Global Solutions to Large-Scale Spherical Constrained Quadratic Minimization via Canonical Dual Approach

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This paper presents global optimal solutions to a nonconvex quadratic minimization problem over a sphere constraint. The problem is well-known as a trust region subproblem and has been studied extensively for decades. The main challenge is the so-called 'hard case', i.e., the problem has multiple solutions on the boundary of the sphere. By canonical duality theory, this challenging problem is able to reform as an one-dimensional canonical dual problem without duality gap. Sufficient and necessary conditions are obtained by the triality theory, which can be used to identify whether the problem is hard case or not. A perturbation method and the associated algorithms are proposed to solve this hard case problem. Theoretical results and methods are verified by large-size examples.

Keywords: global optimization; quadratic minimization problems; canonical duality theory; trust region subproblem

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1. Introduction

We consider the following quadratic minimization problem:

\[(P) \quad \min_{x} P(x) = x^T Q x - 2 f^T x \]  

where the given matrix \(Q \in \mathbb{R}^{n \times n}\) is assumed to be symmetric, \(f \in \mathbb{R}^{n}\) is an arbitrarily given vector, and the feasible region is defined as

\[\mathcal{X} = \{x \in \mathbb{R}^{n} \mid \|x\| \leq r\},\]  

in which, \(r\) is a positive real number.

Problem \((P)\) arises naturally in computational mathematical physics with extensive applications in engineering sciences. From the point of view of systems theory, if the vector \(f \in \mathbb{R}^{n}\) is considered as an input (or source), then the solution \(x \in \mathbb{R}^{n}\) is refereed as the output (or state) of the system. By the fact that the capacity of any given system is limited, the spherical constraint in \(\mathcal{X}\) is naturally required for virtually every real-world system. For example, in engineering structural analysis, if the applied force field \(f \in \mathbb{R}^{\infty}\) is big enough, the stress distribution in the structure will reach its elastic limit and the structure will collapse. For elasto-perfectly plastic materials, the well-known
von Mises yield condition is a quadratic inequality constraint at each material point[1]
(see Chapter 7, [6]). By finite element method, the variational problem in structural
limit analysis can be formulated as a large-size nonlinear optimization problem with
m quadratic inequality constraints (the m depends on the number of total finite elements).
Such problems have been studied extensively in computational mechanics for more than
fifty years and the so-called penalty-duality finite element programming [4, 5] is one of
well-developed efficient methods for solving this type of problems in engineering sciences.

In mathematical programming, the problem (P) is known as a trust region subprob-
lem, which arises in trust region methods [25]. A more general problem with nonconvex
quadratic constraint is considered in [34]. Although the function P(x) can be nonconvex
if the matrix Q has negative eigenvalues, it is proved that the problem (P) is hidden
convex, i.e. (P) is actually equivalent to a convex optimization problem [1]. By the opti-
mization theory we know that the vector  is a solution of (P) if there exists a Lagrange
multiplier such that the following conditions hold [2]:

\[(Q + \bar{\mu}I)x = f\]  \hspace{1cm} (3)
\[\|\bar{x}\| \leq r\]  \hspace{1cm} (4)
\[Q + \bar{\mu}I \succeq 0, \bar{\mu} \geq 0\]  \hspace{1cm} (5)
\[\bar{\mu}(\|\bar{x}\| - r) = 0\]  \hspace{1cm} (6)

Let  be the smallest eigenvalue of the matrix Q. From conditions (5), we know that
\[\bar{\mu} \geq \max\{0, -\lambda_1\}.

If the problem (P) has no solution on the boundary of X, then Q must be positive
definite and \(\|Q^{-1}f\| < r\), which leads to \(\bar{\mu} = 0\). If (P) has a solution on the boundary
of X and \((Q + \bar{\mu}I) > 0\), then we have \(\|(Q + \bar{\mu}I)^{-1}f\| = r\). In this case, the multiplier \(\bar{\mu}\) can be found by using Newton’s method. However, if the solution \(\bar{x}\) is located on
the boundary of X and \(\det(Q + \bar{\mu}I) = 0\), this situation is the so-called ‘hard case’ [24],
which leads to numerical difficulties. In this case, the equation \((Q + \bar{\mu}I)x = f\) has no unique
solution, and all vectors in the form \(x = (Q + \bar{\mu}I)^{1/2}f + \tau\bar{x}\) with \((Q + \bar{\mu}I)x = 0\) are its
solutions. In [24], Moré and Sorensen proposed a safeguarding scheme to update \(\mu\) and
replaced \(\bar{x}\) by the vector \(z\) with \(\|Rz\|\) being an approximation of the smallest singular
value of R, where R is the Cholesky factorisation of \(Q + \mu I\). Many other methods have
been developed to deal with either hard case or large-size problems. Methods through
a parameterized eigenvalue problem are discussed in [3, 26, 27, 30]. At each iteration,
the Lanczos method was used to calculate an approximation of the smallest eigenvalue.
Another kind of methods [19, 20, 31] searches solutions in the Krylov space, which is
gradually expanded during iterations. In [32], the d.c. (difference of convex functions)
algorithm is applied to solve the problem (P).

