

# Solutions to quadratic minimization problems with box and integer constraints

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**Abstract** This paper presents a canonical duality theory for solving quadratic minimization problems subjected to either box or integer constraints. Results show that under Gao and Strang's general global optimality condition, these well-known nonconvex and discrete problems can be converted into smooth concave maximization dual problems over closed convex feasible spaces without duality gap, and can be solved by well-developed optimization methods. Both existence and uniqueness of these canonical dual solutions are presented. Based on a second-order canonical dual perturbation, the discrete integer programming problem is equivalent to a continuous unconstrained Lipschitzian optimization problem, which can be solved by certain deterministic technique. Particularly, an analytical solution is obtained under certain condition. A fourth-order canonical dual perturbation algorithm is presented and applications are illustrated. Finally, implication of the canonical duality theory for the popular semi-definite programming method is revealed.

**Keywords** Canonical duality theory · Quadratic programming · Integer programming · NP-hard problems · Global optimization

## 1 Primal problems and preliminary results

Let us consider the following constrained nonconvex quadratic minimization problem:

$$(\mathcal{P}) : \quad \min \left\{ P(\mathbf{x}) = \frac{1}{2} \langle \mathbf{x}, \mathbf{Q}\mathbf{x} \rangle - \langle \mathbf{x}, \mathbf{c} \rangle \mid \mathbf{x} \in \mathcal{X}_a \right\}, \quad (1)$$

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where  $\mathbf{Q} = \mathbf{Q}^T \in \mathbb{R}^{n \times n}$  is a given indefinite matrix,  $\mathbf{c}$  is a given vector in  $\mathbb{R}^n$ ,  $\mathcal{X}_a \subset \mathbb{R}^n$  is a feasible space, and  $\langle *, * \rangle$  represents a bilinear form on  $\mathbb{R}^n \times \mathbb{R}^n$ . For box constrained problem,  $\mathcal{X}_a$  is defined by

$$\mathcal{X}_a = \{\mathbf{x} \in \mathbb{R}^n \mid -1 \leq x_i \leq 1, \forall i = 1, \dots, n\}. \tag{2}$$

Problem  $(\mathcal{P})$  is probably the most simple global optimization problem, which appears in many applications (see Floudas and Visweswaran [9,10]). Replacing the inequality constraints in  $\mathcal{X}_a$  by equality constraints  $x_i = \pm 1$  ( $i = 1, 2, \dots, n$ ), the problem  $(\mathcal{P})$  is reduced to the well-known integer programming:

$$(\mathcal{P}_{ip}) : \min \left\{ P(\mathbf{x}) = \frac{1}{2} \langle \mathbf{x}, \mathbf{Q}\mathbf{x} \rangle - \langle \mathbf{x}, \mathbf{c} \rangle \mid \text{s.t. } \mathbf{x} \in \partial \mathcal{X}_a \right\}, \tag{3}$$

where the feasible set  $\partial \mathcal{X}_a$  denotes the vertices of  $\mathcal{X}_a$ , i.e.,

$$\partial \mathcal{X}_a = \{\mathbf{x} \in \mathbb{R}^n \mid \mathbf{x} \in \{-1, 1\}^n\}. \tag{4}$$

Due to the nonconvexity of the quadratic function  $P(\mathbf{x})$ , quadratic minimization problems with either box or integer constraints are considered to be NP-hard (see Murty and Kabadi [29], Pardalos and Schnitger [30], Pardalos and Vavasis [31]). Detailed discussions and some important numerical algorithms were given in [1,2,3,7,8,25,26,34,35] as well as in the review article [10].

Canonical duality theory developed in [12,13] is a potentially powerful methodology which can be used to solve a wide class of nonconvex/nonsmooth/discrete problems in non-linear analysis, global optimization, and computational science. The original idea of this theory is from the joint paper by Gao and Strang [22] in *fully nonlinear systems*. Applications of this canonical duality theory in global optimization have been given in [13–15]. Recently, perfect dual problems (with zero duality gap) have been formulated for a class of nonconvex polynomial minimization problems with box and integer constraints [16]. By introducing a quadratic operator  $\epsilon = \Lambda(\mathbf{x}) = \frac{1}{2}\{x_i^2 - 1\}$  such that the linear inequality constraints in  $\mathcal{X}_a$  is re-written in the so-called canonical form  $\epsilon(\mathbf{x}) \leq 0$  (the key step in the canonical dual transformation [13,14]), the canonical dual for box constrained problem has a very simple form

$$(\mathcal{P}^d) : \max \left\{ P^d(\boldsymbol{\sigma}) = -\frac{1}{2} \langle [\mathbf{G}(\boldsymbol{\sigma})]^{-1} \mathbf{c}, \mathbf{c} \rangle - \frac{1}{2} \langle \mathbf{e}, \boldsymbol{\sigma} \rangle \mid \boldsymbol{\sigma} \in S_a^+ \right\}, \tag{5}$$

where  $\mathbf{G}(\boldsymbol{\sigma}) = \mathbf{Q} + \text{Diag}(\boldsymbol{\sigma})$ , the notation  $\text{Diag}(\boldsymbol{\sigma})$  represents a diagonal matrix with  $\sigma_i$ ,  $i = 1, 2, \dots, n$  being its diagonal elements,  $\mathbf{e}$  is an  $n$ -vector of all ones, and the dual feasible space  $S_a^+$  and  $S_a^-$  are defined as

$$S_a^+ = \{\sigma \in \mathbb{R}^n \mid \sigma \geq 0, \mathbf{G}(\sigma) \succ 0\}, \tag{6}$$

$$S_a^- = \{\sigma \in \mathbb{R}^n \mid \sigma \geq 0, \mathbf{G}(\sigma) \prec 0\} \tag{7}$$

The following theorem shows that  $(\mathcal{P}^d)$  is canonically (i.e. with zero duality gap) dual to the primal problem  $(\mathcal{P})$ .

**Theorem 1** ([16]) *The problem  $(\mathcal{P}^d)$  is canonically dual to  $(\mathcal{P})$  in the sense that if  $\bar{\sigma}$  is a critical point of  $P^d(\sigma)$ , the vector  $\bar{\mathbf{x}}(\bar{\sigma}) = [\mathbf{G}(\bar{\sigma})]^{-1}\mathbf{c}$  is a KKT point of the problem  $(\mathcal{P})$  and*

$$P(\bar{\mathbf{x}}) = P^d(\bar{\sigma}). \tag{8}$$

*If the critical point  $\bar{\sigma} > 0$ , then the vector  $\bar{\mathbf{x}} = [\mathbf{G}(\bar{\sigma})]^{-1}\mathbf{c} \in \{-1, 1\}^n$  is a local optimal solution to the integer programming problem  $(\mathcal{P}_{ip})$ .*

*If  $\bar{\sigma} \in S_a^+$ , then  $\bar{\sigma}$  is a global maximizer of  $(\mathcal{P}^d)$ ,  $\bar{\mathbf{x}} = [\mathbf{G}(\bar{\sigma})]^{-1}\mathbf{c}$  is a global minimizer of  $(\mathcal{P})$ , and*

$$P(\bar{\mathbf{x}}) = \min_{\mathbf{x} \in \mathcal{X}_a} P(\mathbf{x}) = \max_{\sigma \in S_a^+} P^d(\sigma) = P^d(\bar{\sigma}). \tag{9}$$

*If the critical point  $\bar{\sigma} \in S_a^+$  and  $\bar{\sigma} > 0$ , then the vector  $\bar{\mathbf{x}} = [\mathbf{G}(\bar{\sigma})]^{-1}\mathbf{c} \in \{-1, 1\}^n$  is a global minimizer to the integer programming problem  $(\mathcal{P}_{ip})$ .*

*If  $\bar{\sigma} \in S_a^-$ , then  $\bar{\sigma}$  is a local minimizer of  $(\mathcal{P}^d)$ , the vector  $\bar{\mathbf{x}} = [\mathbf{G}(\bar{\sigma})]^{-1}\mathbf{c}$  is a local minimizer of  $(\mathcal{P})$ , and on the neighborhood  $\mathcal{X}_o \times S_o$  of  $(\bar{\mathbf{x}}, \bar{\sigma})$ ,*

$$P(\bar{\mathbf{x}}) = \min_{\mathbf{x} \in \mathcal{X}^o} P(\mathbf{x}) = \min_{\sigma \in S_o} P^d(\sigma) = P^d(\bar{\sigma}). \tag{10}$$

This theorem shows that by the canonical duality theory, the box constrained nonconvex minimization problem  $(\mathcal{P})$  can be converted into continuous concave maximization dual problem over a convex set  $S_a^+$  and from the point view of the canonical duality, the integer programming problem  $(\mathcal{P}_{ip})$  is actually a special case of  $(\mathcal{P})$ . Since the canonical dual function  $P^d(\sigma)$  is strictly concave on  $S_a^+$ , if  $S_a^+ \neq \emptyset$ , the problem  $(\mathcal{P}^d)$  can be solved easily to obtain a unique global maximizer of the primal problem  $(\mathcal{P})$ . If  $\bar{\sigma} > 0$ , the vector  $\bar{\mathbf{x}} = [\mathbf{G}(\bar{\sigma})]^{-1}\mathbf{c} \in \{-1, 1\}^n$  is a unique solution to  $(\mathcal{P}_{ip})$ . In finite deformation theory and nonconvex variational analysis, Theorem 1 is known as the *pure complementary variational principle* [11, 28].

Recently, in the study of 0–1 programming [5] and nonconvex constrained optimization [19], it was discovered that for certain given matrix  $\mathbf{Q}$  and vector  $\mathbf{c}$ , the canonical dual problem  $(\mathcal{P}^d)$  may have no critical point in  $S_a^+$ . It is now understood that if the primal problem  $(\mathcal{P})$  is NP-hard, it usually has multiple solutions. In this case, the canonical dual problem  $(\mathcal{P}^d)$  has no solution in  $S_a^+$ . Therefore, the main purpose of this paper is to generalize the results presented in [16] and to study the existence and uniqueness conditions of the canonical dual solutions. In the next section, a general form of the canonical dual problem is presented by the standard canonical dual transformation proposed in [22]. The relation of this transformation with the classical Lagrangian method is discussed. In Sect. 3, both global and local optimality criteria are provided based on the triality theory developed in general nonconvex systems [12]. The existence and uniqueness of the canonical dual solutions are discussed in Sect. 4, where we also demonstrate that the so-called *complementary gap function* discovered by Gao and Strang in general nonconvex and nonsmooth variational analysis plays an important role in identifying the global minimizers of the nonconvex quadratic programming problems. Canonical dual perturbation and analytic solutions to integer programming are discussed in Sect. 5, a new canonical dual problem for convex integer programming is proposed. In Sect. 6,

a Newton-type algorithm is proposed for solving the perturbed canonical dual problem. Applications are illustrated in Sect. 7. Implication of the canonical duality theory for semi-definite programming method is revealed in the last section with some comments, conclusions, and open problems for the future study.

