A Finite Algorithm for Solving General Quadratic Problems

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Abstract. Here we propose a global optimization method for general, i.e. indefinite quadratic problems, which consist of maximizing a non-concave quadratic function over a polyhedron in n-dimensional Euclidean space. This algorithm is shown to be finite and exact in non-degenerate situations. The key procedure uses copositivity arguments to ensure escaping from inefficient local solutions. A similar approach is used to generate an improving feasible point, if the starting point is not the global solution, irrespective of whether or not this is a local solution. Also, definiteness properties of the quadratic objective function are irrelevant for this procedure. To increase efficiency of these methods, we employ pseudoconvexity arguments. Pseudoconvexity is related to copositivity in a way which might be helpful to check this property efficiently even beyond the scope of the cases considered here.

Key words. Copositivity, global optimization, indefinite quadratic problems, pseudoconvexity.

1. Introduction

Indefinite quadratic problems consist of maximizing a non-concave quadratic function over a polyhedron in n-dimensional Euclidean space $\mathbb{R}^n$. They arise in different fields of applications from combinatorial optimization to database problems and VLSI design. The solution of problems of this type is, from the perspective of worst-case complexity, NP-hard [17]; even checking whether a given feasible point is a local solution is also NP-hard [13], [16]. Pardalos [14] pointed out that there is in general no local criterion for global optimality. As an example to illustrate this observation, he chose the convex maximization problem

$$\sum_{j=1}^{n} \left(\tfrac{1}{2}x_j + x_j^2\right) \to \max! \quad \text{subject to} \quad -1 \leq x_i \leq 1\,, \quad 1 \leq i \leq n\,, \tag{1.1}$$

which has 3^n Karush–Kuhn–Tucker points and 2^n local maxima.

A finite algorithm for finding the global maximum of a convex quadratic function over a polyhedron is specified in [3]. This procedure is based on an optimality criterion derived by means of ε-subdifferential calculus (see [8], [9]). However, it has been shown recently [2] that there is a similar criterion also for indefinite quadratic problems. Based upon this result, we develop in this paper a procedure that essentially enables escaping inefficient local maxima. Furthermore, we propose an algorithm which delivers the exact global solution after a finite number of iterations.

The similarity between this algorithm and the algorithm given in [3] for the convex case consists primarily of using a procedure which checks copositivity of an $n \times n$-matrix Q with respect to a polyhedral cone $\Gamma \subseteq \mathbb{R}^n$. Recall that Q is said to be Γ-copositive if (v^T denoting transpose of v)

$$v^T Q v \geq 0 \quad \text{for all} \quad v \in \Gamma . \tag{1.2}$$

However, there is an essential difference between the convex and the indefinite cases. While in the former case the global maximum is attained at a vertex of the feasible set M, in the latter case the solution lies in the interior of a face of M. Hence, a global optimization procedure for indefinite problems cannot consist of an "efficient" search among vertices, e.g., by applying the simplex method to an approximate auxiliary linear program, as done in [3].

The paper is organized as follows: in Section 2, we start from an arbitrary feasible point and show how to obtain an improving feasible point from the criterion in [2], if the starting point is not the global solution, irrespective of whether or not it is a Karush–Kuhn–Tucker point. Also, definiteness properties of the quadratic objective function are irrelevant for this procedure. In Section 3, we employ pseudoconvexity arguments to increase efficiency of the methods developed in Section 2. Pseudoconvexity is related to copositivity in a way which might be helpful to check this property efficiently even beyond the scope of the cases considered here. In Section 4, we present a global optimization procedure which is shown to be finite and exact in nondegenerate situations. Here the nondegeneracy assumption is only needed to ensure finiteness of Lemke's algorithm, which is used as a subroutine in the proposed procedure. The method resembles in some sense the branch-and-bound procedures for global optimization described, e.g. in [10], using the very specific properties of quadratic functions and polytopes in an extensive way.

2. Escaping from Local Solutions

Consider the general quadratic maximization problem

$$g(x) = \tfrac{1}{2} x^T Q x + c^T x \rightarrow \max! \quad \text{subject to} \quad x \in M , \tag{2.1}$$

where

$$M = \{x \in \mathbb{R}^n : Ax \leq b\} . \tag{2.2}$$

Here Q is a symmetric $n \times n$-matrix; $c \in \mathbb{R}^n$; A is an $m \times n$-matrix; and $b \in \mathbb{R}^m$. For the sake of completeness, we recapitulate the characterization of optimality from [2]. To this end, we need some notation: consider a feasible point $\bar{x} \in M$, denote by

$$I(\bar{x}) = \{i \in (1, \ldots, m) : (A\bar{x})_i = b_i\} \tag{2.3}$$

the set of binding constraints at $\bar{x}$; and by

$$\Gamma = \{v \in \mathbb{R}^n : (Av)_i \leq 0 \text{ for all } i \in I(\bar{x})\} \tag{2.4}$$

the tangent cone of M at $\bar{x}$. The idea in [2] now is to proceed as follows:

(a) pick a feasible direction v at $\bar{x}$;

(b) consider the increment

$$\theta_v(\lambda) = g(\bar{x} + \lambda v) - g(\bar{x}) = \frac{v^T Q v}{2} \lambda^2 + v^T(Q\bar{x} + c)\lambda\,, \quad \lambda \geq 0\,; \tag{2.5}$$

(c) determine the extremal feasible point $\bar{x} + \lambda_v v$ on the ray given by v, i.e. the feasible point farthest away from $\bar{x}$ on that ray, and calculate the extremal increment $\theta_v(\lambda_v)$.

