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Sufficient global optimality conditions for non-convex quadratic minimization problems with box constraints

V. Jeyakumar · A. M. Rubinov · Z. Y. Wu

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Abstract In this paper we establish conditions which ensure that a feasible point is a global minimizer of a quadratic minimization problem subject to box constraints or binary constraints. In particular, we show that our conditions provide a complete characterization of global optimality for non-convex weighted least squares minimization problems. We present a new approach which makes use of a global subdifferential. It is formed by a set of functions which are not necessarily linear functions, and it enjoys explicit descriptions for quadratic functions. We also provide numerical examples to illustrate our optimality conditions.

Keywords Quadratic optimization · Global optimality conditions · Non-convex minimization · Weighted least squares · Box constraints · Bivalent programs

AMS subject classification 41A65 · 41A29 · 90C30

V. Jeyakumar (✉)
Department of Applied Mathematics,
University of New South Wales, Sydney 2052, Australia
e-mail: jeya@maths.unsw.edu.au

A. M. Rubinov
School of Information Technology and Mathematical Sciences,
University of Ballarat, Ballarat 3353, Victoria, Australia.
e-mail:a.rubinov@ballarat.edu.au

Z. Y. Wu
Department of Mathematics, Chongqing Normal University,
Chongqing 400047, People's Republic of China.
e-mail: zhiyouwu@maths.unsw.edu.au

1 Introduction

Consider the following quadratic minimization model problem with box constraints

$$\text{(QP)} \qquad \min_{x\in\mathbb{R}^n} \frac{1}{2}x^{\mathrm{T}}Ax + a^{\mathrm{T}}x$$
$$\text{s.t.} \quad x \in \prod_{i=1}^{n}[u_i, v_i]$$

where $u_i, v_i \in \mathbb{R}$ and $u_i \leq v_i, i = 1, \ldots, n$, $a \in \mathbb{R}^n$ and $A \in S^n$, the space of $n \times n$ symmetric real matrices. Model problems of the form (QP) arise in many applications [1, 2]. For instance, a continuous relaxation of a quadratic minimization problem with binary constraints, known as bivalent quadratic programming problems (see [3, 4]) is of the form (QP). Such problems arise in various combinatorial optimization problems such as the max-cut problem and are known to be NP hard (see [5]). Due to the importance of finding global minimizers of quadratic problems of the form (QP), a significant amount of different computational approaches to solving these problems has been developed in the literature [6–10, 1].

In recent years, a great deal of attention has been focused on characterizing global minimizers of quadratic minimization problems (see [11–13, 3] and other references therein). In particular, Beck and Teboulle [3] have given elegant global optimality conditions for bivalent quadratic minimization problems.

The purpose of this paper is to establish conditions which ensure that a feasible point is a global minimizer of a quadratic minimization problem subject to box constraints or binary constraints. Our conditions completely characterize global optimality of weighted least squares minimization problems. Moreover, our sufficient global optimality conditions for bivalent quadratic programming problems generalize the corresponding results of [3].

We examine optimality conditions in terms of a global subdifferential, called L-subdifferential (see [14, 15]). It is formed by functions which are not necessarily linear. This subdifferential enjoys explicit descriptions for quadratic functions and allows us to obtain global optimality conditions for non-convex quadratic minimization problems, including indefinite quadratic minimization problems, in terms of the problem data. We show how an L-subdifferential can be explicitly calculated for quadratic functions and then develop global optimality conditions for (QP). We demonstrate how the L-subdifferential approach can also be used to derive general sufficient global optimality conditions for bivalent quadratic minimization problems, covering the corresponding conditions of [3]. We also give numerical examples to discuss our results.

The layout of the paper is as follows. Section 2 presents the notion of the L-subdifferential and develops sufficient conditions for global minimizers of (QP). Section 3 provides sufficient global optimality conditions for bivalent quadratic minimization problems. Section 4 provides a summary and an outline for future work.

2 *L*-Subdifferentials and quadratic minimization

In this section, we investigate a general quadratic minimization problem with box constraints and derive sufficient global optimality conditions. We begin by presenting basic definitions and notations that will be used throughout the paper.

The real line is denoted by $\mathbb{R}$ and the n-dimensional Euclidean space is denoted by $\mathbb{R}^n$. For vectors $x, y \in \mathbb{R}^n$, $x \geq y$ means that $x_i \geq y_i$, for $i = 1, \ldots, n$. The identity matrix is denoted by I. The notation $A \succeq 0$ means that the matrix A is a positive semi-definite. A diagonal matrix with diagonal elements $\alpha_1, \ldots, \alpha_n$ is denoted by $\mathrm{diag}(\alpha_1, \ldots, \alpha_n)$. Let L be a set of real-valued functions defined on $\mathbb{R}^n$.