### 2 Generalized canonical dual problems

Following the standard procedure of the canonical dual transformation [12], we rewrite the inequality constraints  $-1 \leq x_i \leq 1, i = 1, \dots, n$  in  $\mathcal{X}_a$  in the canonical form:  $\mathbf{x} \circ \mathbf{x} \leq \mathbf{e}$ , where the notation  $\mathbf{s} \circ \mathbf{t} := (s_1t_1, s_2t_2, \dots, s_nt_n)$  denotes the Hadamard product for any two vectors  $\mathbf{s}, \mathbf{t} \in \mathbb{R}^n$ ; by introducing a quadratic *geometrical operator*

$$\xi = \{\xi, \mathbf{e}\} = \Lambda(\mathbf{x}) = \frac{1}{2} \left\{ \mathbf{x}^T \mathbf{Q} \mathbf{x}, \mathbf{x} \circ \mathbf{x} \right\} : \mathbb{R}^n \rightarrow \mathcal{E} = \mathbb{R}^{1+n}, \tag{11}$$

and let

$$V(\xi) = \begin{cases} \xi & \text{if } \mathbf{e} \leq \frac{1}{2}\mathbf{e}, \\ +\infty & \text{otherwise,} \end{cases} \tag{12}$$

the box constrained problem ( $\mathcal{P}$ ) can be reformulated as the following unconstrained canonical form:

$$\min\{\Pi(\mathbf{x}) = V(\Lambda(\mathbf{x})) - \langle \mathbf{x}, \mathbf{c} \rangle \mid \mathbf{x} \in \mathbb{R}^n\}. \tag{13}$$

Since  $V(\xi)$  is convex and lower semi-continuous on  $\mathcal{E}$ , the canonical dual variable  $\xi^*$  can be defined by the following subdifferential *constitutive law* [22]

$$\xi^* \in \partial V(\xi) = \{1, \boldsymbol{\sigma}\} \in \mathcal{E}^* = \mathbb{R}^{1+n}. \tag{14}$$

Let  $\langle \xi; \xi^* \rangle$  denote the bilinear form on  $\mathcal{E} \times \mathcal{E}^*$ , the so-called complementary function  $V^\sharp(\xi^*)$  can be defined by the Fenchel transformation:

$$V^\sharp(\xi^*) = \sup_{\xi \in \mathcal{E}} \{\langle \xi; \xi^* \rangle - V(\xi)\} = \begin{cases} \frac{1}{2} \langle \mathbf{e}, \boldsymbol{\sigma} \rangle & \text{if } \boldsymbol{\sigma} \geq \mathbf{0} \in \mathbb{R}^n, \\ +\infty & \text{otherwise.} \end{cases}$$

Since both  $V(\xi)$  and  $V^\sharp(\xi^*)$  are proper convex functions over their effective domains  $\mathcal{E}_a = \{\xi = \{\xi, \mathbf{e}\} \in \mathcal{E} \mid \mathbf{e} \leq \frac{1}{2}\mathbf{e}\}$  and  $\mathcal{E}_a^* = \{\xi^* = \{1, \boldsymbol{\sigma}\} \in \mathcal{E}^* \mid \boldsymbol{\sigma} \geq \mathbf{0}\}$ , respectively, the following canonical duality relations hold on  $\mathcal{E}_a \times \mathcal{E}_a^*$ :

$$\xi^* \in \partial V(\xi) \Leftrightarrow \xi^* \in \partial V^\sharp(\xi) \Leftrightarrow V(\xi) + V^\sharp(\xi^*) = \langle \xi; \xi^* \rangle. \tag{15}$$

Therefore, by the definition introduced in [12,13], the pair  $(\xi, \xi^*)$  is called a *generalized canonical dual pair* on  $\mathcal{E}_a \times \mathcal{E}_a^*$ . Replacing  $V(\Lambda(\mathbf{x}))$  in the canonical primal problem (13) by the Fenchel-Young equality  $V(\Lambda(\mathbf{x})) = \langle \Lambda(\mathbf{x}); \xi^* \rangle - V^\sharp(\xi^*)$ , the *total complementary function* (see [22])  $\Xi(\mathbf{x}, \boldsymbol{\sigma}) : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}$  associated with the problem ( $\mathcal{P}$ ) can be defined as below

$$\Xi(\mathbf{x}, \boldsymbol{\sigma}) = \langle \Lambda(\mathbf{x}); \xi^* \rangle - V^\sharp(\xi^*) - \langle \mathbf{x}, \mathbf{c} \rangle \tag{16}$$

$$= \frac{1}{2} \langle \mathbf{x}, \mathbf{G}(\boldsymbol{\sigma}) \mathbf{x} \rangle - \frac{1}{2} \langle \mathbf{e}, \boldsymbol{\sigma} \rangle - \langle \mathbf{x}, \mathbf{c} \rangle \quad \text{s.t. } \boldsymbol{\sigma} \in \mathbb{R}_+^n, \tag{17}$$

where  $\mathbb{R}_+^n := \{\sigma \in \mathbb{R}^n \mid \sigma \geq \mathbf{0}\}$ . For a fixed  $\sigma \in \mathbb{R}_+^n$ , the criticality condition  $\nabla_{\mathbf{x}} \Xi(\mathbf{x}, \sigma) = 0$  leads to the *canonical equilibrium equation* [12]:

$$\mathbf{G}(\sigma)\bar{\mathbf{x}} = \mathbf{c}. \tag{18}$$

Clearly, if the matrix  $\mathbf{G}(\sigma)$  is invertible on  $S_a$ , the primal variable  $\bar{\mathbf{x}}$  can be uniquely defined by  $\bar{\mathbf{x}} = \mathbf{G}^{-1}(\sigma)\mathbf{c}$ . Substituting this into (17) the canonical dual problem ( $\mathcal{P}^d$ ) was formulated in [16].

On the other hand, for a given matrix  $\mathbf{Q}$  and  $\sigma \in \mathbb{R}_+^n$ , if the vector  $\mathbf{c}$  is in the column space  $\mathcal{C}_{ol}(\mathbf{G}(\sigma))$  of the matrix  $\mathbf{G}(\sigma)$ , i.e., a linear space spanned by the columns of  $\mathbf{G}(\sigma)$ , the generalized solution  $\bar{\mathbf{x}}$  of the canonical equilibrium equation (18) is well defined by

$$\bar{\mathbf{x}} = \mathbf{G}^\dagger(\sigma)\mathbf{c},$$

where  $\mathbf{G}^\dagger(\sigma)$  denotes the Moore-Penrose generalized inverse of  $\mathbf{G}(\sigma)$ . Substituting this generalized solution into the total complementary function  $\Xi$  and let  $S_g$  be a generalized canonical dual feasible space defined by

$$S_g = \{\sigma \in \mathbb{R}^n \mid \sigma \geq 0, \mathbf{c} \in \mathcal{C}_{ol}(\mathbf{G}(\sigma))\}, \tag{19}$$

the generalized canonical dual function  $P^g : S_g \rightarrow \mathbb{R}$  can be formulated as

$$\begin{aligned} P^g(\sigma) &= \text{sta} \{ \Xi(\mathbf{x}, \sigma) \mid \mathbf{x} \in \mathbb{R}^n \} \\ &= -\frac{1}{2} \langle \mathbf{G}^\dagger(\sigma)\mathbf{c}, \mathbf{c} \rangle - \frac{1}{2} \langle \mathbf{e}, \sigma \rangle. \end{aligned} \tag{20}$$

Therefore, the generalized canonical dual problem ( $\mathcal{P}^g$ ) can be formulated as the following minimal stationary point problem

$$(\mathcal{P}^g) : \min \text{sta} \left\{ P^g(\sigma) = -\frac{1}{2} \langle \mathbf{G}^\dagger(\sigma)\mathbf{c}, \mathbf{c} \rangle - \frac{1}{2} \langle \mathbf{e}, \sigma \rangle \mid \sigma \in S_g \right\}. \tag{21}$$

**Theorem 2** (Complementary-dual principle) *The problem ( $\mathcal{P}^g$ ) is canonically dual to ( $\mathcal{P}$ ) in the sense that if  $\bar{\sigma} \in S_g$  is a feasible solution of ( $\mathcal{P}^g$ ), then the vector*

$$\bar{\mathbf{x}}(\bar{\sigma}) = \mathbf{G}^\dagger(\bar{\sigma})\mathbf{c} \tag{22}$$

*is a feasible solution of the problem ( $\mathcal{P}$ ) and*

$$P(\bar{\mathbf{x}}) = P^g(\bar{\sigma}). \tag{23}$$

*If  $\bar{\sigma} \neq \mathbf{0}$  is a critical point of ( $\mathcal{P}^g$ ), then  $\bar{\mathbf{x}} \in \partial\mathcal{X}_a$  is a feasible solution of ( $\mathcal{P}_{ip}$ ).*

*Proof* By introducing a Lagrange multiplier  $\epsilon \in \mathbb{R}_-^n := \{\epsilon \in \mathbb{R}^n \mid \epsilon \leq \mathbf{0}\}$  to relax the inequality condition  $\sigma \geq \mathbf{0}$  in  $S_g$ , the Lagrangian  $L : S_g \times \mathbb{R}_-^n \rightarrow \mathbb{R}$  associated with the problem ( $\mathcal{P}^g$ ) is

$$L(\sigma, \epsilon) = P^g(\sigma) - \langle \epsilon, \sigma \rangle. \tag{24}$$

It is easy to prove that the criticality condition  $\delta L(\bar{\sigma}, \epsilon; \sigma) = 0 \forall \sigma \in \mathbb{R}^n$  (Gâteaux variational of  $L$  at  $(\bar{\sigma}, \epsilon)$  in the direction of  $\sigma$ , see [12]) leads to the *geometrical equation*

$$\epsilon = \nabla P^g(\bar{\sigma}) = \frac{1}{2} (\bar{\mathbf{x}}(\bar{\sigma}) \circ \bar{\mathbf{x}}(\bar{\sigma}) - \mathbf{e}) = \epsilon(\bar{\mathbf{x}}(\bar{\sigma})) - \frac{1}{2} \mathbf{e} \tag{25}$$

and the KKT conditions

$$0 \leq \bar{\sigma} \perp \epsilon(\bar{\mathbf{x}}) \leq 0, \tag{26}$$

where  $\bar{\mathbf{x}} = \mathbf{G}^\dagger(\bar{\boldsymbol{\sigma}})\mathbf{c}$ , and  $\bar{\boldsymbol{\sigma}} \perp \boldsymbol{\epsilon}$  denotes the complementarity condition, i.e.,

$$\boldsymbol{\epsilon}(\bar{\mathbf{x}}) \perp \bar{\boldsymbol{\sigma}} \Leftrightarrow \frac{1}{2} (x_i^2 - 1) \bar{\sigma}_i = 0, \quad \forall i = 1, \dots, n.$$

This shows that if  $\bar{\boldsymbol{\sigma}}$  is a KKT point of the problem  $(\mathcal{P}^g)$ , then  $\bar{\mathbf{x}} = \mathbf{G}^\dagger(\bar{\boldsymbol{\sigma}})\mathbf{c}$  is a KKT point of the primal problem  $(\mathcal{P})$ .

By the complementarity condition in (26) and  $\bar{\mathbf{x}} = \mathbf{G}^\dagger(\bar{\boldsymbol{\sigma}})\mathbf{c}$ , we have

$$\begin{aligned} P^g(\bar{\boldsymbol{\sigma}}) &= \frac{1}{2} \langle \mathbf{G}^\dagger(\bar{\boldsymbol{\sigma}})\mathbf{c}, \mathbf{c} \rangle - \langle \mathbf{G}^\dagger(\bar{\boldsymbol{\sigma}})\mathbf{c}, \mathbf{c} \rangle - \frac{1}{2} \langle \mathbf{e}, \bar{\boldsymbol{\sigma}} \rangle \\ &= \frac{1}{2} \langle \bar{\mathbf{x}}, \mathbf{Q}\bar{\mathbf{x}} \rangle - \langle \bar{\mathbf{x}}, \mathbf{c} \rangle + \frac{1}{2} \langle \bar{\mathbf{x}} \circ \bar{\mathbf{x}} - \mathbf{e}, \bar{\boldsymbol{\sigma}} \rangle = P(\bar{\mathbf{x}}). \end{aligned}$$

Moreover, if  $\bar{\boldsymbol{\sigma}} \neq 0$ , the complementarity condition  $\boldsymbol{\epsilon}(\bar{\mathbf{x}}) \perp \bar{\boldsymbol{\sigma}}$  in (26) leads to  $\boldsymbol{\epsilon}(\bar{\mathbf{x}}) = \frac{1}{2}(\bar{\mathbf{x}} \circ \bar{\mathbf{x}} - \mathbf{e}) = 0$ , i.e.,  $\nabla P^g(\bar{\boldsymbol{\sigma}}) = 0$ . This shows that if  $\bar{\boldsymbol{\sigma}} \neq 0$  is a critical point of  $P^g(\boldsymbol{\sigma})$ , the associated vector  $\bar{\mathbf{x}}(\bar{\boldsymbol{\sigma}}) = \mathbf{G}^\dagger(\bar{\boldsymbol{\sigma}})\mathbf{c} \in \{-1, 1\}^n$  is a KKT point of the integer programming problem  $(\mathcal{P}_{ip})$ . □

