Triality Theory for General Unconstrained Global Optimization Problems

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Abstract Triality theory is proved for a general unconstrained global optimization problem. The method adopted is simple but mathematically rigorous. Results show that if the primal problem and its canonical dual have the same dimension, the triality theory holds strongly in the tri-duality form as it was originally proposed. Otherwise, both the canonical min-max duality and the double-max duality still hold strongly, but the double-min duality holds weakly in a super-symmetrical form as it was expected. Additionally, a complementary weak saddle min-max duality theorem is discovered. Therefore, an open problem on this statement left in 2003 is solved completely. This theory can be used to identify not only the global minimum, but also the largest local minimum, maximum, and saddle points. Application is illustrated. Some fundamental concepts in optimization and remaining challenging problems in canonical duality theory are discussed.

Key Words: Canonical duality, triality theory, Lagrangian, objectivity, canonical systems, global optimization.

1 Introduction

The general global optimization problem to be solved is proposed in the following form
\[
(P) : \text{ext} \left\{ I(x) = W(x) + \frac{1}{2} \langle x, Ax \rangle - \langle x, f \rangle \mid x \in \mathbb{R}^n \right\},
\]
where \( W(x) \) is a nonconvex function, \( A \in \mathbb{R}^{n \times n} \) is a given symmetric matrix, \( f \in \mathbb{R}^n \) is a given vector (source), \( \langle \ast, \ast \rangle \) is an inner product in \( \mathbb{R}^n \), and the

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notation \( \text{ext}\{\ast\} \) stands for finding global extrema of the function given in \( \{\ast\} \), including both global minimum and the largest local minimum and maximum. In order to have this general problem making sense in reality, the nonconvex function \( W(x) \) should obey certain fundamental rules in systems theory.

Objectivity is a basic concept in science, which is often attributed with the property of scientific measurements that can be measured independently of the observer. General description of the objectivity can be easily found on internet and in many mathematical physics textbooks (see [27,32]). Mathematical definitions of the objective set and objective function are given in the book [9] (Chapter 6, page 288). Let

\[
Q = \{ Q \in \mathbb{R}^{m \times m} | Q^T = Q^{-1}, \det Q = 1 \}
\]

be a proper orthogonal rotation group.

**Definition 1 (Objectivity and Isotropy)** A subset \( Y_a \subset \mathbb{R}^m \) is said to be **objective** if \( Qy \in Y_a \ \forall y \in Y_a \) and \( \forall Q \in Q \).

A real-valued function \( T : Y_a \rightarrow \mathbb{R} \) is said to be **objective** if its domain is objective and

\[
T(Qy) = T(y) \ \forall y \in Y_a \ \text{and} \ \forall Q \in Q. \tag{2}
\]

A subset \( Y_a \subset \mathbb{R}^m \) is said to be **isotropic** if \( yQ^T \in Y_a \ \forall y \in Y_a \) and \( \forall Q \in Q \).

A real-valued function \( T : Y_a \rightarrow \mathbb{R} \) is said to be **isotropic** if its domain is isotropic and

\[
T(yQ^T) = T(y) \ \forall y \in Y_a \ \text{and} \ \forall Q \in Q. \tag{3}
\]

Geometrically speaking, the objectivity means that the function \( T(y) \) does not depend on rotation, but on certain measure (norm) of its variable \( y \). Therefore, the most simple objective function is the \( l_2 \)-norm \( T(y) = \|y\| \) since \( \|Qy\|^2 = y^TQ^TQy = y^Ty = \|y\|^2 \ \forall Q \in Q \). While the isotropy implies that the function \( T(y) \) possesses a certain symmetry. By the fact that \( (xQ^T)(xQ^T)^T = xx^T \succeq 0 \ \forall Q \in Q \), the concept of isotropy plays important role in Semi-Definite Programming (SDP) and integer programming [13,18].

The objectivity in science is also refereed as **frame invariance**, which lays a foundation for mathematical physics and systems theory. In fact, the canonical duality theory was originally developed from this concept [9], which is the reason why this theory can be applied not only for modeling and analysis of complex systems, but also for solving a large class of nonconvex/nonsmooth/discrete problems in both mathematical physics and global optimization. In this paper, we shall need only the following weak assumptions for the nonconvex function \( W(x) \).

(A1). The nonconvex function \( W(x) \) is twice continuously differentiable.

(A2). There exits a geometrical operator

\[
\Lambda(x) = \left\{ \frac{1}{2}x^TB_kx + b_k^Tx \right\} : \mathbb{R}^n \rightarrow \mathbb{R}^m \tag{4}
\]

and a strictly convex function \( V : \mathbb{R}^m \rightarrow \mathbb{R} \) such that

\[
W(x) = V(\Lambda(x)), \tag{5}
\]

where \( B_k \in \mathbb{R}^{n \times n} \) and \( b_k \in \mathbb{R}^n, k = 1, \cdots, m \).
(A3). The critical points of problem (P) are non-singular, i.e., if $\nabla H(\bar{x}) = 0$, then $\det(\nabla^2 H(\bar{x})) \neq 0$.

Based on Assumption (A2), the general problem (1) can be reformulated in the following canonical form:

\[
(P): \text{ext} \left\{ \Pi(x) = V(\Lambda(x)) + \frac{1}{2} \langle x, Ax \rangle - \langle x, f \rangle \mid x \in \mathbb{R}^n \right\}.
\] (6)

This problem arises extensively in many fields of engineering and sciences, including Euclidean distance geometry [4,19], computational biology [5,28,44], numerical methods for solving a large class of nonconvex variational problems in mathematical physics [12,26,34], and much more.