Due to polyhedrality of the feasible set M, the set of feasible directions coincides with the cone Γ defined in (2.4). Observe that $\bar{x}$ is a Karush–Kuhn–Tucker point if and only if $\bar{x}$ satisfies

$$\theta_v'(0) = v^T(Q\bar{x} + c) \leq 0 \quad \text{for all } v \in \Gamma\,. \tag{2.6}$$

It is a straightforward task to determine the extremal point on a ray given by a direction $v \in \Gamma$. If we define

$$z(v) = \begin{cases} \max[\{0\} \cup \{(Av)_i/u_i : i \notin I(\bar{x})\}]\,, & \text{if } v \in \Gamma\,, \\ +\infty\,, & \text{otherwise}\,, \end{cases} \tag{2.7}$$

where we denote by $u_i = b_i - (A\bar{x})_i > 0$ the slack variables at $\bar{x}$ for $i \notin I(\bar{x})$, then for $\lambda \geq 0$ we obtain in the case $z(v) > 0$ that

$$\bar{x} + \lambda v \in M \quad \text{if and only if} \quad \lambda \leq \lambda_v = 1/z(v)\,. \tag{2.8}$$

In this case ($z(v) > 0$) the intersection of M with the ray given by v is bounded and the extremal feasible point on this ray is given by $\bar{x} + \lambda_v v \in M$. So it only remains to calculate the extremal increment via (2.5), (2.7), and (2.8):

$$\theta_v(\lambda_v) = \frac{1}{2z^2(v)} [v^T Q v + 2v^T(Q\bar{x} + c)z(v)]\,. \tag{2.9}$$

Now $z(v)$ is a piecewise linear functional. To obtain linear expressions, we decompose Γ as follows: denote for $i \in \{1, \ldots, m\} \setminus I(\bar{x})$

$$\Gamma_i = \{v \in \Gamma : (Av)_i \geq 0 \text{ and } u_j(Av)_i \geq u_i(Av)_j \text{ for all } j \in \{1, \ldots, m\} \setminus I(\bar{x})\}\,, \tag{2.10}$$

then Γ_i is a polyhedral cone satisfying $\Gamma_i = \{v \in \Gamma : z(v) = (Av)_i/u_i\}$. Similarly,

$$\Gamma_0 = \{v \in \Gamma : (Av)_i \leq 0 \quad \text{for all} \quad i \in \{1, \ldots, m\} \setminus I(\bar{x})\} \tag{2.11}$$

is a polyhedral cone with $\Gamma_0 = \{v \in \mathbb{R}^n : Av \leq o\} = \{v \in \Gamma : z(v) = 0\}$. For a geometric interpretation of the cones Γ_i see Section 4 in [2].

The optimality condition specified below now uses Γ_i-copositivity of Q_i, where the symmetric $n \times n$-matrices Q_i are defined by

$$Q_i = \begin{cases} -Q\,, & \text{if} \quad i = 0\,, \\ B_i - u_i Q\,, & \text{otherwise}\,, \end{cases} \tag{2.12}$$

and

$$B_i = -a_i(Q\bar{x} + c)^T - (Q\bar{x} + c)(a_i)^T\,, \tag{2.13}$$

where $(a_i)^T$ denotes the i-th row of A. The following result is taken from [2].

THEOREM 1. *Let $\bar{x}$ be a feasible point of the problem* (2.1). *Define $I(\bar{x})$, Γ_i, and Q_i as in* (2.3), (2.10), (2.11), (2.12), *and* (2.13), *respectively. Then the following assertions are equivalent*:

(a) *$\bar{x}$ is a global solution to* (2.1);

(b) *$\bar{x}$ is a Karush–Kuhn–Tucker point of* (2.1) *and*

$$Q_i \text{ is } \Gamma_i\text{-copositive for all } i \in \{0, \ldots, m\} \setminus I(\bar{x})\,. \tag{2.14}$$

Proof. The preceding arguments prove that (a) implies (b), since if $\bar{x}$ is a global solution to (2.1), then the inequality $\theta_v(\lambda_v) \leq 0$ results and hence (in the case $z(v) > 0$) the condition

$$v^T Q v + 2v^T(Q\bar{x} + c)z(v) \leq 0 \quad \text{for all} \quad v \in \Gamma \tag{2.15}$$

holds. In the case of an unbounded ray of feasible points (where $z(v) = 0$), an improvement is impossible along this ray if and only if the leading coefficient $v^T Q v \leq 0$ (recall that in case of equality $v^T Q v = 0$, condition (2.6) ensures $\theta_v(\lambda) = v^T(Q\bar{x} + c)\lambda \leq 0$). Hence, in both cases we derive from global optimality of $\bar{x}$ condition (2.15), which can be rephrased into the set of copositivity properties (2.14).

It remains to show that (b) implies (a). To this end consider again at first the case $z(v) > 0$. The Karush–Kuhn–Tucker condition (2.6) guarantees $\theta'_v(0) \leq 0$. Therefore, since θ_v is a quadratic function in λ, it is evident that $\theta_v(\lambda) \leq 0$ holds for all $\lambda \in [0, \lambda_v]$ if and only if $\theta_v(\lambda_v) \leq 0$, i.e. (2.15) holds. This equivalence is valid irrespective of the sign of the leading coefficient $v^T Q v$. In case $z(v) = 0$, conditions (2.6) and (2.15) guarantee $\theta'_v(\lambda) = v^T Q v \lambda + v^T(Q\bar{x} + c) \leq 0$ for all $\lambda \geq 0$, so that we in both cases arrive at the property

$$\theta_v(\lambda) \leq 0 \quad \text{for all} \quad \lambda \geq 0 \quad \text{such that} \quad \bar{x} + \lambda v \in M\,.$$

Evidently $\bar{x}$ then is a global solution to (2.1). □

According to the above theorem, $\bar{x}$ is no global solution if either

- Case I: $\bar{x}$ is a Karush–Kuhn–Tucker point, but (2.14) is violated; or
- Case II: $\bar{x}$ is no Karush–Kuhn–Tucker point.