$L-$Subdifferentials (see [14, 15]). Let $f: \mathbb{R}^n \to \mathbb{R}$ and $x_0 \in \mathbb{R}^n$. An element $l \in L$ is called an L-subgradient of f at a point $x_0 \in \mathbb{R}^n$ if

$$f(x) \geq f(x_0) + l(x) - l(x_0), \ \forall x \in \mathbb{R}^n.$$

The set $\partial_L f(x)$ of all L-subgradients of f at x_0 is referred to as L-subdifferential of f at x_0.

Note that if L is chosen as the set of all linear functions defined on $\mathbb{R}^n$, then for any real-valued convex function f defined on $\mathbb{R}^n$, $\partial_L f(x) = \partial f(x)$, where $\partial f(x)$ is the sub-differential in the sense of convex analysis [16]. Note also that it follows easily from the definition that if $f \in L$, then $\partial_L f(x)$ is non-empty at every x. In the following, we explicitly calculate $\partial_L f(x)$ for quadratic functions by suitably choosing L.

Consider the quadratic minimization problem, given in the introduction:

$$\text{(QP)} \qquad \min_{x \in \mathbb{R}^n} f(x) := \frac{1}{2} x^{\mathrm{T}} A x + a^{\mathrm{T}} x$$
$$\text{s.t.} \ \ x \in S := \prod_{i=1}^{n} [u_i, v_i],$$

where $A \in S^n$, the space of $n \times n$ symmetric real matrices. Without loss of generality, we suppose that $u_i < v_i$. If $u_i = v_i$, we can replace S by $\prod_{j=1}^{i-1} S_j \times \prod_{j=i+1}^{n} S_j$ and replace f by $\bar{f}$, where $\bar{f}(x) = f(\bar{x}), \ \bar{x} = (x_1, \ldots, x_{i-1}, u_i, x_{i+1}, \ldots, x_n)^{\mathrm{T}}$ and $S_j = [u_j, v_j]$.

Unless stated otherwise, throughout the rest of the paper, the set L is given by

$$L = \left\{ \frac{1}{2} x^{\mathrm{T}} Q x + x^{\mathrm{T}} \beta \ \mid \ Q = \mathrm{diag}(\alpha_1, \ldots, \alpha_n), \alpha_i \in \mathbb{R}, \ \beta \in \mathbb{R}^n \right\}.$$

Note that L satisfies the property that $-l \in L$ for each $l \in L$. We begin by calculating $\partial_L f(x)$ for the quadratic function $f(x) = \frac{1}{2} x^{\mathrm{T}} A x + a^{\mathrm{T}} x$.

Proposition 2.1. *Let* $f(x) := \frac{1}{2} x^{\mathrm{T}} A x + a^{\mathrm{T}} x$ *and let* $\bar{x} = (\bar{x}_1, \ldots, \bar{x}_n)^{\mathrm{T}} \in \mathbb{R}^n$. *Then,*

$$\partial_L f(\bar{x}) = \left\{ \frac{1}{2} x^{\mathrm{T}} Q x + \beta^{\mathrm{T}} x \ \middle| \ \begin{array}{c} A - Q \succeq 0, \ Q = \mathrm{diag}(\alpha_1, \ldots, \alpha_n), \alpha_i \in \mathbb{R} \\ \beta = a + (A - Q)\bar{x}, \beta \in \mathbb{R}^n \end{array} \right\}.$$

Proof Note, by definition, that $l_0 \in \partial_L f(\bar{x})$ if and only if

$$l_0(x) - l_0(\bar{x}) \leq f(x) - f(\bar{x}), \quad \forall x \in \mathbb{R}^n. \tag{1}$$

Let $l_0(x) = \frac{1}{2} x^{\mathrm{T}} Q x + \beta^{\mathrm{T}} x$ and let $\varphi(x) = f(x) - l_0(x)$. Then $\varphi(x) = \frac{1}{2} x^{\mathrm{T}} (A - Q) x + (a - \beta)^{\mathrm{T}} x$. By (1), for each $x \in \mathbb{R}^n$,

$$\varphi(x) = \frac{1}{2} x^{\mathrm{T}} (A - Q) x + (a - \beta)^{\mathrm{T}} x \geq f(\bar{x}) - l_0(\bar{x}).$$

Thus, φ is bounded below and attains its minimum at $\bar{x}$. So, $A - Q \succeq 0$. Hence, φ is a convex function on $\mathbb{R}^n$, and so, φ attains its minimum at $\bar{x}$ if and only if $\nabla \varphi(\bar{x}) = 0$. This gives us that

$$(A - Q)\bar{x} + (a - \beta) = 0 \quad \text{and} \quad \beta = a + (A - Q)\bar{x}.$$

□

For (QP), let

$$v := (v_1, \ldots, v_n)^{\mathrm{T}}, \tag{2}$$
$$u := (u_1, \ldots, u_n)^{\mathrm{T}}, \tag{3}$$
$$a := (a_1, \ldots, a_n)^{\mathrm{T}}. \tag{4}$$