The goal of this paper is to solve the problem (P) in any size, especially for the hard
case. Our approach is the canonical duality theory, a newly developed and potentially
powerful methodological theory, which has been used successfully for solving a large class
of nonconvex/nonsmooth/discrete problems in analysis and global optimization within
a unified framework (see [12, 15]). This theory is composed mainly of (1) a canonical
dual transformation; (2) a complementary-dual principle, and (3) a triality theory. We
first show in the next section that by the canonical dual transformation, this constrained
nonconvex problem can be reformulated as a one-dimensional optimization problem. The
complementary-dual principle shows that this one-dimensional problem is canonically

1The Tresca yield condition is equivalent to a box constraint at each material point
(i.e. perfectly) dual to \((P)\) in the sense that both problems have the same set of KKT solutions. While the triality theory (mainly the first statement, i.e. the canonical min-max duality) provides sufficient and necessary conditions for identifying global optimal solutions. In order to solve the hard case, a perturbation method is proposed in Section 4 and, accordingly, a canonical primal-dual algorithm is developed in Section 5. Numerical results presented in Section 6 show that our approach can efficiently solve large-size problems. The paper is ended with some conclusion remarks.

2. Canonical dual problem

According to [15], the canonical dual problem of \((P)\) is given by

\[
\text{sta}\left\{ P^d(\sigma) \mid \sigma \in S_a \right\}, \tag{7}
\]

where the notation sta denotes computing stationary points of the canonical dual function \(P^d(\sigma)\) which is defined as

\[
P^d(\sigma) = -f^T G_a(\sigma)^{-1} f - r^2 \sigma, \tag{8}
\]

in which, \(G_a(\sigma) = Q + \sigma I\) and \(G_a(\sigma)^{-1}\) denotes the inverse of \(G_a(\sigma)\). The feasible set \(S_a\) is defined as

\[
S_a = \{ \sigma \mid \sigma \geq 0, \ f \in C_\text{col}(G_a(\sigma)) \},
\]

and the notation \(C_\text{col}(\cdot)\) represents the column space of \(G_a\).

We note that the canonical dual \(P^d(\sigma)\) is a function of a scalar variable \(\sigma \in \mathbb{R}\), regardless of the dimension of the primal problem. The canonical duality theory demonstrates that there is no duality gap between the primal problem \((P)\) and its canonical dual \((P)\), which is illustrated by the following theorem.

Theorem 2.1 (Analytical Solution and Complementary-Dual Principle [6, 15])

The problem \((P)\) is canonically dual to the problem \((P)\) in the sense that if \(\bar{\sigma} \in S_a\) is a critical point of \(P^d(\sigma)\), then

\[
\bar{x} = G_a(\bar{\sigma})^{-1} f
\]

is a KKT point of the primal problem \((P)\), and we have

\[
P(\bar{x}) = P^d(\bar{\sigma}). \tag{10}
\]

The proof is omitted here, which is analogous with that in [15]. In order to identify global optimal solutions among all the critical points of \(P^d(\sigma)\), a subset of \(S_a\) is needed:

\[
S_a^+ = \{ \sigma \in S_a \mid G_a(\sigma) \succeq 0 \}.
\]

Therefore, the canonical dual problem of \((P)\) can be proposed as the following

\[
(P^d) \quad \max \{ P^d(\sigma) \mid \sigma \in S_a^+ \}. \tag{11}
\]

Theorem 2.2 (Global Optimality Condition [6, 15]) Suppose that \(\bar{\sigma}\) is a critical point of \(P^d(\sigma)\). If \(\bar{\sigma} \in S_a^+\) and \(\det(G_a(\bar{\sigma})) \neq 0\), then \(\bar{\sigma}\) is a global maximal solution of
the problem \((\mathcal{P}^d)\) on \(S_a^+\) and \(\tilde{x} = G_a(\tilde{\sigma})^{-1} f\) is a global minimal solution of the primal problem \((\mathcal{P})\), i.e.

\[ P(\tilde{x}) = \min_{x \in \mathcal{X}} P(x) = \max_{\sigma \in S_a^+} P^d(\sigma) = P^d(\tilde{\sigma}). \] (12)

According to the triality theorem \([6, 17]\), the global optimality condition (12) is called canonical min-max duality. It guarantees that if there is a critical point in the interior of \(S_a^+\), computing the global minimal solution of the nonconvex problem \((\mathcal{P})\) can be converted to a concave maximization problem. Therefore, the so-called hidden convexity discovered in \([1]\) is actually a special case of the canonical duality. Also, by the canonical duality theory, complete solutions of the problem \((\mathcal{P})\) have been discussed by Gao in \([8]\), wherein, Theorem 3 states that if \(P(x)\) is not convex and the Morse index of \(P(x)\) (i.e. the number of negative eigenvalues of \(Q\), see Chapter 5 in \([6]\)) is \(i_d\), then the problem \((\mathcal{P})\) has at most \(2i_d + 1\) KKT points on the boundary of the sphere and they can be calculated from the \(2i_d+1\) KKT points of the dual problem. Moreover, the corresponding primal and dual functions are equal at each of these KKT points. This theorem presents a perfect duality relationship between the problem \((\mathcal{P})\) and its dual problem. By the double-min duality statement in the weak-triality theory proven recently (see \([17, 22, 23]\)), we know that the problem \((\mathcal{P})\) has at most one local minimizer since the canonical dual problem is in one-dimensional space. Similar result is also proven in \([21]\). For the hard case, i.e. the matrix \(G_a(\sigma)\) is singular at the critical point \(\tilde{\sigma}\), the canonical dual \(P^d(\sigma)\) should be replaced by (see \([13]\))