Since this section is devoted to the problem to escape from inefficient local solutions, we at first concentrate on Case I. However, for efficiency reasons it may pay also to deal with Case II, which we will do at the end of this section.

The main ingredient of the escape procedure described below is the copositivity algorithm COPOS from [3] addressed in the introduction, which (a) checks copositivity and (b) generates a direction v violating (1.2) in case of a negative answer. Note that there are several algorithms which achieve (a), see, e.g., [5], [11], [7], [6]. But, to our knowledge, the only one which also performs (b) is the algorithm given in [3].

ESCAPE ($\bar{x}$)

1. Initialization: if $\bar{x}$ is the first point investigated, call COPOS(Q_0, Γ_0); if the answer is negative, stop: the problem is unbounded from above (see (3.16) in [2]). Else $z(v) = 0$ implies $v^T Q_i v \geqslant 0$ for all $v \in \Gamma_i$;
2. for all $i \in \{1, \ldots, m\} \backslash I(\bar{x})$ call COPOS(Q_i, Γ_i); if a direction $v \in \Gamma_i$ with $v^T Q_i v < 0$ (and hence $z(v) > 0$) is generated, calculate the corresponding extremal increment (2.9), which equals
$$\theta_v(\lambda_v) = -\frac{u_i}{2[(Av)_i]^2} v^T Q_i v > 0 . \tag{2.16}$$
If no improvement is obtained in this way, i.e. if all Q_i are Γ_i-copositive, then stop: $\bar{x}$ is the global solution of (2.1).
3. Pick that index i and the corresponding direction v with maximal $\theta_v(\lambda_v)$. Put $\hat{x} = \bar{x} + \lambda_v v = \bar{x} + z(v)^{-1} v$. Then $\hat{x}$ is a feasible point with $g(\hat{x}) > g(\bar{x})$. Return.

Now let us deal with Case II, where there are also locally improving feasible directions available, i.e. $v \in \Gamma$ with $\theta_v'(0) = v^T(Q\bar{x} + c) > 0$, cf. (2.5). If θ_v happens to be strictly concave (i.e. if $v^T Q v < 0$), the extremal value of λ_v might yield a lower improvement (if any) than a λ interior to the interval $[0, \lambda_v]$. In this case, the global maximum of θ_v is attained at $\lambda = \mu_v$, where
$$\mu_v = -\frac{v^T(Q\bar{x} + c)}{v^T Q v} . \tag{2.17}$$

To be precise, one has to replace $\bar{x} + \lambda_v v$ with $\bar{x} + \mu_v v$ if (i) $v^T Q v < 0$ and (ii) $0 < \mu_v \leqslant \lambda_v$, to obtain the highest possible improvement along direction v. Observe that conditions (i) and (ii) can hold simultaneously only if $\bar{x}$ is no

Karush–Kuhn–Tucker point and g is not convex. This is the reason why for convex maximization, the algorithm in [3] cannot be improved in this way. Note further that under (i), the inequality $\mu_v \leqslant \lambda_v$ is equivalent to the piecewise quadratic inequality

$$v^T(Q\bar{x} + c)z(v) \leqslant -v^T Qv ,$$

which reduces to

$$v^T R_i v \geqslant 0 \quad \text{if} \quad v \in \Gamma_i , \tag{2.18}$$

where

$$R_i = B_i - 2u_i Q = Q_i - u_i Q . \tag{2.19}$$

Since the above reasoning makes sense only if $v^T(Q\bar{x} + c) \geqslant 0$, we decompose Γ_i as follows:

$$\begin{aligned} \Gamma^+ &= \{v \in \Gamma : v^T(Q\bar{x} + c) \geqslant 0\} , \\ \Gamma^- &= \{v \in \Gamma : v^T(Q\bar{x} + c) \leqslant 0\} . \end{aligned} \tag{2.20}$$

Then for $i \in \{1, \ldots, m\} \backslash I(\bar{x})$ let $\Gamma_i^\pm = \Gamma_i \cap \Gamma^\pm$.

To sum up, there are two ways to generate an improving feasible point $\hat{x}$, starting from $\bar{x}$ along a direction $v \in \Gamma_i$ (for the sake of completeness, we include also the case where no improvement along v is possible):

$$\hat{x} = \begin{cases} \bar{x} + \mu_v v , & \text{if} \quad v^T R_i v > 0 \quad \text{and} \quad v \in \Gamma_i^+ ; \\ \bar{x} + \lambda_v v , & \text{if} \quad v^T R_i v \leqslant 0 \quad \text{and} \quad v \in \Gamma_i^+ . \\ \bar{x} + \lambda_v v , & \text{if} \quad v^T Q_i v < 0 \quad \text{and} \quad v \in \Gamma_i^- ; \\ \bar{x} + 0v , & \text{if} \quad v^T Q_i v \geqslant 0 \quad \text{and} \quad v \in \Gamma_i^- . \end{cases} \tag{2.21}$$

In the first case (which always implies $v^T Qv < 0$), the resulting improvement is

$$g(\hat{x}) - g(\bar{x}) = \theta_v(\mu_v) = -\frac{[v^T(Q\bar{x} + c)]^2}{2v^T Qv} . \tag{2.22}$$

Note that the curvature of θ_v influences the distinction among the above case only indirectly.