Actually, the assumption (A2) is the so-called canonical transformation introduced in [9]. The idea of this transformation was from Gao and Strang’s original work [21] on nonconvex variational problems in large deformation theory, where the geometrical operator $\Lambda(u) = \frac{1}{2}(\nabla u)^T(\nabla u)$ is a Cauchy-Riemann metric tensor field, which is an objective measure of the deformation gradient $\epsilon = \nabla u$, and $W(\nabla u) = V(\Lambda(u))$ is a stored strain energy. By using finite element discretization for the deformation field $u(x)$, the nonconvex variational problems in infinite dimensional space can be reduced to the canonical global optimization problem (P) (see [26,34]). It is known in continuum physics that the stored energy $W$ is usually a nonconvex function of the linear measure $\nabla u$ (which is not a strain measure), but $V(e)$ is convex in terms of the objective measure $e = \Lambda(u)$. Therefore, by this quadratic objective operator $\Lambda(u)$, a complementary gap function was discovered by Gao and Strang in nonconvex variational analysis, and by which, complementary variational principles were recovered in fully nonlinear equilibrium problems of mathematical physics [4]. They also proved that the nonnegative gap function can be used to identify global minimizer of the nonconvex problem. Seven years later, it was discovered that the negative gap function can be used to identify the largest local minimum and maximum. Therefore, the triality theory was first proposed in nonconvex mechanics [6,7], and then generalized to global optimization [10]. This triality theory is composed of a canonical min-max duality and two pairs of double-min, double-max dualities, which reveals an intrinsic duality pattern in complex systems and has been used successfully for solving a wide class of challenging problems in nonconvex analysis and global optimization [2]. However, it was realized in 2003 [11,12] that the double-min duality holds conditionally under “certain additional conditions”. Recently, this problem is partly solved for a class of fourth order polynomial optimization problems [23,36].

The aim of this paper is to prove the triality theory for the general nonconvex global optimization problem (P). In the following sections, we first provide a brief review on the canonical duality theory and the associated triality theory. We will show that by the canonical transformation, the nonconvex primal problem (P) can be reformulated as a canonical dual problem without duality gap. Section 3 presents a strong triality theory for the case that the primal problem and its

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1 In continuum physics, complementary variational principle means perfect duality since any duality gap will violate certain physical laws. The existence of a complementary variational principle was a well-known debate existing for several decades in large deformation theory (see [30]). This problem was partially solved by Gao and Strang’s work, and solved completely in 1999 [5].
canonical dual have the same dimension, i.e. \( n = m \). We then show in Section 4 that this theory holds weakly for the case \( n \neq m \). The “certain additional conditions” for the double-min duality are provided. Application is illustrated in Section 5. The original definition of Lagrangian, Lagrangian duality and its difference with the canonical duality are discussed in Section 6. The paper is ended with some conclusion remarks and challenging problems.

2 Canonical Duality, Triality, and Open Problem

Let

\[
V_a = \{ \xi \in \mathbb{R}^m | \xi = \Lambda(x) \ \forall x \in \mathbb{R}^n \},
\]

\[
V^*_a = \{ \varsigma \in \mathbb{R}^m | \varsigma = \nabla V(\xi) \ \forall \xi \in V_a \}.
\]

By (A1) and (A2) we know that \( V: V_a \to \mathbb{R} \) is also a twice continuously differentiable. Therefore, its Legendre conjugate \( V^*: V^*_a \to \mathbb{R} \) can be uniquely defined as

\[
V^*(\varsigma) = \text{sta} \{ (\xi, \varsigma) - V(\xi) | \xi \in V_a \},
\]

where \((*,*)\) is an inner product in \( \mathbb{R}^m \) and \( \text{sta} \{ \} \) stands for finding stationary value of the expression given in \( \{ \} \). It is easy to verify that the canonical duality relations

\[
\varsigma = \nabla V(\xi) \iff \xi = \nabla V^*(\varsigma) \iff V(\xi) + V^*(\varsigma) = \langle \xi, \varsigma \rangle
\]

hold on \( V_a \times V^*_a \).

Substituting \( V(\Lambda(x)) = (\Lambda(x); \varsigma) - V^*(\varsigma) \), the primal function \( II(x) \) can be reformulated as the total-complementary function \([9]\)

\[
\Xi(x, \varsigma) = \frac{1}{2} \langle x, G(\varsigma)x \rangle - V^*(\varsigma) - \langle x, F(\varsigma) \rangle,
\]

where

\[
G(\varsigma) = A + \sum_{k=1}^{m} \varsigma_k B^k, \quad F(\varsigma) = f - \sum_{k=1}^{m} \varsigma_k b_k.
\]

For a fixed \( \varsigma \), the criticality condition \( \nabla_x \Xi(x, \varsigma) = 0 \) leads to the following canonical equilibrium equation

\[
G(\varsigma)x = F(\varsigma),
\]

which can be solved analytically to obtain \( x = [G(\varsigma)]^{-1} F(\varsigma) \) for all \( \varsigma \) in the canonical dual feasible space \( S_a \) defined by

\[
S_a = \{ \varsigma \in V^*_a | F(\varsigma) \in \text{Col}(G(\varsigma)) \},
\]

where \( \text{Col}(G(\varsigma)) \) is a space spanned by the columns of \( G(\varsigma) \). Therefore, substituting this solution into the total complementary function \( \Xi \), the canonical dual problem can be formulated as

\[
(P^d): \quad \text{ext} \left\{ II^d(\varsigma) = -\frac{1}{2} \langle [G(\varsigma)]^{-1} F(\varsigma), F(\varsigma) \rangle - V^*(\varsigma) | \varsigma \in S_a \right\}.
\]

The following theorem was originally presented in general nonconvex systems \([9]\).
Theorem 1 (Analytical Solution and Complementary-dual principle)