\[ P^d(\sigma) = -f^T G_a(\sigma)^\dagger f - r^2 \sigma, \] (13)

where \(G_a(\sigma)^\dagger\) stands for a generalized inverse of \(G_a(\sigma)\). Since this function is not strictly concave on \(S_a^+\), it may have multiple critical points located on the boundary of \(S_a^+\). In the following sections, we will first study the existence conditions of these critical points, and then to study associated algorithm for computing these solutions.

3. Existence condition

By the symmetry of the matrix \(Q\), there exist diagonal matrix \(\Lambda\) and orthogonal matrix \(U\) such that \(Q = U \Lambda U^T\). The diagonal entities of \(\Lambda\) are the eigenvalues of the matrix \(Q\) and are arranged in nondecreasing order,

\[ \lambda_1 = \cdots = \lambda_k < \lambda_{k+1} \leq \cdots \leq \lambda_n. \]

The columns of \(U\) are corresponding eigenvectors.

It’s easy to verify that \((Q + \sigma I)^{-1} = U (\Lambda + \sigma I)^{-1} U^T\). Let \(\hat{f} = U^T f\). Therefore, we can rewrite the dual function into

\[ P^d(\sigma) = -\sum_{i=1}^k \frac{\hat{f}_i^2}{\lambda_i + \sigma} - \sum_{i=k+1}^n \frac{\hat{f}_i^2}{\lambda_i + \sigma} - r^2 \sigma, \] (14)

where \(\hat{f}_i\) are elements of \(\hat{f}\). We notice that the function \(P^d(\sigma)\) is always well defined and have stationary points over its domain except that \(f = 0\). Thus, for the case of \(f \neq 0\), the dual problem \((\mathcal{P}^d)\) is well defined. For the case of \(f = 0\), the canonical dual problem can be solved by the perturbation method provided in the next section.

**Proposition 3.1 (Existence Condition)** Suppose that \(\lambda_i\) and \(\hat{f}_i\) are defined as
above and there is a solution of the problem \( (\mathcal{P}) \) on the boundary of \( X \). Then there exists a critical point of \( P^d(\sigma) \) in \( (-\lambda_1, +\infty) \) if and only if either \( \sum_{i=1}^k \hat{f}_i^2 \neq 0 \) or \( \sum_{i=k+1}^n \frac{\hat{f}_i^2}{(\lambda_i - \lambda_1)^2} > r^2 \). If \( P^d(\sigma) \) has a critical point \( \tilde{\sigma} \) in \( (-\lambda_1, +\infty) \), then this critical point is unique and \( \bar{x} = G_a(\tilde{\sigma})^{-1} f \) is a global solution of the problem \( (\mathcal{P}) \).

**Proof:** First, let us prove that \( P^d(\sigma) \) has a critical point in \( (-\lambda_1, +\infty) \) implies either \( \sum_{i=1}^k \hat{f}_i^2 \neq 0 \) or \( \sum_{i=k+1}^n \frac{\hat{f}_i^2}{(\lambda_i - \lambda_1)^2} > r^2 \). Equivalently, we can prove that if \( \sum_{i=1}^k \hat{f}_i^2 = 0 \) and \( \sum_{i=k+1}^n \frac{\hat{f}_i^2}{(\lambda_i - \lambda_1)^2} \leq r^2 \) the dual function \( P^d(\sigma) \) will have no critical points in \( (-\lambda_1, +\infty) \). If \( \sum_{i=1}^k \hat{f}_i^2 = 0 \), the first item vanishes in the expression (14). Since we assume that \( \sum_{i=k+1}^n \frac{\hat{f}_i^2}{(\lambda_i - \lambda_1)^2} < r^2 \), the first-order derivative of the dual function \( P^d(\sigma) \)

\[
(P^d(\sigma))' = \sum_{i=k+1}^n \frac{\hat{f}_i^2}{(\lambda_i + \sigma)^2} - r^2
\]

is always negative in \( (-\lambda_1, +\infty) \). Therefore, the dual function \( P^d(\sigma) \) will have no critical points in \( (-\lambda_1, +\infty) \).

Next we give the proof of the sufficiency, which is divided into two parts:

1) If \( \sum_{i=1}^k \hat{f}_i^2 \neq 0 \), \( \lambda_1 \) is a pole of \( P^d(\sigma) \), which implies that as \( \sigma \) approaches \( -\lambda_1 \) from the right side, the function \( P^d(\sigma) \) approaches \( -\infty \). Also, \( P^d(\sigma) \) approaches \( -\infty \) as \( \sigma \) approaches \( +\infty \). Therefore, \( -P^d(\sigma) \) is coercive on \( (-\lambda_1, +\infty) \). Since, for any \( \sigma \in (-\lambda_1, +\infty) \), \( G_a(\sigma) \) is positive definite, \( P^d(\sigma) \) is strictly concave on \( (-\lambda_1, +\infty) \). Thus there exists a unique critical point on \( (-\lambda_1, +\infty) \).