To avoid superfluous calls of $\mathtt{COPOS}(-R_i, \Gamma_i^+)$, it is reasonable to call first $\mathtt{COPOS}(Q, \Gamma^+)$ because the first case in (2.21) cannot pertain if Q is Γ^+-copositive (cf. Section 3 below). Hence, we propose the following improvement procedure:

$\mathtt{IMPR}(\bar{x})$

1. *Initialization step*: *if* $\bar{x}$ is the first point investigated, call COPOS(Q_0, Γ_0); if the answer is negative, stop: the problem is unbounded from above.
2. Check whether $\bar{x}$ is a Karush–Kuhn–Tucker point or not by applying the simplex method to the linear program

$$v^T(Q\bar{x} + c) \rightarrow \max! \quad \text{subject to} \quad v \in \Gamma . \tag{2.23}$$

   If the optimal objective value of (2.23) is zero, then $\bar{x}$ is a Karush–Kuhn–Tucker point; call ESCAPE($\bar{x}$) and return. Else (2.23) is unbounded. Store a direction $v \in \Gamma$ with $v^T(Q\bar{x} + c) > 0$.
3. Select those i such that $v \in \Gamma_i^+$, i.e. $z(v) = (Av)_i/u_i$, and set

$$\operatorname{imp}(v) = \begin{cases} \theta_v(\mu_v), & \text{if} \quad v^T R_i v > 0, \\ \theta_v(\lambda_v), & \text{if} \quad v^T R_i v \leq 0. \end{cases}$$

4. Call COPOS(Q, Γ^+); if a direction $w \in \Gamma^+$ is generated such that $w^T Q w < 0$, repeat step 3, replacing v with w, and then go to the next step. Else (Q is Γ^+-copositive) skip the next step.
5. For all $j \in \{1, \dots, m\} \backslash I(\bar{x})$ call COPOS($-R_j, \Gamma_j^+$); if a direction $v_j \in \Gamma_j^+$ with $v_j^T R_j v_j > 0$ (and hence $v_j^T Q v_j < 0$) is generated, calculate the corresponding improvement

$$\operatorname{imp}(v_j) = \theta_{v_j}(\mu_{v_j}) .$$

6. For all $j \in \{1, \dots, m\} \backslash I(\bar{x})$ call COPOS(Q_j, Γ_j^-); if a direction $w_j \in \Gamma_j^-$ with $w_j^T Q_j w_j < 0$ is generated, calculate the corresponding improvement

$$\operatorname{imp}(w_j) = \theta_{w_j}(\lambda_{w_j}) .$$

7. Pick that direction, v, or w, or v_j, or w_j, which yields the maximal improvement. Determine $\hat{x}$ according to (2.21). Return.

Observe that steps 4 through 6 above merely serve to improve the objective function additionally. Hence one even could do without them in order to decrease computational cost, or, e.g., include only step 4 etc.

3. Using Pseudoconvexity to Improve Efficiency

Closer inspection of procedure IMPR reveals that in some cases, steps 4 through 6 might yield no further improving feasible direction, so that the only improvement one gets is from step 3. On the other hand, the additional (affirmative) copositivity information obtained in these cases can be used to refine the procedure considerably. To this end we first characterize pseudoconvexity by means of copositivity: recall that a function $g : \mathbb{R}^n \to \mathbb{R}$ is said to be pseudoconvex at $\bar{x} \in \mathbb{R}^n$ with respect to a set $S \subseteq \mathbb{R}^n$ if for any $x \in S$ (∇ denoting the gradient),

$$(x - \bar{x})^T \nabla g(\bar{x}) \geq 0 \quad \text{implies} \quad g(x) \geq g(\bar{x}) . \tag{3.1}$$

A quadratic function $g(x) = \frac{1}{2}x^T Qx + c^T x$ is pseudoconvex at $\bar{x}$ w.r.t. $\mathbb{R}^n$ as a whole if and only if Q is positive semidefinite, i.e., if g is convex. See, e.g. ([12] pp. 147, 152), where the case $S = \mathbb{R}^n$ and $S = \mathbb{R}^n_+$ are treated. Both cases are of restricted interest here as we are dealing with constrained problems, i.e. with the case $S \subseteq M$.

THEOREM 2. *Let* g, M, Γ_i, R_i *and* Γ_i^+ *be as in* (2.1), (2.2), (2.10), (2.19), *and* (2.20), *respectively. Define* $M_i = \{x \in M : x - \bar{x} \in \Gamma_i\}$. *Then*

(a) *g is pseudoconvex at $\bar{x}$ w.r.t. M_i if and only if*

$$-Q_i \text{ is } \Gamma_i^+\text{-copositive} .$$

(b) *If $-R_i$ is Γ_i^+-copositive, then g is pseudoconvex at $\bar{x}$ w.r.t. M_i.*

(c) *If Q is Γ^+-copositive, then g is pseudoconvex at $\bar{x}$ w.r.t. M.*

Proof. (a) First observe that for $S = M_i$, condition (3.1) is equivalent to

$$\theta_v(\lambda) \geq 0 \quad \text{for all} \quad \lambda \in [0, \lambda_v] \quad \text{if} \quad v \in \Gamma_i^+ . \tag{3.2}$$

Indeed, any $x \in M_i$ with $(x - \bar{x})^T \nabla g(\bar{x}) = (x - \bar{x})^T (Q\bar{x} + c) \geq 0$ gives rise to a direction $v \in \Gamma_i^+$ and vice versa. Moreover, a number $\lambda \geq 0$ satisfies $\bar{x} + \lambda v \in M$ if and only if $\lambda \in [0, \lambda_v]$. Hence (3.1) implies (3.2) by definition (2.5). But positivity of θ_v over the interval $[0, \lambda_v]$ is guaranteed if

$$v^T Qv \geq 0$$

or if

$$v^T Qv < 0 \quad \text{and} \quad \lambda_v \leq -\frac{2v^T(Q\bar{x} + c)}{v^T Qv} .$$

As in Section 2, the latter inequality is easily seen to be equivalent to $v^T Q_i v \leq 0$, provided $v^T Qv < 0$. On the other hand, $v^T Qv \geq 0$ entails for any $v \in \Gamma_i^+$ the relation $v^T Q_i v \leq 0$.