Problem \((\mathcal{P}^d)\) is canonically dual to \((\mathcal{P})\) in the sense that if \(\bar{\varsigma}\) is a critical point of \((\mathcal{P}^d)\), then

\[ x = \begin{bmatrix} G(\varsigma) \end{bmatrix}^{-1} F(\varsigma) \tag{12} \]

is a critical point of \((\mathcal{P})\), the pair \((\bar{x}, \bar{\varsigma})\) is a critical point of \(\Xi(x, \varsigma)\), and

\[ \Pi(\bar{x}) = \Xi(\bar{x}, \bar{\varsigma}) = \Pi^d(\bar{\varsigma}). \tag{13} \]

This theorem shows that there is no duality gap between the primal problem \((\mathcal{P})\) and its canonical dual \((\mathcal{P}^d)\). Actually, in \(\Xi(x, \varsigma)\) the first term

\[ G_{ap}(x, \varsigma) = \frac{1}{2} \langle x, G(\varsigma)x \rangle \tag{14} \]

is the complementary gap function, first introduced by Gao and Strang in 1989 [21]. They proved that if this gap function is positive, the critical point \(\bar{\varsigma}\) is a global maximizer of \(\Pi^d\) and the associated \(\bar{x}(\bar{\varsigma})\) is a global minimizer of the primal problem \((\mathcal{P})\). By introducing the following notations

\[ S_a^+ = \{ \varsigma \in S_a \mid G(\varsigma) \succeq 0 \} \tag{15} \]
\[ S_a^- = \{ \varsigma \in S_a \mid G(\varsigma) \prec 0 \} \tag{16} \]

where \(G(\varsigma) \succeq 0\) means that \(G(\varsigma)\) is positive semi-definite and \(G(\varsigma) \prec 0\) means that \(G(\varsigma)\) is negative definite, the Gao and Strang canonical min-max duality theory can be stated as

\[ \Pi(\bar{x}) = \min_{x \in \mathbb{R}^n} \Pi(x) = \max_{\varsigma \in S_a^+} \Pi^d(\varsigma) = \Pi^d(\bar{\varsigma}) \tag{17} \]

This general result has been used extensively in nonconvex analysis and mechanics [9,43]. In 1996, it was discovered by Gao that if the gap function is negative in a neighborhood \(X_o \times S_o \subset \mathbb{R}^n \times S_a^-\) of \((\bar{x}, \bar{\varsigma})\), then either the double-max duality relation

\[ \Pi(\bar{x}) = \max_{x \in X_o} \Pi(x) = \max_{\varsigma \in S_a} \Pi^d(\varsigma) = \Pi^d(\bar{\varsigma}) \tag{18} \]

holds or the double-min duality relation

\[ \Pi(\bar{x}) = \min_{x \in X_o} \Pi(x) = \min_{\varsigma \in S_a} \Pi^d(\varsigma) = \Pi^d(\bar{\varsigma}) \tag{19} \]

Therefore, the triality theorem was formed by these three pairs of dualities and has been used extensively in nonconvex mechanics [9,16] and global optimization [2][3][5][33]. However, it was realized in 2003 [11][12] that if the dimensions of the primal problem and its canonical dual are different, the double-min duality \((19)\) needs “certain additional conditions”. For the sake of mathematical rigor, the double-min duality was not included in the triality theory and these additional constraints were left as an open problem (see Remark 1 in [11], also Theorem 3 and its Remark in a review article by Gao [12]). By the facts that the double-max duality \((18)\) is always true and the double-min duality plays a key role in real-life applications, it was still included in the triality theory in the either-or form in many applications for the purposes of perfection in esthesia and some other reasons in reality. In the following sections, we will show that the triality theorem holds strongly for the problems it was originally proposed. Also we will explain the reasons why the “certain additional conditions” in the double-min duality were ignored.
3 Strong Triality Theory

In the case $n = m$, the triality theorem holds strongly in the following form.

**Theorem 2 (Tri-duality Theorem)** Suppose that $\xi$ is a critical point of the canonical problem ($P^{d}$) and $\bar{x} = [G(\xi)]^{-1}F(\xi)$.

If $\bar{\xi} \in S_{\alpha}^{m}$, then $\bar{\xi}$ is a global maximizer of Problem ($P^{d}$) in $S_{\alpha}^{m}$ if and only if $\bar{x}$ is a global minimizer of Problem ($P$), i.e., the following canonical min-max duality statement holds:

$$\Pi(\bar{x}) = \min_{x \in \mathbb{R}^{n}} \Pi(x) \iff \max_{\xi \in S_{\alpha}} \Pi^{d}(\xi) = \Pi^{d}(\bar{\xi}).$$

(20)

If $\bar{\xi} \in S_{\alpha}$, then there exists a neighborhood $\mathcal{X}_{0} \times S_{0} \subset \mathbb{R}^{n} \times S_{\alpha}$ of $(\bar{x}, \bar{\xi})$ such that we have either the double-min duality statement

$$\Pi(\bar{x}) = \min_{x \in \mathcal{X}_{0}} \Pi(x) \iff \min_{\xi \in S_{0}} \Pi^{d}(\bar{\xi}) = \Pi^{d}(\xi),$$

(21)
or the double-max duality statement

$$\Pi(\bar{x}) = \max_{x \in \mathcal{X}_{0}} \Pi(x) \iff \max_{\xi \in S_{0}} \Pi^{d}(\xi) = \Pi^{d}(\bar{\xi}).$$

(22)