*Remark* Comparing  $(\mathcal{P}^d)$  with  $(\mathcal{P}^g)$  we can see that the constraint  $\det \mathbf{G}(\boldsymbol{\sigma}) \neq 0$  in the original dual feasible space  $\mathcal{S}_a$  is released by using the generalized inverse. Actually,  $\det \mathbf{G}(\boldsymbol{\sigma}) \neq 0$  is not an optimization (variational) constraint as the Lagrange multiplier for this inequality condition is identical zero (see [12]). For the integer programming problem  $(\mathcal{P}_{ip})$ , the inequality constraint  $\boldsymbol{\epsilon} \leq \frac{1}{2}\mathbf{e}$  in Eq. 12 should be replaced by the equality constraint  $\boldsymbol{\epsilon} = \frac{1}{2}\mathbf{x} \circ \mathbf{x} = \frac{1}{2}\mathbf{e}$ , and also the condition  $\mathbf{c} \in \mathcal{C}_{ol}(\mathbf{G}(\boldsymbol{\sigma}))$  is not a constraint (see [18]). Therefore, the canonical dual problem for the integer programming problem  $(\mathcal{P}_{ip})$  can be simply formulated as the following minimal stationary point problem

$$(\mathcal{P}_{ip}^g) : \min \text{sta} \left\{ P^g(\boldsymbol{\sigma}) = -\frac{1}{2} \langle \mathbf{G}^\dagger(\boldsymbol{\sigma})\mathbf{c}, \mathbf{c} \rangle - \frac{1}{2} \langle \mathbf{e}, \boldsymbol{\sigma} \rangle \mid \boldsymbol{\sigma} \neq 0 \right\}. \tag{27}$$

**Corollary 1** *If  $\bar{\boldsymbol{\sigma}}$  is a solution to  $(\mathcal{P}_{ip}^g)$ , then the vector  $\bar{\mathbf{x}} = \mathbf{G}^\dagger(\bar{\boldsymbol{\sigma}})\mathbf{c} \in \{-1, 1\}^n$  is a feasible solution to the integer programming problem  $(\mathcal{P}_{ip})$ .*

*Proof* By the criticality condition  $\delta P^g(\bar{\boldsymbol{\sigma}}; \boldsymbol{\sigma}) = \langle \nabla P^g(\bar{\boldsymbol{\sigma}}), \boldsymbol{\sigma} \rangle = 0 \quad \forall \boldsymbol{\sigma} \neq 0 \in \mathbb{R}^n$ , where  $\delta P^g(\bar{\boldsymbol{\sigma}}; \boldsymbol{\sigma})$  denotes the Gâteaux variation of  $P^g$  at  $\bar{\boldsymbol{\sigma}}$  in the direction  $\boldsymbol{\sigma}$ , we have the canonical complementarity equation

$$(\bar{\mathbf{x}}(\bar{\boldsymbol{\sigma}}) \circ \bar{\mathbf{x}}(\bar{\boldsymbol{\sigma}}) - \mathbf{e}, \boldsymbol{\sigma}) = 0 \quad \forall \boldsymbol{\sigma} \in \mathbb{R}^n, \tag{28}$$

where  $\bar{\mathbf{x}} = \mathbf{G}^\dagger(\bar{\boldsymbol{\sigma}})\mathbf{c}$ . Therefore, under the condition  $\boldsymbol{\sigma} \neq 0$ , the canonical solution  $\mathbf{x} = \mathbf{G}^\dagger(\boldsymbol{\sigma})\mathbf{c}$  is a feasible solution of  $(\mathcal{P}_{ip})$ . □

For the given indefinite matrix  $\mathbf{Q}$ , the inequality constraint  $\boldsymbol{\sigma} \neq 0$  is essential for the canonical dual integer programming problem  $(\mathcal{P}_{ip}^g)$ . But, this condition, as well as the condition  $\mathbf{c} \in \mathcal{C}_{ol}(\mathbf{G}(\boldsymbol{\sigma}))$  in  $\mathcal{S}_g$ , can also be relaxed easily by perturbation methods given in Sect. 5.

### 3 Global optimality and existence criteria

In this section, we shall present both global and local optimality conditions for the nonconvex problems  $(\mathcal{P})$  and  $(\mathcal{P}_{ip})$ . We let

$$S_g^+ = \{\sigma \in S_g \mid \mathbf{G}(\sigma) \succeq 0\}, \quad S_g^- = \{\sigma \in S_g \mid \mathbf{G}(\sigma) \prec 0\}, \tag{29}$$

and consider the following canonical dual problem:

$$(\mathcal{P}_{\max}^g) : \max \left\{ P^g(\sigma) = -\frac{1}{2} \langle \mathbf{G}^\dagger(\sigma) \mathbf{c}, \mathbf{c} \rangle - \frac{1}{2} \langle \mathbf{e}, \sigma \rangle \mid \sigma \in S_g^+ \right\}. \tag{30}$$

**Theorem 3** *For any given matrix  $\mathbf{Q} \in \mathbb{R}^{n \times n}$  and a vector  $\mathbf{c} \in \mathbb{R}^n$ , the canonical dual problem  $(\mathcal{P}_{\max}^g)$  has at least one KKT point  $\bar{\sigma} \in S_g^+$  and the following weak duality relation holds*

$$\min_{\mathbf{x} \in \mathcal{X}_a} P(\mathbf{x}) \geq \max_{\sigma \in S_g^+} P^g(\sigma) = P^g(\bar{\sigma}). \tag{31}$$

*If the KKT point  $\bar{\sigma} \in S_g^+$  is a critical point of  $P^g(\sigma)$ , then the vector  $\bar{\mathbf{x}} = \mathbf{G}^\dagger(\bar{\sigma})\mathbf{c}$  is a global minimizer to the primal problem  $(\mathcal{P})$  and the following strong duality relation holds*

$$P(\bar{\mathbf{x}}) = \min_{\mathbf{x} \in \mathcal{X}_a} P(\mathbf{x}) = \max_{\sigma \in S_g^+} P^g(\sigma) = P^g(\bar{\sigma}). \tag{32}$$

*If  $\bar{\sigma} \in S_g^-$  is a critical point of  $P^g(\sigma)$  and  $\bar{\mathbf{x}} = \mathbf{G}^\dagger(\bar{\sigma})\mathbf{c}$ , then on the neighborhood  $\mathcal{X}_o \times \mathcal{S}_o \subset \mathcal{X}_a \times S_g^-$  of  $(\bar{\mathbf{x}}, \bar{\sigma})$ , we have*

$$P(\bar{\mathbf{x}}) = \min_{\mathbf{x} \in \mathcal{X}_o} P(\mathbf{x}) = \min_{\sigma \in \mathcal{S}_o} P^g(\sigma) = P^g(\bar{\sigma}). \tag{33}$$

*Proof* Since  $S_g^+$  is a closed convex set, for any given  $\sigma \in S_g^+$  such that  $\mathbf{x} = \mathbf{G}^\dagger(\sigma)\mathbf{c}$ , the Hessian matrix of  $P^d(\sigma)$

$$\nabla^2 P^g(\sigma) = -\text{Diag}(\mathbf{x}(\sigma)) \mathbf{G}^\dagger(\sigma) \text{Diag}(\mathbf{x}(\sigma)) \tag{34}$$

is negative semi-definite on  $S_g^+$ . Thus, the canonical dual function  $P^g(\sigma)$  is concave on  $S_g^+$ . By the fact for any given  $\sigma \geq 0 \in \mathbb{R}^n$

$$\lim_{\alpha \rightarrow \infty} P^g(\alpha\sigma) = -\infty, \tag{35}$$

we know that the canonical dual function  $P^g(\sigma)$  is coercive on the closed convex set  $S_g^+$ . Therefore, the canonical dual problem  $(\mathcal{P}_{\max}^g)$  has at least one maximizer  $\bar{\sigma} \in S_g^+$  by the theory of convex analysis [4,32]. Since the total complementary function  $\Xi(\mathbf{x}, \sigma)$  is a saddle function on  $\mathbb{R}^n \times S_g^+$ , we have

$$\min_{\mathbf{x} \in \mathcal{X}_a} P(\mathbf{x}) = \min_{\mathbf{x} \in \mathbb{R}^n} \max_{\sigma \in S_g^+} \Xi(\mathbf{x}, \sigma) \geq \max_{\sigma \in S_g^+} \min_{\mathbf{x} \in \mathbb{R}^n} \Xi(\mathbf{x}, \sigma) = \max_{\sigma \in S_g^+} P^g(\sigma).$$

This leads to the weak duality relation (31).

By Theorem 2 we know that if the vector  $\bar{\sigma} \in S_g$  is a critical point of the canonical dual function  $(P^g)$ , then  $\bar{\mathbf{x}} = \mathbf{G}^\dagger(\bar{\sigma})\mathbf{c}$  is a KKT point of the problem  $(\mathcal{P})$  and

$$P(\bar{\mathbf{x}}) = \Xi(\bar{\mathbf{x}}, \bar{\sigma}) = P^g(\bar{\sigma}). \tag{36}$$

Since the geometrical operator  $\Lambda(\mathbf{x})$  defined in (11) is a (pure) quadratic operator, the quadratic function

$$G_{ap}(\mathbf{x}, \sigma) = \frac{1}{2} \langle \mathbf{x}, \mathbf{G}(\sigma)\mathbf{x} \rangle \tag{37}$$

is the so-called *complementary gap function* first introduced in [22], which is a convex function of  $\mathbf{x} \in \mathbb{R}^n$  for any given  $\sigma \in S_g^+$ . Therefore, the total complementary function  $\Xi : \mathbb{R}^n \times S_g^+ \rightarrow \mathbb{R}$  is a saddle function which is convex in  $\mathbf{x} \in \mathbb{R}^n$  and concave in  $\sigma \in S_g^+$ . Thus, by Theorem 5 proved in [22] we have (32).

On the other hand, if  $\mathbf{G}(\bar{\sigma}) < 0$ , the total complementary function  $\Xi(\mathbf{x}, \sigma)$  defined by (17) is a so-called *super-critical function* (see [12]), i.e., it is locally concave in both  $\mathbf{x}$  and  $\sigma$ . Thus, on the neighborhood  $\mathcal{X}_o \times S_o$  of  $(\bar{\mathbf{x}}, \bar{\sigma})$ , we have, by the triality lemma proposed in [15]

$$\begin{aligned} P(\bar{\mathbf{x}}) &= \min_{\mathbf{x} \in \mathcal{X}_o} P(\mathbf{x}) = \min_{\mathbf{x} \in \mathcal{X}_o} \max_{\sigma \in S_o} \Xi(\mathbf{x}, \sigma) \\ &= \min_{\sigma \in S_o} \max_{\mathbf{x} \in \mathcal{X}_o} \Xi(\mathbf{x}, \sigma) = \min_{\sigma \in S_o} P^g(\sigma) = P^g(\bar{\sigma}). \end{aligned}$$

This proves the statement (33). □

**Corollary 2** *Suppose that  $\bar{\sigma} \in S_g^+$  is a critical point of the canonical dual problem  $(\mathcal{P}_{\max}^g)$  and  $\bar{\mathbf{x}} = \mathbf{G}^\dagger(\bar{\sigma})\mathbf{c}$ .*

*If  $\mathbf{G}(\bar{\sigma}) > 0$ , then  $\bar{\mathbf{x}}$  is a unique global minimizer of the problem  $(\mathcal{P})$ .*

*If  $\bar{\sigma} \in S_g^+$  and  $\bar{\sigma} \neq 0$ , then  $\bar{\mathbf{x}}$  is a global minimizer of the integer programming problem  $(\mathcal{P}_{ip})$ .*

Theoretical results presented in this section show that by the global optimality condition  $G_{ap}(\mathbf{x}, \bar{\sigma}) \geq 0 \ \forall \mathbf{x}$ , proposed in Gao and Strang’s original work [22], the nonconvex minimization problem  $(\mathcal{P})$  can be converted into a concave maximization problem  $(\mathcal{P}_{\max}^g)$  over the convex set  $S_g^+$ , which can be solved by well-developed nonlinear programming methods. If the dual solution  $\bar{\sigma} \in S_a^+$ , it must be a critical point of  $P^d(\sigma)$  and the vector  $\bar{\mathbf{x}} = [\mathbf{G}(\bar{\sigma})]^{-1}\mathbf{c}$  is a unique global minimizer of the problem  $(\mathcal{P})$ . If  $\bar{\sigma} \neq 0$ , then  $\bar{\mathbf{x}} = [\mathbf{G}(\bar{\sigma})]^{-1}\mathbf{c}$  must be located on the vertices of  $\mathcal{X}_a$ , i.e.  $\bar{\mathbf{x}} \in \{-1, 1\}^n$  is a global minimizer to the integer programming problem  $(\mathcal{P}_{ip})$ . Since the primal function  $P(\mathbf{x})$  is nonconvex, to find the global minimizer by traditional direct approaches are fundamentally difficult. Therefore, traditional direct methods for solving such problems are difficult.