(b) follows easily from $-Q_i = -R_i - u_i Q$ and from the above arguments. (c) is obtained in a similar way. □

Hence if in steps 4 (or 5) of IMPR no improving directions w or v_j are generated, we know from Theorem 2 that any direction $w \in \Gamma^+$ (or $v_j \in \Gamma_j^+$) yields an improvement. This knowledge may be exploited, e.g., by applying Lemke's complementary pivoting algorithm to the reduced problem

$$g(x) \to \max! \quad \text{subject to} \quad x \in M^+ , \tag{3.3}$$

where $M^+ = \{x \in M : (x - \bar{x})^T(Q\bar{x} + c) \geq 0\}$. If every basic feasible solution of M^+ is non-degenerate, Lemke's algorithm after finitely many iterations either (i) generates a Karush–Kuhn–Tucker point of problem (3.3), or (ii) terminates with the information that (3.3) is unbounded from above, provided that the matrix $-Q$ is copositive-plus ([1] p. 446). This property means that (a) $-Q$ is $\mathbb{R}^n_+$-copositive; and that (b) $v^TQv = 0$ and $v \in \mathbb{R}^n_+$ imply $Qv = 0$. Of course, the same assertions hold mutatis mutandis for the problems

$$g(x) \to \max! \quad \text{subject to} \quad x \in M_j^+ , \tag{3.4}$$

where $M_j^+ = M_j \cap M^+$. We now show how to transform problems (3.3) and (3.4) to validate these properties of Q.

THEOREM 3. *Let Q be a symmetric $n \times n$-matrix with eigenvalues $\lambda_1 \leq \cdots \leq \lambda_n$ and corresponding orthonormal eigenvectors $q_1, \ldots, q_n$. Assume that $\lambda_k < 0 \leq \lambda_{k+1}$ holds for some $k \in \{1, \ldots, n-1\}$, and that $\lambda_n > 0$, which means that Q is indefinite. Form the basis $b_1, \ldots, b_n$ as follows*:

$$b_i = \begin{cases} q_i , & \text{if } i \leq k , \\ q_k + \delta q_i , & \text{else} , \end{cases}$$

where $\delta = \sqrt{|\lambda_k|/2\lambda_n}$. Let B be the regular $n \times n$-matrix consisting of the columns b_i. Then

(a) *the $n \times n$-matrix $-B^TQB$ is copositive-plus*;

(b) *the point x is a Karush–Kuhn–Tucker point of problem* (3.3) *if and only if the point y is a Karush–Kuhn–Tucker point of the problem*

$$\begin{aligned} &\tfrac{1}{2} y^T(B^TQB)y + (Bc)^Ty \to \max! \\ &\qquad (AB)y \leq b \\ &-(Q\bar{x} + c)^TBy \leq -(Q\bar{x} + c)^T\bar{x} \end{aligned} \tag{3.5}$$

Similarly, (3.3) *is unbounded from above if and only if* (3.5) *is unbounded from above.*

Proof. (a) By construction of b_i, we get for $y = [\alpha_1, \ldots, \alpha_n]^T \in \mathbb{R}^n_+$

$$
\begin{aligned}
y^T B^T Q B y &= \sum_{i=1}^{n} \alpha_i (b_i)^T \left[\sum_{j=1}^{k} \alpha_j \lambda_j q_j + \sum_{j>k} \alpha_j (\lambda_k q_k + \lambda_j \delta q_j) \right] \\
&= \sum_{i=1}^{k} (\alpha_i)^2 \lambda_i + \Big(\sum_{i>k} \alpha_i \Big)^2 \lambda_k + \delta^2 \sum_{i>k} (\alpha_i)^2 \lambda_i \\
&\leqslant \sum_{i=1}^{k} (\alpha_i)^2 \lambda_i + 2 \sum_{i>j>k} \alpha_i \alpha_j \lambda_k + \sum_{i>k} (\alpha_i)^2 \lambda_k + \delta^2 \sum_{i>k} (\alpha_i)^2 \lambda_n \\
&\leqslant \sum_{i=1}^{k} (\alpha_i)^2 \lambda_i + \sum_{i>j>k} \alpha_i \alpha_j \lambda_k + \frac{1}{2} \sum_{i>k} (\alpha_i)^2 \lambda_k \\
&= \sum_{i=1}^{k} (\alpha_i)^2 \lambda_i + \frac{1}{2} \Big(\sum_{i>k} \alpha_i \Big)^2 \lambda_k \leqslant 0
\end{aligned}
$$

with equality only if $y = o$. Hence assertion (a) follows.

(b) is an easy consequence of the fact that the map $y \mapsto x = By$ is invertible. □

To sum up, we start with the following preprocessing procedure, in which we also incorporate the initialization steps from ESCAPE and IMPR:

PREPROC

1. Diagonalize Q. If Q is positive semidefinite, apply the algorithm in [3] and stop. If Q is negative semidefinite, we have a convex minimization problem, where every Karush–Kuhn–Tucker point delivers a solution. Apply, e.g., Lemke's algorithm to problem (2.1) and stop. Else Q is indefinite. Then proceed as in Theorem 3 to ensure that $-B^T QB$ is copositive-plus.
2. Form Q_0 and Γ_0 – which do not depend on any point $\bar{x}$ – as in (2.11) and (2.12). Call COPOS(Q_0, Γ_0); if the answer is negative, stop: the problem is unbounded from above. Else suppress, in all subsequent calls of ESCAPE and IMPR, the initialization steps, and generate a feasible point $\bar{x} \in M$, e.g., via phase I of the simplex method. Return.

