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CANONICAL DUAL APPROACH TO SOLVING 0-1 QUADRATIC PROGRAMMING PROBLEMS

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Abstract. By using the *canonical dual transformation* developed recently, we derive a pair of canonical dual problems for 0-1 quadratic programming problems in both minimization and maximization form. Regardless convexity, when the canonical duals are solvable, no duality gap exists between the primal and corresponding dual problems. Both global and local optimality conditions are given. An algorithm is presented for finding global minimizers, even when the primal objective function is not convex. Examples are included to illustrate this new approach.

1. Introduction.

In this paper, we consider a simple 0-1 quadratic programming problem in the following form:

$$(\mathcal{P}): \qquad \min/\max\left\{P(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T Q\mathbf{x} - \mathbf{f}^T\mathbf{x} \;\mid\; \mathbf{x} \in \mathcal{X}_a\right\}, \tag{1}$$

where $\mathbf{x}$ and $\mathbf{f}$ are real n-vectors, $Q \in \mathbb{R}^{n\times n}$ is a symmetrical matrix of order n and

$$\mathcal{X}_a = \{\mathbf{x} \in \mathbb{R}^n \mid 0 \le x_i \le 1, \; i = 1, 2, ..., n\} \cap \mathcal{I}^n. \tag{2}$$

with $\mathcal{I}^n = \{\mathbf{x} \in \mathbb{R}^n | \;\; x_i \text{ is an integer}, \;\; i = 1, 2, ..., n\}$. Since the Q matrix in the objective function $P(\mathbf{x})$ can be indefinite, we use the notation "min/max" to indicate that we are interested in finding both minimizers and maximizers.

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Integer programming and quadratic programming problems appear naturally in system science and engineering with wide applications [16, 1]. Our primal problem is a very simple version. Nevertheless, it still possesses the main difficulties in integer programming problems, namely, the 0-1 integer requirement results in combinatorial complexity and the nonconvexity of the object function complicates the finding of a global solution (see [12, 13]). Classical dual approaches [14, 15] may suffer from having potential duality gaps.

The goal of this paper is to explore the potential of using the recently developed *canonical duality theory* [2] to characterize the solutions of our primal problem and design a solution procedure for finding global optimizers. The canonical duality theory was originally developed for handling general nonconvex and/or nonsmooth systems. It is composed mainly of a canonical dual transformation and an associated *triality theory*. The canonical dual transformation may convert some nonconvex and/or nonsmooth primal problems into smooth canonical dual problems without generating any duality gap, while the triality theory provides hints to identify both global and local extremum solutions. The canonical duality theory has shown its potential for global optimization and nonconvex nonsmooth analysis [3, 4, 6, 7]. Comprehensive reviews of the canonical duality theory and its applications for finite and infinite dimensional systems can be found in [5, 10].

The rest of this paper is arranged as follows. In Section 2, we show that the canonical dual transformation can lead our nonconvex 0-1 programming problem to a pair of dual problems in the continuous space with zero duality gap. Then a set of KKT solutions to the primal problem are obtained. The extremality conditions of these KKT solutions are explicitly specified in Section 3 using the associated triality theory. Some examples are given in Section 4 to illustrate this new approach. Finally, we present an algorithm for finding a global solution to large scale 0-1 quadratic programming problems in Section 5. Some concluding remarks are made in the last section.

2. **Canonical dual approach.** For easy manipulation, we first consider the minimization problem and rewrite our primal problem $(\mathcal{P})$ as

$$(\mathcal{P}_{\min}): \quad \min\left\{P(\mathbf{x}) = W(\mathbf{x}) + \frac{1}{2}\mathbf{x}^T Q\mathbf{x} - \mathbf{f}^T\mathbf{x} \;\mid\; \mathbf{x} \in \mathcal{I}^n\right\}, \tag{3}$$

where $W(\mathbf{x})$ is an indicator of the box constraints $0 \leq x_i \leq 1, \quad i = 1, 2, ..., n$, defined by

$$W(\mathbf{x}) = \begin{cases} 0 & \text{if } 0 \leq x_i \leq 1, \;\; i = 1, 2, ..., n, \\ +\infty & \text{otherwise.} \end{cases} \tag{4}$$

By the standard canonical dual transformation (see [2, 4, 7]), we introduce a nonlinear transformation (i.e. the so-called *geometrical mapping*) $\mathbf{y} = \Lambda(\mathbf{x}) \in \mathbb{R}^n$ with $y_i = x_i(x_i - 1)$ and let

$$V(\mathbf{y}) = \begin{cases} 0 & \text{if } \mathbf{y} \leq \mathbf{0} \in \mathbb{R}^n, \\ +\infty & \text{otherwise.} \end{cases} \tag{5}$$

Clearly, we have $W(\mathbf{x}) = V(\Lambda(\mathbf{x}))$. Thus, the primal problem $(\mathcal{P})$ can be written in the following canonical form [4, 7]:

$$(\mathcal{P}_{\min}): \quad \min\left\{P(\mathbf{x}) = V(\Lambda(\mathbf{x})) + \frac{1}{2}\mathbf{x}^T Q\mathbf{x} - \mathbf{f}^T\mathbf{x} \mid \; \mathbf{x} \in \mathcal{I}^n\right\}. \tag{6}$$

According to the Fenchel transformation, the sup-conjugate $V^\sharp$ of the function $V(\mathbf{y})$ is defined by

$$V^\sharp(\boldsymbol{\sigma}) = \sup_{\mathbf{y}\in\mathbb{R}^n} \{\mathbf{y}^T\boldsymbol{\sigma} - V(\mathbf{y})\} = \begin{cases} 0 & \text{if } \boldsymbol{\sigma} \geq \mathbf{0} \in \mathbb{R}^n, \\ +\infty & \text{otherwise.} \end{cases}$$

Since $V(\mathbf{y})$ is a proper closed convex function over $\mathbb{R}^n_- := \{\mathbf{y} \in \mathbb{R}^n | \ \mathbf{y} \leq \mathbf{0}\}$, we know that

$$\boldsymbol{\sigma} \in \partial V(\mathbf{y}) \quad \Leftrightarrow \quad \mathbf{y} \in \partial V^\sharp(\boldsymbol{\sigma}) \quad \Leftrightarrow \quad V(\mathbf{y}) + V^\sharp(\boldsymbol{\sigma}) = \mathbf{y}^T\boldsymbol{\sigma}. \tag{7}$$

The pair of $(\mathbf{y}, \boldsymbol{\sigma})$ is called a *generalized canonical dual pair* on $\mathbb{R}^n_- \times \mathbb{R}^n_+$ as defined in [2, 3]. By the definition of sub-differential, it is easy to verify that the canonical duality relations of (7) are equivalent to

$$\mathbf{y} \leq \mathbf{0}, \;\; \boldsymbol{\sigma} \geq \mathbf{0}, \;\; \mathbf{y}^T\boldsymbol{\sigma} = 0.$$

In particular, if $\boldsymbol{\sigma} > \mathbf{0}$ then the complementarity condition $\mathbf{y}^T\boldsymbol{\sigma} = 0$ leads to $\mathbf{y} = \mathbf{0}$, and consequently $\mathbf{x} \in \mathcal{X}_a$. Thus, for our 0-1 integer program, the dual feasible space is an open convex cone

$$\mathcal{S}_\sharp = \{\boldsymbol{\sigma} \in \mathbb{R}^n \mid \boldsymbol{\sigma} > \mathbf{0}\}.$$

Following the idea of [11], we let $\mathcal{X} = \mathbb{R}^n$ and replace $V(\Lambda(\mathbf{x}))$ in equation (6) by the Fenchel-Young equality $V(\Lambda(\mathbf{x})) = \Lambda(\mathbf{x})^T\boldsymbol{\sigma} - V^\sharp(\boldsymbol{\sigma})$. Then the so-called *total complementary function* $\Xi(\mathbf{x}, \boldsymbol{\sigma}) : \mathcal{X} \times \mathcal{S}_\sharp \to \mathbb{R}$ associated with the problem $(\mathcal{P}_{min})$ can be defined as below

$$\Xi(\mathbf{x}, \boldsymbol{\sigma}) = \Lambda(\mathbf{x})^T\boldsymbol{\sigma} - V^\sharp(\boldsymbol{\sigma}) + \frac{1}{2}\mathbf{x}^T Q\mathbf{x} - \mathbf{f}^T\mathbf{x}.$$

By the definition of $\Lambda(\mathbf{x})$ and $V^\sharp(\boldsymbol{\sigma})$, we have

$$\Xi(\mathbf{x}, \boldsymbol{\sigma}) = \frac{1}{2}\mathbf{x}^T Q_d(\boldsymbol{\sigma})\mathbf{x} - \mathbf{x}^T(\mathbf{f} + \boldsymbol{\sigma}), \tag{8}$$

where

$$Q_d(\boldsymbol{\sigma}) = Q + 2\text{Diag }(\boldsymbol{\sigma})$$

and Diag $(\boldsymbol{\sigma}) \in \mathbb{R}^{n\times n}$ ia a diagonal matrix with σ_i, $i = 1, 2, ..., n$, being its diagonal elements. Thus, for any given $\boldsymbol{\sigma} \in \mathcal{S}_\sharp$, the canonical dual function $P^d(\boldsymbol{\sigma})$ can be defined by $\Xi(\bar{\mathbf{x}}, \boldsymbol{\sigma})$ with $\bar{\mathbf{x}}$ being a stationary point of $\Xi(\mathbf{x}, \boldsymbol{\sigma})$ with respect to $\mathbf{x} \in \mathcal{X}$. Notice that the total complementary function $\Xi(\mathbf{x}, \boldsymbol{\sigma})$ is a quadratic function of $\mathbf{x} \in \mathcal{X}$ and for any given $\boldsymbol{\sigma} \in \mathbb{R}^n$ such that $\det Q_d(\boldsymbol{\sigma}) \neq 0$, $\Xi(\mathbf{x}, \boldsymbol{\sigma})$ has a unique stationary (critical) point $\mathbf{x} = [Q_d(\boldsymbol{\sigma})]^{-1}(\mathbf{f} + \boldsymbol{\sigma})$. Thus, on the dual feasible space $\mathcal{S}^a_\sharp \subset \mathcal{S}_\sharp$ defined as

$$\mathcal{S}^a_\sharp := \{\boldsymbol{\sigma} \in \mathbb{R}^n \mid \boldsymbol{\sigma} > \mathbf{0}, \;\; \det Q_d(\boldsymbol{\sigma}) \neq 0\},$$

the stationary solution of $\Xi(\mathbf{x}, \boldsymbol{\sigma})$ over $\mathbf{x} \in \mathcal{X}$ happens at $\mathbf{x} = [Q_d(\boldsymbol{\sigma})]^{-1}(\mathbf{f} + \boldsymbol{\sigma})$ with a value of

$$P^d(\boldsymbol{\sigma}) = -\frac{1}{2}(\mathbf{f} + \boldsymbol{\sigma})^T Q_d^{-1}(\boldsymbol{\sigma})(\mathbf{f} + \boldsymbol{\sigma}). \tag{9}$$