Theorem 3 shows that a vector  $\bar{\mathbf{x}} = \mathbf{G}^\dagger(\bar{\sigma})\mathbf{c}$  is a global minimizer of the problem  $(\mathcal{P})$  if  $\bar{\sigma}$  is a critical solution of  $(\mathcal{P}_{\max}^g)$ . For certain given matrix  $\mathbf{Q}$  and vector  $\mathbf{c} \in \mathbb{R}^n$ , the canonical dual function might have no critical point in  $S_g^+$ . In the case that  $\det \mathbf{G}(\bar{\sigma}) = 0$ , the problem  $(\mathcal{P}_{\max}^g)$  may have multiple KKT points  $\bar{\sigma}$  on the boundary of  $S_g^+$ . In this case, the primal problems  $(\mathcal{P})$  and  $(\mathcal{P}_{ip})$  may have multiple solutions. Detailed discussion will be given in the following section.

#### 4 Existence and uniqueness conditions

The weak duality theorem (31) shows that the canonical dual problem  $(\mathcal{P}_{\max}^g)$  provides a lower bound for the box/integer constrained problems. In order to study existence and uniqueness



of the canonical dual problems, we introduce a singular hyper-surface defined by

$$\mathcal{G}_a = \{ \boldsymbol{\sigma} \in \mathbb{R}^n \mid \det \mathbf{G}(\boldsymbol{\sigma}) = 0 \}. \tag{38}$$

**Theorem 4** (Existence and uniqueness criterion) *Suppose that for a given symmetric matrix  $\mathbf{Q}$  and a vector  $\mathbf{c}$  such that  $\mathcal{S}_g^+ \neq \emptyset$  and  $\mathcal{G}_a \subset \mathcal{S}_g^+$ . If for any given  $\boldsymbol{\sigma}_o \in \mathcal{G}_a$  and  $\boldsymbol{\sigma} \in \mathcal{S}_a^+$ ,*

$$\lim_{\alpha \rightarrow 0^+} P^g(\boldsymbol{\sigma}_o + \alpha \boldsymbol{\sigma}) = -\infty, \tag{39}$$

*then the canonical dual problem ( $\mathcal{P}_{\max}^g$ ) has a unique critical point  $\bar{\boldsymbol{\sigma}} \in \mathcal{S}_a^+$  and  $\bar{\mathbf{x}} = \mathbf{G}^{-1}(\bar{\boldsymbol{\sigma}})\mathbf{c}$  is a global minimizer to the primal problem ( $\mathcal{P}$ ). If  $\bar{\boldsymbol{\sigma}} \neq 0$ , then  $\bar{\mathbf{x}}$  is a global minimizer to the integer programming problem ( $\mathcal{P}_{ip}$ ).*

*Proof* If  $\mathcal{G}_a \subset \mathcal{S}_g^+$ , then  $\mathcal{S}_g^+$  is a closed convex subset of  $\mathbb{R}_+^n$ . Since  $P^g : \mathcal{S}_g^+ \rightarrow \mathbb{R}$  is concave and the condition (35) holds, if (39) holds, the canonical dual function  $P^g(\boldsymbol{\sigma})$  is coercive on the open convex set  $\mathcal{S}_a^+$ . Therefore, the canonical dual problem ( $\mathcal{P}^g$ ) has a unique maximizer  $\bar{\boldsymbol{\sigma}} \in \mathcal{S}_a^+$ .  $\square$

Clearly, if  $\mathbf{Q} \succ 0$ , the quadratic objective function  $P(\mathbf{x})$  is convex and the solution to the box constrained primal problem ( $\mathcal{P}$ ) could be a stationary point in the box  $\mathcal{X}_a$ . If  $\mathbf{Q} \prec 0$ , the primal function  $P(\mathbf{x})$  is concave and its global minimizer  $\bar{\mathbf{x}}$  must be located on the boundary of the feasible space  $\mathcal{X}_a$ . In this case, the box constrained problem ( $\mathcal{P}$ ) is identical to the integer constrained problem ( $\mathcal{P}_{ip}$ ), and both of them are considered to be NP-hard. However, by the fact that  $\mathcal{G}_a \subset \mathcal{S}_g^+$  and for any given  $\mathbf{c} \in \mathbb{R}^n$ , the dual feasible space  $\mathcal{S}_g^+ \neq \emptyset$ , the canonical dual problem ( $\mathcal{P}_{\max}^g$ ) could be much easier to solve. Detailed discussion is given in the next section.

In the case that  $\mathbf{Q} = \text{Diag}(\mathbf{q})$  is a diagonal matrix with  $\mathbf{q} = \{q_i\} \in \mathbb{R}^n$  being its diagonal elements, the canonical dual function  $P^d(\boldsymbol{\sigma})$  has a simple form

$$P^d(\boldsymbol{\sigma}) = - \sum_{i=1}^n \left( \frac{c_i^2}{2(q_i + \sigma_i)} + \frac{1}{2} \sigma_i \right). \tag{40}$$

The criticality condition  $\delta P^d(\boldsymbol{\sigma}) = 0$  leads to the dual solutions

$$\sigma_i = -q_i \pm |c_i|, \quad \forall i = 1, 2, \dots, n. \tag{41}$$

Clearly, for any given  $\mathbf{q} \in \mathbb{R}^n$ , if  $c_i \neq 0 \quad \forall i = 1, \dots, n$ , the condition (39) holds. Therefore, by Theorems 3 and 4, we have the following result.

**Corollary 3** *For any given diagonal matrix  $\mathbf{Q} = \text{Diag}(\mathbf{q})$  and a vector  $\mathbf{c} \in \mathbb{R}^n$  such that  $c_i \neq 0 \quad \forall i = 1, \dots, n$ , then*

$$\mathbf{x} = \left\{ \begin{array}{l} c_i \\ |c_i| \end{array} \right\} \text{ is a global minimizer of } (P_{ip}) \text{ if } \boldsymbol{\sigma} = \{-q_i + |c_i|\} > 0;$$

$$\mathbf{x} = \left\{ \begin{array}{l} -c_i \\ |c_i| \end{array} \right\} \left\{ \begin{array}{l} \text{is a local minimizer of } (P_{ip}) \text{ if } \boldsymbol{\sigma} = \{-q_i - |c_i|\} > 0, \\ \text{is a local maximizer of } (P_{ip}) \text{ if } \boldsymbol{\sigma} = \{-q_i - |c_i|\} < 0. \end{array} \right.$$

### 5 Perturbations and analytical solutions

For any given indefinite symmetrical matrix  $\mathbf{Q} \in \mathbb{R}^{n \times n}$ , there exists a parametrical vector  $\boldsymbol{\alpha} \in \mathbb{R}^n$  such that  $\mathbf{Q} + \text{Diag}(\boldsymbol{\alpha})$  is either positive definite or negative definite. By the fact that

$\mathbf{x} \circ \mathbf{x} = \mathbf{e}$ , the integer programming problem  $(\mathcal{P}_{ip})$  is identical to the following perturbed problem

$$(\mathcal{P}_\alpha) : \min \left\{ P_\alpha(\mathbf{x}) = \frac{1}{2} \langle \mathbf{x}, (\mathbf{Q} + \text{Diag}(\boldsymbol{\alpha}))\mathbf{x} \rangle - \langle \mathbf{x}, \mathbf{c} \rangle - d_\alpha \mid \mathbf{x} \in \partial \mathcal{X}_\alpha \right\}, \quad (42)$$

where  $d_\alpha = \frac{1}{2} \langle \mathbf{e}, \boldsymbol{\alpha} \rangle$ . Clearly, if we choose  $\boldsymbol{\alpha} \in \mathbb{R}^n$  such that  $\mathbf{Q}_\alpha = \mathbf{Q} + \text{Diag}(\boldsymbol{\alpha}) \prec 0$ , the primal function  $P_\alpha(\mathbf{x})$  is strictly concave and its global minimizers must be located on the boundary  $\partial \mathcal{X}_\alpha$ . In this case, the condition  $\mathbf{G}_\alpha(\boldsymbol{\sigma}) = \mathbf{Q} + \text{Diag}(\boldsymbol{\alpha} + \boldsymbol{\sigma}) \geq 0$  implies  $\boldsymbol{\sigma} > 0$ . Therefore, on the perturbed dual feasible space

$$S_\alpha^+ = \{ \boldsymbol{\sigma} \in \mathbb{R}^n \mid \mathbf{G}_\alpha(\boldsymbol{\sigma}) \geq 0 \}, \quad (43)$$

the perturbed canonical dual problem is

$$(\mathcal{P}_\alpha^g) : \max \text{sta} \left\{ P_\alpha^g(\boldsymbol{\sigma}) = -\frac{1}{2} \langle \mathbf{G}_\alpha^\dagger(\boldsymbol{\sigma})\mathbf{c}, \mathbf{c} \rangle - \frac{1}{2} \langle \mathbf{e}, \boldsymbol{\sigma} \rangle - d_\alpha \mid \boldsymbol{\sigma} \in S_\alpha^+ \right\}. \quad (44)$$

Since the inequality constraint  $\boldsymbol{\sigma} \neq 0$  is relaxed by the  $\alpha$ -concave perturbation  $\mathbf{Q} + \text{Diag}(\boldsymbol{\alpha}) \prec 0$ , this perturbed canonical dual problem is easier than  $(\mathcal{P}_{ip}^g)$ . Still, for certain given  $\mathbf{c} \in \mathbb{R}^n$ , the function  $P_\alpha^g(\boldsymbol{\sigma})$  may have no critical point in  $S_\alpha^+$ . Therefore, a nonsmooth  $\alpha$ -perturbed canonical dual problem was proposed in [17]

$$(\mathcal{P}_\alpha^d) : \min \text{sta} \left\{ P_\alpha^d(\boldsymbol{\sigma}) = -\frac{1}{2} \langle \mathbf{Q}_\alpha^{-1} \boldsymbol{\sigma}, \boldsymbol{\sigma} \rangle - \sum_{i=1}^n |c_i - \sigma_i| - d_\alpha \mid \boldsymbol{\sigma} \in \mathbb{R}^n \right\}, \quad (45)$$

where  $|t_i| = \max\{t_i, -t_i\}$  represents the absolute value of  $t_i$ .

**Theorem 5** (Analytic solution to integer programming problem  $(\mathcal{P}_{ip})$ ) *For a given  $\boldsymbol{\alpha} \in \mathbb{R}^n$  such that  $\det \mathbf{Q}_\alpha \neq 0$ . Then the problem  $(\mathcal{P}_\alpha^d)$  is canonically dual to the integer programming  $(\mathcal{P}_{ip})$  in the sense that if  $\bar{\boldsymbol{\sigma}} = \{\bar{\sigma}_i\}^n$  is a solution to  $(\mathcal{P}_\alpha^d)$ , then the vector  $\bar{\mathbf{x}} = \{\bar{x}_i\}^n$  defined by*

$$\bar{\mathbf{x}}(\bar{\boldsymbol{\sigma}}) = \left\{ \begin{array}{l} c_i - \bar{\sigma}_i \\ |c_i - \bar{\sigma}_i| \end{array} \right\}^n \quad (46)$$

is a feasible solution to  $(\mathcal{P}_{ip})$ , and  $P(\bar{\mathbf{x}}) = P_\alpha^d(\bar{\boldsymbol{\sigma}})$ .

*If  $\mathbf{Q}_\alpha > 0$ , the dual problem  $(\mathcal{P}_\alpha^d)$  has at most one solution  $\bar{\boldsymbol{\sigma}}$ , which is a global maximizer of  $P_\alpha^d(\boldsymbol{\sigma})$ , the vector  $\bar{\mathbf{x}}(\bar{\boldsymbol{\sigma}})$  is a unique global minimizer of  $(\mathcal{P}_{ip})$ , and*

$$P_\alpha(\bar{\mathbf{x}}) = \min_{\mathbf{x} \in \{-1, 1\}^n} P_\alpha(\mathbf{x}) = \max_{\boldsymbol{\sigma} \in \mathbb{R}^n} \text{sta} P_\alpha^d(\boldsymbol{\sigma}) = P_\alpha^d(\bar{\boldsymbol{\sigma}}). \quad (47)$$

*If  $\mathbf{Q}_\alpha < 0$ , the dual problem  $(\mathcal{P}_\alpha^d)$  exists at least one solution  $\bar{\boldsymbol{\sigma}}$ , the vector  $\bar{\mathbf{x}}(\bar{\boldsymbol{\sigma}})$  is a global minimizer of  $(\mathcal{P}_{ip})$ , and*

$$P_\alpha(\bar{\mathbf{x}}) = \min_{\mathbf{x} \in \{-1, 1\}^n} P_\alpha(\mathbf{x}) = \min_{\boldsymbol{\sigma} \in \mathbb{R}^n} P_\alpha^d(\boldsymbol{\sigma}) = P_\alpha^d(\bar{\boldsymbol{\sigma}}). \quad (48)$$

*Proof* The first part of theorem can be proved easily by the complementary-dual principle. If  $\mathbf{Q}_\alpha > 0$ , then  $P_\alpha^d(\boldsymbol{\sigma})$  is strictly concave and the canonical dual problem  $(\mathcal{P}_\alpha^d)$  is equivalent to

$$\max \text{sta} \left\{ P_\alpha^d(\boldsymbol{\sigma}) \mid \boldsymbol{\sigma} \in \mathbb{R}^n \right\}, \quad (49)$$

which has at most one solution  $\bar{\sigma}$  over  $\mathbb{R}^n$ . By the canonical duality theory, the feasible solution  $\bar{\mathbf{x}}(\bar{\sigma})$  is a global minimizer of  $(P_{ip})$ .