Next we try to make IMPR more efficient along the lines indicated above.

EFFIMPR($\bar{x}$)

1. Perform steps 2 through 4 of IMPR($\bar{x}$).
2. (this is a modification of step 5 in IMPR)
   For all $j \in \{1, \ldots, m\} \setminus I(\bar{x})$ call COPOS($-R_j, \Gamma_j^+$); if a direction $v_j \in \Gamma_j^+$ with $v_j^T R_j v_j > 0$ (and hence $v_j^T Q v_j < 0$) is generated, calculate the corresponding improvement

   $$\operatorname{imp}(v_j) = \theta_{v_j}(\mu_{v_j}) .$$

Else ($-R_j$ is Γ_j^+-copositive) apply Lemke's method to problem (3.4). If the resulting Karush–Kuhn–Tucker point y satisfies $g(y) > g(\bar{x})$, then for $y - \bar{x} \in \Gamma_j^+$ record

$$\operatorname{imp}(y - \bar{x}) = g(y) - g(\bar{x}) > 0\,.$$

3. (this is a modification of step 6 in IMPR)
   If Q is Γ^+-copositive (cf. step 4 in IMPR), then apply Lemke's algorithm to the problem (3.3) and proceed with the resulting Karush–Kuhn–Tucker point y as in step 2 above. For all $j \in \{1, \ldots, m\} \backslash I(\bar{x})$ call COPOS(Q_j, Γ_j^-); if a direction $w_j \in \Gamma_j^-$ with $w_j^T Q_j w_j < 0$ is generated, calculate the corresponding improvement

$$\operatorname{imp}(w_j) = \theta_{w_j}(\lambda_{w_j})\,.$$

4. Pick that direction, v, or w, or v_j, or w_j, or $y - \bar{x}$, which yields the maximal improvement. Determine $\hat{x}$ as in (2.21), or put $\hat{x} = y$, accordingly. Return.

Similarly one could use the information that Q_j is Γ_j^--copositive obtained in step 6 of IMPR: this means that $g(x) \leq g(\bar{x})$ for all $x \in \Gamma_j^-$, so that one could replace M with $M \backslash \Gamma_j^-$. This procedure might be interpreted as performing several deep cuts simultaneously, cf. ([10] pp. 86, 195, 205). However, $M \backslash \Gamma_j^-$ is no more a polyhedron in general, so that this method rather resembles branch-and-bound procedures for global optimization as described, e.g., in ([10] pp. 111ff.).

4. A Finite Global Optimization Procedure

We begin with a rather simple argument. Let PRIMALG denote the primitive method to start with PREPROC and then iterate procedure EFFIMPR, replacing $\bar{x}$ with $\hat{x}$. Then this algorithm terminates after a finite number of iterations, provided that the following assumption holds:

$$\left.\begin{array}{l}\text{for any choice of the starting point } x_0 \in M, \text{ PRIMALG generates} \\ \text{a Karush–Kuhn–Tucker point of (2.1) after finitely many steps}\,.\end{array}\right\} \tag{4.1}$$

Under assumption (4.1), finiteness of PRIMALG follows from the following elementary result:

LEMMA 4. *The set*

$$V = \{g(\bar{x}) : \bar{x} \text{ is a Karush–Kuhn–Tucker point of } (2.1)\}$$

of objective values at Karush–Kuhn–Tucker points has less than $2^m + 1$ *elements.*

Proof. Let $\bar{x}$ and $\bar{y}$ be two Karush–Kuhn–Tucker points located at the relative interior of the same facet of M. This simply means $I(\bar{x}) = I(\bar{y})$. Then $v = \bar{y} - \bar{x}$

satisfies $\bar{x} + \lambda v \in M$ and $\bar{y} - \lambda v \in M$ irrespective of the sign of λ, provided $|\lambda|$ is small enough. Hence from the first-order optimality conditions we obtain $\theta_v'(0) = 0$ and $\tau_v'(0) = 0$ where $\theta_v(\lambda) = g(\bar{x} + \lambda v) - g(\bar{x})$ and $\tau_v(\lambda) = g(\bar{y} - \lambda v) - g(\bar{y})$. But $\tau_v(\lambda) = \theta_v(1 - \lambda) + g(\bar{x}) - g(\bar{y})$, so that we conclude $\theta_v'(1) = 0$. Hence θ_v is constant, and we get $g(\bar{y}) = g(\bar{x})$. Since there are 2^m possibilities to choose $I \subset \{1, \ldots, m\}$, the result follows. □

With the same technique one can show that for two Karush–Kuhn–Tucker points $\bar{x}$ and $\bar{y}$ of (2.1),

$$I(\bar{x}) \subset I(\bar{y}) \quad \text{implies} \quad g(\bar{x}) \leq g(\bar{y}) \,. \tag{4.2}$$

An easy consequence of property (4.2) is the well-known fact that the global maximum of a non-concave quadratic function is attained at the boundary of the feasible polyhedron M, see, e.g. ([15] p. 39).