2) If \( \sum_{i=1}^k \hat{f}_i^2 = 0 \) and \( \sum_{i=k+1}^n \frac{\hat{f}_i^2}{(\lambda_i - \lambda_1)^2} > r^2 \), \( (P^d(\sigma))' \) is positive at \( \sigma = -\lambda_1 \). Moreover, \( (P^d(\sigma))' \) approaches \( -r^2 \) as \( \sigma \) approaches \( \infty \). Therefore, there exists at least one root for the equation \( (P^d(\sigma))' = 0 \) over \( (-\lambda_1, +\infty) \), which means \( P^d(\sigma) \) has at least one critical point in \( (-\lambda_1, +\infty) \). Similarly, because of the strict concavity of \( P^d(\sigma) \) over \( (-\lambda_1, +\infty) \), the critical point is unique.

Let \( \tilde{\sigma} \) denote the critical point. If \( \lambda_1 \leq 0 \), we have \( \tilde{\sigma} \in S_\sigma^+ \). Then, from Theorem \ref{thm:existence}, we further have that \( \bar{x} = G_a(\tilde{\sigma})^{-1} f \) is a global solution of the problem \( (\mathcal{P}) \). If \( \lambda_1 > 0 \), from equations \ref{eq:existence} \ref{eq:existence}, we know that the dual variable \( \bar{\mu} \) satisfying \( \| (Q + \bar{\mu} I)^{-1} f \| = r \) is the critical point \( \tilde{\sigma} \). Thus \( \bar{x} = G_a(\tilde{\sigma})^{-1} f = (Q + \bar{\mu} I)^{-1} f \) is a global solution of the problem \( (\mathcal{P}) \).

The proposition is proved.

\[\square\]

### 4. Perturbation method

This section is devoted to the solutions for hard case, where \( \sum_{i=1}^k \hat{f}_i^2 = 0 \) and \( \sum_{i=k+1}^n \frac{\hat{f}_i^2}{(\lambda_i - \lambda_1)^2} \leq r^2 \), i.e. the existence condition obtained in the previous section is violated. This case leads to challenges for solving the problem \( (\mathcal{P}) \) via (pure) mathematical analysis. Our approach is the perturbation method, which has been used successfully in canonical duality theory for solving nonlinear algebraic equations \cite{28}, chaotic dynamical systems \cite{29}, as well as a class of NP-hard problems in global optimization \cite{13, 33}. In order to reinforce the existence condition, a set of perturbation parameters

\[\alpha_i \neq 0, \quad \text{for some } i \in \{1, \ldots, k\}, \quad (16)\]
is introduced, and we let

\[ p = f + \sum_{i=1}^{k} \alpha_i u_i, \quad \hat{p} = U^T p, \quad P_\alpha(x) = x^T Q x - 2p^T x. \]

Then the perturbed problem can be defined as

\[ (P_\alpha) \min_{x \in X} P_\alpha(x) \quad \text{s.t.} \quad x \in X. \quad (17) \]

It is true that the existence condition holds for the perturbed problem since (16) will guarantee \( \sum_{i=1}^{k} p_i^2 \neq 0 \).

The following theorem states that for certain appropriate \( \{\alpha_i\}_{i=1}^{k} \), the optimal solution of the perturbed problem converges to that of the primal problem \( (P) \).

**Theorem 4.1** Suppose that \( \lambda_1 \leq 0 \), and \( \bar{x} \) and \( \bar{x}^* \) are optimal solutions of the problems \((P)\) and \((P_\alpha)\), respectively, on the boundary of \( X \). Then, for any \( \varepsilon > 0 \), if the parameters \( \{\alpha_i\} \) satisfy

\[ \sum_{i=1}^{k} \alpha_i^2 \leq (\lambda_2 - \lambda_1)^2 \left( r^2 - \sum_{i=k+1}^{n} \frac{\hat{f}_i^2}{(\lambda_i - \lambda_1)^2} \right) \left( \frac{1}{\sqrt{2(1 - \cos(\varepsilon/r) - 1)} - 2}, \right) \]

we have \( \|\bar{x}^* - \bar{x}\| \leq \varepsilon \).

**Proof:** For simplicity, we rotate the coordinate system and substitute \( x \) with \( U y \) in the problem \((P)\). As \( \hat{f}_i = 0 \) for \( i = 1, \ldots, k \), variables \( y_i \) for \( i = 1, \ldots, k \) appear in the form of squares in the target function. Since it is assumed that \( \bar{x} \) and \( \bar{x}^* \) are optimal solutions on the boundary of \( X \), both should satisfy the equality constraint in \( X \). Let \( y_{k+1} = \{y_i\}_{i=k+1}^{n} \). On the boundary of \( X \), the problem \((P)\) is equivalent to the following problem in \( \mathbb{R}^{n-k} \):

\[ \min_{\|y_{k+1}\| \leq r} P(y_{k+1}) = \sum_{i=k+1}^{n} (\lambda_i - \lambda_1) y_i^2 - \sum_{i=k+1}^{n} 2\hat{f}_i y_i + \lambda_1 r^2. \quad (19) \]