Now, we use the notation

$$\text{sta}\{h(\mathbf{x}) \mid \; \mathbf{x} \in \mathcal{X}\},$$

to represent the task of finding stationary points of a given function $h(\mathbf{x})$ with respect to $\mathbf{x} \in \mathcal{X}$. The *canonical dual* problem for our primal problem $(\mathcal{P}_{min})$ can be proposed as follows:

$$(\mathcal{P}^d_\sharp): \;\; \text{sta}\left\{P^d(\boldsymbol{\sigma}) = -\frac{1}{2}(\mathbf{f} + \boldsymbol{\sigma})^T[Q_d(\boldsymbol{\sigma})]^{-1}(\mathbf{f} + \boldsymbol{\sigma}) \;\mid\; \boldsymbol{\sigma} \in \mathcal{S}^a_\sharp\right\}. \tag{10}$$

The following theorem characterizes a key primal-dual relationship:

Theorem 1. *The canonical dual problem* ($\mathcal{P}^d_\sharp$) *is perfectly dual to the primal problem* ($\mathcal{P}_{\min}$) *in the sense that if* $\bar{\boldsymbol{\sigma}}$ *is a critical point of* $P^d(\boldsymbol{\sigma})$ *and* $\bar{\boldsymbol{\sigma}} > 0$*, then the vector*

$$\bar{\mathbf{x}} = [Q_d(\bar{\boldsymbol{\sigma}})]^{-1}(\mathbf{f} + \bar{\boldsymbol{\sigma}}) \tag{11}$$

is a KKT point of ($\mathcal{P}_{\min}$) *and*

$$P(\bar{\mathbf{x}}) = P^d(\bar{\boldsymbol{\sigma}}). \tag{12}$$

Proof. By introducing the Lagrange multiplier vector $\boldsymbol{\gamma} \in \mathbb{R}^n$ to relax the inequality constraint $\boldsymbol{\sigma} > \mathbf{0}$ in $\mathcal{S}^a_\sharp$, the Lagrangean function associated with the total complementary function $\Xi(\mathbf{x}, \boldsymbol{\sigma})$ defined by (8) becomes

$$L(\mathbf{x}, \boldsymbol{\sigma}; \boldsymbol{\gamma}) = \Xi(\mathbf{x}, \boldsymbol{\sigma}) + \boldsymbol{\gamma}^T \boldsymbol{\sigma}.$$

Then the KKT conditions of the primal problem ($\mathcal{P}$) become

$$\frac{\partial L}{\partial \mathbf{x}} = Q_d(\bar{\boldsymbol{\sigma}})\bar{\mathbf{x}} - (\mathbf{f} + \bar{\boldsymbol{\sigma}}) = 0, \tag{13}$$

$$\frac{\partial L}{\partial \boldsymbol{\sigma}} = \bar{\mathbf{x}} \circ [\bar{\mathbf{x}} - \mathbf{e}] + \boldsymbol{\gamma} = \mathbf{0}, \tag{14}$$

$$\boldsymbol{\gamma} \leq \mathbf{0}, \;\; \bar{\boldsymbol{\sigma}} > 0, \;\; \boldsymbol{\gamma}^T \bar{\boldsymbol{\sigma}} = 0, \tag{15}$$

where $\mathbf{e}$ is an n-vector of all ones and the notation $\mathbf{s} \circ \mathbf{t} := (s_1 t_1, s_2 t_2, \ldots, s_n t_n)$ denotes the Madamard product for any two vectors $\mathbf{s}, \mathbf{t} \in \mathbb{R}^n$. The first condition leads to $\bar{\mathbf{x}} = [Q_d(\bar{\boldsymbol{\sigma}})]^{-1}(\mathbf{f} + \bar{\boldsymbol{\sigma}})$. The complementary condition $\boldsymbol{\gamma}^T \bar{\boldsymbol{\sigma}} = 0$ in (15) shows that if $\bar{\boldsymbol{\sigma}} > \mathbf{0}$, then the Lagrange multiplier $\boldsymbol{\gamma} = \mathbf{0}$. Consequently, the second condition leads to the integer requirement

$$\bar{\mathbf{x}} \circ (\bar{\mathbf{x}} - \mathbf{e}) = \mathbf{0}. \tag{16}$$

Replacing $\bar{\mathbf{x}}$ by $[Q_d(\bar{\boldsymbol{\sigma}})]^{-1}(\mathbf{f} + \bar{\boldsymbol{\sigma}})$ in (16) we have

$$[Q_d(\bar{\boldsymbol{\sigma}})]^{-1}(\mathbf{f} + \bar{\boldsymbol{\sigma}}) \circ \left([Q_d(\bar{\boldsymbol{\sigma}})]^{-1}(\mathbf{f} + \bar{\boldsymbol{\sigma}}) - \mathbf{e}\right) = \mathbf{0},$$

which is exactly the critical point condition of $\nabla P^d(\bar{\boldsymbol{\sigma}}) = 0$. This proved that if $\bar{\boldsymbol{\sigma}} > 0$ is a critical point of $P^d(\boldsymbol{\sigma})$, the vector $\bar{\mathbf{x}}(\bar{\boldsymbol{\sigma}})$ defined by (11) is a KKT point of the primal problem ($\mathcal{P}_{\min}$).

Moreover, the equation (16) implies $\bar{\mathbf{y}} = \Lambda(\bar{\mathbf{x}}) = \mathbf{0}$. This leads to $V(\bar{\mathbf{y}}) = 0$ by (5). Since $\bar{\boldsymbol{\sigma}} > 0$, we also have $V^\sharp(\bar{\boldsymbol{\sigma}}) = 0$. Therefore,

$$\begin{aligned}\Xi(\bar{\mathbf{x}}, \bar{\boldsymbol{\sigma}}) &= \Lambda(\bar{\mathbf{x}})^T \bar{\boldsymbol{\sigma}} - V^\sharp(\bar{\boldsymbol{\sigma}}) + \frac{1}{2}\bar{\mathbf{x}}^T Q \bar{\mathbf{x}} - \bar{\mathbf{x}}^T \mathbf{f} \\ &= \frac{1}{2}\bar{\mathbf{x}}^T Q \bar{\mathbf{x}} - \bar{\mathbf{x}}^T \mathbf{f} = P(\bar{\mathbf{x}}).\end{aligned}$$

On the other hand,

$$\begin{aligned}\Xi(\bar{\mathbf{x}}, \bar{\boldsymbol{\sigma}}) &= \frac{1}{2}\bar{\mathbf{x}}^T Q_d(\bar{\boldsymbol{\sigma}})\bar{\mathbf{x}} - \bar{\mathbf{x}}^T(\mathbf{f} + \bar{\boldsymbol{\sigma}}) \\ &= \frac{1}{2}\bar{\mathbf{x}}^T(\mathbf{f} + \bar{\boldsymbol{\sigma}}) - \bar{\mathbf{x}}^T(\mathbf{f} + \bar{\boldsymbol{\sigma}}) \\ &= -\frac{1}{2}\bar{\mathbf{x}}^T(\mathbf{f} + \bar{\boldsymbol{\sigma}}) = P^d(\bar{\boldsymbol{\sigma}}).\end{aligned}$$

This completes the proof. □

Now let us consider the maximization of the problem $(\mathcal{P})$ by letting

$$(\mathcal{P}_{\max}): \quad \max\left\{P(\mathbf{x}) = -W(\mathbf{x}) + \frac{1}{2}\mathbf{x}^T Q\mathbf{x} - \mathbf{f}^T\mathbf{x} \;\mid\; \mathbf{x} \in \mathcal{I}^n\right\}, \tag{17}$$

In this case, we take the canonical function (5) in the form of

$$V(\mathbf{y}) = \begin{cases} 0 & \text{if } \mathbf{y} \leq \mathbf{0}, \\ -\infty & \text{otherwise,} \end{cases} \tag{18}$$

then it is a proper closed concave function with the following Fenchel inf-conjugate

$$V^\flat(\boldsymbol{\sigma}) = \inf_{\mathbf{y}\in\mathbb{R}^n}\{\mathbf{y}^T\boldsymbol{\sigma} - V(\mathbf{y})\} = \begin{cases} 0 & \text{if } \boldsymbol{\sigma} \leq 0, \\ -\infty & \text{otherwise.} \end{cases}$$

Dual to $\mathcal{S}_\sharp$, we let

$$\mathcal{S}_\flat = \{\boldsymbol{\sigma} \in \mathbb{R}^n \mid \boldsymbol{\sigma} < \mathbf{0}\}.$$

Then the corresponding generalized complementary function $\Xi(\mathbf{x}, \boldsymbol{\sigma}) : \mathcal{X} \times \mathcal{S}_\flat \to \mathbb{R}$ can be written as

$$\begin{aligned} \Xi(\mathbf{x}, \boldsymbol{\sigma}) &= \Lambda(\mathbf{x})^T\boldsymbol{\sigma} - V^\flat(\boldsymbol{\sigma}) + \frac{1}{2}\mathbf{x}^T Q\mathbf{x} - \mathbf{f}^T\mathbf{x}, \\ &= \frac{1}{2}\mathbf{x}^T Q_d(\boldsymbol{\sigma})\mathbf{x} - \mathbf{x}^T(\mathbf{f} + \boldsymbol{\sigma}). \end{aligned} \tag{19}$$