**Proof.** If $(\bar{x}, \bar{\xi})$ is a critical point of the total complementary function $\Xi(x, \xi)$, then by Theorem 1, we have $\bar{x} = [G(\xi)]^{-1}F(\xi)$, and

$$\nabla^{2} \Pi^{d}(\xi) = -(\nabla A(\bar{x}))^{T}[G(\xi)]^{-1}\nabla A(\bar{x}) - \nabla^{2}V^{*}(\bar{\xi}),$$

(23)

$$\nabla^{2} \Pi(\bar{x}) = G(\bar{\xi}) + \nabla A(\bar{x})\nabla^{2}V(\nabla A(\bar{x}))(\nabla A(\bar{x}))^{T}.$$ 

(24)

By the assumption (A2) we know that $V(\xi)$ is strictly convex, then,

$$\nabla^{2}(V(\nabla A(\bar{x}))) = (\nabla^{2}V^{*}(\bar{\xi}))^{-1} > 0,$$

(25)

where $\bar{\xi} = A(\bar{x})$. Substituting (23) into (24), we obtain

$$\nabla^{2} \Pi(\bar{x}) = G(\bar{\xi}) + \nabla A(\bar{x})(\nabla^{2}V^{*}(\bar{\xi}))^{-1}(\nabla A(\bar{x}))^{T}.$$ 

(26)

Proof of the canonical min-max duality statement (20) (this proof is a finite-dimensional version of Gao and Strang's original proof of Theorem 2 in non-convex analysis [21]).

Suppose that $\bar{\xi} \in S_{\alpha}^{m}$ is a critical point. Since $\Pi^{d}(\bar{\xi})$ is concave on $S_{\alpha}^{m}$, the critical point $\bar{\xi} \in S_{\alpha}^{m}$ must be a global maximizer of $\Pi^{d}(\bar{\xi})$ on $S_{\alpha}^{m}$.

On the other hand, if $\bar{\xi} \in S_{\alpha}^{m}$, the gap function $G_{ap}(x, \xi) = \frac{1}{2}\langle x, G(\xi)x \rangle$ is convex in $x \in \mathbb{R}^{n}$. By the convexity of $V : \mathcal{V}_{0} \rightarrow \mathbb{R}$, we have [21]

$$\Pi(x) - \Pi(\bar{x}) \geq \langle \nabla V(A(\bar{x})) ; (A(x) - A(\bar{x})) \rangle + \frac{1}{2}\langle x, Ax \rangle - \frac{1}{2}\langle \bar{x}, A\bar{x} \rangle - \langle x - \bar{x}, f \rangle$$

$$= G_{ap}(x, \xi) - G_{ap}(\bar{x}, \bar{\xi}) - \langle x - \bar{x}, F(\bar{\xi}) \rangle$$

$$\geq \langle x - \bar{x}, G(\xi)\bar{x} - F(\xi) \rangle = 0 \ \forall x \in \mathbb{R}^{n}.$$

Thus, $\bar{x} = [G(\xi)]^{-1}F(\xi)$ is a global minimizer of problem ($P$). Furthermore, $\bar{\xi}$ is also a global maximizer of Problem ($P^{d}$) in $S_{\alpha}^{m}$ and the statement (20) holds by Theorem 1.
Proof of the double-min duality statement (21).

Suppose that $\bar{\varsigma} \in S^{-a}$ and $\bar{\varsigma}$ is a local minimizer of problem $(P^d)$. Then, we have $\nabla^2 II^d(\bar{\varsigma}) \succeq 0$ and

$$-(\nabla A(\bar{x}))^T [G(\bar{\varsigma})]^{-1} \nabla A(\bar{x}) \succeq \nabla^2 V^*(\bar{\varsigma}) \succ 0.$$ 

Thus, $\nabla A(\bar{x})$ is invertible, which leads to

$$-G(\bar{\varsigma}) \leq \nabla A(\bar{x})(\nabla^2 V^*(\bar{\varsigma}))^{-1}(\nabla A(\bar{x}))^T.$$ 

(27)

Therefore, we have

$$\nabla^2 \Pi(\bar{x}) = G(\bar{\varsigma}) + \nabla A(\bar{x})(\nabla^2 V^*(\bar{\varsigma}))^{-1}(\nabla A(\bar{x}))^T \succ 0.$$ 

(28)

By the assumption (A3), $\bar{x} = [G(\bar{\varsigma})]^{-1} F(\bar{\varsigma})$ is also a local minimizer of problem $(P)$. The reversed statement can be proved in the similar way. Thus, (21) holds.

Proof of the double-max duality statement (22).

Suppose that $\bar{\varsigma} \in S^{-a}$ and $\bar{\varsigma}$ is a local maximizer of problem $(P^d)$. Then, $\nabla^2 II^d(\bar{\varsigma}) \preceq 0$. By Theorem 1, $\bar{x} = [G(\bar{\varsigma})]^{-1} F(\bar{\varsigma})$ is a critical point of problem $(P)$. Due to the assumption (A3), $\nabla^2 II(\bar{x})$ is invertible. By the well-known Sherman-Morrison-Woodbury identity [3], $\nabla^2 II^d(\bar{\varsigma})$ is also invertible. Furthermore,

$$(\nabla^2 II(\bar{x}))^{-1} = G(\bar{\varsigma})^{-1} + G(\bar{\varsigma})^{-1} \nabla A(\bar{x})(\nabla^2 II^d(\bar{\varsigma}))^{-1}(\nabla A(\bar{x}))^T G(\bar{\varsigma})^{-1} \prec 0.$$ 

Thus, $\bar{x} = [G(\bar{\varsigma})]^{-1} F(\bar{\varsigma})$ is also a local maximizer of problem $(P)$. Similarly, we can prove the reversed statement. Therefore, the triality theorem holds strongly for the case $n = m$. □

Remark 1 The tri-duality theorem provides global extremum criteria for three types solutions of the nonconvex problem $(P)$: a global minimizer $\bar{x}(\bar{\varsigma})$ if $\bar{\varsigma} \in S^+_a$ and a pair of the largest-valued local extrema, i.e., $\bar{x}(\bar{\varsigma})$ is a global maximizer (resp. minimizer) if $\bar{\varsigma} \in S^-a$ is a local maximizer (resp. minimizer). This pair of largest local extrema plays a critical role in nonconvex mechanics and phase transitions.