For $\bar{x} = (\bar{x}_1, \ldots, \bar{x}_n)^{\mathrm{T}} \in S$, define

$$\widetilde{x}_i := \begin{cases} -1 & \text{if } \bar{x}_i = u_i \\ 1 & \text{if } \bar{x}_i = v_i \\ a_i + (A\bar{x})_i & \text{if } \bar{x}_i \in (u_i, v_i), \end{cases} \tag{5}$$
$$\widetilde{X} := \operatorname{diag}(\widetilde{x}_1, \ldots, \widetilde{x}_n). \tag{6}$$

For $Q = \operatorname{diag}(\alpha_1, \ldots, \alpha_n),\ \alpha_i \in \mathbb{R}, i = 1, \ldots, n$, define

$$\widehat{\alpha}_i := \min\{0, \alpha_i\} = \begin{cases} 0 & \text{if } \alpha_i \geq 0 \\ \alpha_i & \text{if } \alpha_i < 0, \end{cases} \tag{7}$$
$$\widehat{Q} := \operatorname{diag}(\widehat{\alpha}_1, \ldots, \widehat{\alpha}_n). \tag{8}$$

Using Proposition 2.1, we obtain the following sufficient optimality condition for (QP).

Theorem 2.1. *For* (QP)*, let* $\bar{x} = (\bar{x}_1, \ldots, \bar{x}_n)^{\mathrm{T}} \in S$*. Suppose that there exists a diagonal matrix* $Q := \operatorname{diag}(\alpha_1, \ldots, \alpha_n),\ \alpha_i \in \mathbb{R}^n, i = 1, \ldots, n$ *such that* $A - Q \succeq 0$ *and*

$$\widetilde{X}(a + A\bar{x}) - \frac{1}{2}\widehat{Q}(v - u) \leq 0. \tag{9}$$

Then $\bar{x}$ *is a global minimizer of problem* (QP).

Proof Let $Q := \operatorname{diag}(\alpha_1, \ldots, \alpha_n),\ \alpha_i \in \mathbb{R}^n, i = 1, \ldots, n$ such that $A - Q \succeq 0$ and (9) holds. Let $\beta := a + (A - Q)\bar{x}$. Then, by Proposition 2.1, $l = \frac{1}{2}x^{\mathrm{T}}Qx + \beta^{\mathrm{T}}x \in \partial_L f(\bar{x})$, i.e.,

$$f(x) - f(\bar{x}) \geq l(x) - l(\bar{x}), \quad \forall x \in \mathbb{R}^n.$$

If $l(x) - l(\bar{x}) \geq 0$ for each $x \in S$, then $\bar{x}$ is a global minimizer of (QP). To see this, we first note from (7) that, for each $i = 1, \ldots, n$,

$$\alpha_i \geq \widehat{\alpha}_i.$$

By (9), for each $i = 1, \ldots, n$,

$$-\frac{\widehat{\alpha}_i}{2}(v_i - u_i) + \widetilde{x}_i(a_i + (A\bar{x})_i) \leq 0.$$

Since $\widehat{\alpha}_i \leq 0$, for each $x_i \in [u_i, v_i],\ i = 1, \ldots, n$,

$$-\frac{\widehat{\alpha}_i}{2}(x_i - u_i) + \widetilde{x}_i(a_i + (A\bar{x})_i) \leq 0 \quad \text{and} \quad \frac{\widehat{\alpha}_i}{2}(x_i - v_i) + \widetilde{x}_i(a_i + (A\bar{x})_i) \leq 0.$$

We now consider the following three cases:

Case 1 Let $\bar{x}_i \in (u_i, v_i)$. Then $\widetilde{x}_i = a_i + (A\bar{x})_i$. So, $\widehat{\alpha}_i = 0$ and $a_i + (A\bar{x})_i = 0$. This gives us that

$$\begin{aligned} &\frac{\alpha_i}{2}(x_i - \bar{x}_i)^2 + (a_i + (A\bar{x})_i)(x_i - \bar{x}_i) \\ &\geq \frac{\widehat{\alpha}_i}{2}(x_i - \bar{x}_i)^2 \\ &= 0. \end{aligned}$$

Case 2 Let $\bar{x}_i = u_i$. Then

$$\begin{aligned}
&\frac{\alpha_i}{2}(x_i - \bar{x}_i)^2 + (a_i + (A\bar{x})_i)(x_i - \bar{x}_i) \\
&\geq \frac{\widehat{\alpha}_i}{2}(x_i - \bar{x}_i)^2 + (a_i + (A\bar{x})_i)(x_i - \bar{x}_i) \\
&= -\left[-\frac{\widehat{\alpha}_i}{2}(x_i - u_i) + \widetilde{x}_i(a_i + (A\bar{x})_i)\right](x_i - u_i) \\
&= -\left[-\frac{\widehat{\alpha}_i}{2}(x_i - u_i) + \widetilde{x}_i(a_i + (A\bar{x})_i)\right](x_i - u_i) \\
&\geq 0.
\end{aligned}$$