Parallel to what we did before, we can define another *canonical dual* problem for the primal problem $(\mathcal{P})$ as follows:

$$(\mathcal{P}^d_\flat): \text{ sta}\left\{P^d(\boldsymbol{\sigma}) = -\frac{1}{2}(\mathbf{f} + \boldsymbol{\sigma})^T[Q_d(\boldsymbol{\sigma})]^{-1}(\mathbf{f} + \boldsymbol{\sigma}) \;\mid\; \boldsymbol{\sigma} \in \mathcal{S}^a_\flat\right\}, \tag{20}$$

where

$$\mathcal{S}^a_\flat := \{\boldsymbol{\sigma} \in \mathbb{R}^n \mid \boldsymbol{\sigma} < \mathbf{0}, \;\; \det Q_d(\boldsymbol{\sigma}) \neq 0\}.$$

Moreover, the following result follows:

Theorem 2. *The canonical dual problem $(\mathcal{P}^d_\flat)$ is perfectly dual to the primal problem $(\mathcal{P}_{\max})$ in the sense that if $\bar{\boldsymbol{\sigma}}$ is a critical point of $P^d(\boldsymbol{\sigma})$ and $\bar{\boldsymbol{\sigma}} < 0$, then the vector $\bar{\mathbf{x}}(\bar{\boldsymbol{\sigma}}) = [Q_d(\bar{\boldsymbol{\sigma}})]^{-1}(\mathbf{f} + \bar{\boldsymbol{\sigma}})$ is a KKT point of $(\mathcal{P}_{\max})$ and*

$$P(\bar{\mathbf{x}}) = P^d(\bar{\boldsymbol{\sigma}}). \tag{21}$$

The proof of this theorem parallels to the proof of the theorem 1.

Observation 1. *Theorems 1 and 2 show that by using the canonical dual transformation, the discrete integer problems $(\mathcal{P}_{\min})$ and $(\mathcal{P}_{\max})$ can be converted respectively into continuous dual problems $(\mathcal{P}^d_\sharp)$ and $(\mathcal{P}^d_\flat)$, a critical point solution of $\nabla P^d(\bar{\boldsymbol{\sigma}}) = 0$ with either $\bar{\boldsymbol{\sigma}} > 0$ or $\bar{\boldsymbol{\sigma}} < 0$ provides a KKT point of $\bar{\mathbf{x}}(\bar{\boldsymbol{\sigma}})$ as defined by (11) for the 0-1 quadratic programming problem $(\mathcal{P})$. The inequality of* $\det Q_d(\boldsymbol{\sigma}) \neq 0$ *in the dual feasible spaces $\mathcal{S}^a_\sharp$ and $\mathcal{S}^a_\flat$ is essentially not a constraint as indicated in* [7]. *Actually, the singularity* $\det Q_d(\boldsymbol{\sigma}) = 0$ *plays an important role in nonconvex analysis* [8].

However, the KKT conditions are only necessary conditions for local minimizers to satisfy for nonconvex programming problems. To identify a global minimizer among all KKT points $\bar{\mathbf{x}}(\bar{\boldsymbol{\sigma}})$ remains a key task for us to address in the next section.

3. **Global and local optimality conditions.** In order to study the extremality conditions for both local and global optimal solutions, by combining the properties associated with the pair of the canonical dual problems, we introduce the following four sets for consideration:

$$\mathcal{S}_\sharp^+ = \{\boldsymbol{\sigma} \in \mathbb{R}^n | \ \boldsymbol{\sigma} > 0, \ \ Q_d(\boldsymbol{\sigma}) \text{ is positive definite}\}, \tag{22}$$

$$\mathcal{S}_\sharp^- = \{\boldsymbol{\sigma} \in \mathbb{R}^n | \ \boldsymbol{\sigma} > 0, \ \ Q_d(\boldsymbol{\sigma}) \text{ is negative definite}\}, \tag{23}$$

$$\mathcal{S}_\flat^- = \{\boldsymbol{\sigma} \in \mathbb{R}^n | \ \boldsymbol{\sigma} < 0, \ \ Q_d(\boldsymbol{\sigma}) \text{ is negative definite}\}, \tag{24}$$

$$\mathcal{S}_\flat^+ = \{\boldsymbol{\sigma} \in \mathbb{R}^n | \ \boldsymbol{\sigma} < 0, \ \ Q_d(\boldsymbol{\sigma}) \text{ is positive definite}\}. \tag{25}$$

Then we have the following result on the global and local optimality conditions:

Theorem 3. *Let Q be a symmetrix matrix and $\mathbf{f} \in \mathbb{R}^n$. Assume that $\bar{\boldsymbol{\sigma}}$ is critical point of $P^d(\boldsymbol{\sigma})$ and $\bar{\mathbf{x}} = [Q_d(\bar{\boldsymbol{\sigma}})]^{-1}(\mathbf{f} + \bar{\boldsymbol{\sigma}})$.*

(a) If $\bar{\boldsymbol{\sigma}} \in \mathcal{S}_\sharp^+$, then $\bar{\mathbf{x}}$ is a global minimizer of $P(\mathbf{x})$ over $\mathcal{X}_a$ and $\bar{\boldsymbol{\sigma}}$ is a global maximizer of $P^d(\boldsymbol{\sigma})$ over $\mathcal{S}_\sharp^+$ with

$$P(\bar{\mathbf{x}}) = \min_{\mathbf{x} \in \mathcal{X}_a} P(\mathbf{x}) = \max_{\boldsymbol{\sigma} \in \mathcal{S}_\sharp^+} P^d(\boldsymbol{\sigma}) = P^d(\bar{\boldsymbol{\sigma}}). \tag{26}$$

(b) If $\bar{\boldsymbol{\sigma}} \in \mathcal{S}_\sharp^-$, then $\bar{\mathbf{x}}$ is a local minimizer of $P(\mathbf{x})$ over $\mathcal{X}_a$ if and only if $\bar{\boldsymbol{\sigma}}$ is a local minimizer of $P^d(\boldsymbol{\sigma})$ over $\mathcal{S}_\sharp^-$, i.e., in a neighborhood $\mathcal{X}_o \times \mathcal{S}_o \subset \mathcal{X}_a \times \mathcal{S}_\sharp^-$ of $(\bar{\mathbf{x}}, \bar{\boldsymbol{\sigma}})$,

$$P(\bar{\mathbf{x}}) = \min_{\mathbf{x} \in \mathcal{X}_o} P(\mathbf{x}) = \min_{\boldsymbol{\sigma} \in \mathcal{S}_o} P^d(\boldsymbol{\sigma}) = P^d(\bar{\boldsymbol{\sigma}}). \tag{27}$$

(c) If $\bar{\boldsymbol{\sigma}} \in \mathcal{S}_\flat^-$, then $\bar{\mathbf{x}}$ is a global maximizer of $P(\mathbf{x})$ over $\mathcal{X}_a$ and $\bar{\boldsymbol{\sigma}}$ is a global minimizer of $P^d(\boldsymbol{\sigma})$ over $\mathcal{S}_\flat^-$ with

$$P(\bar{\mathbf{x}}) = \max_{\mathbf{x} \in \mathcal{X}_a} P(\mathbf{x}) = \min_{\boldsymbol{\sigma} \in \mathcal{S}_\flat^-} P^d(\boldsymbol{\sigma}) = P^d(\bar{\boldsymbol{\sigma}}). \tag{28}$$

(d) If $\bar{\boldsymbol{\sigma}} \in \mathcal{S}_\flat^+$, then $\bar{\mathbf{x}}$ is a local maximizer of $P(\mathbf{x})$ over $\mathcal{X}_a$ if and only if $\bar{\boldsymbol{\sigma}}$ is a local maximizer of $P^d(\boldsymbol{\sigma})$ over $\mathcal{S}_\flat^+$, i.e., in a neighborhood $\mathcal{X}_o \times \mathcal{S}_o \subset \mathcal{X}_a \times \mathcal{S}_\flat^+$ of $(\bar{\mathbf{x}}, \bar{\boldsymbol{\sigma}})$,

$$P(\bar{\mathbf{x}}) = \max_{\mathbf{x} \in \mathcal{X}_o} P(\mathbf{x}) = \max_{\boldsymbol{\sigma} \in \mathcal{S}_o} P^d(\boldsymbol{\sigma}) = P^d(\bar{\boldsymbol{\sigma}}). \tag{29}$$

Proof. (a) Notice that the canonical dual function $P^d(\boldsymbol{\sigma})$ is concave on $\mathcal{S}_\sharp^+$. For a critical point $\bar{\boldsymbol{\sigma}} \in \mathcal{S}_\sharp^+$, it must be a global maximizer of $P^d(\boldsymbol{\sigma})$ on $\mathcal{S}_\sharp^+$. By the fact that for any given $\boldsymbol{\sigma} \in \mathcal{S}_\sharp^+$, the complementary function $\Xi(\mathbf{x}, \boldsymbol{\sigma})$ is convex in $\mathbf{x}$ and concave in $\boldsymbol{\sigma}$, the critical point $(\bar{\mathbf{x}}, \bar{\boldsymbol{\sigma}}) \in \mathcal{X}_a \times \mathcal{S}_\sharp^+$ is a saddle point of Ξ with

$$\begin{aligned}
P^d(\bar{\boldsymbol{\sigma}}) &= \max_{\boldsymbol{\sigma} \in \mathcal{S}_\sharp^+} P^d(\boldsymbol{\sigma}) \\
&= \max_{\boldsymbol{\sigma} \in \mathcal{S}_\sharp^+} \min_{\mathbf{x} \in \mathbb{R}^n} \Xi(\mathbf{x}, \boldsymbol{\sigma}) = \min_{\mathbf{x} \in \mathbb{R}^n} \max_{\boldsymbol{\sigma} \in \mathcal{S}_\sharp^+} \Xi(\mathbf{x}, \boldsymbol{\sigma}) \\
&= \min_{\mathbf{x} \in \mathbb{R}^n} \left\{ \frac{1}{2}\mathbf{x}^T Q \mathbf{x} - \mathbf{f}^T \mathbf{x} + \max_{\boldsymbol{\sigma} \in \mathcal{S}_\sharp^+} \left\{ \sum_{i=1}^n (x_i^2 - x_i)\sigma_i \right\} \right\} \\
&= \min_{\mathbf{x} \in \mathcal{X}_a} P(\mathbf{x}).
\end{aligned}$$

The last equation in the above expression is obtained because the following result of linear programming

$$\max_{\boldsymbol{\sigma}\in\mathcal{S}_\sharp^+}\left\{\sum_{i=1}^n (x_i^2 - x_i)\sigma_i\right\} = \begin{cases} 0 & \text{if } x \in \mathcal{X}_a, \\ \infty & \text{otherwise.}\end{cases}$$

leads to the canonical function $V(\Lambda(\mathbf{x}))$, which has a finite value in the open domain $\mathcal{S}_\sharp^+$ if and only if $\mathbf{x} \in \mathcal{X}_a$. Then Theorem 1 assures (26).