Remark 2 The tri-duality theorem can also be used to identify saddle points of the primal problem, i.e., $\bar{\varsigma} \in S^-a$ is a saddle point of $II(\bar{\varsigma})$ if and only if $\bar{x} = [G(\bar{\varsigma})]^{-1} F(\bar{\varsigma})$ is a saddle point of $II(\bar{x})$. By the facts that the saddle points are not stable and do not exist physically, these points are excluded from the triality theory.

The triality theory was first discovered in post-buckling analysis of a large deformed elastic beam model proposed by Gao in 1996 [6,7], where the primal functional is a double-well potential of a 2-dimensional displacement field, and its canonical dual is the so-called pure complementary energy defined on a 2-dimensional stress field. Therefore, the triality theory was first proposed in its strong form, i.e. the tri-duality theorem.
4 Triality Theory for General Case

We now consider the general case $m \neq n$. Suppose that $\bar{x}$ and $\bar{\xi}$ are the critical points of problem (P) and (P$_d$), respectively, where $\bar{x} = [G(\bar{\xi})]^{-1}F(\bar{\xi})$ and $G(\bar{\xi})$ is invertible. In this case, we also can show that

$$
\nabla^2 \Pi(\bar{x}) = G(\bar{\xi}) + \nabla A(\bar{x})(\nabla^2 V^*(\bar{\xi}))^{-1}(\nabla A(\bar{x}))^T,
$$

and

$$
\nabla^2 \Pi^d(\bar{\xi}) = - (\nabla A(\bar{\xi}))^T [G(\bar{\xi})]^{-1} \nabla A(\bar{x}) - \nabla^2 V^*(\bar{\xi}).
$$

Suppose that $m < n$. By the Sherman-Morison-Woodbury Theorem in [3] and the assumption (A3), we have

$$
[\nabla^2 \Pi(\bar{x})]^{-1} = [G(\bar{\xi})]^{-1} + [G(\bar{\xi})]^{-1} \nabla A(\bar{x})(\nabla^2 \Pi^d(\bar{\xi}))^{-1}(\nabla A(\bar{x}))^T[G(\bar{\xi})]^{-1}.
$$

This shows that $\nabla^2 \Pi^d(\bar{\xi})$ is invertible. Similarly, we can show that $\nabla^2 \Pi^d(\bar{\xi})$ is also invertible if $m > n$.

**Lemma 1** Suppose that $m < n$, the critical point $\bar{\xi} \in S_n$ is a local minimizer of problem (P$_d$). Then, $\nabla^2 \Pi(\bar{x})$ has $m$ positive eigenvalues and $n - m$ negative eigenvalues, i.e., there exists two matrices $P_1 \in \mathbb{R}^{n \times m}$ and $P_2 \in \mathbb{R}^{n \times (n - m)}$ such that

$$
P_1^T \nabla^2 \Pi(\bar{x}) P_1 > 0 \text{ and } P_2^T \nabla^2 \Pi(\bar{x}) P_2 < 0.
$$

**Proof.** Since $\nabla^2 V^*(\bar{\xi}) > 0$, there exists an invertible matrix $R \in \mathbb{R}^{m \times m}$ such that $\nabla^2 V^*(\bar{\xi}) = R^T R$. Thus, we have

$$
- (\nabla A(\bar{x}) R^{-1})^T [G(\bar{\xi})]^{-1} \nabla A(\bar{x}) R^{-1} - I_{m \times m} > 0.
$$

Note that $G(\bar{\xi}) < 0$ and $\nabla A(\bar{x}) R^{-1}(\nabla A(\bar{x}) R^{-1})^T \geq 0$. There exists a matrix $T$ such that

$$
T^T G(\bar{\xi}) T = \text{Diag}(-\lambda_1, \ldots, -\lambda_n),
$$

and

$$
T^T \nabla A(\bar{x}) R^{-1}(\nabla A(\bar{x}) R^{-1})^T T = \text{Diag}(a_1, \ldots, a_m, 0, \ldots, 0),
$$

where $\lambda_k > 0$, $k = 1, \ldots, n$, and $a_k > 0$, $k = 1, \ldots, m$. According to the decomposition theory of singular matrices, we know that there exist orthogonal matrices $U \in \mathbb{R}^{n \times n}$ and $E \in \mathbb{R}^{m \times m}$ such that

$$
T^T \nabla A(\bar{x}) R^{-1} = U \begin{pmatrix}
\sqrt{a_1} \\ & \ddots \\ & & \sqrt{a_m}
\end{pmatrix} E.
$$

In light of (33), we know that $U = I_{n \times n}$. Then, we have

$$
(R^{-1})^T \nabla^2 \Pi^d(\bar{\xi}) R^{-1} = - (T^T \nabla A(\bar{x}) R^{-1})^T [G(\bar{\xi})]^{-1} \nabla A(\bar{x}) R^{-1} - I_{m \times m}
$$

$$
= - (T^T \nabla A(\bar{x}) R^{-1})^T [T^T G(\bar{\xi}) T]^{-1} T \nabla A(\bar{x}) R^{-1} - I_{m \times m}
$$

$$
= E^T \text{Diag} \left( \frac{a_1}{\lambda_1} - 1, \ldots, \frac{a_m}{\lambda_m} - 1 \right) E > 0.
$$
Thus, \( a_k > \lambda_k, \ k = 1, \ldots, m \). It is easy to verify that
\[
T^T \nabla^2 \Pi(\bar{x}) T = \text{Diag}(a_1 - \lambda_1, \ldots, a_m - \lambda_m, -\lambda_{m+1}, \ldots, -\lambda_n). \tag{37}
\]
This shows that \( \nabla^2 \Pi(\bar{x}) \) has \( m \) positive eigenvalues and \( n - m \) negative eigenvalues. Therefore, the matrix \( P_3 \) can be obtained by collecting all the eigenvectors corresponding to the positive eigenvalues and \( P_2 \) can be obtained by collecting all the eigenvectors corresponding to the negative eigenvalues. □

In a similar way, we can prove the following lemma.