However, we are not aware of simple conditions which guarantee that assumption (4.1) holds. Therefore, we have to include an anti-jamming device in the following algorithm. To this end, we need some further notation: For $I \subseteq \{1, \ldots, m\}$, let $F_I = \{x \in M : I \subset I(x)\}$ be the corresponding facet of M, and let $F_I^o = \{x \in M : I(x) = I\}$ be its relative interior. Then for any $\bar{x} \in F_I^o$, the set of feasible directions leading to a point in F_I coincides with

$$\Gamma_I = \{v \in \mathbb{R}^n : (Av)_i = 0 \text{ for all } i \in I\} \,.$$

COPOSGLOBAL

1. Call PREPROC.
2. If $\bar{x}$ is the feasible point generated, let $I = I(\bar{x})$ and call COPOS$(-Q, \Gamma_I)$.
   2a. If $-Q$ is Γ_I-copositive, then

$$g(x) \to \max! \quad \text{subject to} \quad x \in F_I \tag{4.3}$$

   is a concave quadratic maximization problem. Apply Lemke's procedure to (4.3), which (under non-degeneracy) after finitely many steps either stops with the information that (4.3) – and hence (2.1) – is unbounded from above, or delivers a global solution x_I of (4.3). In the latter case, call EFFIMPR, replacing $\bar{x}$ with x_I, and go to step 3.
   2b. Else a direction $v \in \Gamma_I$ is generated with $v^T Q v > 0$. Since also $-v \in \Gamma_I$, convexity of the function θ_v yields $\max\{\theta_v(\lambda_v), \theta_{-v}(\lambda_{-v})\} > 0$ (note that PREPROC would have stopped before if $\pm v \in \Gamma_0$). If $\theta_v(\lambda_v) \geq \theta_{-v}(\lambda_{-v}) > 0$, then put $\hat{x} = \bar{x} + \lambda_v v$; otherwise let $\hat{x} = \bar{x} - \lambda_{-v} v$. Go to step 3.
3. Replace $\bar{x}$ with the obtained improving feasible point $\hat{x}$, and repeat step 2.

THEOREM 5. *Suppose that every basic feasible solution occurring during the use of Lemke's procedure in algorithm* COPOSGLOBAL *is non-degenerate. Then this* *algorithm stops after finitely many iterations, either with the information that* (2.1) *is unbounded from above, or delivering the global solution of* (2.1).

Proof. The non-degeneracy assumption together with the transformation performed in PREPROC ensures that Lemke's procedure is finite and exact whenever it is used during the algorithm (cf. Theorem 3). Whenever branch 2b of COPOSGLOBAL is entered, the set I is enlarged by at least one element, because

$$I(\bar{x} \pm \lambda_{\pm v} v) = I(\bar{x}) \cup \{i\}$$

where $i \not\in I(\bar{x})$ satisfies $z(\pm v) = \pm(Av)_i/u_i$. Hence this can happen successively in at most m iterations, whereafter we would obtain $I = \{1, \ldots, m\}$. But then $\Gamma_I \subset \Gamma_0$, so that branch 2a will pertain in the next iteration (otherwise PREPROC would have stopped before). On the other hand, every successful execution of branch 2a guarantees the strict inequality

$$g(\hat{x}) > g(\bar{x}) = g(x_I) \geqslant g(x) \quad \text{for all} \quad x \in F_I\,,$$

so that the facet F_I will never be visited again during the following iterations. Since M is the finite union of its facets, the assertion is proved. □

EXAMPLE. Consider the problem from Example X.5. in ([10] p. 578). Here $n = 2$; $m = 4$;

$$Q = \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}; \quad c = \begin{bmatrix} 1 \\ 1 \end{bmatrix}; \quad A = \begin{bmatrix} -6 & 3 & -1 & 0 \\ 8 & -1 & 0 & -1 \end{bmatrix}^T; \quad \text{and}$$
$$b = [3, 3, 0, 0]^T\,.$$

For the sake of argument, let us assume that COPOS(Q, Γ) contains an additional shortcut method consisting of (a) checking whether an eigenvector corresponding to a negative eigenvalue belongs to Γ and (b) of checking whether the extremal rays of Γ violate (1.2). If one of these cases happens, the corresponding direction v is returned. Note that these shortcuts are not mentioned explicitly in [3]. Directions w and v in iterations 1 and 2 below are generated according to (a), while directions v_1 and v_2 in iteration 1 originate from case (b), since the eigenvectors do not belong to the corresponding cones Γ_j^+. The algorithm COPOSGLOBAL now proceeds as follows:

1. PREPROC yields indefiniteness of Q and $\Gamma_0 = \{o\}$. Hence Q_0 is trivially Γ_0-copositive. The first feasible point generated is the vertex $x_0 = o$.

Iteration 1:

2. For $\bar{x} = x_0$, we have $I = \{3, 4\}$. Since x_0 is a vertex, $\Gamma_I = \{o\}$ and hence $-Q$ is copositive w.r.t. this cone. Case 2a holds, and problem (4.3) is trivial. $x_I = x_0$ and EFFIMPR(x_0) is called:

1. Since $v=[1,0]^T \in \Gamma$ satisfies $v^T(Qx_0+c)=1>0$, x_0 is no Karush–Kuhn–Tucker point, and

   $\mathrm{imp}\,(v)=\theta_v(\lambda_v)=1$.

   Furthermore, $\Gamma^+=\mathbb{R}^2_+$, thus Q is not Γ^+-copositive, and $\mathrm{COPOS}(Q,\Gamma^+)$ generates $w=[1,1]^T$, yielding the improvement

   $\mathrm{imp}\,(w)=\theta_w(\mu_w)=1$.

2. Next we determine

   $$R_1=\begin{bmatrix}12 & 4\\ 4 & -16\end{bmatrix} \quad \text{and} \quad R_2=\begin{bmatrix}-6 & 4\\ 4 & 2\end{bmatrix}$$

   as well as $\Gamma_j^+=\Gamma_j$, which have the extremal rays $[1,1]^T$, $[0,1]^T$ for $j=1$, and $[1,1]^T$, $[1,0]^T$ for $j=2$, respectively (see Figure 1). Then $\mathrm{COPOS}(-R_1,\Gamma_1^+)$ and $\mathrm{COPOS}(-R_2,\Gamma_2^+)$ both yield the same improving direction $v_1=v_2=w$.
3. Thereafter, we investigate $\Gamma_j^-=\{o\}$ and obtain Γ_j^--copositivity of Q_j for $j=1,2$.
4. By coincidence both directions $v=[1,0]^T$ and $w=[1,1]^T$ obtained so far yield the same improvement. For didactic reasons, we choose $\hat{x}=x_0+\mu_w w=[1,1]^T$. Note that if we chose $\hat{x}=x_0+\lambda_v v=[1,0]^T$, then the procedure would terminate at the global solution in the next iteration.