Case 3 Let $\bar{x}_i = v_i$. Then

$$\begin{aligned}
&\frac{\alpha_i}{2}(x_i - \bar{x}_i)^2 + (a_i + (A\bar{x})_i)(x_i - \bar{x}_i) \\
&\geq \frac{\widehat{\alpha}_i}{2}(x_i - \bar{x}_i)^2 + (a_i + (A\bar{x})_i)(x_i - \bar{x}_i) \\
&= \left[\frac{\widehat{\alpha}_i}{2}(x_i - v_i) + \widetilde{x}_i(a_i + (A\bar{x})_i)\right](x_i - v_i) \\
&\geq 0.
\end{aligned}$$

Hence, if (9) holds, then

$$l(x) - l(\bar{x}) = \sum_{i=1}^{n} \frac{\alpha_i}{2}(x_i - \bar{x}_i)^2 + (a + A\bar{x})^{\mathrm{T}}(x - \bar{x}) \geq 0. \qquad \square$$

Let us examine how we can obtain a simple sufficient condition for global optimality of (QP) using (9). Recall that a matrix $A := (a_{ij}) \in S^n$ is said to be *diagonally dominant* if $|a_{ii}| \geq \sum_{j\neq i, j=1}^{n} |a_{ij}|$, for $i = 1, \ldots, n$. Every diagonally dominant matrix $A \in S^n$ with non-negative diagonal elements is positive semi-definite. For details see [17]. Let $A = (a_{ij}) \in S^n$ and let

$$\bar{a}_i := a_{ii} - \sum_{j\neq i, j=1}^{n} |a_{ij}|, \tag{10}$$

$$\bar{a} := (\bar{a}_1, \ldots, \bar{a}_n)^{\mathrm{T}}, \tag{11}$$

$$\bar{A} := \mathrm{diag}(\bar{a}_1, \ldots, \bar{a}_n). \tag{12}$$

Let $\mu_i, i = 1, \ldots, n$ be the eigenvalues of A and let

$$\mu = \min\{\mu_i \mid i = 1, \ldots, n\}. \tag{13}$$

Clearly $A \succeq 0$ if and only if $\mu \geq 0$. For $\lambda \in [0, 1]$, let

$$A_\lambda := \lambda\bar{A} + (1 - \lambda)(\mu I) = \mathrm{diag}(\alpha_{1,\lambda}, \ldots, \alpha_{n,\lambda}) \tag{14}$$

and

$$\widehat{A}_\lambda := \mathrm{diag}(\widehat{\alpha}_{1,\lambda}, \ldots, \widehat{\alpha}_{n,\lambda}), \tag{15}$$

where $\alpha_{i,\lambda} = \lambda\bar{a}_i + (1 - \lambda)\mu$ and $\widehat{\alpha}_{i,\lambda} = \min\{0, \alpha_{i,\lambda}\}$, for $i = 1, \ldots, n$. We now derive a sufficient condition for global optimality.

Corollary 2.1. *For* (QP), *let* $\bar{x} \in S$.

1°. *If* $\mu \geq 0$ *then* $\bar{x}$ *is a global minimizer of* (QP) *if and only if*

$$\widetilde{X}(A\bar{x} + a) \leq 0.$$

2°. *If* $\mu < 0$ *and if there exists* $\lambda \in [0, 1]$ *such that*

$$\widetilde{X}(A\bar{x} + a) - \frac{1}{2}\widehat{A}_\lambda(v - u) \leq 0, \tag{16}$$

then $\bar{x}$ *is a global minimizer of* (QP).

Proof 1°. Let $\mu \geq 0$. Then A is positive semi-definite. If $\widetilde{X}(A\bar{x} + a) \leq 0$ then by choosing $Q = \widehat{Q} = 0$, (9) holds and so, by Theorem 2.1, $\bar{x}$ is a global minimizer of (QP). Conversely, if $\bar{x}$ is a global minimizer then $-\partial f(\bar{x}) \cap N_S(\bar{x}) \neq \emptyset$. So, $-A\bar{x} - a \in N_S(\bar{x})$. Thus, for each $x \in S$, $(A\bar{x} + a)^{\mathrm{T}}(x - \bar{x}) \geq 0$. Using the same line of arguments as in the proof of Theorem 2.1, we obtain that $\widetilde{X}(A\bar{x} + a) \leq 0$.