**Lemma 2** Suppose that \( m > n \) and the critical point \( \bar{x} = [G(\bar{\xi})]^{-1} F(\bar{\xi}) \) is a local minimizer of Problem \( (P) \), where \( \bar{\xi} \in S_m^+ \). Then, \( \nabla^2 \Pi^d(\bar{\xi}) \) has \( n \) positive eigenvalues and \( m - n \) negative eigenvalues, i.e., there exists two matrices \( Q_3 \in \mathbb{R}^{m \times n} \) and \( Q_2 \in \mathbb{R}^{m \times (m-n)} \) such that
\[
Q_3^T \nabla^2 \Pi^d(\bar{\xi}) Q_3 \succ 0 \quad \text{and} \quad Q_2^T \nabla^2 \Pi^d(\bar{\xi}) Q_2 \prec 0. \tag{38}
\]

Let the \( m \) column vectors of \( P_3 \) be \( p_1^d, \ldots, p_m^d \) and the \( n \) column vectors of \( Q_3 \) be \( q_1^d, \ldots, q_n^d \), respectively. Clearly, \( p_1^d, \ldots, p_m^d \) and \( q_1^d, \ldots, q_n^d \) are two sets of linearly independent vectors, respectively. By introducing two subspaces
\[
X_0 = \{ x \in \mathbb{R}^n \mid x = \bar{x} + \theta_1 p_1^d + \cdots + \theta_m p_m^d, \ \theta_i \in \mathbb{R}, \ i = 1, \ldots, m \}, \tag{39}
\]
\[
S_0 = \{ \xi \in \mathbb{R}^m \mid \xi = \bar{\xi} + \theta_1 q_1^d + \cdots + \theta_n q_n^d, \ \theta_i \in \mathbb{R}, \ i = 1, \ldots, n \}, \tag{40}
\]
the triality theory holds for general case in the following refined form.

**Theorem 3 (Triality Theorem)**

Suppose that \( \bar{\xi} \) is a critical point of problem \( (P^d) \) and \( \bar{x} = [G(\bar{\xi})]^{-1} F(\bar{\xi}) \).

If \( \bar{\xi} \in S_m^+ \), then the canonical min-max duality holds in the strong form of
\[
\Pi(\bar{x}) = \min_{x \in X_0} \Pi(x) \Leftrightarrow \max_{\xi \in S_0} \Pi^d(\bar{\xi}) = \Pi^d(\bar{\xi}). \tag{41}
\]

If \( \bar{\xi} \in S_m^+ \), then there exists a neighborhood \( X_0 \times S_0 \subset \mathbb{R}^n \times S_m^+ \) of \( (\bar{x}, \bar{\xi}) \) such that the double-max duality holds in the strong form of
\[
\Pi(\bar{x}) = \max_{x \in X_0} \Pi(x) \Leftrightarrow \max_{\xi \in S_0} \Pi^d(\bar{\xi}) = \Pi^d(\bar{\xi}). \tag{42}
\]
However, the double-min duality statement holds conditionally in the following symmetrical forms.

1. If \( m < n \) and \( \bar{\xi} \in S_m^+ \) is a local minimizer of \( \Pi^d(\bar{\xi}) \), then \( \bar{x} = [G(\bar{\xi})]^{-1} F(\bar{\xi}) \) is a saddle point of \( \Pi(x) \) and the double-min duality holds weakly on \( X_0 \cap X_0 \times S_0 \), i.e.
\[
\Pi(\bar{x}) = \min_{x \in X_0 \cap X_0} \Pi(x) = \min_{\xi \in S_0} \Pi^d(\bar{\xi}) = \Pi^d(\bar{\xi}). \tag{43}
\]

2. If \( m > n \) and \( \bar{\xi} = [G(\bar{\xi})]^{-1} F(\bar{\xi}) \) is a local minimizer of \( \Pi(x) \), then \( \bar{\xi} \) is a saddle point of \( \Pi^d(\bar{\xi}) \) and the double-min duality holds weakly on \( X_0 \times S_0 \cap S_0 \), i.e.
\[
\Pi(\bar{x}) = \min_{x \in X_0} \Pi(x) = \min_{\xi \in S_0 \cap S_0} \Pi^d(\bar{\xi}) = \Pi^d(\bar{\xi}). \tag{44}
\]
Proof. The proof of min-max duality statement (11) and the double-max duality statement (12) are the same to the proof of (20) and (22). We only need to prove (13) and (14).