If  $\mathbf{Q}_\alpha < 0$ , the function  $P_\alpha(\mathbf{x})$  is strictly concave and the primal problem  $(P_\alpha)$  has at least one global minimizer located on  $\partial\mathcal{X}_\alpha$ . By the complementary-dual principle, the unconstrained dual problem  $(P_\alpha^d)$  has at least a stationary point which minimizes  $P_\alpha^d(\sigma)$  over  $\mathbb{R}^n$ .  $\square$

Theorem 5 shows that for convex perturbation  $\mathbf{Q}_\alpha > 0$ , the canonical dual problem  $(P_\alpha^d)$  is a unconstrained concave maximization problem (49). Therefore, if the primal problem has a unique global minimizer, it can be obtained easily by solving the convex perturbation canonical dual problem (49). However, for certain given  $\mathbf{Q}$  and  $\mathbf{c}$ , this problem may have no critical solution.

On the other hand, for concave perturbation  $\mathbf{Q}_\alpha < 0$ , the global minimizers of  $(P_\alpha^d)$  must be critical points. Therefore, the integer programming problem  $(P_{ip})$  is equivalent to the following unconstrained nonconvex/nonsmooth minimization problem

$$\min \left\{ P_\alpha^d(\sigma) \mid \sigma \in \mathbb{R}^n \right\}, \tag{50}$$

which can be solved by certain deterministic methods (may be not in polynomial times), such as the DIRECT method [20]. Combining Theorems 3 and 5, the condition for existence of unique solution can be given by the following result.

**Theorem 6** (Unique analytic solution) *For a given matrix  $\mathbf{Q} = \{q_{ij}\} \in \mathbb{R}^{n \times n}$  and a vector  $\mathbf{c} = \{c_i\} \in \mathbb{R}^n$ , let  $\alpha = \{\alpha_i\} \in \mathbb{R}^n$  be a parametrical vector such that either  $\mathbf{Q} + \text{Diag}(\alpha) > 0$  or  $\mathbf{Q} + \text{Diag}(\alpha) < 0$ . If*

$$|c_i| > \sum_{j=1}^n |\alpha_i \delta_{ij} + q_{ij}| \quad \forall i = 1, \dots, n, \tag{51}$$

where  $\delta_{ij} = 1$  if  $i = j$ , 0 if  $i \neq j$  is Kronecker delta, the integer programming problem  $(P_{ip})$  has a unique global minimizer  $\bar{\mathbf{x}} = \{\bar{x}_i\}^n$  determined by

$$\bar{x}_i = \begin{cases} 1 & \text{if } c_i > \sum_{j=1}^n |\alpha_i \delta_{ij} + q_{ij}|, \\ -1 & \text{if } c_i < -\sum_{j=1}^n |\alpha_i \delta_{ij} + q_{ij}|. \end{cases} \tag{52}$$

*Proof* By the criticality condition  $\nabla P_\alpha^d(\bar{\sigma}) = 0$  we have

$$(G_\alpha^{-1}(\bar{\sigma})\mathbf{c}) \circ (G_\alpha^{-1}(\bar{\sigma})\mathbf{c}) = \mathbf{e}, \tag{53}$$

or in the component form  $(G_\alpha^{-1}(\bar{\sigma})\mathbf{c})_i^2 = 1$ . Thus we have  $G_\alpha^{-1}(\bar{\sigma})\mathbf{c} = \mathbf{t}$ , where  $\mathbf{t} = \{\pm 1\}^n$ . This leads to the linear equation  $\bar{\sigma} \circ \mathbf{t} = \mathbf{c} - \alpha \circ \mathbf{t} - \mathbf{Qt}$ , or equivalently,

$$\bar{\sigma} = (\mathbf{c} - \alpha \circ \mathbf{t} - \mathbf{Qt}) \circ \mathbf{t}.$$

If the condition (51) holds and let  $\mathbf{t} = \bar{\mathbf{x}} = \{\bar{x}_i\}^n$ , where  $\bar{x}_i$  is defined by (52), then we have  $\bar{\sigma} > 0$ . This leads to  $G_\alpha(\bar{\sigma}) > 0$  since  $\mathbf{Q} + \text{Diag}(\alpha) > 0$ . By Corollary 2 we know that  $\bar{\mathbf{x}} = G_\alpha^{-1}(\bar{\sigma})\mathbf{c} = \{\bar{x}_i\}^n$  given by (52) is a global minimizer to the integer minimization problem  $(P_{ip})$ .

On the other hand, if  $\mathbf{Q} + \text{Diag}(\boldsymbol{\alpha}) \prec 0$  and the condition (51) holds, the dual problem  $(\mathcal{P}_\alpha^d)$  has a unique critical point  $\bar{\boldsymbol{\sigma}} = \mathbf{G}_\alpha \bar{\mathbf{x}}$ . Therefore, the vector defined by (52) must be a unique solution of  $(\mathcal{P}_{ip})$ .  $\square$

Theorem 6 shows that the existence of a unique analytical solution depends mainly on the given input  $\mathbf{c}$ . If  $\mathbf{c}$  is very small or even zero (for example, max-cut problems), the primal problem  $(\mathcal{P}_{ip})$  is usually NP-hard and has more than one global minimizer. Therefore, in order to use the canonical dual problem  $(\mathcal{P}_\alpha^g)$  for solving the integer programming problem, a  $\beta$ -perturbed canonical dual problem can be proposed as the following

$$(\mathcal{P}_{\alpha\beta}^d) : \max \left\{ P_{\alpha\beta}^d(\boldsymbol{\sigma}) = -\frac{1}{2} \langle \mathbf{G}_\alpha^{-1}(\boldsymbol{\sigma})\mathbf{c}, \mathbf{c} \rangle - \frac{1}{2} \sum_{i=1}^n \left( \frac{\sigma_i^2}{\beta_i} + \sigma_i \right) - d_\alpha \mid \mathbf{G}_\alpha(\boldsymbol{\sigma}) \succ 0 \right\}, \tag{54}$$

where  $\boldsymbol{\beta} \in \mathbb{R}_+^n$  is a given perturbation vector.

**Theorem 7** (Canonical dual perturbation) *Suppose that for the given  $\mathbf{Q} \in \mathbb{R}^{n \times n}$ ,  $\mathbf{c} \in \mathbb{R}^n$ , and a perturbation vector  $\boldsymbol{\alpha} \in \mathbb{R}^n$  such that  $\mathbf{Q} + \text{Diag}(\boldsymbol{\alpha}) \prec 0$ . Then there exists a vector  $\tilde{\boldsymbol{\beta}} > 0$  such that for any given  $\boldsymbol{\beta} \geq \tilde{\boldsymbol{\beta}}$ , the  $\beta$ -perturbed canonical dual problem has a unique solution  $\boldsymbol{\sigma}_\beta \in \mathcal{S}_\alpha^+$ . If  $\bar{\mathbf{x}}_\beta = \mathbf{G}_\alpha^{-1}(\bar{\boldsymbol{\sigma}}_\beta)\mathbf{c} \in \{-1, 1\}^n$ , then  $\bar{\mathbf{x}}_\beta$  is a global minimizer to  $(\mathcal{P}_{ip})$ .*

*Proof* For any given  $\mathbf{Q} \in \mathbb{R}^{n \times n}$  and  $\mathbf{c} \in \mathbb{R}^n$ , there exists a vector  $\boldsymbol{\alpha} \in \mathbb{R}^n$  such that  $\mathbf{Q} + \text{Diag}(\boldsymbol{\alpha}) \prec 0$  and  $\mathcal{S}_\alpha^+ \subset \mathcal{S}_g^+ \neq \emptyset$ . Therefore, by Theorem 4 we know that for any given  $\boldsymbol{\beta} \in \mathbb{R}_+^n$ , the  $\beta$ -perturbed canonical dual problem  $(\mathcal{P}_{\alpha\beta}^d)$  has a unique solution  $\bar{\boldsymbol{\sigma}}_\beta$ . By the complementary-dual principle and the penalty method we know that if  $\bar{\mathbf{x}}_\beta \in \{-1, 1\}^n$ , then  $\bar{\mathbf{x}}_\beta$  should be a solution to  $(\mathcal{P}_{ip})$ .  $\square$

### 6 Canonical duality algorithm

Deterministic methods for solving the nonsmooth  $\alpha$ -perturbed canonical dual problem  $(\mathcal{P}_\alpha^d)$  will be given in an another paper. In this section, we shall discuss the algorithm for the  $\beta$ -perturbed canonical dual problem  $(\mathcal{P}_{\alpha\beta}^d)$ . Since for a given perturbation vector  $\boldsymbol{\beta}_k \in \mathbb{R}_+^n$ , the canonical dual function  $P_{\alpha\beta}^d(\boldsymbol{\sigma})$  is smooth and strictly concave on  $\mathcal{S}_\alpha^+$ , the problem  $(\mathcal{P}_{\alpha\beta}^d)$  can be solved easily by Newton-type methods. An important step in nonlinear iteration algorithms is to choose a good initial vector  $\boldsymbol{\sigma}_0 \in \mathcal{S}_\alpha^+$ . By the canonical duality theory for solving quadratic minimization over a sphere  $\frac{1}{2} \|\mathbf{x}\|^2 \leq 1$  developed in [15], we can let  $\boldsymbol{\sigma}_0 = \boldsymbol{\sigma}_0 \mathbf{e}$ , where  $\sigma_0$  is a solution to the one-dimensional problem

$$(\mathcal{P}_s^d) : \max \left\{ P_s^d(\sigma) = -\frac{1}{2} \langle \mathbf{G}_\alpha^{-1}(\sigma)\mathbf{c}, \mathbf{c} \rangle - \sigma - d_\alpha \mid \mathbf{G}_\alpha(\sigma) \succ 0 \right\}, \tag{55}$$

in which,  $\mathbf{G}_\alpha(\sigma) = \mathbf{Q} + \text{Diag}(\boldsymbol{\alpha}) + \sigma I$ . By using this initial solution, an algorithm can be proposed to solve the problem  $(\mathcal{P}_{ip})$ .

**Algorithm 1 (Canonical dual perturbation for integer programming)**

*Step 0:* Let  $\sigma_0 = \sigma_0 I$ , compute  $\mathbf{x}_0 = \mathbf{G}_\alpha^{-1}(\sigma_0)\mathbf{c}$  and  $P_{\alpha\beta}^d(\sigma_0)$ . Also let  $k = 0$ , choose  $\beta_0 \in \mathbb{R}_+^n$ ,  $\omega > 1$ , and  $\delta > 0$ .

*Step 1:* Compute the canonical dual solution  $\sigma_{k+1}$  by solving

$$P_{\alpha\beta}^d(\sigma_{k+1}) = \max \left\{ P_{\alpha\beta}^d(\sigma) \mid \mathbf{G}_\alpha(\sigma) > 0 \right\} \tag{56}$$

with  $\sigma_k$  as a starting point.

*Step 2:* Compute the primal solution by

$$\mathbf{x}_{k+1} = \mathbf{G}_\alpha^{-1}(\sigma_{k+1})\mathbf{c}.$$

*Step 3:* If either  $|P_{\alpha\beta}^d(\sigma_{k+1}) - P_{\alpha\beta}^d(\sigma_k)| > \delta$  or  $|P(\mathbf{x}_{k+1}) - P_{\alpha\beta}^d(\sigma_{k+1})| > \delta$ , let  $\beta_{k+1} = \omega\beta_k$  and  $k = k + 1$ , go to Step 1.

Otherwise, stop the algorithm, the vector  $\sigma_{k+1}$  is the optimal solution of  $(\mathcal{P}_{\alpha\beta}^d)$ . If  $\mathbf{x}_{k+1} \in \{-1, 1\}^n$ , it is the optimal solution for the integer programming problem  $(\mathcal{P}_{ip})$ . Otherwise, round the current  $\mathbf{x}_{k+1}$  to the nearest integer vector and report the rounded solution.

