Global optimal solutions to nonconvex optimisation problems with a sum of double-well and log-sum-exp functions

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Abstract
This paper presents a canonical dual approach for solving a nonconvex global optimisation problem with a sum of double-well and log-sum-exp functions. Such a problem arises extensively in mechanics, robot designing, information theory and network communication systems. It includes fourth-order polynomial minimisation problems and minimax problems. Based on the canonical duality theory, this nonconvex problem is transformed to an equivalent dual problem, and the triality theory explicates that under certain condition the dual problem can be solved easily and, correspondingly, the global solution of the primal problem can be obtained analytically from the dual solution. It also discusses the relationships between local extremums of the primal problem and the dual problem. Furthermore, two specific problems, a fourth-order polynomial minimisation problem and a minimax problem, are discussed and situations when the condition in the triality theory holds are presented. In the end, several numerical examples are provided to illustrate the application of canonical duality theory on this problem.

Keywords
Global optimization, canonical duality theory, double-well function, log-sum-exp function, polynomial minimisation, minimax problems

1 Introduction
In this paper, we are interesting in the following nonconvex global optimization problem:

$$\min \left\{ H(x) := \frac{1}{2} x^T A x - f^T x + W(x) + T(x) \mid x \in \mathbb{R}^n \right\}$$

in which $A \in \mathbb{R}^{n \times n}$ is a symmetric matrix, $f \in \mathbb{R}^n$, and the log-sum-exp function $T(x)$ and the double-well function $W(x)$ are defined as

$$W(x) := \sum_{i=1}^p \frac{\alpha_i}{2} \left( \frac{1}{2} x^T B_i x - b_i^T x + c_i \right)^2,$$

$$T(x) := \frac{1}{\beta} \log \left[ 1 + \sum_{i=1}^p \exp \left( \beta \left( \frac{1}{2} x^T Q_i x - q_i^T x + d_i \right) \right) \right],$$

where $Q_i \in \mathbb{R}^{n \times n}$ and $B_i \in \mathbb{R}^{n \times n}$ are symmetric matrices, $q_i \in \mathbb{R}^n$, $b_i \in \mathbb{R}^n$, $d_i$ and $c_i$ are any real numbers, and $\alpha_i$ and $\beta$ are positive real numbers.

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The double-well function is well known in modelling potential energy, for example, in [19], it was used to model post-buckling of beams. Whereas the log-sum-exp function is one of the fundamental functions in numerical analysis, and it is widely applied to deal with minimax problems [22, 23, 24, 26], which arise broadly in regions including plasticity theory [27], non smooth variational problems [18], structural optimisation problems [3], robot manipulator designing [1, 2, 25] and so on. Another significant application of the log-sum-exp function is in geometric programming, where objective and constraint functions are posynomial or monomial functions and they are rewritten as convex log-sum-exp functions [5, 6, 20].

The canonical duality theory was originally developed for handling general nonconvex and/or nonsmooth systems [8]. The canonical duality theory has been applied successfully to many problems arising in global optimization and nonconvex nonsmooth analysis, such as quadratic problems [7, 10, 12, 14], polynomial optimisation [11], transportation problems [15], location problems [13], and max-cut problem [28]. There are also some efficient algorithms developed which are based on the canonical duality theory [16].

The purpose of this paper is to apply the canonical duality theory to solve globally the nonconvex optimisation problem presented above. By introducing geometrical operators and canonical functions, the canonical dual problem can be constructed, which is equivalent to the primal problem. The triality theory explicates that under certain condition the dual problem can be solved easily. This condition is the appearance of a critical point in the positive semidefinite region of the feasible space of the dual problem. Correspondingly, the global solution of the primal problem can be obtained analytically from the critical point. This is called min-max duality. The triality theory also discusses the relationships between local extremums of the primal problem and the dual problem, which are stated as the double-min and double-max dualities. Then, two problems, a fourth-order polynomial minimisation problem and a minimax problem, are particularly discussed. For these two specific problems, the conditions of a critical point existing in the interior of the positive semidefinite region are presented, which are derived from the coefficients of the primal problems. In the end of the paper, several numerical examples are provided to illustrate the application of the canonical duality theory to the problems discussed in this paper.

The rest of this paper is arranged as follows. In Section 2, the canonical duality theory is applied to the problem (P). The relationships of solutions of the primal and dual problems are discussed by the triality theory in Section 3. Then, in Section 4, two specific problems, a fourth-order polynomial minimisation problem and a minimax problem, is discussed. In Section 5, several examples are provided to illustrate the canonical duality theory. Finally, some conclusions are given in Section 6.

2 Canonical dual problem and analytical solutions

In this section, we apply the canonical duality theory to the problem (P). We first introduce the following two geometrical operators:

\[ \xi(x) := \left\{ \frac{1}{2} x^T Q_i x - q_i^T x + d_i \right\}_{i=1}^p : \mathbb{R}^n \to \mathcal{E}_1 \subseteq \mathbb{R}^p, \]  

(4)

\[ \eta(x) := \left\{ \frac{1}{2} x^T B_i x - b_i^T x + c_i \right\}_{i=1}^r : \mathbb{R}^n \to \mathcal{E}_2 \subseteq \mathbb{R}^r, \]  

(5)

and the following two canonical functions:

\[ V_1(\xi) := \frac{1}{\beta} \log \left[ 1 + \sum_{i=1}^p \exp (\beta \xi_i) \right], \]  

(6)

\[ V_2(\eta) := \sum_{i=1}^r \frac{\alpha_i}{2} \eta_i^2, \]  

