, \widetilde{d}, \widetilde{h}$, and α, which in turn depends on the values at which the variables have been fixed, as the right hand side term b is affected by the fixings. These vectors can however be updated quickly in an incremental fashion.

As a final remark, we want to point out that it is also possible to use the kernel representation of the equality constraints as $\{x \in \mathbb{R}^n \mid Ax = b\} = \{x \in \mathbb{R}^n \mid x = Vy + w,\ y \in \mathbb{R}^k\}$, where $V \in \mathbb{R}^{n\times k}$ is an orthonormal matrix defining a basis for $\ker(A)$ and $w \in \mathbb{R}^n$ is any vector satisfying $Aw = b$. By substituting x by $Vy + w$ in (2) and by further manipulations of the expressions, we get again a trust region type problem. The main difference between the two approaches consists in the computations needed to define the trust region relaxation at each node of the branch-and-bound tree, but the resulting bounds both agree with (2) and are hence the same.

3. Penalty approach

In the second approach we take inspiration from an old idea based on Lagrangian relaxation, in which the squared violation of linear constraints $\|Ax - b\|^2$ is lifted to the quadratic objective function (see [7] and references therein). Indeed Poljak et al. [7] prove the existence of a value $\bar{M}$ such that problem (1) is equivalent to

$$\min_{x\in X} q(x) + M\|Ax - b\|^2 \quad \text{for all } M \ge \bar{M}$$

whenever X is a finite set. In the following we explain how to obtain a finite value of $\bar{M}$ for which this equivalence holds.

More generally, consider the problem

$$\begin{aligned} q(x^*) = \min\ & q(x) = x^\top Qx + c^\top x \\ \text{s.t.}\ & x \in \mathcal{F} \cap X \end{aligned} \tag{5}$$

where $X \subseteq \mathbb{R}^n$ is again a finite set and $\mathcal{F} \subseteq \mathbb{R}^n$ is arbitrary. Let $d_{\mathcal{F}}(x) : \mathbb{R}^n \to \mathbb{R}_0^+$ be a function such that

$$\begin{aligned} d_{\mathcal{F}}(x) &= 0 \quad \text{if } x \in \mathcal{F}; \\ d_{\mathcal{F}}(x) &> 0 \quad \text{otherwise}. \end{aligned}$$

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