The concave maximization problem (56) can be solved easily by the Newton method:

$$\sigma_{k+1} = \sigma_k - H_{k+1} \nabla P_{\alpha\beta}^d(\sigma_k), \tag{57}$$

where  $\nabla P_{\alpha\beta}^d(\sigma_k) = \mathbf{x}_k \circ \mathbf{x}_k - \mathbf{e} - \sigma_k/\beta_k$  and  $H_{k+1}$  is the inverse Hessian matrix of  $P_{\alpha\beta}^d(\sigma_k)$  which can be simply given by

$$H_{k+1} = \left( \nabla^2 P_{\alpha\beta}^d(\sigma_k) \right)^{-1} = \left[ -\text{Diag}(\mathbf{x}_k)\mathbf{G}_\alpha^{-1}(\sigma_k)\text{Diag}(\mathbf{x}_k) - \text{Diag}(1/\beta_k) \right]^{-1}. \tag{58}$$

For high dimensional problems, the BFGS method is suggested.

**7 Applications**

*Example 1 One-D concave minimization.* First of all, let us consider one dimensional concave minimization problem:

$$\min \left\{ P(x) = \frac{1}{2}qx^2 - cx \mid -1 \leq x \leq 1 \right\}. \tag{59}$$

Clearly, if  $q < 0$ , the global minimizer of  $P(x)$  has to be one of boundary points  $\bar{x} = \pm 1$ . Since  $q \neq 0$ , the canonical dual function  $P^d(\sigma) = P^g(\sigma)$  is

$$P^d(\sigma) = -\frac{1}{2}c^2/(q + \sigma) - \frac{1}{2}\sigma. \tag{60}$$

The criticality condition  $\delta P^d(\sigma) = \frac{1}{2}c^2/(q + \sigma)^2 - \frac{1}{2} = 0$  has two roots:  $\bar{\sigma}_{1,2} = -q \pm |c|$  and  $\bar{x}_{1,2} = \pm c/|c| \in \{-1, 1\}^2$  are two KKT points of  $(\mathcal{P})$ . By Theorem 1 we know that  $\bar{\sigma}_1 = -q + |c| > -q > 0$  is a unique global maximizer of  $P^d$  on  $\mathcal{S}_\alpha^+ = \{\sigma \in \mathbb{R} \mid \sigma \geq 0, q + \sigma > 0\}$ .

The canonical dual function  $P_\alpha^d(\sigma)$  in this example is a nonconvex/nonsmooth function

$$P_\alpha^d(\sigma) = -\frac{1}{2}q^{-1}\sigma^2 - |c - \sigma|, \tag{61}$$

which has at most two critical points:  $\bar{\sigma}_1 = q$  if  $c > q$  and  $\bar{\sigma}_2 = -q$  if  $c < -q$ .

If we choose  $c = 0.5$ ,  $q = -1$ , the dual solution  $\bar{\sigma}_1 = 1.5$  for the problem  $(\mathcal{P}^d)$  gives the global minimizer  $\bar{x}_1 = c/(q + \bar{\sigma}_1) = 1$ . It is easy to check that  $P(\bar{x}_1) = -1 = P^d(\bar{\sigma}_1)$ . While  $\bar{\sigma}_2 = 0.5$  is a minimizer of  $P^d$  on  $S_a^- = \{\sigma \in \mathbb{R} \mid \sigma \geq 0, q + \sigma < 0\}$ , which gives a local minimizer  $\bar{x}_2 = -1$  and we have  $P(\bar{x}_2) = 0 = P^d(\bar{\sigma}_2)$ . The graphs of  $P(x)$  and  $P^d(\sigma)$  are shown in Fig. 1a.

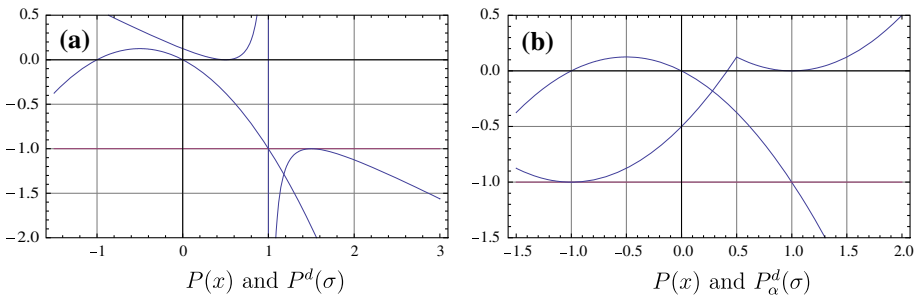
The graphs of  $P(x)$  and  $P^d_\alpha(\sigma)$  are shown in Fig. 1b. As we can see that the graph of  $P^d_\alpha(\sigma)$  is nonconvex/nonsmooth and has two critical points  $\bar{\sigma}_1 = -1$  and  $\bar{\sigma}_2 = 1$ . By the analytical solution (46) we have  $\bar{x}_1 = 1$  and  $\bar{x}_2 = -1$ . It is easy to verify that  $P(\bar{x}_1) = P^d_\alpha(\bar{\sigma}_1) = -1$  and  $P(\bar{x}_2) = P^d_\alpha(\bar{\sigma}_2) = 0$ .

If we choose  $c = 1.5$ ,  $q = -1$ , the canonical dual problem  $(\mathcal{P}^d)$  has two critical points:  $\bar{\sigma}_1 = 2.5$  and  $\bar{\sigma}_2 = -0.5$ . By the fact that  $\bar{\sigma}_1 \in S_a^+$ , therefore  $\bar{x}_1 = c/(q + \bar{\sigma}_1) = 1$  is a global minimizer and  $P(\bar{x}_1) = -2 = P^d(\bar{\sigma}_1)$ . Since  $\bar{\sigma}_2 = -0.5 < 0$ , by Corollary 3  $\bar{x}_2$  is a local maximizer (see Fig. 2a). In this case, the canonical dual problem  $(\mathcal{P}^d_\alpha)$  has only one critical point  $\bar{\sigma} = -1$  which is a global minimizer of  $P^d_\alpha(\sigma)$ . By Theorem 5 we know that  $\bar{x} = 1$  is a global minimizer of  $(\mathcal{P}_{ip})$  and  $P(\bar{x}) = -2 = P^d_\alpha(\bar{\sigma})$ .

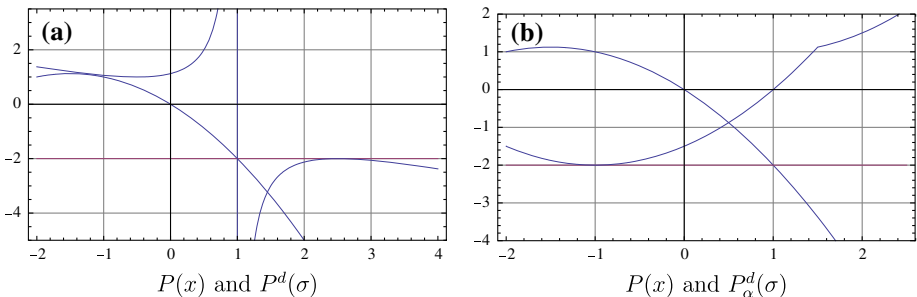
**Example 2 Two-D nonconvex programming problem.** We now consider the following quadratic programming within a convex set:

$$\min P(x_1, x_2) = \frac{1}{2} (q_1x_1^2 + q_2x_2^2 + 2q_3x_1x_2) - c_1x_1 - c_2x_2 \tag{62}$$

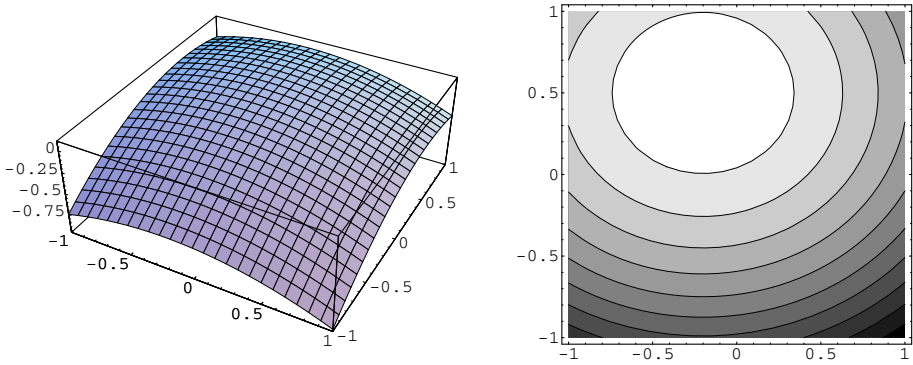
$$s.t. -1 \leq x_i \leq 1, \quad i = 1, 2. \tag{63}$$



**Fig. 1** Graphs of  $P(x)$  and its dual functions for Example 1 with  $c = 0.5$



**Fig. 2** Graphs of  $P(x)$  and its dual functions for Example 1 with  $c = 1.5$



**Fig. 3** Graph of the concave function  $P(x_1, x_2)$  and its contour for Example 2 (I)

The canonical dual function has the form of

$$P^g(\sigma_1, \sigma_2) = -\frac{1}{2}[c_1, c_2] \begin{bmatrix} q_1 + \sigma_1 & q_3 \\ q_3 & q_2 + \sigma_2 \end{bmatrix}^\dagger \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} - \frac{1}{2}(\sigma_1 + \sigma_2). \tag{64}$$

Three cases will be considered.

**Case I.**  $q_1 \leq 0, q_2 \leq 0,$  and  $q_3 = 0$ . In this case,  $P(\mathbf{x})$  is concave. If we let  $\mathbf{c} = (0.1, -0.3), q_1 = -0.5, q_2 = -0.6,$  the dual function  $P^g(\boldsymbol{\sigma}) = P^d(\boldsymbol{\sigma})$  has four critical points:

$$\boldsymbol{\sigma}_1 = \{0.6, 0.9\}, \boldsymbol{\sigma}_2 = \{0.4, 0.3\}, \boldsymbol{\sigma}_3 = \{0.4, 0.9\}, \boldsymbol{\sigma}_4 = \{0.6, 0.3\}.$$

It is easy to check that critical point

$$\boldsymbol{\sigma}_1 = \{0.6, 0.9\} \in S_a^+ = \{\boldsymbol{\sigma} \in \mathbb{R}^2 \mid \sigma_1 > 0.5, \sigma_2 > 0.6\},$$

and

$$\boldsymbol{\sigma}_2 = \{0.4, 0.3\} \in S_a^- = \{\boldsymbol{\sigma} \in \mathbb{R}^2 \mid 0 \leq \sigma_1 < 0.5, 0 \leq \sigma_2 < 0.6\}.$$

By Theorem 2, we know that  $\mathbf{x}_1 = \{c_i/(q_i + \sigma_i)\} = \{1.0, -1.0\}$  is a global minimizer, and  $\mathbf{x}_2 = \{-1.0, 1.0\}$  is a local minimizer on the boundary. It is easy to verify that

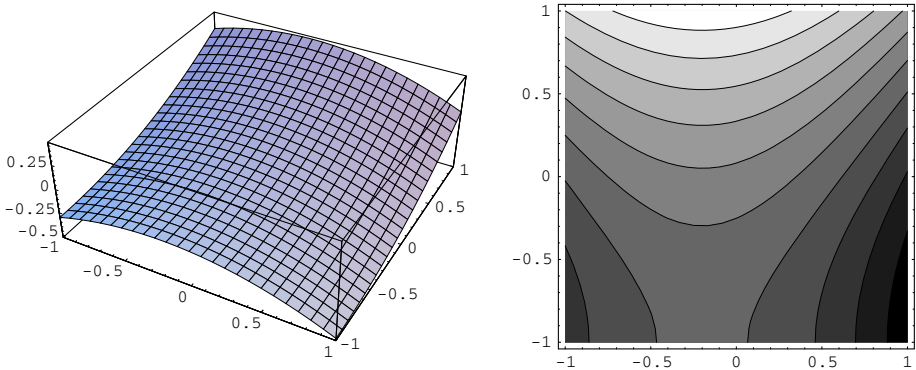
$$P(\mathbf{x}_1) = P^d(\boldsymbol{\sigma}_1) = -0.95 < P(\mathbf{x}_2) = P^d(\boldsymbol{\sigma}_2) = -0.15.$$

The other two solutions  $\boldsymbol{\sigma}_3 = \{0.4, 0.9\}, \boldsymbol{\sigma}_4 = \{0.6, 0.3\}$  give  $\mathbf{x}_3 = \{-1, -1\},$  and  $\mathbf{x}_4 = \{1, 1\},$  respectively. We have  $P(\mathbf{x}_3) = P^d(\boldsymbol{\sigma}_3) = -0.75, P(\mathbf{x}_4) = P^d(\boldsymbol{\sigma}_4) = -0.35.$  (see Fig. 3).