Similarly, the perturbed problem \((17)\) with the equality constraint is equivalent to

\[ \min_{\|y_{k+1}\| \leq r} P_\alpha(y_{k+1}) = \sum_{i=k+1}^{n} (\lambda_i - \lambda_1) y_i^2 - \sum_{i=k+1}^{n} 2\hat{f}_i y_i + \lambda_1 r^2 \]

\[ - 2\sqrt{\sum_{i=1}^{k} \alpha_i^2 \left( r^2 - \sum_{i=k+1}^{n} y_i^2 \right)}. \quad (20) \]

Then it is not difficult to verify that \( \bar{y}_{k+1} = \{\bar{y}_i = U^T \bar{x}\}_{i=k+1}^{n} \) and \( \bar{y}_{k+1}^* = \{\bar{y}_i = U^T \bar{x}^*\}_{i=k+1}^{n} \) are optimal solutions of problems \((19)\) and \((20)\), respectively. Since \( P(y_{k+1}) \) is a strictly convex function, it has a unique stationary point, which is \( \{\hat{f}_i\}_{i=k+1}^{n} \). Combining with the assumption, we know that this stationary point is the global optimal solution of the problem \((19)\), i.e.

\[ \bar{y}_i = \frac{\hat{f}_i}{\lambda_i - \lambda_1}, \quad i = k+1, \ldots, n. \]
The function $P^u_\alpha(y_\ell)$ is also strictly convex. Furthermore, for any $\|y_\ell\| < r$, we have $P^u_\alpha(y_\ell) < P^u(y_\ell)$, and for any $\|y_\ell\| = r$, we have $P^u_\alpha(y_\ell) = P^u(y_\ell)$, which indicates that the unique stationary point of $P^u_\alpha(y_\ell)$ is in the interior of $\|y_\ell\| \leq r$. Thus it is the global optimal solution of the problem (20) and $\tilde{y}_\ell$ satisfies

$$\tilde{y}_i^* = \frac{\tilde{f}_i}{\lambda_i - \lambda_1 + \sqrt{\sum_{i=1}^k \alpha_i^2 (r^2 - \sum_{i=k+1}^n (\tilde{y}_i^*)^2)^{-\frac{1}{2}}}}, \quad i = k + 1, \ldots, n.$$ 

Obviously,

$$|\tilde{y}_i^*| < |\tilde{y}_i|, \quad i = k + 1, \ldots, n. \quad (21)$$

We have the inequality

$$\tilde{y}^T y = \sqrt{r^2 - \tilde{y}_\ell^T y_\ell} \sqrt{r^2 - \tilde{y}_\ell^T y_\ell + \tilde{y}_\ell^T y_\ell} \leq \frac{1}{2} (r^2 - \tilde{y}_\ell^T y_\ell^* + r^2 - \tilde{y}_\ell^T y_\ell) + \tilde{y}_\ell^T y_\ell = r^2 - \frac{1}{2} \|\tilde{y}_\ell^* - \tilde{y}_\ell\|^2,$$

which further implies that

$$\|\tilde{y}_\ell^* - \tilde{y}_\ell\| \leq r \arccos \left( \frac{\tilde{y}_\ell^T y_\ell}{r^2} \right) \leq r \arccos \left( \frac{r^2 - \frac{1}{2} \|\tilde{y}_\ell^* - \tilde{y}_\ell\|^2}{r^2} \right). \quad (22)$$

Thus, if we want $\|\tilde{y}_\ell^* - \tilde{y}_\ell\| \leq \epsilon$, it is necessary to make sure $\|\tilde{y}_\ell^* y_\ell\|^2 \leq 2r^2(1 - \cos \frac{\epsilon}{r})$. Because of the inequality

$$\|\tilde{y}_\ell^* - \tilde{y}_\ell\|^2 \leq \frac{r^2}{(\lambda_2 - \lambda_1) \sqrt{r^2 - \tilde{y}_\ell^T y_\ell} \sqrt{\sum_{i=1}^k \alpha_i^2}} 2,$$ 

if we let its right side be less than or equal to $2r^2(1 - \cos \frac{\epsilon}{r})$, we obtain

$$\sum_{i=1}^k \alpha_i^2 \leq \frac{(\lambda_2 - \lambda_1)^2 (r^2 - \tilde{y}_\ell^T y_\ell)}{(1/\sqrt{2(1 - \cos \frac{\epsilon}{r})} - 1)^2}. \quad (24)$$

Hence, combining with relations in (21), we can state that $\|\tilde{y}_\ell^* - \tilde{y}_\ell\| \leq \epsilon$ if the following inequality is true

$$\sum_{i=1}^k \alpha_i^2 \leq \frac{(\lambda_2 - \lambda_1)^2 (r^2 - \sum_{i=k+1}^n \tilde{f}_i^2)}{(1/\sqrt{2(1 - \cos \frac{\epsilon}{r})} - 1)^2}. \quad (25)$$

Since $\|\tilde{x}_\ell^* - \tilde{x}_\ell\| = \|\tilde{y}_\ell^* - \tilde{y}_\ell\|$, the theorem is proved. \hfill \Box