2°. Let $\mu < 0$. Then, $A - \mu I \succeq 0$. Also, it is easy to verify that $A - \bar{A}$ is a diagonally dominant matrix with non-negative diagonal elements, and so, $A - \bar{A} \succeq 0$. Hence, $A - A_\lambda \succeq 0$. The conclusion now follows from Theorem 2.1 by taking $Q = A_\lambda$ and $\widehat{Q} = \widehat{A}_\lambda$. □

We now show, for certain special class of quadratic minimization problems, that Theorem 2.1 yields complete characterization of global optimality. Consider the problem

$$(\mathrm{QP}_0) \qquad \min_{x \in \mathbb{R}^n} \sum_{i=1}^{n} \frac{\gamma_i}{2} x_i^2 + \sum_{i=1}^{n} a_i x_i$$
$$\text{s.t.} \quad x \in S := \prod_{i=1}^{n} [u_i, v_i],$$

where $\gamma_i, a_i \in \mathbb{R}$, $u_i, v_i \in \mathbb{R}$ and $u_i \leq v_i$, $i = 1, \ldots, n$. Define

$$\widehat{\gamma_i} := \min\{0, \gamma_i\} = \begin{cases} 0 & \text{if } \gamma_i \geq 0 \\ \gamma_i & \text{if } \gamma_i < 0. \end{cases} \tag{17}$$

Corollary 2.2. *For* (QP_0), *let* $\bar{x} \in S$ *and let* $\widetilde{x}_i, \widehat{\gamma_i}$ *be defined by* (5) *and* (17), *respectively. Then* $\bar{x}$ *is a global minimizer of* (QP_0) *if and only if, for each* $i = 1, \ldots, n$,

$$\widetilde{x}_i(a_i + \gamma_i \bar{x}_i) - \frac{1}{2}\widehat{\gamma_i}(v_i - u_i) \leq 0. \tag{18}$$

Proof Let $f(x) := \sum_{i=1}^{n} \frac{\gamma_i}{2} x_i^2 + \sum_{i=1}^{n} a_i x_i$. By the definition, $\bar{x}$ is a global minimizer of (QP_0) if and only if, for each $x \in S = \prod_{i=1}^{n}[u_i, v_i]$,

$$\begin{aligned} f(x) - f(\bar{x}) &= \sum_{i=1}^{n} \frac{\gamma_i}{2} x_i^2 + \sum_{i=1}^{n} a_i x_i - \left[\sum_{i=1}^{n} \frac{\gamma_i}{2} \bar{x}_i^2 + \sum_{i=1}^{n} a_i \bar{x}_i\right] \\ &= \sum_{i=1}^{n} \frac{\gamma_i}{2}(x_i - \bar{x}_i)^2 + \sum_{i=1}^{n}(a_i + \gamma_i \bar{x}_i)(x_i - \bar{x}_i) \\ &\geq 0. \end{aligned}$$

Thus, $\bar{x}$ is a global minimizer of (QP_0) if and only if, for each $i = 1, \ldots, n$, $x_i \in [u_i, v_i]$,

$$\frac{\gamma_i}{2}(x_i - \bar{x}_i)^2 + (a_i + \gamma_i \bar{x}_i)(x_i - \bar{x}_i) \geq 0. \tag{19}$$

We now show that (19) implies (18). Assume that (19) holds.

Case 1 Let $\bar{x}_i = u_i$. Then

$$\frac{\gamma_i}{2}(x_i - u_i) + (a_i + \gamma_i \bar{x}_i) \geq 0, \quad \text{for each } x_i \in [u_i, v_i]. \tag{20}$$

If $\gamma_i \geq 0$, then (20) holds if and only if $a_i + \gamma_i \geq 0$. If $\gamma_i < 0$, (20) holds if and only if $\frac{\gamma_i}{2}(v_i - u_i) + (a_i + \gamma_i \bar{x}_i) \geq 0$.

Case 2 Let $\bar{x}_i = v_i$. Then

$$\frac{\gamma_i}{2}(x_i - v_i) + (a_i + \gamma_i \bar{x}_i) \leq 0, \quad \text{for each } x_i \in [u_i, v_i]. \tag{21}$$

If $\gamma_i \geq 0$, (21) holds if and only if $a_i + \gamma_i \bar{x}_i \leq 0$. If $\gamma_i < 0$, Eq. (21) holds if and only if $\frac{\gamma_i}{2}(u_i - v_i) + (a_i + \gamma_i \bar{x}_i) \leq 0$.

Case 3 Let $\bar{x}_i \in (u_i, v_i)$. Then $\gamma_i \geq 0$ and $a_i + \gamma_i \bar{x}_i = 0$. Thus, (18) holds. To prove the converse implication, choose $Q = \text{diag}(\gamma_1, \ldots, \gamma_n)$. Then (18) collapses to (9). □

Let us now give two numerical examples to apply our results to quadratic program.