(7)

where \( \xi_i \) is the \( i \)th component of \( \xi \), and \( \eta_i \) is the \( i \)th component of \( \eta \). It is easy to verify that \( \xi(x) \) and \( \eta(x) \) are twice Gâteaux differentiable, and \( V_1(\xi) \) and \( V_2(\eta) \) are convex.
We define the following two operators
\[
\tau := \nabla V_1(\xi) = \left\{ \exp(\beta \xi_i) \over 1 + \sum_{k=1}^p \exp(\beta \xi_k) \right\}_{i=1}^p : \mathcal{E}_1 \to \mathcal{E}_1^*,
\]
\[
\sigma := \nabla V_2(\eta) = \{ a_i \eta_i \}_{i=1}^r : \mathcal{E}_2 \to \mathcal{E}_2^*,
\]
where \( \mathcal{E}_1^* \subseteq \{ \tau \in \mathbb{R}^p \mid \tau > 0, \, e^T \tau < 1 \} \), and \( \mathcal{E}_2^* \subseteq \mathbb{R}^r \). Thus, from the Legendre transformation, we have the following relationships:
\[
V_1(\xi) + V_1^*(\tau) = \xi^T \tau, \\
V_2(\eta) + V_2^*(\sigma) = \eta^T \sigma,
\]
where \( V_1^* \) and \( V_2^* \) are the conjugate functions of \( V_1 \) and \( V_2 \), respectively,
\[
V_1^*(\tau) := {1 \over \beta} \left[ \sum_{i=1}^p \tau_i \log(\tau_i) + (1 - \sum_{i=1}^p \tau_i) \log(1 - \sum_{i=1}^p \tau_i) \right],
\]
\[
V_2^*(\sigma) := \sum_{i=1}^r {1 \over 2a_i} \sigma_i^2.
\]

Let
\[
m = p + r, \quad \zeta = (\tau, \sigma), \quad \mathcal{E}_a = \mathcal{E}_1 \times \mathcal{E}_2, \quad \text{and} \quad \mathcal{E}_a^* = \mathcal{E}_1^* \times \mathcal{E}_2^*.
\]
The so-called generalized total complementary function \( \Xi : \mathbb{R}^n \times \mathcal{E}_a^* \to \mathbb{R} \) can be defined as
\[
\Xi(x, \zeta) := V_1(\xi(x)) + V_2(\eta(x)) + {1 \over 2} x^T A x - f^T x
\]
\[
= \tau^T \xi(x) - V_1^*(\tau) + \sigma^T \eta(x) - V_2^*(\sigma) + {1 \over 2} x^T A x - f^T x
\]
\[
= {1 \over 2} x^T G_a x - f_a^T x + d^T \tau - V_1^*(\tau) + c^T \sigma - V_2^*(\sigma),
\]
where \( G_a := A + \sum_{i=1}^p \tau_i Q_i + \sum_{i=1}^r \sigma_i B_i \) and \( f_a := f + \sum_{i=1}^p \tau_i q_i + \sum_{i=1}^r \sigma_i b_i \).

Thus, for any given \( \zeta \in \mathcal{E}_a^* \), the canonical dual function \( II^d(\zeta) \) is defined as
\[
II^d(\zeta) := \text{sta}\{ \Xi(x, \zeta) \mid x \in \mathbb{R}^n \},
\]
where the notation \( \text{sta}\{ \cdot \} \) represents the task of finding stationary points of \( \Xi(x, \zeta) \) with respect to \( x \). Notice that for any given \( \zeta \), the total complementary function \( \Xi(x, \zeta) \) is a quadratic function of \( x \) and its stationary points are the solutions of the following equation system
\[
\nabla_x \Xi(x, \zeta) = G_a x - f_a = 0.
\]
If \( f_a \in C_{ad}(G_a) \), then \( x \) can be solved analytically as \( x = G_a^T f_a \), in which \( G_a^T \) denotes the generalized inverse of \( G_a \). Thus the canonical dual function \( II^d(\zeta) \) can be written explicitly as
\[
II^d(\zeta) = {1 \over 2} f_a^T G_a^T f_a + c^T \sigma - \sum_{i=1}^r {1 \over 2a_i} \sigma_i^2 + d^T \tau
\]
\[
- {1 \over \beta} \left[ \sum_{i=1}^p \tau_i \log(\tau_i) + (1 - \sum_{i=1}^p \tau_i) \log(1 - \sum_{i=1}^p \tau_i) \right].
\]

Let
\[
S_a := \{ \zeta \mid \zeta \in \mathcal{E}_a^*, \quad f_a \in C_{ad}(G_a) \}.
\]
The canonical dual problem for the primal problem \( (P) \), therefore, is defined as follows:
\[
(P^d) : \quad \text{sta}\{ II^d(\zeta) \mid \zeta \in S_a \}.
\]

The following theorem states that there is no duality gap between the primal problem \( (P) \) and the canonical dual problem \( (P^d) \). The proof is omitted here, which is analogous with that in [9].
Suppose that Lemma 2 in \cite{17}.

Suppose that Lemma 3.

\[ x = G_a^\dagger f_a \] (19)

is a critical point of \( \Pi(x) \), the pair \((\bar{x}, \zeta)\) is a critical point of \( \Xi(x, \zeta) \), and we have

\[ \Pi(\bar{x}) = \Xi(\bar{x}, \zeta) = \Pi^d(\zeta). \] (20)

3 Triality theory

In this section we study the conditions for local and global optima of the primal and dual problems. We focus the discussion on the following two regions of the dual space:

\[ S^+_a := \{ \zeta \in S_a \mid G_a \preceq 0 \}, \]

\[ S^-_a := \{ \zeta \in S_a \mid G_a \prec 0 \}. \]