Theorem 4.1 shows that with certain proper parameters $\{\alpha_i\}_{i=1}^k$, the existence condition is guaranteed for the perturbed problem such that the perturbation method can be used to solve the hard case. As we know that in hard case, the primal problem ($P$)
may have multiple solutions \( \{ \bar{x} \} \) on the boundary of the feasible region \( \mathcal{X} \). By the fact that the perturbed problem \( (P_\alpha) \) is strictly convex in the neighborhood of \( \bar{x}^* \) and its global minimal solution \( \bar{x}^* \) will approach to one of these \( \{ \bar{x} \} \), depending on the parameters \( \{ \alpha_i \} \). From the projection theorem, we know that the nearest points to \( \bar{x} \) and \( \bar{x}^* \) in the subspace spanned by \( \{ U_1, \ldots, U_k \} \) are \( \sum_{i=1}^{k} (\bar{x}^* U_i) U_i \) and \( \sum_{i=1}^{k} (\bar{x}^* U_i) U_i \), respectively, which have the following relationship

\[
\| \bar{x}^* - \sum_{i=1}^{k} (\bar{x}^* U_i) U_i \|^2 < \| \bar{x} - \sum_{i=1}^{k} (\bar{x}^* U_i) U_i \|^2. \tag{26}
\]

Therefore, the perturbed solution \( \bar{x}^* \) is closer to the subspace spanned by \( \{ U_1, \ldots, U_k \} \) than the solution \( \bar{x} \).

5. Canonical primal-dual algorithm

Based on the results in the previous section, we are ready to present an algorithm. The Lanczos method is employed to compute approximately the smallest eigenvalue and the corresponding eigenvector, which will be used to construct the safeguarding and perturbation. A canonical primal-dual iterative scheme is introduced, which is matrix inverse free. The essential cost of this algorithm is only the matrix-vector multiplication.

The key step of this algorithm is to solve the following perturbed canonical dual problem:

\[
(P^d_\alpha) : \max \left\{ P^d_\alpha(\sigma) = -p^T G_\alpha(\sigma)^{-1} p - r^2 \sigma \mid \sigma \in S^+_\alpha \right\} \tag{27}
\]

Let \( \psi(\sigma) \) be its first-order derivative, i.e.,

\[
\psi(\sigma) = (P^d_\alpha(\sigma))' = p^T G_\alpha(\sigma)^{-1} G_\alpha(\sigma)^{-1} p - r^2.
\]

The critical point of \( P^d_\alpha(\sigma) \) in \( S^+_\alpha \) is a unique solution to the equation \( \psi(\sigma) = 0 \) in \( S^+_\alpha \). Thus we need to compute the zero of \( \psi(\sigma) \) in \( S^+_\alpha \) to find the critical point. The first and second order derivatives of \( \psi(\sigma) \) are

\[
\psi'(\sigma) = -2p^T G_\alpha(\sigma)^{-1} G_\alpha(\sigma)^{-1} G_\alpha(\sigma)^{-1} p, \tag{28}
\]

\[
\psi''(\sigma) = 6p^T G_\alpha(\sigma)^{-1} G_\alpha(\sigma)^{-1} G_\alpha(\sigma)^{-1} G_\alpha(\sigma)^{-1} p. \tag{29}
\]

It is noticed that \( \psi(\sigma) \) is strictly decreasing and strictly convex over \( S^+_\alpha \), \( \psi(\sigma) \) will approach \( -r^2 \) as \( \sigma \) approaches infinity and \( \sigma = -\lambda_1 \) is a pole of \( \psi(\sigma) \). Here we use the Lanczos method to compute an approximation of the smallest eigenvalue of \( Q \) and the corresponding eigenvector, denoted by \( \bar{\lambda}_1 \) and \( \bar{U}_1 \), respectively. Clearly, we have \( \| \bar{U}_1 \| = 1 \).

If \( \lambda_1 > 0 \), we can conclude that \( \lambda_1 > 0 \) since \( \bar{\lambda}_1 \) is always smaller than \( \lambda_1 \). The dual feasible region is \( S^+_\alpha = [0, +\infty) \). Thus, if \( \psi(0) \leq 0 \), the maximiser of the dual function over \( S^+_\alpha \) is \( \sigma = 0 \) and \( x = G_\alpha(0)^{-1} f \) is the global solution of the primal problem \( (P) \). If \( \psi(0) > 0 \), there exists a critical point in \( S^+_\alpha \), which is also the unique critical point in \( (-\lambda_1, +\infty) \).

If \( \lambda_1 \leq 0 \), we always intend to calculate the critical point in \( (-\lambda_1, +\infty) \). However, \( (-\lambda_1, +\infty) \) may be not the \( S^+_\alpha \), because it is possible that \( \lambda_1 > 0 \), especially when a large error tolerance is chosen. Thus, we should check whether the critical point is on the right side of 0. If not, the maximiser in \( S^+_\alpha \) should be \( \sigma = 0 \). When the problem is
in the hard case, it is rather rational to choose $\alpha \tilde{U}_1$ with a proper scaling parameter $\alpha$ as a perturbation to $f$.