Example 2.1. Consider the following problem:

$$\text{(EP1)} \qquad \min_{x \in \mathbb{R}^3} f(x) = -\frac{1}{2}x_1^2 - x_2^2 - \frac{3}{2}x_3^2 + x_1 - x_2 + 2x_3$$
$$\text{s.t.} \quad x \in S = \prod_{i=1}^{3}[-1, 1].$$

Let $\gamma_1 = -1, \gamma_2 = -2, \gamma_3 = -3, a_1 = 1, a_2 = -1$ and $a_3 = 2$. Let $\bar{x} = (-1, 1, -1)^{\mathrm{T}}$ and $\bar{y} = (-1, -1, -1)^{\mathrm{T}}$. It is easy to check that (18) of Corollary 2.2 is satisfied at $\bar{x}$, but not at $\bar{y}$. Thus, $\bar{x}$ is a global minimizer of (EP1) and $\bar{y}$ is not a global minimizer of (EP1).

Example 2.2. Consider the following problem:

$$\text{(EP2)} \qquad \min_{x \in \mathbb{R}^4} f(x) = -\frac{1}{2}x_1^2 + 2x_1x_2 + x_1x_4 - \frac{1}{2}x_2^2 + x_2x_3 + 3x_3^2$$
$$-x_3x_4 - x_4^2 + 4x_1 + \frac{9}{2}x_2 - x_3 - x_4$$
$$\text{s.t.} \quad x \in S = \prod_{i=1}^{4}[-1, 1].$$

Let

$$A = \begin{pmatrix} -1 & 2 & 0 & 1 \\ 2 & -1 & 1 & 0 \\ 0 & 1 & 6 & -1 \\ 1 & 0 & -1 & -2 \end{pmatrix}$$

and $a_1 = 4, a_2 = \frac{9}{2}, a_3 = -1, a_4 = -1$, $u_i = -1$ and $v_i = 1, i = 1, 2, 3, 4$. Let $\bar{x} = (-1, -1, \frac{1}{2}, 1)^{\mathrm{T}}$. Then $A\bar{x} = (0, -\frac{1}{2}, 1, -\frac{7}{2})^{\mathrm{T}}$ and $\widehat{A}_\lambda = \text{diag}(-4, -4, 0, -4)$ with $\lambda = 1$. Then,

$$\widetilde{X}(A\bar{x} + a) - \frac{1}{2}\widehat{A}_\lambda(v - u) = \left(0, 0, 0, -\frac{1}{2}\right)^{\mathrm{T}} \leq 0.$$

So, $\bar{x}$ satisfies (16) for $\lambda = 1$. Indeed, $\bar{x}$ is a global minimizer of (EP2).

3 Bivalent quadratic programming

In this section, we will apply the technique, developed in Sect. 2, to bivalent non-convex quadratic minimization problem of the form:

$$\text{(BQP)} \qquad \min_{x\in\mathbb{R}^n} \; f(x) = \frac{1}{2}x^{\mathrm{T}}Ax + a^{\mathrm{T}}x$$
$$\text{s.t.} \quad x \in \prod_{i=1}^{n}\{u_i, v_i\},$$

where $a \in \mathbb{R}^n$ and $A \in S^n$, $u_i < v_i, i = 1,\ldots,n$ are given real numbers. Let $S^i_{\mathrm{B}} := \{u_i, v_i\}, i = 1,\ldots,n$ and let $S_{\mathrm{B}} := \prod_{i=1}^n S^i_{\mathrm{B}} = \prod_{i=1}^n\{u_i, v_i\}$. Using the same line of arguments as in the proof of Theorem 2.1, we obtain sufficient global optimality conditions for (BQP).

Theorem 3.1. *Let* $\bar{x} = (\bar{x}_1,\ldots,\bar{x}_n)^{\mathrm{T}} \in S_{\mathrm{B}}$. *Suppose that there exists a diagonal matrix* $Q := \mathrm{diag}(\alpha_1,\ldots,\alpha_n),\ \alpha_i \in \mathbb{R}^n, i = 1,\ldots,n$ *such that* $A - Q \succeq 0$ *and*

$$\widetilde{X}(a + A\bar{x}) - \frac{1}{2}Q(v-u) \le 0. \tag{22}$$

Then, $\bar{x}$ *is a global minimizer of problem* (BQP).

Proof Let $Q := \mathrm{diag}(\alpha_1,\ldots,\alpha_n),\ \alpha_i \in \mathbb{R}^n, i = 1,\ldots,n$ such that $A - Q \succeq 0$ and (22) holds. Let $\beta := a + (A-Q)\bar{x}$. Then, by Proposition 2.1, $l = \frac{1}{2}x^{\mathrm{T}}Qx + \beta^{\mathrm{T}}x \in \partial_L f(\bar{x})$, i.e.,

$$f(x) - f(\bar{x}) \ge l(x) - l(\bar{x}), \quad \forall x \in \mathbb{R}^n.$$

If $l(x) - l(\bar{x}) \ge 0$ for each $x \in S_{\mathrm{B}}$, then $\bar{x}$ is a global minimizer of problem (BQP). For each $i = 1,\ldots,n$, $x_i \in \{u_i, v_i\}$, we now consider the following two cases.
Case 1 Let $\bar{x}_i = u_i$. Then

$$\frac{\alpha_i}{2}(x_i - \bar{x}_i)^2 + (a_i + (A\bar{x})_i)(x_i - \bar{x}_i) \ge 0$$

if and only if

$$\frac{\alpha_i}{2}(v_i - u_i)^2 + (a_i + (A\bar{x})_i)(v_i - u_i) = \left[\frac{\alpha_i}{2}(v_i - u_i) - \widetilde{x}_i(a_i + (A\bar{x})_i)\right](v_i - u_i) \ge 0.$$