For convenience, we firstly give the first and second derivatives of functions \( \Pi(x) \) and \( \Pi^d(\zeta) \):

\begin{align*}
\nabla \Pi(x) &= G_a x - f_a, \tag{21} \\
\nabla^2 \Pi(x) &= G_a + FD F^T, \tag{22} \\
\nabla \Pi^d(\zeta) &= \left[ \frac{1}{2} f_a^T G_a^\dagger Q_a G_a^\dagger f_a - q_i^T G_a^\dagger f_a + d_i - \frac{1}{\sigma_i} \log \left( 1 + \sum_{j=1}^p r_j \right) \right]_{i=1}^p, \tag{23} \\
\nabla^2 \Pi^d(\zeta) &= -F^T G_a^\dagger F - D^{-1}, \tag{24}
\end{align*}

where \( F \in \mathbb{R}^{n \times m} \) and \( D \in \mathbb{R}^{m \times m} \) are defined as

\[ F := \begin{bmatrix} Q_1 x - q_1, \ldots, Q_p x - q_p, B_1 x - b_1, \ldots, B_r x - b_r \end{bmatrix}, \]

\[ D := \begin{bmatrix} \beta \left( \text{diag}(\tau) - \tau \tau^T \right) & 0 \\ 0 & \text{diag}(\alpha) \end{bmatrix}. \]

We also need the following two lemmas. Their proofs are omitted, which are analogous with that in \cite{17}.

Lemma 2 Suppose that \( m < n \), \( \zeta \in S^-_a \) is a critical point and a local minimizer of \( \Pi^d(\zeta) \), and \( \bar{x} = G_a^\dagger f_a \). Then, there exists a matrix \( L \in \mathbb{R}^{n \times m} \) with \( \text{rank}(L) = m \) such that

\[ L^T \nabla^2 \Pi(\bar{x}) L \succeq 0. \] (25)

Lemma 3 Suppose that \( m > n \), \( \bar{\zeta} \in S^-_a \) is a critical point of \( \Pi^d(\zeta) \), and \( \bar{x} = G_a^\dagger f_a \) is a local minimizer of \( \Pi(x) \). Then, there exists a matrix \( P \in \mathbb{R}^{m \times n} \) with \( \text{rank}(P) = n \) such that

\[ P^T \nabla^2 \Pi^d(\bar{\zeta}) P \succeq 0. \] (26)

Since \( \text{rank}(L) = m \), the columns of matrix \( L \) are linearly independent. Similarly, the columns of matrix \( P \) are linearly independent too. We defined the column spaces of \( L \) and \( P \), respectively, as:

\[ X_L := \{ x \in \mathbb{R}^n \mid \bar{x} + L \theta, \ \theta \in \mathbb{R}^m \}, \]

\[ S_P := \{ \zeta \in \mathbb{R}^m \mid \bar{\zeta} + P \vartheta, \ \vartheta \in \mathbb{R}^n \}. \]

Theorem 4 (Triality Theorem) Suppose that \( \bar{\zeta} \) is a critical point of \( \Pi^d(\zeta) \), and \( \bar{x} = G_a^\dagger f_a \).

1. If \( \bar{\zeta} \in S^+_a \), then the canonical min-max duality holds in the form of

\[ \Pi(\bar{x}) = \min_{x \in \mathbb{R}^n} \Pi(x) = \max_{\zeta \in S^+_a} \Pi^d(\zeta) = \Pi^d(\bar{\zeta}). \] (27)
2. If $\bar{\zeta} \in S^n_+$, then there exists a neighborhood $X_0 \times S_0 \subset \mathbb{R}^n \times S^n_-$ of $(\bar{x}, \bar{\zeta})$ such that the double-max duality holds in the form of

$$II(\bar{x}) = \max_{x \in X_0} II(x) = \max_{\zeta \in S_0} II^d(\zeta) = II^d(\bar{\zeta}).$$

(28)

3. If $\bar{\zeta} \in S^n_-$, then the double-min duality statement holds conditionally as:

(a) if $m = n$, then there exists a neighborhood $X_0 \times S_0 \subset \mathbb{R}^n \times S^n_-$ of $(\bar{x}, \bar{\zeta})$ such that

$$II(\bar{x}) = \min_{x \in X_0} II(x) = \min_{\zeta \in S_0} II^d(\zeta) = II^d(\bar{\zeta}).$$

(29)

(b) if $m < n$ and $\bar{\zeta}$ is a local minimizer of $II^d(\zeta)$, then $\bar{x}$ is a saddle point of $II(x)$, and there exists a neighborhood $(X_0 \cap X_L) \times S_0 \subset \mathbb{R}^n \times S^n_-$ of $(\bar{x}, \bar{\zeta})$ such that

$$II(\bar{x}) = \min_{x \in X_0 \cap X_L} II(x) = \min_{\zeta \in S_0} II^d(\zeta) = II^d(\bar{\zeta});$$

(30)

(c) if $m > n$ and $\bar{x}$ is a local minimizer of $II(x)$, then $\bar{\zeta}$ is a saddle point of $II^d(\zeta)$, and there exists a neighborhood $X_0 \times (S_0 \cap S_P) \subset \mathbb{R}^n \times S^n_-$ of $(\bar{x}, \bar{\zeta})$ such that

$$II(\bar{x}) = \min_{x \in X_0} II(x) = \min_{\zeta \in S_0 \cap S_P} II^d(\zeta) = II^d(\bar{\zeta}).$$

(31)

Proof:

1. Since $\bar{\zeta} \in S^n_+$, we have $G_a \succeq 0$ and $D \succeq 0$, which implies that $II^d(\zeta)$ is strictly concave on $S^n_+$. Thus, $\bar{\zeta}$ is a global maximizer of $II^d(\zeta)$ on $S^n_+$. Similarly, it can be proved that $\Xi(x, \bar{\zeta})$ is convex on $\mathbb{R}^n$, which, plus the fact that $\bar{x}$ is a critical point of $\Xi(x, \bar{\zeta})$, implies that for any $x \in \mathbb{R}^n$, we have $\Xi(x, \bar{\zeta}) \geq \Xi(\bar{x}, \bar{\zeta})$. Furthermore, from the Fenchel’s inequality, it is true that $\Xi(x, \bar{\zeta}) \leq II(x)$, $\forall (x, \bar{\zeta}) \in \mathbb{R}^n \times S_0$. Therefore, for any $x \in \mathbb{R}^n$, we have

$$II(x) \geq \Xi(x, \bar{\zeta}) \geq \Xi(\bar{x}, \bar{\zeta}) = II(\bar{x}),$$

(32)

where the last equality has been proved in Theorem 1, which also has proved that $II(\bar{x}) = II^d(\bar{\zeta})$. Thus, $\bar{x}$ is a global minimizer of $II(x)$, and equation (27) is true.

2. Suppose $\bar{\zeta}$ is a local maximizer of $II^d(\zeta)$ on $S^n_-$. Then we have $\nabla^2 II(\bar{\zeta}) = -FTG_a^{-1}F - D^{-1} \preceq 0$, and there exists a neighborhood $S_0 \subset S_-$ such that for all $\zeta \in S_0$, $\nabla^2 II(\zeta) \preceq 0$. Since for any $\zeta \in S_0$, the matrix $G_a$ is nonsingular, thus the map $x = G_a^{-1}f_a : S_0 \rightarrow \mathbb{R}^n$ is one-to-one. Let $X_0$ be the image of the map $x = G_a^{-1}f_a$ on $S_0$. Obviously, $X_0$ is a neighborhood of $\bar{x}$. Next, we want to prove that for any $x \in X_0$, $\nabla^2 II(x) \preceq 0$, which plus the fact that $\bar{x}$ is a critical point of $II(x)$ implies that $\bar{x}$ is a maximizer of $II(x)$ over $X_0$. For any $x \in X_0$, let $\zeta$ be the corresponding point under the map $x = G_a^{-1}f_a$. Thus, $\nabla^2 II(\zeta) = -FTG_a^{-1}F - D^{-1} \preceq 0$. By singular value decomposition, there exists orthogonal matrices $E \in \mathbb{R}^{n \times n}$, $K \in \mathbb{R}^{m \times m}$ and $R \in \mathbb{R}^{n \times m}$ with

$$R_{ij} = \begin{cases} \delta_i, & i = j \text{ and } i = 1, \ldots, r, \\ 0, & \text{otherwise,} \end{cases}$$

(33)

where $\delta_i > 0$ for $i = 1, \ldots, r$ and $r = \text{rank}(F)$, such that

$$FD^{-\frac{1}{2}} = ERK.$$  

(34)

Then we have

$$- D^{-\frac{1}{2}} - D^{-\frac{1}{2}}K^TERTG_a^{-1}ERKD^{-\frac{1}{2}} \preceq 0.$$  

(35)

Being multiplied by $K D^{-\frac{1}{2}}$ from the left and $D^{-\frac{1}{2}}K^T$ from the right, the equation (35) can be converted equivalently into

$$-I_m - RTERTG_a^{-1}ER \preceq 0,$$

(36)
which, by Lemma 7 in Appendix, is further equivalent to

\[ E^T G_a E + RRT \preceq 0. \tag{37} \]

Multiplying the equation (37) by \(E\) from the left and \(E^T\) from the right, we obtain

\[ 0 \succeq G_a + E R K D^{-\frac{1}{2}} D D^{-\frac{1}{2}} K^T R^T E = G_a + F D F^T = \nabla^2 \Pi(x). \tag{38} \]

Therefore, \(\bar{x}\) is a maximizer of \(\Pi(x)\) over \(S_0\).

Similarly, we can prove that if \(\bar{\zeta}\) is a maximizer of \(\Pi^d(\zeta)\) over \(X_0\), \(\bar{x}\) is a maximizer of \(\Pi^d(\zeta)\) over \(S_0\). The equation (28) can be proved similarly as the equation (27).

3. Then we prove the double-min duality.

(a) Suppose that \(m = n\) and \(\bar{\zeta}\) is a local minimizer of \(\Pi^d(\zeta)\) over \(S_0^\ast\). Then there exists a neighborhood \(S_0 \subset S_0\) of \(\zeta\) such that for any \(\zeta \in S_0\), \(\nabla^2 \Pi^d(\zeta) \succeq 0\). Denote \(X_0\) as the image of the map \(x = G_a^{-1} f_a\) over \(S_0\). For any \(x \in X_0\), let \(\zeta\) be the corresponding point under the map \(x = G_a^{-1} f_a\). From \(\nabla^2 \Pi^d(\zeta) = -F^T G_a^{-1} F - D^{-1} \succeq 0\), we have

\[ -F^T G_a^{-1} F \succeq D^{-1} \succ 0, \tag{39} \]

which is further equivalent to

\[ -G_a^{-1} \succeq (F^T)^{-1} D^{-1} F^{-1}. \tag{40} \]

Thus, we prove that \(\nabla^2 \Pi(x) = G_a + F D F^T \succeq 0\). The converse can be proved similarly. The equation (29) can be proved similarly as the equation (27).

(b) Suppose that \(m < n\) and \(\bar{\zeta}\) is a local minimizer of \(\Pi^d(\zeta)\) over \(S_0^\ast\). We claim that \(\bar{x}\) is not a local minimizer of \(\Pi(x)\). If \(\bar{x}\) is a local minimizer of \(\Pi(x)\), we would have

\[ \nabla^2 \Pi(x) = G_a + F D F^T \succeq 0, \]

which implies that the matrix \(F\) is invertible. Then we obtain

\[ -G_a^{-1} \succeq (F^T)^{-1} D^{-1} F^{-1}, \tag{41} \]

which is a contradiction. Therefore, plus the previous discussion, \(\bar{x}\) must be a saddle point of \(\Pi(x)\).