3. Now $x_1=[1,1]^T$ is the starting point for

Iteration 2:

2. x_1 is interior to M so that $I=\emptyset$, and thus $\Gamma_I=\mathbb{R}^2$. Hence, case 2b holds.

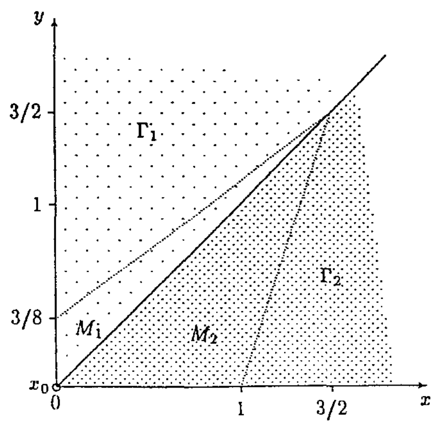

Fig. 1. Cones at x_0 (for M_i cf. Thm 2).

COPOS($-Q, \mathbb{R}^2$) yields $v = [1, -1]^T$. Then $\theta_v(\lambda_v) = \frac{1}{16} > \theta_{-v}(\lambda_{-v}) = \frac{1}{196}$, and $\hat{x} = x_1 + \lambda_v v = [\frac{5}{4}, \frac{3}{4}]^T$.

3. Now $x_2 = [\frac{5}{4}, \frac{3}{4}]^T$ is the starting point for

Iteration 3:

2. Now $I = \{2\}$ and $\Gamma_I = \{v \in \mathbb{R}^2 : v_2 = 3v_1\}$. Moreover, $-Q$ is Γ_I-copositive. Since this cone is a straight line, the corresponding problem (4.3) is easily solved, resulting in $x_3 = x_I = [\frac{7}{6}, \frac{1}{2}]^T$. Again, EFFIMPR($x_3$) is called.
1. Since (2.23) has optimal value zero, x_3 is a Karush–Kuhn–Tucker point. Now $I = \{1, 3, 4\}$, and ESCAPE(x_3) has to call COPOS(Q_i, Γ_i) for all $i \in I$. Here

$$Q_1 = \begin{bmatrix} 6 & 1 \\ 1 & 8/3 \end{bmatrix}; \quad Q_3 = \begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix}; \quad \text{and} \quad Q_4 = \begin{bmatrix} 0 & 1 \\ 1 & -1/3 \end{bmatrix}.$$

Now Q_1 is positive definite; Q_3 has positive entries and is thus copositive w.r.t. $\mathbb{R}^2_+$ and hence also w.r.t $\Gamma_3 \subset -\mathbb{R}^2_+$; finally, any direction $v \in \Gamma_4$ satisfies $v_2 = -(Av)_4 \leq 0$ and thus $6v_1 - v_2 \leq 6v_1 - 2v_2 = 2(Av)_2 \leq 0$, so that $3v^T Q_4 v = v_2(6v_1 - v_2) \geq 0$ (the cones are depicted in Figure 2). Hence all Q_i are Γ_i-copositive, and the algorithm stops, delivering the global maximizer $x_3 = [\frac{7}{6}, \frac{1}{2}]^T$ with objective value $\frac{13}{12}$.

The path generated by COPOSGLOBAL is shown in Figure 3.

Apart from efficiently selecting an improving feasible direction, the proposed algorithm frequently uses the simplex algorithm. This fact, together with quite encouraging numerical experiments with the central copositivity procedure COPOS, which consist of data-driven recursive schemes using again the simplex method [3], suggests that in the average case (cf. [4]) the computational costs of

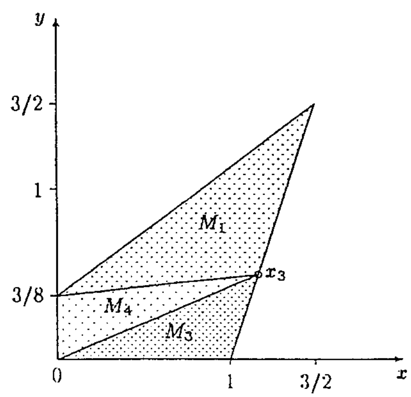

Fig. 2. Partition of M induced by cones at x_3.

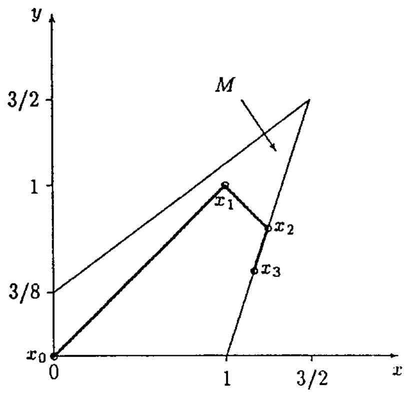

Fig. 3. Path generated by COPOS-GLOBAL.

COPOSGLOBAL can be held within reasonable limits. The observation that the similar optimization procedure in [3] delivers the solution of (1.1) after at most n steps may further support this assertion.

As mentioned already in the introduction, problem (2.1) is NP-hard from the worst-case complexity point of view. However, our approach shows that there is no essential difference between the complexities of checking local optimality and of checking global optimality, despite the fears expressed in [13].

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