(b) For $\bar{\boldsymbol{\sigma}} \in \mathcal{S}_\sharp^-$, the matrix $Q_d(\bar{\boldsymbol{\sigma}}) = Q + 2\ \mathrm{Diag}\ (\bar{\boldsymbol{\sigma}})$ is negative definite. In this case, the total complementary function $\Xi(\mathbf{x}, \boldsymbol{\sigma})$ is a so-called *super-critical function* (see [2]). It is locally concave in both $\mathbf{x} \in \mathbb{R}^n$ and $\boldsymbol{\sigma} \in \mathcal{S}_\sharp^-$. By the super-Lagrangian duality developed in [2, 6], if $(\bar{\mathbf{x}}, \bar{\boldsymbol{\sigma}})$ is a critical point of $\Xi(\mathbf{x}, \boldsymbol{\sigma})$, then in a neighborhood $\mathcal{X}_o \times \mathcal{S}_o \subset \mathbb{R}^n \times \mathcal{S}_\sharp^-$ of $(\bar{\mathbf{x}}, \bar{\boldsymbol{\sigma}})$ the following super-Lagrangian duality relation holds:

$$\min_{\mathbf{x}\in\mathcal{X}_o}\max_{\boldsymbol{\sigma}\in\mathcal{S}_o}\Xi(\mathbf{x},\boldsymbol{\sigma}) = \min_{\boldsymbol{\sigma}\in\mathcal{S}_o}\max_{\mathbf{x}\in\mathcal{X}_o}\Xi(\mathbf{x},\boldsymbol{\sigma}). \tag{30}$$

Since for each $\boldsymbol{\sigma} \in \mathcal{S}_o \subset \mathcal{S}_\sharp^-$, the total complementary function $\Xi(\mathbf{x}, \boldsymbol{\sigma})$ is locally concave in $\mathbf{x} \in \mathcal{X}_o$, we have

$$\max_{\mathbf{x}\in\mathcal{X}_o}\Xi(\mathbf{x},\boldsymbol{\sigma}) = P^d(\boldsymbol{\sigma}), \ \ \forall \boldsymbol{\sigma} \in \mathcal{S}_o \subset \mathcal{S}_\sharp^-.$$

On the other hand, if $\mathcal{X}_o$ is a subset of $\mathcal{X}_a$, then

$$\max_{\boldsymbol{\sigma}\in\mathcal{S}_o}\Xi(\mathbf{x},\boldsymbol{\sigma}) = P(\mathbf{x}), \ \ \forall \mathbf{x} \in \mathcal{X}_o \subset \mathcal{X}_a.$$

Thus, the equality (30) leads to (27).

The proof of statements (c) and (d) are parallel to that of (a) and (b), respectively, using Theorem 2. □

Several observations can be made here:

Observation 2. *When the integer constraints in $\mathcal{X}_a$ is relaxed, the problem $(\mathcal{P})$ becomes the following quadratic minimization problem with box constraints as studied in* [7]*:*

$$(\mathcal{P}_{box}): \quad \min/\max\left\{P(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T Q\mathbf{x} - \mathbf{x}^T\mathbf{f} \ \mid \ 0 \le \mathbf{x} \le 1\right\}. \tag{31}$$

Its canonical dual problem is

$$(\mathcal{P}_{box}^d): \ \ \mathrm{sta}\left\{P^d(\boldsymbol{\sigma}) \mid \boldsymbol{\sigma} \in \mathbb{R}^n, \ \det Q_d(\boldsymbol{\sigma}) \neq 0\right\}. \tag{32}$$

The following result follows immediately:

Corollary 1. *If $\bar{\boldsymbol{\sigma}}$ is a critical point of the problem $(\mathcal{P}_{box}^d)$, then the vector*

$$\bar{\mathbf{x}} = [Q_d(\bar{\boldsymbol{\sigma}})]^{-1}(\mathbf{f} + \bar{\boldsymbol{\sigma}}) \tag{33}$$

is a KKT point of $(\mathcal{P}_{box})$ and

$$P(\bar{\mathbf{x}}) = P^d(\bar{\boldsymbol{\sigma}}). \tag{34}$$

Moreover, if $\bar{\boldsymbol{\sigma}} \ge 0$ and $Q_d(\bar{\boldsymbol{\sigma}})$ is positive definite, then $\bar{\mathbf{x}}$ is a global minimizer of the problem $(\mathcal{P}_{box})$; if $\bar{\boldsymbol{\sigma}} \le 0$ and $Q_d(\bar{\boldsymbol{\sigma}})$ is negative definite, then $\bar{\mathbf{x}}$ is a global maximizer of the problem $(\mathcal{P}_{box})$.

Observation 3. *Theorem 3 says that when the matrix* $Q_d(\boldsymbol{\sigma}) = Q + 2Diag\ (\boldsymbol{\sigma})$ *is positive-definite, the canonical dual problem in equation (26) is a concave maximization problem over a convex open domain* $\mathcal{S}^+_\sharp$. *In general, for any given* $\mathbf{f} \in \mathbb{R}^n$, *if the matrix* Q *is "principal diagonal dominated" such that, for any given* $\boldsymbol{\sigma} \in \mathcal{S}^+_\sharp$, *the vector* $\mathbf{f} + \boldsymbol{\sigma}$ *falls in the column space of* $Q + 2Diag\ (\boldsymbol{\sigma})$, *then the canonical dual problem could have a unique global maximizer* $\bar{\boldsymbol{\sigma}} \in \mathcal{S}^+_\sharp$. *This leads to a global minimizer of the primal problem. However, if* Q *is not principal diagonal dominated, then for certain given* $\mathbf{f} \in \mathbb{R}^n$, *the canonical dual feasible domain* $\mathcal{S}^+_\sharp$ *could become empty. In this case, we can always choose a sufficiently large parameter* $\alpha > 0$ *such that* $Q + \alpha I \succ 0$ *and replace* $\mathbf{f}$ *by* $\mathbf{f} + \frac{1}{2}\alpha\mathbf{e}$ *due to the fact that* $\frac{1}{2}\alpha\mathbf{x} \circ \mathbf{x} = \frac{1}{2}\alpha\mathbf{x}$.

In many applications, the canonical dual solutions $\bar{\boldsymbol{\sigma}}$ could locate on the boundary of $\mathcal{S}^+_\sharp$, i.e. $\det Q_d(\bar{\boldsymbol{\sigma}}) = 0$. In this case, the primal problem may have more than one global minimizers. According to the generalized canonical duality theory (see equation (5.83) in [3]), the canonical dual problem should be replaced by

$$(\mathcal{P}^d_g): \ \max \left\{ P^d(\boldsymbol{\sigma}) = -\frac{1}{2}(\mathbf{f} + \boldsymbol{\sigma})^T [Q_d(\boldsymbol{\sigma})]^+ (\mathbf{f} + \boldsymbol{\sigma}) \mid \forall\ \boldsymbol{\sigma} \in \mathcal{S}^+_g \right\}, \qquad (35)$$

where $[Q_d(\boldsymbol{\sigma})]^+$ represents the Moore-Penrose generalized inverse of $Q_d(\boldsymbol{\sigma})$ and the canonical dual feasible space $\mathcal{S}^+_g$ is defined as

$$\mathcal{S}^+_g = \{\boldsymbol{\sigma} \in \mathbb{R}^n \mid \boldsymbol{\sigma} > 0,\ Q_d(\boldsymbol{\sigma}) \succeq 0\}.$$

Since the geometrical mapping $\Lambda(\mathbf{x})$ is a quadratic operator, the quadratic function $\frac{1}{2}\mathbf{x}^T Q_d(\boldsymbol{\sigma})\mathbf{x}$ is the Gao-Strang *complementary gap function*. According to the general theory developed in [11], if $\bar{\boldsymbol{\sigma}}$ is a KKT point of $(\mathcal{P}^d_g)$, the vector $\bar{\mathbf{x}} = [Q_d(\boldsymbol{\sigma})]^+(\mathbf{f} + \bar{\boldsymbol{\sigma}})$ is a global minimizer of $P(\mathbf{x})$ on $\mathcal{X}_a$. Detailed study on this generalized canonical dual problem is given in [9].

In case $Q = \text{Diag}\ (\mathbf{q})$, a diagonal matrix with q_i, $i = 1, 2, ...n$, being the diagonal elements, the criticality condition of $\nabla P^d(\bar{\boldsymbol{\sigma}}) = 0$ leads to 2^n dual critical solutions

$$\bar{\sigma}_i = \frac{1}{2}\{-q_i \pm (q_i - 2f_i)\} \ \text{ or equivalently, } \ \bar{\sigma}_i = -f_i \ \text{or} \ f_i - q_i, \ \ i = 1, 2, \ldots, n. \qquad (36)$$

Notice that $q_i + 2(-f_i) = q_i - 2f_i$ when $\bar{\sigma}_i = -f_i$, and $q_i + 2(f_i - q_i) = 2f_i - q_i$ when $\bar{\sigma}_i = f_i - q_i$. Therefore, if $\mathbf{q} \neq 2\mathbf{f}$, then $Q_d(\bar{\boldsymbol{\sigma}})$ must be invertible for such $\bar{\boldsymbol{\sigma}}$. Moreover, one of such $Q_d(\bar{\boldsymbol{\sigma}})$ is positive definite, another one is negative definite, and the rest $2^n - 2$ are indefinite. Each of these dual solutions provides a primal solution

$$\bar{\mathbf{x}} = Q_d^{-1}(\bar{\boldsymbol{\sigma}})(\mathbf{f} + \bar{\boldsymbol{\sigma}}) = \left\{ \frac{f_i + \bar{\sigma}_i}{q_i + 2\bar{\sigma}_i} \right\}. \qquad (37)$$

This leads to the next result.