Suppose that $m < n$ and $\xi \in S_\alpha^-$ is not only a local minimizer, but also a critical point of problem $\langle P^d \rangle$. By Lemma 1 we know that $\nabla^2 \Pi(\bar{x})$ has both positive and negative eigenvalues. Thus, $\bar{x} = [G(\bar{x})]^{-1} F(\bar{x})$ is a saddle point of problem $\langle P \rangle$. We let

$$\varphi(t_1, \ldots, t_m) = \Pi(\bar{x} + t_1 p_1^\flat + \cdots + t_m p_m^\flat),$$

(45)

where $p_1^\flat, \ldots, p_m^\flat$ are the column vectors of $P_\flat$ defined in Lemma 1. By direct verification, we have

$$\nabla \varphi(0, \ldots, 0) = (\nabla \Pi(\bar{x}))^T P_\flat = 0$$

(46)

and

$$\nabla^2 \varphi(0, \ldots, 0) = P_\flat^T \nabla^2 \Pi(\bar{x}) P_\flat > 0.$$ (47)

Thus, $(0, \ldots, 0)$ is a local minimizer of $\varphi(t_1, \ldots, t_m)$. Hence, the equation (13) holds. The statement (14) can be proved in the similar way. □

Remark 3 (NP-hard Problems and Perturbation) The canonical min-max duality (11) shows that the nonconvex minimization problem is equivalent to a concave maximization dual problem over a closed convex set $S_\alpha^+$. If $\Pi^d(\xi)$ has at least one critical point in $S_\alpha^+$, the global minimizer of $\Pi(x)$ can be easily obtained by the canonical duality theory. However, if $\Pi^d(\xi)$ has no critical points in $S_\alpha^+$, to find global minimizer for nonconvex function $\Pi(x)$ could be very difficult. If the vector $f = 0 \in \mathbb{R}^n$, the problem $\langle P \rangle$ is homogenous. Moreover, if $b_0 = 0 \in \mathbb{R}^n \forall k = 1, \ldots, m$, then the geometrical operator $A(x)$ is a pure quadratic measure (i.e. an objective measure in certain space). In this case, the vector $F(\xi) = 0$, the set $S_\alpha^+$ is empty, and the canonical dual function $\Pi^d(\xi) = -V^*(\xi)$ is concave, which has only a unique maximizer $\xi$. By the double-max duality we know that the corresponding primal solution $\bar{x} = 0$ is a local maximizer if $\xi \in S_\alpha^-$. From the point view of systems theory, the pure quadratic operator $A(x)$ means that the system possesses certain symmetry. If there is no input ($f = 0$), the primal function $\Pi(x)$ could have multiple global minimizers. It was indicated in (13) that a nonconvex minimization problem could be NP-hard if its canonical dual has no KKT (or critical) point in $S_\alpha^+$. In order to solve this type problems, several perturbation methods have been suggested in (15)(33)(22). It is shown very recently that by the canonical duality theory, a class of NP-hard box/integer constrained programming problems are equivalent to unconstrained canonical dual problems in continuous space, which can be solved via deterministic methods (22).

Dual to $\lambda_\xi$ and $\lambda_\Pi$, we can let

$$\lambda_\xi^+ = \{x \in \mathbb{R}^n \mid x = \bar{x} + \theta_1 p_1^\flat + \cdots + \theta_{n-m} p_{n-m}^\flat, \theta_i \in \mathbb{R}, i = 1, \ldots, n - m\},$$

$$\lambda_\Pi^+ = \{\xi \in \mathbb{R}^m \mid \xi = \bar{\xi} + \theta_1 q_1^\flat + \cdots + \theta_{m-n} q_{m-n}^\flat, \theta_i \in \mathbb{R}, i = 1, \ldots, m - n\},$$

where $\{p_i^\flat\}$ and $\{q_i^\flat\}$ are column vectors of $P_\Pi$ and $Q_\Pi$, respectively. Then, complementary to the weak double-min duality statements (13) and (14), we have the following weak saddle min-max duality theorem.
Theorem 4 (Weak Saddle Duality Theorem)

Suppose that \( \bar{\xi} \in S^{-}_{a} \) is a critical point of problem \((P_{d})\), the vector \( \bar{x} = [G(\bar{\xi})]^{-1}F(\bar{\xi}) \), and \( X_{o} \times S_{o} \subset \mathbb{R}^{n} \times S^{-}_{a} \) is a neighborhood of \((\bar{x}, \bar{\xi})\).

1. If \( m < n \) and \( \bar{\xi} \in S^{-}_{a} \) is a local minimizer of \( \Pi^{d}(\xi) \), then \( \bar{x} = [G(\bar{\xi})]^{-1}F(\bar{\xi}) \) is a saddle point of \( \Pi(x) \) and the saddle max-min duality holds weakly on \( X_{o} \cap X'_{a} \times S_{o} \), i.e.

\[
\Pi(\bar{x}) = \max_{x \in X_{o}} \Pi(x) = \min_{\xi \in S_{o}} \Pi^{d}(\xi) = \Pi^{d}(\bar{\xi}).
\]

(48)

2. If \( m > n \) and \( \bar{x} = [G(\bar{\xi})]^{-1}F(\bar{\xi}) \) is a local minimizer of \( \Pi(x) \), then \( \bar{\xi} \) is a saddle point of \( \Pi^{d}(\xi) \) and the saddle min-max duality holds weakly on \( X_{o} \times S_{o} \cap S_{\#} \), i.e.

\[
\Pi(\bar{x}) = \min_{x \in X_{o}} \Pi(x) = \max_{\xi \in S_{o} \cap S_{\#}} \Pi^{d}(\xi) = \Pi^{d}(\bar{\xi}).
\]

(49)

Remark 4

Theorem 3 shows that both the canonical min-max and double-max duality statements hold strongly for general cases; the double-min duality holds strongly for \( n = m \) but weakly for \( n \neq m \) in a symmetrical form. The “certain additional conditions” are simply the intersection \( X_{o} \cap X'_{a} \) for \( n > m \) and \( S_{o} \cap S_{\#} \) for \( n < m \). Therefore, the open problem on the double-min duality left in 2003 [11,12] is now solved! While from Theorem 4 we know that if \( G(\bar{\xi}) \prec 0 \) and \( n \geq m \), the solution \( \bar{x}(\bar{\xi}) \) could be a saddle point. Mathematically speaking, nonstable critical points do not produce any computational difficulties in numerical optimization. Also, in real-life problems the saddle point is not considered as a phase state and does not physically exist. These are the part of reasons why the saddle point in \( S^{-}_{a} \) is ignored by the triality theory.