Case 2 Let $\bar{x}_i = v_i$. Then

$$\frac{\alpha_i}{2}(x_i - \bar{x}_i)^2 + (a_i + (A\bar{x})_i)(x_i - \bar{x}_i) \ge 0$$

if and only if

$$\frac{\alpha_i}{2}(u_i - v_i)^2 + (a_i + (A\bar{x})_i)(u_i - v_i) = \left[-\frac{\alpha_i}{2}(v_i - u_i) + \widetilde{x}_i(a_i + (A\bar{x})_i)\right](u_i - v_i) \ge 0.$$

Thus, if (22) holds, then

$$l(x) - l(\bar{x}) = \sum_{i=1}^{n} \frac{1}{2}\alpha_i(x_i - \bar{x}_i)^2 + (a_i + (A\bar{x})_i)(x_i - \bar{x}_i) \ge 0$$

and so, $\bar{x}$ is a global minimizer of (BQP). □

Corollary 3.1. *Let* $\bar{x} = (\bar{x}_1, \ldots, \bar{x}_n)^{\mathrm{T}} \in S_{\mathrm{B}}$*; let* A_λ *be defined by* (14). *Suppose that there exists* $\lambda \in [0, 1]$ *such that*

$$\widetilde{X}(A\bar{x} + a) - \frac{1}{2}A_\lambda(v - u) \leq 0. \tag{23}$$

Then $\bar{x}$ *is a global minimizer of* (BQP).

Proof (i) Let $Q_1 = \mu I$ and let $Q_2 = \bar{A}$. Then, we can easily verify that $A - Q_i \succeq 0$, $i = 1, 2$. Let $Q = A_\lambda$. Then $A - Q$ is also a positive semi-definite matrix. The conclusion now follows from Theorem 3.1. □

Let us consider certain special cases of (BQP). Firstly, consider the problem

$$(\mathrm{BQP}_0) \qquad \min_{x \in \mathbb{R}^n} \sum_{i=1}^{n} \frac{1}{2}\gamma_i x_i^2 + \sum_{i=1}^{n} a_i x_i$$
$$\text{s.t.} \quad x \in S_{\mathrm{B}} := \prod_{i=1}^{n} \{u_i, v_i\},$$

where $\gamma_i, a_i \in \mathbb{R}$, $u_i, v_i \in \mathbb{R}$ and $u_i \leq v_i$, $i = 1, \ldots, n$.

Corollary 3.2. *For the problem* (BQP_0)*, let* $\bar{x} \in S_{\mathrm{B}}$. *Let* $\widetilde{x}_i$ *be defined by* (5). *Then* $\bar{x}$ *is a global minimizer of* (BQP_0) *if and only if for each* $i = 1, \ldots, n$,

$$\widetilde{x}_i(a_i + \gamma_i \bar{x}_i) - \frac{\gamma_i}{2}(v_i - u_i) \leq 0. \tag{24}$$

Proof The proof is as similar to the proof of Theorem 2.2 and so it is omitted. □

Now, consider the following special case of (BQP), where for each $i = 1, \ldots, n$, $u_i = u_0$ and $v_i = v_0$.

$$(\mathrm{BQP}_1) \qquad \min_{x \in \mathbb{R}^n} f(x) = \frac{1}{2}x^{\mathrm{T}}Ax + a^{\mathrm{T}}x$$
$$\text{s.t.} \quad x \in S_{\mathrm{B}} = \prod_{i=1}^{n} \{u_0, v_0\},$$

where $a \in \mathbb{R}^n$ and $A \in S^n$, $u_0 < v_0$ are given real numbers. Let $e = (1, \ldots, 1)^{\mathrm{T}}$.

The following Corollary extends Theorem 2.3 of [3].

Corollary 3.3. *Let* $\bar{x} = (\bar{x}_1, \ldots, \bar{x}_n)^{\mathrm{T}}$ *be a feasible point of* (BQP_1). *Let* A_λ *be defined by* (14). *Suppose that there exists* $\lambda \in [0, 1]$ *such that*

$$\widetilde{X}(A\bar{x} + a) - \tfrac{1}{2}A_\lambda(v_0 - u_0)e \leq 0. \tag{25}$$

Then $\bar{x}$ *is a global minimizer of* (BQP_1).