Theorem 4. *For a 0-1 quadratic programming problem with any given* $\mathbf{q} \in \mathbb{R}^{\mathbf{n}}$ *such that* $Q = Diag\ (\mathbf{q})$ *and* $2\mathbf{f} \neq \mathbf{q}$, *if*

$$\boldsymbol{\sigma}^\sharp = \{\max\{-f_i, f_i - q_i\}\}, \qquad (38)$$

$$\boldsymbol{\sigma}^\flat = \{\min\{-f_i, f_i - q_i\}\}, \qquad (39)$$

and

$$\mathbf{x}^\sharp = Q_d^{-1}(\boldsymbol{\sigma}^\sharp)(\mathbf{f} + \boldsymbol{\sigma}^\sharp), \qquad (40)$$

$$\mathbf{x}^\flat = Q_d^{-1}(\boldsymbol{\sigma}^\flat)(\mathbf{f} + \boldsymbol{\sigma}^\flat), \qquad (41)$$

then the following statements hold:

(a) If $\boldsymbol{\sigma}^\sharp > \mathbf{0}$*, then* $\mathbf{x}^\sharp$ *is a global minimizer of* $P(\mathbf{x})$ *over* $\mathcal{X}_a$*.*
(b) If $\boldsymbol{\sigma}^\flat > \mathbf{0}$*, then* $\mathbf{x}^\flat$ *is a local minimizer of* $P(\mathbf{x})$ *over* $\mathcal{X}_a$*.*
(c) If $\boldsymbol{\sigma}^\flat < \mathbf{0}$*, then* $\mathbf{x}^\flat$ *is a global maximizer of* $P(\mathbf{x})$ *over* $\mathcal{X}_a$*.*
(d) If $\boldsymbol{\sigma}^\sharp < \mathbf{0}$*, then* $\mathbf{x}^\sharp$ *is a local maximizer of* $P(\mathbf{x})$ *over* $\mathcal{X}_a$

Proof. Notice that the larger λ_i is, so is $q_i + 2\lambda_i$. Since $q_i + 2\lambda_i$ is either $q_i - 2f_i$ or $2f_i - q_i$, by the assumption of $\mathbf{q} \neq 2\mathbf{f}$, $\boldsymbol{\sigma}^\sharp$ must correspond to the case with a positive definite $Q_d(\boldsymbol{\sigma}^\sharp)$. Similarly, we know $Q_d(\boldsymbol{\sigma}^\flat)$ is negative definite.

Theorem 3 then implies that (a) If $\boldsymbol{\sigma}^\sharp > 0$, then $\boldsymbol{\sigma}^\sharp \in \mathcal{S}_\sharp^+$ and $\mathbf{x}^\sharp$ is a global minimizer of $P(\mathbf{x})$ over $\mathcal{X}_a$; (b) If $\boldsymbol{\sigma}^\flat > 0$, then $\boldsymbol{\sigma}^\flat \in \mathcal{S}_\sharp^-$ and $\mathbf{x}^\flat$ is a local minimizer of $P(\mathbf{x})$ over $\mathcal{X}_a$; (c) If $\boldsymbol{\sigma}^\flat < 0$, then $\boldsymbol{\sigma}^\flat \in \mathcal{S}_\flat^-$ and $\mathbf{x}^\flat$ is a global maximizer of $P(\mathbf{x})$ over $\mathcal{X}_a$; and (d) If $\boldsymbol{\sigma}^\sharp < 0$, then $\boldsymbol{\sigma}^\sharp \in \mathcal{S}_\flat^+$ and $\mathbf{x}^\sharp$ is a local maximizer of $P(\mathbf{x})$ over $\mathcal{X}_a$. □

4. **Examples.** In this section, we use some examples to illustrate the theorems developed in the previous sections.

4.1. **One-dimensional problems.** For $n = 1$, we have the following primal problem

$$\min / \max \left\{ P(x) = \frac{1}{2} q x^2 - f x \;\mid\; x \in \{0, 1\} \right\}. \tag{42}$$

It is a concave minimization problem for $q < 0$. Its canonical dual problem becomes

$$\text{sta}\{P^d(\sigma) = -0.5(f + \sigma)^2/(q + 2\sigma) \mid\; q + 2\sigma \neq 0\}. \tag{43}$$

The criticality condition

$$\frac{\partial P^d(\sigma)}{\partial \sigma} = -\frac{(f+\sigma)(q+2\sigma) - (f+\sigma)^2}{(q+2\sigma)^2} = 0$$

has two real roots $\sigma_1 = -f$ and $\sigma_2 = f - q$.

Take it as an example with $q = -1$, $f = 0.5$ such that $q \neq 2f$. Then $\sigma^\sharp = \max\{-f, f - q\} = 1.5 > 0$ and $\sigma^\flat = \min\{-f, f - q\} = -0.5 < 0$. Using $\bar{x} = (f + \bar{\sigma})/(q + 2\bar{\sigma})$ results in

$$x^\sharp = 1, \;\; x^\flat = 0.$$

By Theorem 4 we know that $x^\sharp = 1$ is a global minimizer since $\sigma^\sharp = 1.5 \in \mathcal{S}_\sharp^+$, and $x^\flat = 0$ is a global maximizer since $\sigma^\flat \in \mathcal{S}_\flat^-$. It is easy to verify that

$$P(x_1) = -1 = P^d(\sigma_1) \;\text{ and }\; P(x_2) = 0 = P^d(\sigma_2).$$

The graph of $P^d(\sigma)$ is shown in Fig. 1. We can see that the canonical dual function $P^d(\sigma)$ is strictly concave for $\sigma > -q/2 = 0.5$.

4.2. **Two-dimensional problems.** Consider the instance with

$$P(\mathbf{x}) = \frac{1}{2}(x_1, x_2)\begin{pmatrix} q_{11} & q_{12} \\ q_{21} & q_{22} \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} - (f_1 x_1 + f_2 x_2), \tag{44}$$

and

$$P^d(\boldsymbol{\sigma}) = -\frac{1}{2}(f_1 + \sigma_1, f_2 + \sigma_2)\begin{pmatrix} q_{11} + 2\sigma_1 & q_{12} \\ q_{21} & q_{22} + 2\sigma_2 \end{pmatrix}^{-1}\begin{pmatrix} f_1 + \sigma_1 \\ f_2 + \sigma_2 \end{pmatrix}. \tag{45}$$

We focus on three interesting cases.

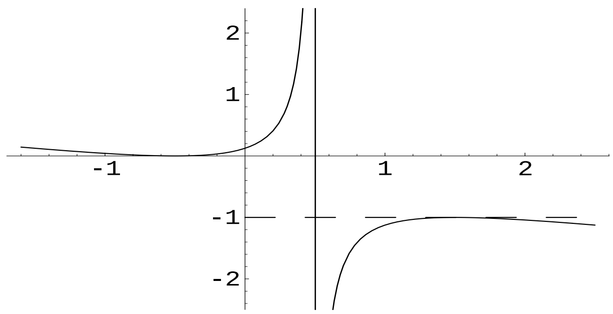

FIGURE 1. Graphs of $P^d(\sigma)$: Concave for $\sigma > 0.5$ and convex for $\sigma < 0.5$

Case 1. (Q is negative definite). Let $q_{11} = -7,\ q_{22} = -2,\ q_{12} = q_{21} = 1$. The eigenvalues of Q are $q_1 = -7.19$ and $q_2 = -1.8$. For $f_1 = -3$ and $f_2 = -2$, the dual function $P^d(\boldsymbol{\sigma})$ has four critical points:

$$\bar{\boldsymbol{\sigma}}_1 = (4,\ 3),\ \ \bar{\boldsymbol{\sigma}}_2 = (3, 2),\ \ \bar{\boldsymbol{\sigma}}_3 = (4,\ 0),\ \ \bar{\boldsymbol{\sigma}}_4 = (3, -1).$$

By the fact that $\bar{\boldsymbol{\sigma}}_1 \in \mathcal{S}_\sharp^+$, we know that it is a global maximizer of $P^d(\boldsymbol{\sigma})$ over $\mathcal{S}_\sharp^+$ and $\bar{\mathbf{x}}_1 = (1, 0)$ is a global minimizer of $P(\mathbf{x})$. Since both $\bar{\boldsymbol{\sigma}}_2$ and $\bar{\boldsymbol{\sigma}}_3$ lead to an indefinite matrix $Q + 2\text{Diag}\ (\bar{\boldsymbol{\sigma}})$, $\bar{\mathbf{x}}_2 = (0, 0)$ and $\bar{\mathbf{x}}_3 = (0, 1)$ are local KKT points. For $\bar{\boldsymbol{\sigma}}_4 = (3, -1)$, $Q + 2\text{Diag}\ (\bar{\boldsymbol{\sigma}}_4)$ is negative definite but $\bar{\boldsymbol{\sigma}}_4$ does not belong to $\mathcal{S}_\sharp^-$ or $\mathcal{S}_\flat^-$. In fact, the corresponding solution $\bar{\mathbf{x}}_4 = (1, 1)$ is a saddle point. It is a local minimizer in the x-direction, while a local maximizer in the y-direction. We have

$$P(\bar{\mathbf{x}}_1) = -0.5 < P(\bar{\mathbf{x}}_2) = 0 < P(\bar{\mathbf{x}}_3) = 1 < P(\bar{\mathbf{x}}_4) = 1.5$$

Case 2. (Q is indefinite.) Let $q_{11} = 2,\ q_{22} = -2$ and $q_{12} = q_{21} = 1$. Then the eigenvalues of Q are $q_1 = 2.2361$ and $q_2 = -2.2361$. For $f_1 = 0.5,\ f_2 = 1$, the dual function $P^d(\boldsymbol{\sigma})$ has four critical points:

$$\bar{\boldsymbol{\sigma}}_1 = (0.5,\ 3),\ \ \bar{\boldsymbol{\sigma}}_2 = (-2.5, 2),\ \ \bar{\boldsymbol{\sigma}}_3 = (-0.5,\ -1),\ \ \bar{\boldsymbol{\sigma}}_4 = (-1.5, 0).$$