Although the perturbed canonical dual problem ($P^d_\alpha$) is strictly concave on the closed domain $S_+^+$, its derivative $\psi(\sigma)$ could be ill-conditioned when $\sigma$ approaches to the pole. Therefore, instead of nonlinear optimization techniques, a bisection method is used to find the zero of $\psi(\sigma)$ in $(-\lambda_1, +\infty)$.

For moderate-size problems, it is possible to calculate $G_a(\sigma)^{-1}p$ by computing the inverse or decomposition of $G_a(\sigma)$, but it is not possible for very large-size problems, especially when the memory is very limited. One alternative approach is to solve the following strictly convex minimisation problem,

$$\min_{x \in \mathbb{R}^n} x^T G_a(\sigma)x - 2p^T x,$$  \hspace{1cm} (30)

whose optimal solution is $x = G_a(\sigma)^{-1}p$. Actually, during iterations, we do not need to calculate $\psi(\sigma)$ every time, especially for $\sigma$ being on the left side of the zero and close to the pole. We discover that for a given $\sigma$, the value of $\psi(\sigma)$ is equal to the optimal value of the following unconstrained concave maximization problem

$$\max_{z \in \mathbb{R}^n} -z^T G_a(\sigma)G_a(\sigma)z + 2p^T z - r^2.$$  \hspace{1cm} (31)

By the fact that the value of the target function will increase during the iterations, we can stop solving the problem (31) if the target function is larger than a threshold and then claim that the $\sigma$ must be at the left side of the zero. Thus, the ill-condition in computing $\psi(\sigma)$ as $\sigma$ approaching to the pole can be prevented.

An uncertainty interval should be initialized before the bisection method is applied, and it is used to safeguard that the interval contains the critical point. For the right end of the interval, any large enough number can be chosen. Actually, an upper bound of the critical point can be calculated, then it can be the right end of the uncertainty interval. Denote $\sigma^* \in (-\lambda_1, +\infty)$ be the critical point of $P^d_\alpha(\sigma)$. From the definition of $\psi(\sigma)$, we get

$$\frac{1}{(\lambda_1 + \sigma^*)^2} \sum_{i=1}^{n} \hat{p}_i^2 - r^2 \geq 0.$$  

Hence, $\sqrt{\sum_{i=1}^{n} \hat{p}_i^2}/r = \|p\|/r$ can be an upper bound. However, the bound $\|p\|/r$ may be not tight. A practical way is to let $\sigma = -\lambda_1$ as a starting point and then to update $\sigma$ recursively by moving a certain step to its right each time. If the first $\sigma$ that makes the value of $\psi(\sigma)$ be negative is smaller than the upper bound $\|p\|/r$, it will be set to the right end of the uncertainty interval; otherwise, the upper bound will be the right end.

**Algorithm 1 – Initialization**

*Input:* coefficients $Q$, $f$ and $r$; a given error tolerance $\varepsilon$.

*The smallest eigenvalue:* Use the Lanczos method to obtain $\tilde{\lambda}_1$ and $\tilde{U}_1$.

*Perturbation:*

If the existence condition does not hold, a perturbation is introduced and let

$$p = f + \alpha \tilde{U}_1;$$

Else set $p = f$;

End if
Uncertainty interval: set an update size \( s_t \) and a threshold \( \varepsilon_t \); let \( \sigma = \sigma_t = -\tilde{\lambda}_1 \);

**step 1:** Solve the problem (31). If the value of the target function is larger the threshold \( \varepsilon_t \), the iteration stops, let \( \sigma = \sigma + s_t \) and go to step 1; otherwise, go to step 2.

**step 2:** Calculating the value of \( \psi(\sigma) \).
- If \( \psi(\sigma) > 0 \), set \( \sigma = \sigma, \sigma = \sigma + s_t \) and go to step 2;
- Else \( \sigma_u = \sigma \) and STOP.

End if

As the uncertainty interval \([\sigma_\ell, \sigma_u]\) is obtained, the bisection method is applied to find the next iterate for \( \sigma \), i.e. set \( \sigma \) be the middle point of the uncertainty interval. The main part of our algorithm is given as follows.

**Algorithm 2 – Main**

Do
- set \( \sigma = (\sigma_\ell + \sigma_u)/2 \) and calculate the value of \( \psi(\sigma) \);
- If \( |\psi(\sigma)| < \varepsilon \), then STOP and return \( \sigma \) and \( x \);
- Else if \( \psi(\sigma) > 0 \), update \( \sigma_\ell = \sigma \);
- Else update \( \sigma_u = \sigma \);
End if
End do

6. Numerical experiments

Let us first present two small-size examples to show the application of the canonical duality theory; we then list some large-size examples randomly generated to demonstrate the efficiency of our method.