**Case II.**  $q_1 \leq 0, q_2 \geq 0,$  and  $q_3 = 0$ . In this case,  $P(\mathbf{x})$  is a saddle function. If we let  $\mathbf{c} = (0.1, -0.3), q_1 = -0.5, q_2 = 0.3,$  the dual function  $P^d$  has four critical points

$$\boldsymbol{\sigma}_1 = \{0.6, 0.0\}, \boldsymbol{\sigma}_2 = \{0.4, 0.0\}, \boldsymbol{\sigma}_3 = \{0.4, -0.6\}, \boldsymbol{\sigma}_4 = \{0.6, -0.6\}.$$

Since  $\boldsymbol{\sigma}_1 \in S_a^+ = \{\boldsymbol{\sigma} \in \mathbb{R}^2 \mid \sigma_1 > 0.5, \sigma_2 \geq 0\},$  and  $\boldsymbol{\sigma}_2 \in S_a^- = \{\boldsymbol{\sigma} \in \mathbb{R}^2 \mid 0 \leq \sigma_1 < 0.5, \sigma_2 \geq 0\}$  are KKT points, by Theorem 1, we know that



**Fig. 4** Graph of the saddle function  $P(x_1, x_2)$  and its contour for Example 2 (II)

$\mathbf{x}_1 = \{1.0, -1.0\} \in \mathcal{X}_a$  is a global minimizer, and  $\mathbf{x}_2 = \{-1.0, -1.0\} \in \mathcal{X}_a$  is a local minimizer. It is easy to verify that

$$P(\mathbf{x}_1) = P^d(\boldsymbol{\sigma}_1) = -0.5 < P(\mathbf{x}_2) = P^d(\boldsymbol{\sigma}_2) = -0.3.$$

Since  $\boldsymbol{\sigma}_3$  and  $\boldsymbol{\sigma}_4$  are not KKT points,  $\mathbf{x}_3 = \{-1.0, 1.0\}$  and  $\mathbf{x}_4 = \{1.0, 1.0\}$  are not local extrema (see Fig. 4).

**Case III.** General matrix  $\mathbf{Q} \in \mathbb{R}^{2 \times 2}$  with integer Solutions.

We let  $\mathbf{c} = \{1, -2\}$ ,  $q_1 = -2$ ,  $q_2 = -1$ ,  $q_3 = -3$ . In this case, the eigenvalues of  $\mathbf{Q}$  are  $\{-4.54138, 1.54138\}$ , i.e. the primal problem is nonconvex. The dual problem has four critical points

$$\boldsymbol{\sigma}_1 = \{4, 6\}, \quad \boldsymbol{\sigma}_2 = \{6, 2\}, \quad \boldsymbol{\sigma}_3 = \{0, 0\}, \quad \boldsymbol{\sigma}_4 = \{-2, -4\},$$

from which, we have

$$\mathbf{x}_1 = \{-1, -1\}, \quad \mathbf{x}_2 = \{1, 1\}, \quad \mathbf{x}_3 = \{1, -1\}, \quad \mathbf{x}_4 = \{-1, 1\}.$$

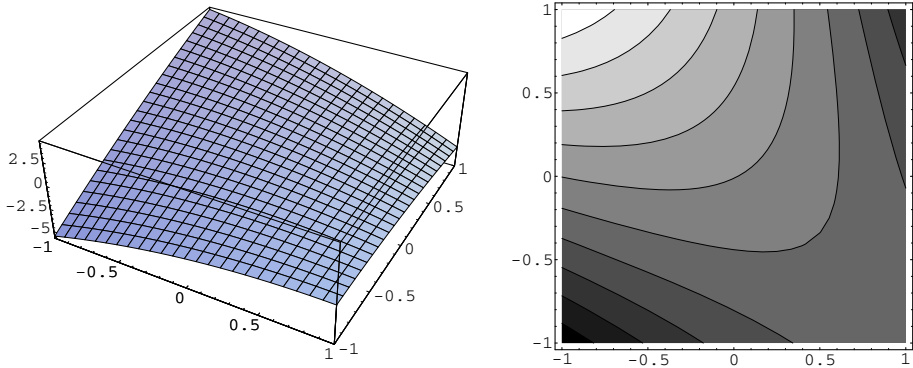
on the four corners of the box  $\mathcal{X}_a = \{\mathbf{x} \in \mathbb{R}^2 \mid -1 \leq x_1 \leq 1, -1 \leq x_2 \leq 1\}$ . Since  $\boldsymbol{\sigma}_1 \in \mathcal{S}_a^+$ , we know that  $\mathbf{x}_1 \in \mathcal{X}_a$  is a global minimizer (see Fig. 5), and

$$P(\mathbf{x}_1) = -5.5 < P(\mathbf{x}_2) = -3.5 < P(\mathbf{x}_3) = -1.5 < P(\mathbf{x}_4) = 4.5.$$

**Case IV.** General matrix  $\mathbf{Q} \in \mathbb{R}^{2 \times 2}$  with mixed solutions.

We choose  $q_1 = -4$ ,  $q_2 = 10$ ,  $q_3 = -2$ , the eigenvalues of  $\mathbf{Q}$  are  $\{10.3, -4.3\}$ , i.e. the primal problem is nonconvex. If we let  $\mathbf{c} = \{-8, 10\}$ , the dual solution is  $\boldsymbol{\sigma} = \{10.4, 0\} \in \mathcal{S}_a^+$ . Since  $\boldsymbol{\sigma}_2 = 0$ , the constraint  $-1 \leq x_2 \leq 1$  is inactive. The corresponding primal solution  $\mathbf{x} = \{-1.0, 0.8\}$  is not on the corner of the feasible set  $\mathcal{X}_a$  (see Fig. 6), but we still have  $P(\mathbf{x}) = -1.3 = P^d(\boldsymbol{\sigma})$ .





**Fig. 5** Graph of the saddle function  $P(x_1, x_2)$  and its contour for Example 2 (III)

**Example 3 High dimensional integer programming problem**

We now let  $n = 10$  and randomly choose  $Q$  and  $c$  as

$$Q = \begin{bmatrix} -6 & 2 & -1 & -3 & 1 & 1 & -3 & -3 & 0 & -1 \\ 2 & -10 & -1 & 2 & 1 & 0 & 2 & 1 & -3 & -4 \\ -1 & -1 & -5 & 0 & 3 & -1 & 1 & 0 & -1 & -4 \\ -3 & 2 & 0 & -6 & 1 & 1 & 1 & -2 & 0 & 0 \\ 1 & 1 & 3 & 1 & -7 & 0 & -4 & -1 & -1 & 2 \\ 1 & 0 & -1 & 1 & 0 & -6 & -2 & 1 & 3 & -1 \\ -3 & 2 & 1 & 1 & -4 & -2 & -8 & -1 & 0 & 0 \\ -3 & 1 & 0 & -2 & -1 & 1 & -1 & -3 & 0 & 0 \\ 0 & -3 & -1 & 0 & -1 & 3 & 0 & 0 & -7 & -4 \\ -1 & -4 & -4 & 0 & 2 & -1 & 0 & 0 & -4 & -6 \end{bmatrix},$$

$$c = \{-9.49, 6.14, 9.13, 0.0525, -2.54, 6.69, 0.847, -8.36, 6.31, -2.69\}.$$

Direct method for solving this size problem need  $2^{10}$  times enumerations. However, the canonical dual problem can be solved with a few steps of iterations to obtain the global maximizer

$$\sigma = 2\{12.2, 16.0, 12.0, 6.0, 8.8, 6.3, 7.6, 10.2, 8.7, 8.7\}.$$

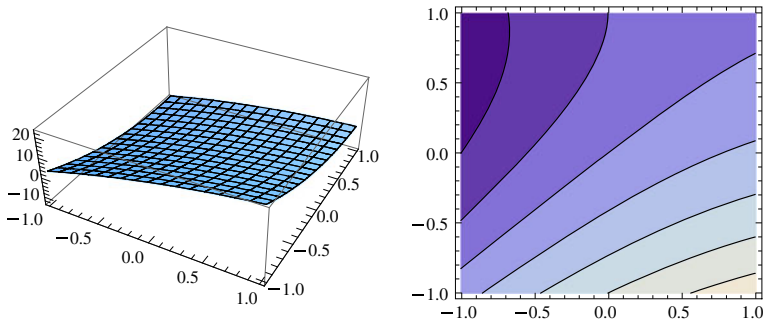
The global minimizer of the primal problem ( $\mathcal{P}$ ) is then

$$x = \{-1, 1, 1, -1, -1, 1, -1, -1, 1, 1\}$$

and  $P^d(\sigma) = -119.1 = P(x)$ .

**8 Conclusion remarks and open problems**

We have presented a detailed application of the canonical duality theory for solving box and integer constrained quadratic optimization problems ( $\mathcal{P}$ ) and ( $\mathcal{P}_{ip}$ ). By using the canonical dual transformation, several canonical dual problems and their perturbations are proposed.



**Fig. 6** Graph of the function  $P(x_1, x_2)$  and its contour for Example 2 (IV)

Since the canonical dual problem  $(\mathcal{P}_{\max}^g)$  and its perturbation form  $(\mathcal{P}_{\alpha\beta}^d)$  are smooth concave maximization over convex feasible spaces, which can be solved easily for certain given  $\mathbf{Q}$  and  $\mathbf{c}$ . Existence and uniqueness criteria are given by Theorem 4. If  $\mathbf{Q}$  and  $\mathbf{c}$  satisfy the condition (51), unique analytical solution can be obtained by Theorem 6.

Theorem 5 is particularly useful, which shows that for any given  $\mathbf{Q}$  and  $\mathbf{c}$ , the discrete integer constrained problem  $(\mathcal{P}_{ip})$  is equivalent to the continuous unconstrained canonical dual problem  $(\mathcal{P}_{\alpha}^d)$ . For convex-perturbation  $\mathbf{Q} + \text{Diag}(\alpha) \succ 0$ , if the concave maximization problem

$$(\mathcal{P}_{\alpha}^{\sharp}) : \max \left\{ P_{\alpha}^d(\sigma) \mid \sigma \in \mathbb{R}^n \right\}. \tag{65}$$

has a critical solution, the discrete problem  $(\mathcal{P}_{ip})$  can be solved uniquely. Otherwise, the nonsmooth problem  $(\mathcal{P}_{\alpha}^{\sharp})$  provides a lower bound for box constrained problem  $(\mathcal{P})$ . For concave-perturbation  $\mathbf{Q} + \text{Diag}(\alpha) \prec 0$ , the problem  $(\mathcal{P}_{\alpha}^d)$  can be simply written as

$$(\mathcal{P}_{\alpha}^b) : \min \left\{ P_{\alpha}^d(\sigma) \mid \sigma \in \mathbb{R}^n \right\}. \tag{66}$$

This continuous unconstrained Lipschitzian optimization has at least one critical solution, which can be obtained by certain deterministic techniques, for example, the well-known DIRECT (DIviding RECTangles) algorithm [27]. Therefore, we have the following conclusions:

*The primal problems  $(\mathcal{P})$  and  $(\mathcal{P}_{ip})$  can be solved in polynomial times if the canonical dual  $(\mathcal{P}^g)$  has a critical point in  $\mathcal{S}_g^+$ . The discrete problem  $(\mathcal{P}_{ip})$  is equivalent to the continuous dual problem  $(\mathcal{P}_{\alpha}^d)$  which can be solved deterministically.*

However, for certain given  $\mathbf{Q}$  and  $\mathbf{c}$ , the canonical dual problem  $(\mathcal{P}^g)$  may have no critical point in  $\mathcal{S}_g^+$ . In this case, the primal problems  $(\mathcal{P})$  and  $(\mathcal{P}_{ip})$  could be NP-hard. In order to solve the following equivalent canonical dual problems,

$$\min \text{sta} \left\{ P^g(\sigma) \mid \sigma \in \mathcal{S}_g \right\}, \quad \min \text{sta} \left\{ P^g(\sigma) \mid \sigma \neq 0 \right\} \tag{67}$$

several perturbation forms  $(\mathcal{P}_{\alpha}^g)$ ,  $(\mathcal{P}_{\alpha}^d)$ , and  $(\mathcal{P}_{\alpha\beta}^d)$ , as well as the related theorems have been proposed in this paper.