By the fact of $\bar{\boldsymbol{\sigma}}_1 \in \mathcal{S}_\sharp^+$, we know it is a global maximizer of $P^d(\boldsymbol{\sigma})$ over $\mathcal{S}_\sharp^+$ and $\bar{\mathbf{x}}_1 = (0, 1)$ is a global minimizer of $P(\mathbf{x})$. Moreover, $\bar{\boldsymbol{\sigma}}_2$ and $\bar{\boldsymbol{\sigma}}_3$ lead to an indefinite matrix $Q_d(\bar{\boldsymbol{\sigma}})$, while $\bar{\boldsymbol{\sigma}}_4$ leads to a negative definite $Q_d(\bar{\boldsymbol{\sigma}})$. However, $\bar{\boldsymbol{\sigma}}_4$ is not in $\mathcal{S}_\sharp^-$ or $\mathcal{S}_\flat^-$. The solution $\bar{\mathbf{x}}_4 = (1, 0)$ is still a global maximizer of $P(\mathbf{x})$ though. Finally, we have

$$P(\bar{\mathbf{x}}_1) = -2 < P(\bar{\mathbf{x}}_2) = -0.5 < P(\bar{\mathbf{x}}_3) = 0 < P(\bar{\mathbf{x}}_4) = 0.5$$

Case 3. (Q is not principal diagonal dominated). Let $q_{11} = 1,\ q_{22} = -2,\ q_{12} = q_{21} = 9$ and $f_1 = 1,\ f_2 = 1$. The dual function $P^d(\boldsymbol{\sigma})$ has four critical points:

$$\bar{\boldsymbol{\sigma}}_1 = (8,\ 3),\ \ \bar{\boldsymbol{\sigma}}_2 = (0,\ 8),\ \ \bar{\boldsymbol{\sigma}}_3 = (-1, -1),\ \ \bar{\boldsymbol{\sigma}}_4 = (-9, -6)$$

Notice that $\bar{\boldsymbol{\sigma}}_1, \bar{\boldsymbol{\sigma}}_2, \bar{\boldsymbol{\sigma}}_3$ lead to an indefinite matrix $Q_d(\bar{\boldsymbol{\sigma}})$ whereas $\bar{\boldsymbol{\sigma}}_4$ lead to a negative definite $Q_d(\bar{\boldsymbol{\sigma}})$. Since $\bar{\boldsymbol{\sigma}}_4 < 0$, Theorem 3 indicates that it is the global minimizer of $P^d(\boldsymbol{\sigma})$ over $\mathcal{S}_\flat^-$, while the corresponding $\bar{\mathbf{x}}_4 = (1, 1)$ is the global maximizer over $\mathcal{X}_a$. To verify that $\bar{\boldsymbol{\sigma}}_4$ is indeed a global minimizer, we found that $\bar{\boldsymbol{\sigma}}_4$ is an interior point of $\mathcal{S}_\flat^-$ and it is the unique critical point. Moreover, the

Hessian matrix of $P^d(\boldsymbol{\sigma})$ at $\bar{\boldsymbol{\sigma}}_4$ is positive definite. To verify that $\bar{\mathbf{x}}_4$ is the global maximizer, we use the grid method to find that

$$P(\bar{\mathbf{x}}_1) = -2 < P(\bar{\mathbf{x}}_2) = -0.5 < P(\bar{\mathbf{x}}_3) = 0 < P(\bar{\mathbf{x}}_4) = 6.5$$

4.3. **Three-dimensional problems.** Let

$$Q = \begin{bmatrix} -22 & 9 & 1 \\ 9 & -140 & 6 \\ 1 & 6 & -80 \end{bmatrix}, \qquad \mathbf{f} = \begin{bmatrix} -2 \\ -6 \\ -1 \end{bmatrix}. \tag{46}$$

Notice that Q is a negative definite matrix with eigenvalues at -141.25, -79.466 and -21.281. There are eight primal 0-1 solutions shown as below:

x_1	0	0	0	0	1	1	1	1
x_2	0	0	1	1	0	0	1	1
x_3	0	1	0	1	0	1	0	1
$P(\mathbf{x})$	0	-39	-64	-97	-9	-47	-64	-96

The corresponding dual solutions are:

σ_1	2	3	11	12	20	19	11	10
σ_2	6	12	134	128	15	21	125	119
σ_3	1	79	7	73	2	78	8	72
$P^d(\boldsymbol{\sigma})$	0	-39	-64	-97	-9	-47	-64	-96

The eigenvalues for $Q + 2\text{Diag}\ (\boldsymbol{\sigma})$ are listed below:

$eig.val_1$	-129.41	-116.98	-66.193	1.2895	-111.61	-98.905	-64.214	-2.8068
$eig.val_2$	-77.359	-15.221	-0.62461	65.29	-75.038	16.67	-0.7274	62.976
$eig.val_3$	-17.232	78.203	128.82	117.42	18.651	76.235	110.94	99.83
	neg.def.	indef.	indef.	p.def.	indef.	indef.	indef.	indef.

From the tables, we see that $\bar{\boldsymbol{\sigma}}_1 = (2, 6, 1) \in \mathcal{S}_\sharp^-$ and $\bar{\boldsymbol{\sigma}}_4 = (12, 128, 73) \in \mathcal{S}_\sharp^+$. The corresponding $\bar{\mathbf{x}}_1 = (0, 0, 0)$ is the maximum integer solution and $\bar{\mathbf{x}}_4 = (0, 1, 1)$ is the minimum integer solution. Actually, $\bar{\mathbf{x}}_1$ is a local minimizer of $P(\mathbf{x})$ over a subregion $[0, 0.01] \times [0, 0.01] \times [0, 0.01] \subset \mathcal{X}_a$. Also notice that the Hessian matrix of the dual objective function is

$$\nabla^2 P^d(\boldsymbol{\sigma}) = -(I - 2\text{Diag}\ (\mathbf{x}(\boldsymbol{\sigma})))[Q_d(\boldsymbol{\sigma})]^{-1}(I - 2\text{Diag}\ (\mathbf{x}(\boldsymbol{\sigma}))).$$

where $\mathbf{x}(\boldsymbol{\sigma}) = [Q_d(\boldsymbol{\sigma})]^{-1}(\mathbf{f} + \boldsymbol{\sigma})$. Since $Q_d(\bar{\boldsymbol{\sigma}}_1)$ is negative definite, $\nabla^2 P^d(\bar{\boldsymbol{\sigma}}_1)$ must be positive definite. This implies that $\bar{\boldsymbol{\sigma}}_1$ is a local minimizer of $P^d(\boldsymbol{\sigma})$ over $\mathcal{S}_\sharp^-$. Thus Theorem 3 is explained.

5. **Algorithm for large scale problems.** Theorem 3 tells us that, if $\mathcal{S}_\sharp^+$ is not empty, the solution $\bar{\boldsymbol{\sigma}}$ of the canonical dual problem

$$\max_{\boldsymbol{\sigma} \in \mathcal{S}_\sharp^+} P^d(\boldsymbol{\sigma}) \tag{47}$$

leads to a global minimizer $\bar{\mathbf{x}} = Q_d^{-1}(\bar{\boldsymbol{\sigma}})(\mathbf{f} + \bar{\boldsymbol{\sigma}})$ of the primal problem $(\mathcal{P})$. In this case, since the canonical dual function $P^d(\boldsymbol{\sigma})$ is concave on $\mathcal{S}_\sharp^+$, the problem can be solved by any commonly used nonlinear programming methods.

Notice that the the inverse of the Hessian matrix for $P^d(\boldsymbol{\sigma})$,

$$[\nabla^2 P^d(\boldsymbol{\sigma})]^{-1} = -(I - 2\text{Diag }(\mathbf{x}(\boldsymbol{\sigma})))^{-1} Q_d(\boldsymbol{\sigma})(I - 2\text{Diag }(\mathbf{x}(\boldsymbol{\sigma})))^{-1},$$

is particularly simple because $(I - 2\text{Diag }(\mathbf{x}(\boldsymbol{\sigma})))$ is a diagonal matrix. It is then reasonable to apply Newton's method for solving the canonical dual problem. We may choose

$$\boldsymbol{\sigma}^\sharp = \{\max\{-f_i, f_i - q_{ii}\}\}$$

where q_{ii} is the i^{th} diagonal element of Q as the initial point to start Newton's method. The algorithm will then stop at one of the 2^n dual critical points. For a minimization problem, if the termination point happens to reside in $\mathcal{S}_\sharp^+$, then Theorem 3 assures that its corresponding primal solution must be the global minimizer. Similar situation can be developed for the maximization problem and we leave it to the readers.

Here we propose using Newton method to solve the canonical dual for the minimization problem.

Algorithm.
Step 0 (Initialization): Let $\boldsymbol{\sigma}^\sharp = \{\max\{-f_i, f_i - q_{ii}\}\}$ where q_{ii} is the i^{th} diagonal element of Q. Also let $k = 0$, $\boldsymbol{\sigma}_0 = \boldsymbol{\sigma}^\sharp$ and choose $\delta > 0$.
Step 1 (Newton steps to maximize $P^d(\boldsymbol{\sigma}) = -\dfrac{1}{2}(\mathbf{f} + \boldsymbol{\sigma})^T Q_d^{-1}(\boldsymbol{\sigma})(\mathbf{f} + \boldsymbol{\sigma})$):
Compute the corresponding primal solution:

$$\mathbf{x}(\boldsymbol{\sigma}_k) = Q_d^{-1}(\boldsymbol{\sigma}_k)(\mathbf{f} + \boldsymbol{\sigma}_k);$$

the gradient vector of $P^d(\boldsymbol{\sigma})$:

$$\nabla P^d(\boldsymbol{\sigma}_k) = \mathbf{x}(\boldsymbol{\sigma}_k) \circ [\mathbf{x}(\boldsymbol{\sigma}_k) - \mathbf{e}];$$

and the inverse Hessian:

$$[\nabla^2 P^d(\boldsymbol{\sigma}_k)]^{-1} = -(I - 2\text{Diag }(\boldsymbol{\sigma}_k))^{-1} Q_d(\boldsymbol{\sigma}_k)(I - 2\text{Diag }(\boldsymbol{\sigma}_k))^{-1}.$$

Step 2 (Stopping rule and purification):
If $\|\nabla P^d(\boldsymbol{\sigma}_k)\|_\infty < \delta$, stop the algorithm. Round the current $\mathbf{x}$ solution to the nearest integer vector and report the *rounded solution.* (Note that a zero gradient of $\nabla P^d(\boldsymbol{\sigma}_k)$ means the same as each component of $\mathbf{x}(\boldsymbol{\sigma}_k)$ being either 0 or 1.)
Step 3 (Newton iteration): Update

$$\boldsymbol{\sigma}_{k+1} := \boldsymbol{\sigma}_k - [\nabla^2 P^d(\boldsymbol{\sigma}_k)]^{-1} \nabla P^d(\boldsymbol{\sigma}_k);$$

$$k := k + 1;$$

Go to Step 1.