6.1. Small-size examples

**Example 1** The given data are

\[
Q = \begin{pmatrix}
-1 & 0 \\
0 & 1
\end{pmatrix}, \quad f = \begin{pmatrix}
0 \\
-1.8
\end{pmatrix}, \quad r = 1.
\]

The existence condition does not hold for this example. There are two global solutions, \( \bar{x}_1 = (0.437, -0.9) \) and \( \bar{x}_2 = (-0.437, -0.9) \), which are red points shown in Figure 1. In order to show how the perturbation method works, we first introduced a big perturbation in the linear coefficient \( f \) and let \( p = (0.5, -1.8) \). The graph of the dual function of the perturbed problem is shown in the Figure 1. There is a critical point in the interior in \( S_+^\alpha \), which is \( \bar{\sigma} = 1.676 \), and the corresponding optimal solution for the perturbed problem is \( \bar{x}^* = (0.74, -0.673) \), which is the green point in the Figure 1. We then reduce the perturbation by letting \( p = (0.01, -1.8) \). The critical point is \( \bar{\sigma} = 1.022 \) and the corresponding solution is \( \bar{x}^* = (0.456, -0.89) \). Figure 2 shows that the perturbed solution \( \bar{x}^* \) approaches \( \bar{x}_1 \).

**Example 2** The matrix \( Q \) and radius \( r \) are same with that in Example 1 and \( f \) is changed to

\[
f = \begin{pmatrix}
0 \\
-3
\end{pmatrix}.
\]
Figure 1. \( \mathbf{p} = (0.5, -1.8) \). (a): The contours of the primal function and the boundary of the sphere; (b): graph of the dual function.

Figure 2. \( \mathbf{p} = (0.01, -1.8) \). (a): The contours of the primal function and the boundary of the sphere; (b): graph of the dual function.

Figure 3. (a): Contours of the primal function and boundary of the sphere; (b): graph of the dual function.

which is in the same direction of that in Example 1 but has a larger length. We notice that though \( \sum_{i=1}^{k} f_i^2 \neq 0 \) is violated, the condition \( \sum_{i=k+1}^{n} \frac{f_i^2}{(\lambda_i - \lambda_1)^2} > r^2 \) holds. Thus, it is not in the hard case. There is a critical point in the interior of \( S^+ \), which is shown in Figure 3(b) and it is corresponding to the unique global solution of the primal problem, which is the green point in Figure 3(a).
6.2. **Large-size examples**

A hundred of examples are randomly generated, containing fifty examples of the general case and fifty examples of the hard case. Both cases have ten examples for dimensions of 500, 1000, 2000, 3000 and 5000. All elements of the coefficients, $Q$, $f$ and $r$, are integer numbers in $[-100, 100]$. For each example of the hard case, a matrix $Q$ with the multiplicity of $\lambda_1 = 1$ is chosen. The corresponding vector $f$ is constructed such that $f$ is perpendicular to the eigenvector $U_1$. Then a proper radius $r$ is calculated such that the existence conditions are violated.

Two approaches are used to calculate the value of $\psi(\sigma)$. One is using decomposition methods to calculate $G_\alpha(\sigma)^{-1}p$, for which we use the ‘left division’ of Matlab. Another is solving the problem (30), for which we use the function ‘quadprog’ of Matlab. For the function ‘quadprog’, the tolerance parameter ‘TolFun’ is set as 1e-12. The Matlab is of version 7.13 and runned in the platform with Linux 64-bit system and quad CPUs.

A perturbation item $\alpha U_1$ is added into the target function for the hard case, and two values of $\alpha$, 1e-3 and 1e-4, are tried. In the main part of the algorithm, the termination tolerance on the value of $\psi(\sigma)$ is set to be 1e-8.

Results are shown in Table 1, 2, 3 and 4, and they contain the number of examples which are successfully solved (Succ.Solv.), the distance of the optimal solution to the boundary of the sphere (Dist.Boun.), the number of iteration of the Algorithm: Main (Numb.Iter.) and the running time of the algorithm (Runn.Time). The values in the columns of Dist.Boun., Numb.Iter. and Runn.Time are averages of the examples successfully solved. We compare the results of the algorithm adopting ‘left division’ and that of the algorithm adopting ‘quadprog’ in the same table, where LD denotes left division and QP denotes quadprog.

We can see that the examples are solved very accurately with error allowance being less than 1e-09, except few instances which are not solved successfully. For general cases, all the examples can be solved within no more than 30 iterations, whiles for hard cases, the number of iterations is around 40. From the running time, we notice that our method is capable to handle large-size problems in reasonable time. The algorithms using ‘left
division’ and ‘quadprog’ have similar performances in the accuracy and the number of iterations. While the one using ‘left division’ needs much less time than that of the one using ‘quadprog’. However, the one using ‘quadprog’ is able to solve more examples successfully.

7. Conclusion Remarks

We have presented a detailed study on the quadratic minimization problem with a sphere constraint. By the canonical duality, this nonconvex optimization is equivalent to a concave maximization dual problem over a convex domain $S^+_a$, which is true also for many other global optimization problems (see [7, 9–11, 14, 16, 18]). Therefore, the so-called hidden convexity discovered by Ben-Tal and Teboulle in [1] is indeed a special case of the canonical duality theory. Based on this canonical dual problem, sufficient and necessary conditions are obtained for both general and hard cases. In order to solve hard case problems, a perturbation method and the associated algorithm are proposed. Numerical results for large-size examples demonstrate the efficiency of the proposed approach. Combining with the trust region method, the results presented in this paper can be used for efficiently solving general global optimizations.

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