The canonical duality theory was originally developed for general complex systems [12, 22], which has been successfully applied for solving a class of nonconvex/nonsmooth variational/boundary value problems [11]. Complete sets of solutions to a class of well-known

problems in finite deformation mechanics and phase transitions of solids have been obtained [18]. Recent applications in finite dimensional systems shown that this theory is potentially useful for solving both continuous and discrete global optimization problems [6, 14, 16, 17, 19, 21].

As indicated in [12–14], the key step in the canonical dual transformation is to choose the (nonlinear) geometrical operator  $\Lambda(\mathbf{x})$ . Different forms of  $\Lambda(\mathbf{x})$  may lead to different (but equivalent) canonical dual problems (see [23]). It is now realized that the popular semi-definite programming (SDP) method for solving integer programming and network optimization problems is actually a special application of the general complementary-dual principle proposed in [22]. To see this, instead of the vector-valued (pure) quadratic geometrical operator  $\Lambda(\mathbf{x}) = \frac{1}{2} \{\mathbf{x}^T \mathbf{Q} \mathbf{x}, \mathbf{x} \circ \mathbf{x}\}$  given in (11), we simply let  $\Lambda(\mathbf{x})$  be a matrix-valued geometrical operator:

$$\xi = \Lambda(\mathbf{x}) = \frac{1}{2} \mathbf{x} \mathbf{x}^T : \mathbb{R}^n \rightarrow \mathcal{E} = \mathbb{R}^{n \times n}. \tag{68}$$

Then, both the primal problems ( $\mathcal{P}$ ) and ( $\mathcal{P}_{ip}$ ) can be written in the following unified canonical form

$$\min\{\Pi(\mathbf{x}) = V(\Lambda(\mathbf{x})) - \langle \mathbf{x}, \mathbf{c} \rangle \mid \mathbf{x} \in \mathbb{R}^n\}, \tag{69}$$

where the canonical function  $V : \mathcal{E} \rightarrow \mathbb{R} \cup \{+\infty\}$  is defined by

$$V(\xi) = \langle \mathbf{Q}; \xi \rangle + \begin{cases} 0 & \text{if } \xi \in \mathcal{E}_a \\ \infty & \text{if } \xi \notin \mathcal{E}_a. \end{cases} \tag{70}$$

For box constrained problem, the effective domain  $\mathcal{E}_a$  of  $V(\xi)$  is defined

$$\mathcal{E}_a = \{\xi \in \mathcal{E} \mid \xi = \xi^T, \xi \geq 0, 2\xi_{ii} \leq 1 \ \forall i \in \{1, \dots, n\}, \xi \text{ rank-one}\}. \tag{71}$$

While for integer constrained problem, the inequality  $2\xi_{ii} \leq 1$  in  $\mathcal{E}_a$  should be replaced by equality. The bilinear form  $\langle \xi; \xi^* \rangle : \mathcal{E} \times \mathcal{E}^* \rightarrow \mathbb{R}$  is defined

$$\langle \xi; \xi^* \rangle = \text{trace}(\xi^T \xi^*) = \sum_{i=1}^n \sum_{j=1}^n \xi_{ij} \xi_{ij}^*. \tag{72}$$

Using  $\sigma \in \mathbb{R}^n$  to relax the inequality condition  $\xi_{ii} \leq \frac{1}{2}$  and let  $\xi = \frac{1}{2} \mathbf{x} \mathbf{x}^T$  to relax  $\xi = \xi^T, \xi \geq 0$ , and rank-one conditions in  $\mathcal{E}_a$ , the Fenchel sup-conjugate of the canonical function  $V(\xi)$  can be obtained as

$$\begin{aligned} V^\sharp(\xi^*) &= \sup_{\xi \in \mathcal{E}} \{\langle \xi; \xi^* \rangle - V(\xi)\} = \sup_{\xi \in \mathcal{E}_a} \{\langle \xi; \xi^* - \mathbf{Q} \rangle\} \\ &= \sup_{\mathbf{x} \in \mathbb{R}^n} \left\{ \frac{1}{2} \langle \mathbf{x}, (\xi^* - \mathbf{Q}) \mathbf{x} \rangle - \sum_{i=1}^n \frac{1}{2} \sigma_i (\mathbf{x}_i^2 - 1) \right\} \\ &= \begin{cases} \frac{1}{2} \langle \mathbf{e}, \sigma \rangle & \text{if } \xi^* \in \mathcal{E}_a^* \\ +\infty & \text{otherwise,} \end{cases} \end{aligned}$$

where

$$\mathcal{E}_a^* = \{\xi^* \in \mathcal{E}_a^* = \mathbb{R}^{n \times n} \mid \xi^* = \mathbf{Q} + \text{Diag}(\sigma), \sigma \in \mathbb{R}_+^n\}. \tag{73}$$

Therefore, in term of  $\sigma$ , the standard total complementary function

$$\Xi(\mathbf{x}, \xi^*) = \langle \Lambda(\mathbf{x}); \xi^* \rangle - V^\sharp(\xi^*) - \langle \mathbf{x}, \mathbf{c} \rangle$$

has exactly the same form as  $\Xi(\mathbf{x}, \boldsymbol{\sigma})$  given in (17). Since the geometrical operator  $\Lambda(\mathbf{x}) = \frac{1}{2}\mathbf{xx}^T$  is pure quadratic tensor-valued function of  $\mathbf{x}$ , its Gâteaux variation at  $\bar{\mathbf{x}}$  in the direction of  $\mathbf{x}$  is  $\delta\Lambda(\bar{\mathbf{x}}; \mathbf{x}) = \Lambda_t(\bar{\mathbf{x}})\mathbf{x} = \mathbf{x}\bar{\mathbf{x}}^T$ , where  $\Lambda_t(\bar{\mathbf{x}}) = \nabla\Lambda(\bar{\mathbf{x}})$  denotes the Gâteaux derivative of  $\Lambda(\mathbf{x})$  at  $\bar{\mathbf{x}}$ . Its complementary operator is defined as  $\Lambda_c(\mathbf{x}) = \Lambda(\mathbf{x}) - \Lambda_t(\mathbf{x}) = -\frac{1}{2}\mathbf{xx}^T$  (see [22], where  $\Lambda, \Lambda_t, \Lambda_c$  were denoted as  $A, T, N$ , respectively). By  $\Lambda_t$ , the canonical equilibrium condition (i.e. the virtual work principle (17) in [22])

$$\langle \Lambda_t(\bar{\mathbf{x}})\mathbf{x}; \boldsymbol{\xi}^* \rangle = \langle \mathbf{x}, \mathbf{c} \rangle \quad \forall \mathbf{x} \in \mathbb{R}^n$$

leads to the analytical solution form  $\bar{\mathbf{x}} = \mathbf{G}^\dagger(\boldsymbol{\sigma})\mathbf{c}$ . While by  $\Lambda_c$ , the complementary gap function (equation (39) in [22]) is given as

$$G_{ap}(\mathbf{x}, \boldsymbol{\xi}^*) = \langle -\Lambda_c(\mathbf{x}); \boldsymbol{\xi}^* \rangle = \frac{1}{2}\langle \mathbf{xx}^T; \mathbf{Q} + \text{Diag}(\boldsymbol{\sigma}) \rangle = \frac{1}{2}\langle \mathbf{x}, \mathbf{G}(\boldsymbol{\sigma})\mathbf{x} \rangle$$

which has exactly the same form as  $G_{ap}(\mathbf{x}, \boldsymbol{\sigma})$  given in (37). Clearly, the sufficient condition  $G_{ap}(\mathbf{x}, \boldsymbol{\sigma}) \geq 0 \quad \forall \mathbf{x} \in \mathbb{R}^n$  for global minimizer of the primal problem leads to the semi-positive definite condition  $\mathbf{G}(\boldsymbol{\sigma}) \succeq 0$ . Therefore, by Theorem 5 proposed in [22], we have the canonical min-max duality theorem (32), i.e.,

$$\min_{\mathbf{x} \in \mathcal{X}_a} P(\mathbf{x}) = \max_{\boldsymbol{\sigma} \in \mathcal{S}_g^+} P^d(\boldsymbol{\sigma}).$$

Thus, we have shown again that the equivalent (or the same) canonical dual problem can be obtained by using different quadratic geometrical operator  $\Lambda(\mathbf{x})$ .

In finite deformation theory and differential geometry, the pure quadratic geometrical measure  $\boldsymbol{\xi} = \Lambda(\mathbf{x})$  is similar to the Cauchy-Riemann type metric tensor, which has been used extensively in the canonical duality theory [12]. In semi-definite optimization, the bilinear form  $\langle \boldsymbol{\xi}; \boldsymbol{\xi}^* \rangle$  is denoted by  $\boldsymbol{\xi} \bullet \boldsymbol{\xi}^*$ . Therefore, in a very special case of  $\mathbf{c} = 0$ , the canonical primal problem (69) for integer programming can be written (in term of  $\mathbf{X} = 2\boldsymbol{\xi} = \mathbf{xx}^T$ ) as:

$$(\mathcal{P}_{mc}) : \min \frac{1}{2}\mathbf{Q} \bullet \mathbf{X}, \quad s.t. \quad \mathbf{X} \succeq 0, \quad X_{ii} = 1, \quad \mathbf{X} = \mathbf{X}^T, \quad \mathbf{X} \text{ rank-one}. \quad (74)$$

If both the symmetrical and rank-one constraints are ignored, this problem is exactly a semi-definite programming problem [36]. However, we must emphasize that for quadratic integer programming problems, these two conditions imply that  $\mathbf{X} = \mathbf{xx}^T$  and can not be ignored. Otherwise, the problem (74) will have  $n \times n$  unknowns, and the dual variable of  $\mathbf{X}$  should be also a tensor  $\mathbf{X}^* \in \mathbb{R}^{n \times n}$ , instead of a vector in  $\mathbb{R}^n$ . Therefore, by introducing Lagrange multiplier  $\boldsymbol{\sigma} \in \mathbb{R}^n$  to relax the equality and rank-one conditions, we have

$$\left(\mathcal{P}_{mc}^d\right) : \max \left\{ -\frac{1}{2}\langle \mathbf{e}, \boldsymbol{\sigma} \rangle \mid \mathbf{G}(\boldsymbol{\sigma}) \succeq 0, \quad \boldsymbol{\sigma} \neq 0 \right\}, \quad (75)$$

which is clearly a special case of the canonical dual problem  $(\mathcal{P}_{max}^g)$ .

From Theorems 4 and 6 we know that the vector  $\mathbf{c}$  plays a fundamental role for unique solution of the nonconvex quadratic programming problems. From point view of systems theory,  $\mathbf{c}$  represents input (or source) while  $\mathbf{x}$  the output (or state). If there is no input, the system either has trivial solution ( $\mathbf{x} = 0$ ) or more than one solution. The reason for multi-solutions is due to the symmetry of the systems. The input usually destroys certain symmetry and leads to the possibility of unique solution. It turns out that there is a limitation for the SDP method. It was shown in [24] that the best ratio of the optimal values of the max-cut problem and its SDP relaxation is usually about 0.878. By introducing a linear cost  $\langle \mathbf{x}, \mathbf{c} \rangle$  in  $(\mathcal{P}_{mc})$ , a linear-perturbation canonical dual approach method was proposed for solving

general homogeneous nonconvex systems [33] and max-cut problems [37]. It was shown in [37] that for certain given inputs  $\mathbf{c}$ , the integer programming problem  $(\mathcal{P}_{ip})$  and the max-cut problem have the same solution set and can be perfectly obtained by the canonical dual approach.

The  $\alpha$ -perturbed problem  $(\mathcal{P}_\alpha)$  is actually a quadratic perturbation which was proposed in [33] for solving general Euclidean distance geometry problems in network optimization. While the  $\beta$ -perturbed problem  $(\mathcal{P}_{\alpha\beta}^d)$  is a fourth-order perturbation and is a natural application of the canonical duality theory for solving general nonconvex minimization problems with double-well structures. Based on  $(\mathcal{P}_{\alpha\beta}^d)$ , the canonical dual algorithm proposed in Sect. 6 can be used for solving a class of nonconvex/discrete problems. However, how to choose the perturbation vector  $\alpha$  and the series  $\{\beta_k\}$  is fundamentally important and deserves further investigation.

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