Using the Newton method incorporating the purification (rounding) strategy in Step 2, we can solve large quadratic integer programs. We implemented the algorithm in MATLAB 7.4 and run with a Pentium M 1.6 GHz CPU and 1.25GB RAM. Here we show three examples. The first one has 10 variables and the others have 25.

For the case with 10 variables,

$$Q = \begin{bmatrix} 384 & 12 & -10 & -8 & 17 & 33 & 34 & -46 & 5 & -14 \\ 12 & 370 & 13 & -10 & 6 & -9 & 77 & 26 & -27 & 9 \\ -10 & 13 & -208 & 88 & 10 & -29 & -18 & 8 & -23 & -4 \\ -8 & -10 & 88 & 490 & -72 & 8 & -57 & -66 & 112 & 79 \\ 17 & 6 & 10 & -72 & 214 & 11 & 13 & -21 & 21 & -43 \\ 33 & -9 & -29 & 8 & 11 & -168 & 31 & 35 & 0 & -27 \\ 34 & 77 & -18 & -57 & 13 & 31 & 252 & -17 & 26 & 15 \\ -46 & 26 & 8 & -66 & -21 & 35 & -17 & 232 & 18 & -8 \\ 5 & -27 & -23 & 112 & 21 & 0 & 26 & 18 & -236 & 14 \\ -14 & 9 & -4 & 79 & -43 & -27 & 15 & -8 & 14 & -208 \end{bmatrix}; \quad (48)$$

$$\mathbf{f} = [-10, -33, -16, -70, -50, -48, -19, -22, -11, -20].$$

The proposed algorithm took 6 iterations in 0.701 cpu seconds to obtain a dual critical solution

$$\bar{\boldsymbol{\sigma}} = (24, 19, 248, 357, 49, 176, 73, 75, 234, 205),$$

which corresponds to the primal 0-1 solution

$$\mathbf{x}(\bar{\boldsymbol{\sigma}}) = (0, 0, 1, 0, 0, 1, 0, 0, 1, 1).$$

It can be easily verified that $\bar{\boldsymbol{\sigma}} \in \mathcal{S}_\sharp^+$ is indeed the only element in $\mathcal{S}_\sharp^+$. By Theorem 2, the primal solution $\mathbf{x}(\bar{\boldsymbol{\sigma}})$ is a global minimizer of the 0-1 quadratic programming problem. A complete enumeration over $2^{10} = 1024$ possible solutions taking 0.16023 cpu seconds on the same machine confirms that $\mathbf{x}(\bar{\boldsymbol{\sigma}})$ is truly a global minimum solution.

To show that the proposed algorithm does work effectively, we randomly choose a case with 25 variables. The matrix $Q \in \mathbb{R}^{25\times 25}$ is shown on the next page and

$$\begin{aligned}\mathbf{f} = \ [\ & 76.9, -12.4, 126, -230, -81, -411, 108, 403, -509, 461, 117, -100, \\ & 365, -303, 484, -453, -425, -472, -299, 141, 335, -69, 28.4, -105, -240]^T.\end{aligned}$$

To solve the primal problem directly, it took Matlab more than 27 cpu minutes to complete a total of 33, 554, 432 enumerations. The optimal integer solution is

$$\bar{\mathbf{x}} = (1, 0, 1, 0, 0, 0, 1, 1, 0, 1, 1, 0, 1, 0, 1, 0, 0, 0, 0, 1, 1, 0, 1, 0, 0)$$

with a corresponding dual critical solution

$$\begin{aligned}\bar{\boldsymbol{\sigma}} = (&89.4, 12.4, 111, 230, 83, 412, 117.5, 389, 511, 469.5, 101.5, 97, \\ &372.5, 312, 487.5, 454, 423, 472, 301, 113, 327.5, 64, 17.9, 104, 244).\end{aligned}$$

Our Newton method took 0.015 second to find the dual optimal solution which falls in $\mathcal{S}_\sharp^+$. In fact, the initial dual feasible solution $\boldsymbol{\sigma}^\sharp$, when converted to its primal correspondence, is already very close to the optimal integer solution. Therefore, a simple purification leads to the desired solution.

Another example has 25 variables with matrix $Q \in \mathbb{R}^{25\times 25}$ shown on a separate page and

$$\begin{aligned}\mathbf{f} \ = \ & [-10, 33, 16, -7, -50, 48, 19, 22, 11, 20, 11, 26, \\ & -33, 5, 23, 18, -8, 12, 42, 29, -37, 29, 36, -3, 17]^T.\end{aligned}$$

$$
\begin{bmatrix}
-11.5 & 1 & -2 & 0 & -2 & -1 & -1 & -1 & 0 & -1 & 0 & 2 & 1 & 1 & 2 & 0 & -2 & 0 & -1 & 2 & -1 & -1 & 0 & 1 & 0 \\
1 & 7 & 0 & 0 & 1 & 1 & 0 & 0 & -1 & 0 & 0 & -1 & 0 & 1 & -1 & 0 & 1 & 1 & 0 & 2 & -1 & 0 & -1 & -1 & 0 \\
-2 & 0 & 13 & -2 & 2 & 0 & 1 & 0 & -2 & 0 & 1 & -1 & 0 & 1 & 1 & -2 & 0 & -1 & 1 & 2 & -2 & -1 & 1 & -2 & 1 \\
0 & 0 & -2 & 13 & 0 & 1 & 0 & 1 & 1 & -1 & 0 & -1 & 2 & 2 & 1 & -1 & -1 & 0 & 0 & -1 & 1 & 0 & -1 & 2 & -1 \\
-2 & 1 & 2 & 0 & -10.5 & 0 & 0 & -2 & 1 & 2 & 1 & -1 & 0 & 0 & 1 & 0 & -1 & -1 & 1 & 0 & 1 & -1 & -1 & 0 & 2 \\
-1 & 1 & 0 & 1 & 0 & -11 & 0 & 1 & 0 & 2 & 1 & 1 & 0 & -1 & 2 & 0 & 0 & 0 & 0 & -2 & -2 & 0 & 0 & 0 & 1 \\
-1 & 0 & 1 & 0 & 0 & 0 & -10.5 & -117 & 26 & 15 & -2 & -2 & 1 & 2 & 1 & 1 & 0 & 1 & -2 & 2 & -2 & -1 & 0 & 1 & 1 \\
-1 & 0 & 0 & 1 & -2 & 1 & 1 & 11 & 1 & 2 & 1 & -2 & 0 & -1 & -1 & -1 & 1 & 0 & 0 & 1 & -1 & 0 & 1 & 2 & 1 \\
0 & -1 & -2 & 1 & 1 & 0 & 1 & 1 & 12 & 2 & 1 & 1 & 0 & 1 & 0 & -2 & 0 & 0 & 1 & 0 & -1 & 1 & 0 & 0 & 1 \\
-1 & 0 & 0 & -1 & 2 & 2 & 0 & 2 & 2 & -10.5 & 0 & -1 & -1 & 2 & 1 & 0 & 0 & 1 & -2 & 1 & 1 & 0 & -1 & 0 & 0 \\
0 & 0 & 1 & 0 & 1 & 1 & -2 & 1 & 1 & 0 & 11.5 & 1 & 0 & 2 & 2 & 0 & 0 & -2 & 2 & 2 & -1 & 0 & 1 & -2 & -1 \\
2 & -1 & -1 & -1 & -1 & 1 & -2 & -2 & 1 & -1 & 1 & 15.5 & -1 & 1 & 0 & 2 & 0 & 0 & 0 & 2 & 0 & 1 & -1 & 1 & 2 \\
1 & 0 & 0 & 2 & 0 & 0 & 1 & 0 & 0 & -1 & 0 & -1 & -8.5 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & -2 \\
1 & 1 & 1 & 2 & 0 & -1 & 2 & -1 & 1 & 2 & 2 & 1 & 1 & 15 & 0 & 1 & 0 & 0 & 0 & 1 & 2 & -1 & -2 & -1 & 0 \\
2 & -1 & 1 & 1 & 1 & 2 & 1 & -1 & 0 & 1 & 2 & 0 & 0 & 0 & -11.5 & 2 & -1 & 2 & 2 & 1 & 0 & 0 & 1 & 0 & 1 \\
0 & 0 & -2 & -1 & 0 & 0 & 1 & -1 & -2 & 0 & 0 & 2 & 0 & 1 & 2 & -13 & -2 & 1 & 0 & -1 & 1 & -1 & 1 & 1 & 0 \\
-2 & 1 & 0 & -1 & -1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & -2 & 9 & -2 & 0 & -1 & 1 & -1 & 0 & 2 & 2 \\
0 & 1 & -1 & 0 & -1 & 0 & 1 & 0 & 0 & 1 & -2 & 0 & 0 & 0 & 2 & 1 & -2 & 8.5 & 1 & 1 & 0 & 0 & -2 & -1 & -2 \\
-1 & 0 & 1 & 0 & 1 & 0 & -2 & 0 & 1 & -2 & 2 & 0 & 0 & 0 & 2 & 0 & 0 & 1 & 13 & 2 & -1 & 0 & 1 & 2 & -1 \\
2 & 2 & 2 & -1 & 0 & -2 & 2 & 1 & 0 & 1 & 2 & 2 & 1 & 1 & 1 & -1 & -1 & 1 & 2 & 14 & 2 & 0 & 0 & 0 & 1 \\
-1 & -1 & -2 & 1 & 1 & -2 & -2 & -1 & -1 & 1 & -1 & 0 & -1 & 2 & 0 & 1 & 1 & 0 & -1 & 2 & 12.5 & -2 & 0 & -1 & 2 \\
-1 & 0 & -1 & 0 & -1 & 0 & -1 & 0 & 1 & 0 & 0 & 1 & 0 & -1 & 0 & -1 & -1 & 0 & 0 & 0 & -2 & 9 & 0 & 0 & 1 \\
0 & -1 & 1 & -1 & -1 & 0 & 0 & 1 & 0 & -1 & 1 & -1 & 0 & -2 & 1 & 1 & 0 & -2 & 1 & 0 & 0 & 0 & 7.5 & 0 & 0 \\
1 & -1 & -2 & 2 & 0 & 0 & 1 & 2 & 0 & 0 & -2 & 1 & 0 & -1 & 0 & 1 & 2 & -1 & 2 & 0 & -1 & 0 & 0 & -11 & -2 \\
0 & 0 & 1 & -1 & 2 & 1 & 1 & 1 & 1 & 0 & -1 & 2 & -2 & 0 & 1 & 0 & 2 & -2 & -1 & 1 & 2 & 1 & 0 & -2 & 12.5
\end{bmatrix}
$$