Let

\[ \varphi(t) = \Pi(\bar{x} + Lt). \tag{42} \]

It can be proved that \(0 \in \mathbb{R}^m\) is a local minimizer of the function \(\varphi(t)\), because we have

\[ \nabla \varphi(0) = L^T \nabla \Pi(\bar{x}) = 0, \tag{43} \]

\[ \nabla^2 \varphi(0) = L^T \nabla^2 \Pi(\bar{x}) L \succeq 0. \tag{44} \]

Thus the equation (30) is proved.

(c) The proof is similar to case (b) and it is omitted.

The theorem is proved.

\[ \square \]

4 Two specific problems

In this section, two specific problems, a fourth-order polynomial minimisation problem and a minimax problem, will be discussed. For these two problems, existence conditions for the critical point in \(S_0^+\) are derived, which also can be used to separate easy and hard problems.
4.1 A fourth-order polynomial minimisation problem

The fourth-order polynomial minimisation problem considered here is

\[
(P_p) \min_{x \in \mathbb{R}^n} II_p(x) = \frac{1}{2} x^T Ax - f^T x + \frac{\alpha}{2} \left(\frac{1}{2} x^T Bx - b^T x + c\right)^2
\]  

(45)

where matrix \( B \) is symmetric and positive definite. Without loss of generality, we can assume \( B = I \), the identity matrix, and \( b = 0 \).

Let

\[G_a = A + \sigma I, \quad \text{and} \quad S_a^+ = \{\sigma \mid G_a \succeq 0, \sigma \geq \alpha c\}.\]

The canonical dual problem for the problem (45) is defined as

\[
(P_{pd}) \min_{\sigma \in S_a^+} II_{pd}(\sigma) = -\frac{1}{2} f^T G_a^{-1} f + c\sigma - \frac{1}{2\alpha}\sigma^2
\]

(46)

From the symmetry of the matrix \( A \), we have a diagonal matrix \( A \) and an orthogonal matrix \( U \) such that \( A = UA^T \). The diagonal entities of \( A \) are the eigenvalues of the matrix \( A \) in non-decreasing order,

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

The columns of \( U \) are the corresponding eigenvectors. If we let \( f = U^T f \), the dual function can be rewritten as

\[II_{pd}(\sigma) = \frac{1}{2} \sum_{i=1}^n \frac{f_i^2}{\lambda_i + \sigma} - \frac{1}{2\alpha}\sigma^2
\]

(47)

The first-order and second-order derivatives of the dual function \( II_{pd}(\sigma) \) are

\[\delta II_{pd}(\sigma) = \frac{1}{2} \sum_{i=1}^n \frac{f_i^2}{(\lambda_i + \sigma)^2} - \frac{1}{\alpha}\sigma
\]

\[\delta^2 II_{pd}(\sigma) = -\frac{1}{2} \sum_{i=1}^n \frac{f_i^2}{(\lambda_i + \sigma)^3} - \frac{1}{\alpha}
\]

Since \( \alpha \) is assumed to be positive, \( \delta^2 II_{pd}(\sigma) \) is negative over \( S_a^+ \). Thus the dual function is concave in \( S_a^+ \). If \( \alpha c > -\lambda_1 \), \( S_a^+ = [\alpha c, +\infty) \) and the maximiser of \( II_{pd}(\sigma) \) in \( S_a^+ \) is corresponding to the unique global solution of the primal problem, since \( G_a \) is positive definite. If \( \alpha c \leq -\lambda_1 \), \( S_a^+ = [-\lambda_1, +\infty) \) and we have the following theorem about the existence of a critical point in \( S_a^+ \). Its proof is similar to that in [4].

**Proposition 5 (Existence Condition)** Suppose that \( \lambda_i \) are defined as above and \( -\lambda_1 \leq \alpha c \).

Then there exist a critical point of \( II_{pd}(\tau) \) in the interior of \( S_a^+ \) if and only if \( \sum_{i=1}^k \tilde{f}_i^2 \neq 0 \) or \( \frac{1}{2} \sum_{i=k+1}^n \tilde{f}_i^2/(-\lambda_1 + \lambda_i)^2 + \lambda_1/\alpha > 0 \). If \( II_{pd}(\tau) \) has a critical point in \( S_a^+ \), the critical point is unique. Let \( \sigma^* \) denote the critical point. Then \( x^* = G_a^{-1} f \) is a global solution of the problem \((P_p)\).

4.2 A minimax problem

In this section, we consider an minimax problem

\[
\min_{x \in \mathbb{R}^n} \max \left\{ \frac{1}{2} x^T A_1 x - f_1^T x + d_1, \frac{1}{2} x^T A_2 x - f_2^T x + d_2 \right\}
\]

(48)

where the matrix \( A_1 \) and the matrix \( A_2 \) are symmetric. Since \( A_1 \) is positive definite, we can rotate and move the coordinate system such that \( A_1 \) becomes the identity matrix and \( f_1 \) vanishes. Thus not losing any generality, we consider the following problem with simpler formulation:

\[
\min_{x \in \mathbb{R}^n} \max \left\{ \frac{1}{2} x^T x + d_1, \frac{1}{2} x^T A_2 x - f_2^T x + d_2 \right\}
\]

(49)
In order to make sure that the problem is not trivial, we further assume that \( d_2 > d_1 \).

For the problem \((\mathcal{P}_m)\), an existing condition for a critical point being in the positive semidefinite region \(S_a^+\) will be presented. Furthermore, if the existing condition does not hold, perturbations are introduced and the perturbed problem will always have a critical point in \(S_a^+\).