Proof The conclusion easily follows from Corollary 3.1 by taking $u_i = u_0$ and $v_i = v_0$, for each $i = 1, 2, \ldots, n$. □

Note from Corollary 3.3 that if

$$\frac{\mu}{2}(v_0 - u_0)e - \widetilde{X}(A\bar{x} + a) \geq 0, \tag{26}$$

at a feasible point $\bar{x} = (\bar{x}_1, \ldots, \bar{x}_n)^{\mathrm{T}}$ of (BQP_1) then $\bar{x}$ is a global minimizer of (BQP_1), since (25) holds for $\lambda = 0$.

Observe that (26) collapses to the condition that

$$\left(\frac{v_0 - u_0}{2}\right)\mu e \geq \left(\frac{v_0 - u_0}{2}\right)\widetilde{X}A\widetilde{x} + \widetilde{X}a + \left(\frac{v_0 + u_0}{2}\right)\widetilde{X}Ae, \tag{27}$$

where $\widetilde{x} = \left(\frac{2}{v_0 - u_0}\right)\bar{x} + \left(\frac{v_0+u_0}{2}\right)e$. So, (27) is just (2.7) of [3].

Corollary 3.4. (Theorem 2.3 [3]) *For* (BQP_1), *let* $u_0 = -1$ *and* $v_0 = 1$. *Let* $\bar{x} = (\bar{x}_1, \ldots, \bar{x}_n)^T$ *be a feasible point of* (BQP_1). *If*

$$\mu e - \widetilde{X}(A\bar{x} + a) \geq 0 \tag{28}$$

then $\bar{x}$ *is a global minimizer of problem* (BQP_1).

Proof The inequality (28) gives us that (25) holds for $\lambda = 0, u_0 = -1$ and $v_0 = 1$. The conclusion follows from Corollary 3.3 by taking $\lambda = 0$, $u_0 = -1$ and $v_0 = 1$. □

The following example illustrates the case where (28) is not satisfied at a global minimizer, whereas (25) holds at a global minimizer.

Example 3.1. Consider the following problem:

$$\text{(EP3)} \qquad \min_{x \in \mathbb{R}^4} f(x) = -\frac{1}{2}x_1^2 + 2x_1x_2 + x_1x_4 - \frac{1}{2}x_2^2 + x_2x_3 + 3x_3^2 - x_3x_4 - x_4^2 + 4x_1 + \frac{9}{2}x_2 - x_3 - x_4$$

$$\text{s.t.} \quad x \in S_B = \prod_{i=1}^{4}\{-1, 1\},$$

where the objective function is the same as in Example 2.2. Let

$$A = \begin{pmatrix} -1 & 2 & 0 & 1 \\ 2 & -1 & 1 & 0 \\ 0 & 1 & 6 & -1 \\ 1 & 0 & -1 & -2 \end{pmatrix}$$

and $a_1 = 4, a_2 = \frac{9}{2}, a_3 = -1, a_4 = -1$, $u_i = -1$ and $v_i = 1, i = 1, 2, 3, 4$. Let $\bar{x} = (-1, -1, 1, 1)^T$. Then $A\bar{x} = (0, 0, 4, -4)^T$ and $\widehat{A}_\lambda = \text{diag}(-4, -4, 4, -4)$ with $\lambda = 1$. Thus,

$$\widetilde{X}(A\bar{x} + a) - \frac{1}{2}A_\lambda(v - u) = \left(0, -\frac{1}{2}, -1, -1\right)^T \leq 0,$$

and so, $\bar{x}$ satisfies (25) for $\lambda = 1$ and is a global minimizer of (EP3). Using MATLAB, we obtain that the least eigenvalue of A is $\mu = -3.4$. Thus, A is an indefinite matrix. But $\bar{x} = (-1, -1, 1, 1)^T$ does not satisfy (28) since for $i = 3$, $\mu = -3.4 < a_3 + (A\bar{x})_3 = 3$. It is easy to check that $\bar{x} = (-1, -1, 1, 1)^T$ is not a global minimizer of (EP2) with the box constraints.

4 Conclusion and future work

In this paper, we have established conditions which ensure that a feasible point is a global minimizer of a general quadratic minimization problem with box constraints or binary constraints. Our global optimality conditions apply to concave quadratic minimization problems as well as to indefinite quadratic programs and they completely characterize global optimality for weighted least squares problems. We have presented a new approach to studying global minimizers of non-convex quadratic optimization problems using a global subdifferential. We have shown how a global subdifferential can be calculated for a quadratic function.

This approach together with the well-known Lagrangian method would allow us to characterize global minimizers of quadratic optimization problems involving quadratic inequality constraints. On the other hand, the problem of calculating L-subdifferentials for suitably chosen L, which is formed by not necessary quadratic functions, remains open. An affirmative response to this problem will result in the development of global optimality conditions for more general non-convex optimization problems. These problems will be treated elsewhere.

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