2146	22	-10	-8	17	33	34	-46	5	-14	23	81	-101	-61	31	18	-64	80	15	-58	-37	46	-83	42	-17
22	1624	13	-10	6	-9	77	26	-27	9	-40	-33	97	-44	29	-80	32	92	103	129	-61	214	79	-38	13
-10	13	-2044	88	10	-29	-18	8	-23	-4	-138	22	-110	-51	-45	11	-92	14	-57	25	169	-309	145	-95	158
-8	-10	88	2630	-72	8	-57	-66	112	79	186	160	91	-94	-52	194	257	-86	-315	-168	107	163	-98	141	183
17	6	10	-72	-1670	-101	13	-21	-21	-43	229	-143	124	65	22	-133	-88	59	106	32	-10	-22	135	-4	-194
33	-9	-29	8	-101	-2274	81	135	-30	-27	-280	-46	301	224	120	69	13	192	-19	35	-121	-6	48	322	-16
34	77	-18	-57	13	81	2238	-117	26	15	-43	176	-68	-89	118	174	198	361	-120	156	25	99	-27	137	-108
-46	26	8	-66	-21	135	-117	1660	18	-8	69	-36	251	29	16	130	55	-90	78	24	128	-116	27	-195	107
5	-27	-23	112	-21	-30	26	18	2246	14	44	-40	81	159	-266	211	235	171	-102	54	77	7	33	-34	107
-14	9	-4	79	-43	-27	15	-8	14	-1684	-95	212	-246	14	32	191	-117	53	20	194	224	-6	-29	44	78
23	-40	-138	186	229	-280	-43	69	44	-95	1430	163	21	303	-88	11	61	-94	106	72	65	41	-58	187	-85
81	-33	22	160	-143	-46	176	-36	-40	212	163	-2934	-138	75	171	-292	317	139	94	-172	-213	150	31	4	-26
-101	97	-110	91	124	301	-68	251	81	-246	21	-138	-2640	-43	-85	180	172	17	73	47	111	-106	-115	48	3
-61	-44	-51	-94	65	224	-89	29	159	14	303	75	-43	-1964	70	100	-98	41	-119	34	121	12	74	-30	-13
31	29	-45	-52	22	120	118	16	-266	32	-88	171	-85	70	1900	66	-1	-47	-241	-9	73	10	142	129	37
18	-80	11	194	-133	69	174	130	211	191	11	-292	180	100	66	2896	107	33	0	92	-22	-85	272	-300	124
-64	32	-92	257	-88	13	198	55	235	-117	61	317	172	-98	-1	107	-2810	-297	60	-142	0	210	0	-27	166
80	92	14	-86	59	192	361	-90	171	53	-94	139	17	41	-47	33	-297	2254	-98	-73	46	28	16	8	-118
15	103	-57	-315	106	-19	-120	78	-102	20	106	94	73	-119	-241	0	60	-98	2014	128	12	0	-14	115	-20
-58	129	25	-168	32	35	156	24	54	194	72	-172	47	34	-9	92	-142	-73	128	-1950	74	-63	121	0	17
-37	-61	169	107	-10	-121	25	128	77	224	65	-213	111	121	73	-22	0	46	12	74	2104	-222	97	58	-30
46	214	-309	163	-22	-6	99	-116	7	-6	41	150	-106	12	10	-85	210	28	0	-63	-222	-2300	0	384	0
-83	79	145	-98	135	48	-27	27	33	-29	-58	31	-115	74	142	272	0	16	-14	121	97	0	2064	224	196
42	-38	-95	141	-4	322	137	-195	-34	44	187	4	48	-30	129	-300	-27	8	115	0	58	384	224	2634	68
-17	13	158	183	-194	-16	-108	107	107	78	-85	-26	3	-13	37	124	166	-118	-20	17	-30	0	196	68	-1884

Our Newton method took 2 iterations in 0.08 cpu second to obtain the following correct solution:

$$\bar{\mathbf{x}} = (0, 0, 1, 0, 1, 1, 0, 0, 0, 1, 0, 1, 1, 1, 0, 0, 1, 0, 0, 1, 0, 1, 0, 0, 1).$$

It is interesting to note that the dual critical solution

$$\bar{\boldsymbol{\sigma}} = (-138, 394, 2440, 702, 1980, 1974, 436, 406, 532, 1649, 281, 2709,$$
$$2603, 1750, 299, 346, 2461, 43, 224, 1972, 140, 2469, 570, 717, 1728)$$

corresponding to $\bar{\mathbf{x}}$ is not in $\mathcal{S}_\sharp^+$, since $\bar{\boldsymbol{\sigma}}$ contains one negative component. Yet, the proposed algorithm still found the optimal solution.

Our computational experience further indicates that the proposed algorithm indeed converges very fast. When $\mathcal{S}_\sharp^+$ is non-empty, since the canonical dual problem is a concave maximization problem over a convex open feasible space, the proposed algorithm surely works very well. However, when $\mathcal{S}_\sharp^+$ is empty, no theorem guarantees that the canonical dual problem is concave. As a result, the proposed algorithm may or may not find a global minimizer. According to our observations, the solvability is highly related to the structure of Q matrix and the vector $\mathbf{f}$. In general, the proposed algorithm works well with those Q matrix being "diagonally dominated" (i.e.,$|q_{ii}| \gg \sum_{j\neq i} q_{ij}$) while it works poorly for those Q matrix being "nondiagonally dominated" (i.e., $|q_{ii}| \ll \sum_{j\neq i} q_{ij}$).

6. **Concluding remarks.**

1. We have successfully constructed a pair of canonical dual problems for the 0-1 quadratic programming problems. No duality gap exists in this dual approach. Some optimality conditions for both local and global optimizers have been given based on the triality theory. We have also proposed an algorithm to handle large scale problems with $\mathcal{S}_\sharp^+$ or $\mathcal{S}_\flat^-$ being nonempty.

2. It is possible to construct an example such that the four regions $\mathcal{S}_\sharp^+, \mathcal{S}_\sharp^-, \mathcal{S}_\flat^+, \mathcal{S}_\flat^-$ are simultaneously empty. For example, let

$$Q = \begin{bmatrix} 100 & 9 & 10 \\ 9 & 120 & 3 \\ 10 & 3 & -140 \end{bmatrix} \text{ and } \mathbf{f} = \begin{bmatrix} -10 \\ 10 \\ -1 \end{bmatrix}. \tag{49}$$

The primal 0-1 solutions are listed below:

x_1	0	0	0	0	1	1	1	1
x_2	0	0	1	1	0	0	1	1
x_3	0	1	0	1	0	1	0	1
$P(\mathbf{x})$	0	-69	50	-16	60	1	119	63

The dual information is given as follows:

σ_1	10	20	19	29	-110	-120	-119	-129
σ_2	-10	-7	-110	-113	-1	2	-119	-122
σ_3	1	139	4	136	11	129	14	126
$P^d(\boldsymbol{\sigma})$	0	-69	50	-16	60	1	119	63

The eigenvalues for $Q + 2\text{Diag }(\boldsymbol{\sigma})$ are given in the following table:

$eig.val_1$	-138.42	103.76	-132.59	-106.34	-129.14	-140.68	-143.71	-160.53
$eig.val_2$	96.549	129.48	-100.13	128.6	-109.25	116.88	-118.73	-121.88
$eig.val_3$	123.87	150.76	138.72	161.74	118.39	125.81	-105.56	112.42
	indef.	p.def.	indef.	indef.	indef.	indef.	neg.def.	indef.

Since there is no dual solution whose components are entirely positive or entirely negative, the four regions that we defined in Theorem 2 are empty. However, $Q_d(\bar{\boldsymbol{\sigma}}_2)$ is positive definite, so $\nabla^2 P^d(\bar{\boldsymbol{\sigma}}_2)$ is negative definite and $\bar{\boldsymbol{\sigma}}_2$ is a local maximizer of $P^d(\boldsymbol{\sigma})$. The corresponding $\bar{\mathbf{x}}_2 = (0, 0, 1)$ is the minimum integer solution. On the other hand, $\bar{\boldsymbol{\sigma}}_7$ is a local minimizer of $P^d(\boldsymbol{\sigma})$ whose corresponding $\bar{\mathbf{x}}_7 = (1, 1, 0)$ is the maximum integer solution.

3. A fundamental question to ask is about the properties of Q and $\mathbf{f}$ that ensure the non-emptiness of $\mathcal{S}_\sharp^+, \mathcal{S}_\sharp^-, \mathcal{S}_\flat^+, \mathcal{S}_\flat^-$. So far we have no luck to get a complete characterization. This could be a topic for future research.

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