If we let \( Q = A_2 - I \), \( q = f_2 \) and \( d = d_2 - d_1 \), then the problem \((\mathcal{P}_m)\) can be approximated as the problem \((\mathcal{P})\) with \( p = 1 \), \( r = 0 \), \( f = 0 \) and \( A = I \).

\[
(\mathcal{P}_m) \quad \min_{x \in \mathbb{R}^n} \Pi_m(x) = \frac{1}{2} x^T x + d_1 + \frac{1}{\beta} \log \left[ 1 + \exp \left( \beta \left( \frac{1}{2} x^T Qx - q^T x + d \right) \right) \right].
\]

The dual function will be an univariate function, the matrix \( G_a \) and the vector \( f_a \) are simplified as
\[
G_a = I + \tau Q, \quad \text{and} \quad f_a = \tau q.
\]

We are only interesting in the behaviour of the dual function on the positive semidefinite region in the dual space, which, for this specific case, is defined as
\[
S_a^+ = \{ \tau \mid 0 < \tau < 1, G_a \geq 0 \}.
\]

The canonical dual problem is defined as
\[
(\mathcal{P}_m^d) \quad \max_{\tau \in S_a^+} \Pi_m^d(\tau) = -\frac{1}{2} f_a^T G_a^{-1} f_a + d \tau - \frac{1}{\beta} [\tau \log(\tau) + (1 - \tau) \log(1 - \tau)] + d_1
\]

Similar with the discussion in last subsection, we denote the eigendecomposition of \( Q \) as \( Q = U \Sigma U^T \). The diagonal entities of \( \Sigma \) are the eigenvalues of the matrix \( Q \) in nondecreasing order,
\[
\lambda_1 = \cdots = \lambda_k < \lambda_{k+1} \leq \cdots \leq \lambda_n.
\]

The columns of \( U \) are the corresponding eigenvectors. If we let \( \hat{q} = U^T q \) and \( \hat{f}_a = \tau \hat{q} \), the dual function can be rewritten as
\[
\Pi_m^d(\tau) = -\frac{\tau^2}{2} \left( \sum_{i=1}^{k} \frac{\hat{q}_i^2}{1 + \tau \lambda_i} + \sum_{i=k+1}^{n} \frac{\hat{q}_i^2}{1 + \tau \lambda_i} \right) + d \tau - \frac{1}{\beta} [\tau \log(\tau) + (1 - \tau) \log(1 - \tau)] + d_1
\]

It can be noticed that if \( \lambda_1 \geq -1 \), the matrix \( G_a \) is always positive definite as \( \tau \in (0,1) \). We then can prove that if \( \lambda_1 \geq -1 \), the dual function \( \Pi_m^d(\tau) \) has a critical point on \( S_a^+ \). The first-order and second-order derivatives of \( \Pi_m^d(\tau) \) are
\[
\delta \Pi_m^d(\tau) = -1/\tau - \lambda_1/2 \sum_{i=1}^{k} \frac{\hat{q}_i^2}{(1 + \tau \lambda_i)^2} - \sum_{i=k+1}^{n} \frac{-1/\tau - \lambda_i/2}{(1 + \tau \lambda_i)^2} \hat{q}_i^2 + \frac{1}{\beta} \log(1/\tau - 1) + d
\]
\[
\delta^2 \Pi_m^d(\tau) = -(QG_a^{-1} f_a - q)^T G_a^{-1} (QG_a^{-1} f_a - q) - \frac{1}{\beta} \left( \frac{1}{\tau} + \frac{1}{1 - \tau} \right)
\]

We notice that \( \delta^2 \Pi_m^d(\tau) \) is negative in \( S_a^+ \), which indicates that \( \Pi_m^d(\tau) \) is concave over \( S_a^+ \). As \( \tau \) is close enough to 1, the value of \( \delta \Pi_m^d(\tau) \) will be negative, and as \( \tau \) approaches to 0, the first two items in \( \delta \Pi_m^d(\tau) \) will approach to zero and the value of \( \delta \Pi_m^d(\tau) \) will be positive with large enough \( \beta \). Thus, with large enough \( \beta \), there will be a critical point of the dual function \( \Pi_m^d(\tau) \) on \( S_a^+ \).

Next we consider the situation where \( \lambda_1 < -1 \). The following proposition gives the conditions for the existence of the critical point of the dual function \( \Pi_m^d(\tau) \) on \( S_a^+ \). Its proof is similar to that in [4] and omitted.

**Proposition 6 (Existence Condition)** Suppose that \( \lambda_i \) and \( \hat{q}_i \) are defined as above and \( \lambda_1 < -1 \). Then there exist a critical point of \( \Pi_m^d(\tau) \) in the interior of \( S_a^+ \) if and only if \( \sum_{i=1}^{k} \hat{q}_i^2 (\lambda_1 - \lambda_i)/2 \neq 0 \) or \( \sum_{i=k+1}^{n} \hat{q}_i^2 (\lambda_1 - \lambda_i)/2 \neq 0 \). If \( \Pi_m^d(\tau) \) has a critical point in the interior of \( S_a^+ \), the critical point is unique. Let \( \tau^* \) denote the critical point. Then \( x^* = G_a^{-1} f_a \) is a global solution of the problem \((\mathcal{P}_m)\).
5 Examples

In this section, several examples are provided to illustrate the perfect duality of the canonical duality theory.

Example 1

Consider the 1-dimensional problem:

$$\min_{x \in \mathbb{R}} \Pi(x) = \log [1 + \exp (0.5x^2 - 0.1)] + 5 (x^2 - 1)^2 - 0.8x.$$

The corresponding canonical dual function is given by

$$\Pi^d(\tau, \sigma) = -\frac{0.32}{\tau + 2\sigma} - \sigma - 0.05\sigma^2 - 0.1\tau - [\tau \log(\tau) + (1 - \tau) \log(1 - \tau)].$$

The graph of function $\Pi(x)$ is shown in Figure 1, and the graph and contour plot of $\Pi^d(\tau, \sigma)$ is shown in Figure 2.

There are three critical points of the dual function $\Pi^d(\tau, \sigma)$:

$$\left(\hat{\tau}_1, \hat{\sigma}_1\right) = \left(0.599866, 0.098119\right), \quad \left(\hat{\tau}_2, \hat{\sigma}_2\right) = \left(0.475231, -9.983154\right), \quad \text{and} \quad \left(\hat{\tau}_3, \hat{\sigma}_3\right) = \left(0.590128, -0.71007\right).$$

They are corresponding to the solutions of the primal problem:

$$\bar{x}_1 = 1.004894, \quad \bar{x}_2 = -0.041044, \quad \text{and} \quad \bar{x}_3 = -0.963843.$$

It is noticed that $(\hat{\tau}_1, \hat{\sigma}_1)$ is in the region $S_a^+$ and $\bar{x}_1$ is the global solution of the primal problem, which is the min-max duality. The double-max duality can be seen from the fact that $(\hat{\tau}_2, \hat{\sigma}_2)$
and $\bar{x}_2$ are local maximisers of functions $\Pi(x)$ and $\Pi^d(\tau, \sigma)$. Since $n = 1$, $m = 2$ and $\bar{x}_3$ is a local minimiser of the function $\Pi(x)$, the fact that $(\bar{\tau}_3, \bar{\sigma}_3) \in S^-_a$ is a saddle point of the function $\Pi^d(\tau, \sigma)$ illustrates the double-min duality. Moreover, we have

$$
\Pi(\bar{x}_1) = \Pi^d(\bar{\tau}_1, \bar{\sigma}_1) = 0.112521, \\
\Pi(\bar{x}_2) = \Pi^d(\bar{\tau}_2, \bar{\sigma}_2) = 5.660800, \\
\Pi(\bar{x}_3) = \Pi^d(\bar{\tau}_3, \bar{\sigma}_3) = 1.688196.
$$

Example 2

Consider a randomly generated fourth-order polynomial problem:

$$
\min_{x \in \mathbb{R}^n} \Pi(x) = \frac{1}{2} x^T A x - f^T x + \frac{\alpha}{2} \left( \frac{1}{2} x^T x + c \right)^2
$$

with

$$
A = \begin{pmatrix}
-16 & -5 \\
-5 & -14
\end{pmatrix}, 
\begin{pmatrix}
f_1 \\
f_2
\end{pmatrix} = \begin{pmatrix}
14 \\
-6
\end{pmatrix}, 
\begin{pmatrix}
c_1 \\
c_2
\end{pmatrix} = \begin{pmatrix}
1 \\
-14
\end{pmatrix}, \text{ and } \alpha = 10;
$$

The contour plot of $\Pi(x)$ and the graph of the dual function are shown in Figure 3. There are five critical points of the dual function:

$$
\bar{\sigma}_1 = 19.093, \bar{\sigma}_2 = 14.495, \bar{\sigma}_3 = -13.184, \bar{\sigma}_4 = -16.459, \text{ and } \bar{\sigma}_5 = -139.945.
$$

The eigenvalues of the corresponding matrix $G_a$ are

$$
\lambda_1 = \begin{pmatrix}
2.282 \\
33.904
\end{pmatrix}, \lambda_2 = \begin{pmatrix}
-2.32 \\
29.31
\end{pmatrix}, \lambda_3 = \begin{pmatrix}
-29.99 \\
1.63
\end{pmatrix}, \lambda_4 = \begin{pmatrix}
-33.27 \\
-1.65
\end{pmatrix}, \text{ and } \lambda_5 = \begin{pmatrix}
-156.76 \\
-125.13
\end{pmatrix},
$$

and the corresponding critical points of the primal problem are:

$$
x_1 = \begin{pmatrix}
5.6 \\
0.07
\end{pmatrix}, x_2 = \begin{pmatrix}
-5.44 \\
-1.16
\end{pmatrix}, x_3 = \begin{pmatrix}
0.38 \\
-5.02
\end{pmatrix}, x_4 = \begin{pmatrix}
-1.18 \\
4.83
\end{pmatrix}, \text{ and } x_5 = \begin{pmatrix}
-0.09 \\
0.05
\end{pmatrix}.
$$

We notice that $\bar{\sigma}_1$ is in $S^+_a$ and $x_1$ is the global solution of the primal problem, which illustrates the min-max duality. Both $\bar{\sigma}_4$ and $\bar{\sigma}_5$ are in $S^-_a$, the double-min duality is demonstrated by the fact that $\bar{\sigma}_4$ is a local minimiser and $x_4$ is a saddle point, and the double-max duality is demonstrated by the fact that $\bar{\sigma}_5$ is a local maximiser and $x_5$ is a local maximiser. Moreover, the values of the primal function and dual function are equal on each pair of solutions.
Example 3 ([21])

We consider a nonconvex and nonsmooth optimisation problem:

$$\min_{x \in \mathbb{R}^2} \max \left\{ x_1^2 + x_2^2 - x_2, -x_1^2 - x_2^2 + 3x_2 \right\}. $$

It’s easy to verify that the optimal solution is $(0, 0)$ with value $0$. Here, we use the log-sum-exp function to approximate the function $\max \{ \cdot, \cdot \}$, and then get the following smooth optimisation problem:

$$\min_{x \in \mathbb{R}^2} \Pi(x) = \frac{1}{\beta} \log \left[ 1 + \exp \left( \beta \left( 2x_1^2 + 2x_2^2 - 4x_2 \right) \right) \right] - x_1^2 - x_2^2 + 3x_2.$$

Its canonical dual function is

$$\Pi^d(\tau) = -\frac{1}{2} \left( \frac{4\tau - 3)^2}{4\tau - 2} \right) - \frac{1}{\beta} \left[ \tau \log \tau + (1 - \tau) \log(1 - \tau) \right].$$

The graphs of the approximation function $\Pi(x)$ and the dual function $\Pi^d(\tau)$ are shown in Figure 4.

With $\beta = 100$, the two critical points of the dual function $\Pi^d(\tau)$ are

$$\tau_1 = 0.749318, \text{ and } \tau_2 = 0.249308.$$  

The corresponding solutions of the primal problem are

$$\bar{x}_1 = \begin{pmatrix} 0 \\ -0.002734 \end{pmatrix}, \text{ and } \bar{x}_2 = \begin{pmatrix} 0 \\ 1.99724 \end{pmatrix}.$$  

The min-max duality is true by the fact that $\tau_1 \in S^+_a$ and $x_1$ is the global solution of the primal problem. The double-min duality is also true because of the fact that $m = 1, n = 2, \tau_2 \in S^-_a$ is a local minimiser and $x_2$ is a saddle point of the primal function. Moreover, we have

$$\Pi(x_1) = \Pi^d(\tau_1) = 0.005627, \text{ and } \Pi(x_2) = \Pi^d(\tau_2) = 2.00562.$$  

6 Conclutions

A very general nonconvex global optimisation problem with a sum of double-well and log-sum-exp functions is discussed. The canonical duality theory is applied to solve this challenging problem. For the general problem, the triality theory concludes that if there is a critical point in the positive semidefinite region $S^+_a$, the dual problem can be solved easily and, correspondingly, the global solution of the primal problem can be found analytically from this critical point. For the
two specific problems, a fourth-order polynomial minimisation problem and a minimax problem, existence conditions for the critical point are presented. If these conditions hold, there must be a critical point in the positive semidefinite region and the global solution of the primal problem can be easily obtained by solving the dual problem. The numerical examples demonstrate the efficiency of the canonical duality approach.

Besides the duality about the global solution, which is called the min-max duality, the triality theory also discusses the relationships of local extremums, which are called double-min duality and double-max duality. But the saddle points which are not in the $S^+_0$ and $S^-_0$ have not been clarified. There are some interesting phenomena, which hint that these saddle points may can be sorted according to certain orders. Thus, our next work about this problem is to investigate the order of the extremums in the dual space. Another work would be constructing existence conditions of a critical point for the general problem.

References


The following lemma is a generalization of Lemma 6 in [17].

**Lemma 7** Suppose that $P \in \mathbb{R}^{n \times n}$, $U \in \mathbb{R}^{m \times m}$ and $D \in \mathbb{R}^{n \times m}$ are given symmetric matrices with

$$P = \begin{bmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{bmatrix} \prec 0, \quad U = \begin{bmatrix} U_{11} & 0 \\ 0 & U_{22} \end{bmatrix} \succ 0, \quad \text{and} \quad D = \begin{bmatrix} D_{11} & 0 \\ 0 & 0 \end{bmatrix},$$

where $P_{11}$, $U_{11}$ and $D_{11}$ are $r \times r$-dimensional matrices, and $D_{11}$ is nonsingular. Then,

$$P + DUU^T \preceq 0 \iff -D^TP^{-1}D - U^{-1} \preceq 0. \quad (54)$$

**Proof:** Obviously, $P + DUU^T \preceq 0$ is equivalent to

$$-P - DUU^T = \begin{bmatrix} -P_{11} - D_{11}U_{11}D_{11}^T & -P_{12} \\ -P_{21} & -P_{22} \end{bmatrix} \succeq 0. \quad (55)$$

Since $P \prec 0$, we have $P_{22} \prec 0$. By Schur lemma, equation (55) is equivalent to

$$-P_{11} - D_{11}U_{11}D_{11}^T + P_{12}P_{22}^{-1}P_{21} \succeq 0. \quad (56)$$
The inverse of matrix $P$ is

$$P^{-1} = \begin{bmatrix}
(P_{11} - P_{12}P_{22}^{-1}P_{21})^{-1} & -P_{11}^{-1}P_{12}(P_{22} - P_{21}P_{11}^{-1}P_{12})^{-1} \\
-(P_{22} - P_{21}P_{11}^{-1}P_{12})^{-1}P_{21}P_{11}^{-1} & (P_{22} - P_{21}P_{11}^{-1}P_{12})^{-1}
\end{bmatrix}.$$  

Then, it is easy to prove that $-P_{11} + P_{12}P_{22}^{-1}P_{21} \succ 0$. Since $D_{11}$ is nonsingular and $U_{11} \succ 0$, we have $D_{11}U_{11}D_{11}^T \succ 0$. Thus, by lemma ??, the equation (56) is equivalent to

$$(-P_{11} + P_{12}P_{22}^{-1}P_{21})^{-1} \preceq (D_{11}U_{11}D_{11}^T)^{-1},$$  \hspace{1cm} (57)

which is further equivalent to

$$D_{11}^T(-P_{11} + P_{12}P_{22}^{-1}P_{21})^{-1}D_{11} \preceq U_{11}^{-1}. \hspace{1cm} (58)$$

Since $D_{11}^T(-P_{11} + P_{12}P_{22}^{-1}P_{21})^{-1}D_{11} = -D^TP^{-1}D$ and $U_{22} \succ 0$, the equation (58) is equivalent to

$$-D^TP^{-1}D - U^{-1} \preceq 0. \hspace{1cm} (59)$$

The lemma is proved.