The triality theory has been challenged recently by a large number of counter-examples in a series of more than seven papers (see [38,40] and references cited therein). It was written in [38] that “Because our counter-examples are very simple, using quadratic functions defined on whole Hilbert (even finite dimensional) spaces, it is difficult to reinforce the hypotheses of the above mentioned results in order to keep the same conclusions and not obtain trivialities.” It turns out that in addition to many conceptual mistakes (see Section 6), most of these counter-examples simply discuss the saddle points in \( S^{-}_{a} \) for the case \( n \neq m \). In fact, these counter-examples address the same type of open problem for the double-min duality left unaddressed in [11,12]. Indeed, by Theorem 3 we know that the double-min duality holds conditionally when \( n \neq m \). Based on Theorems 2 and 3, we know that the saddle points could exist in \( S^{-}_{a} \) for the case \( n \neq m \); While by Theorem 4 one can easily construct many other \( V-Z \) type counter-examples which are physically useless.

5 Application

Let us consider the following quadratic-log optimization problem:

\[
(P) : \text{ext} \left\{ \Pi(x) = \frac{1}{2} x^{T}Ax - \sum_{k=1}^{m} \log \left( \frac{1}{2} x^{T}B^{k}x + d^{k} \right) - x^{T}f \mid x \in \mathbb{R}^{n} \right\},
\]

(50)

It is interesting to note that the references [11,12] never been cited in any one of this set of papers.
where $A$ is a positive definite matrix, $B^k, k = 1, \cdots, m$ are positive semi-definite matrices and $d^k > 0, k = 1, \cdots, m$. In this case, its canonical dual problem can be expressed as:

$$(P^d) : \operatorname{ext} \left\{ \Pi^d(\varsigma) = -\frac{1}{2} f^T G(\varsigma)^{-1} f + \sum_{k=1}^{m} (d^k \varsigma_k + 1 + \log(-\varsigma_k)) \mid \varsigma \in S_\alpha \right\},$$

where $S_\alpha = \{ \varsigma = \{\varsigma_i\} \in \mathbb{R}^m \mid -\frac{1}{d^k} \leq \varsigma_k < 0, k = 1, \cdots, m \}$. Let $n = 2, m = 1$, and

$$A = \begin{pmatrix} 1 \\ 2 \end{pmatrix}, B_1 = \begin{pmatrix} 5 \\ 4 \end{pmatrix}, f = \begin{pmatrix} 0.5 \\ 0.1 \end{pmatrix} \text{ and } d^1 = 1.$$

In this case, we have $S_\alpha = \{ \varsigma \in \mathbb{R} \mid -1 \leq \varsigma < 0 \}$ and

$$\Pi^d(\varsigma) = -\frac{1}{2} \left( \frac{0.5^2}{1 + 5\varsigma} + \frac{0.1^2}{2 + 4\varsigma} + \varsigma + 1 + \log(-\varsigma) \right).$$

From Fig. 1 we can see that $\Pi^d(\varsigma)$ has one critical point $\bar{\varsigma}_1 = -0.13696432$ in $S^+_\alpha = (-0.2, 0)$ and two critical points $\bar{\varsigma}_2 = -0.54470504$ and $\bar{\varsigma}_3 = -0.95209751$ in $S^-_\alpha = (-1, -0.5)$. Thus, by the triality theorem we know that $\bar{x}_1 = (A + \bar{\varsigma}_1 B^1)^{-1} f = [1.58640312, 0.06886375]^T$ is the global minimizer to the problem $(P)$. Since $\bar{\varsigma}_1 \in S^+_\alpha$ is a local minimizer, $\bar{\varsigma}_3 \in S^-_\alpha$ is a local maximizer to the problem $(P^d)$, and $m = 1 < n = 2$, by Theorem 3 we know that $\bar{x}_2 = (A + \bar{\varsigma}_2 B^1)^{-1} f = [-0.2901031, -0.5592211]^T$ is a saddle point of $\Pi(x)$, while $\bar{x}_3 = (A + \bar{\varsigma}_3 B^1)^{-1} f = [-0.13296148, -0.0552978]^T$ is a local maximizer to the problem $(P)$. More applications can be found in [24].
6 Some Fundamental Concepts in Canonical Systems

Global optimization problem in mathematics is usually formulated in the following general form

$$\min \{ f(x) | x \in X \subset \mathbb{R}^n \},$$

where the real-valued function $f(x)$ is simply assumed to be nonconvex (or Lipschitz, differentiable, etc.) on its feasible space $X \subset \mathbb{R}^n$, in which certain constraints are given. It is known that this problem could have a large number of local extrema and to identify global optima is a main challenging task in global optimization. If there is no detailed information available for the given function $f(x)$, it is difficult (may be impossible) to have a general theory and method for solving this general problem effectively. Also, to find the largest local extrema is fundamentally important in many real-life applications.

Mathematics and physics (mechanics) have been complementary partners since Newton’s time. It is known that the calculus of variation and mathematical optimization were originally developed from Euler-Lagrange mechanics. Also, the modern mathematical theory of convex analysis was started from J.J. Moreau’s pioneering work in contact mechanics [31]. However, as V.I. Arnold pointed out [1]: “In the middle of the twentieth century it was attempted to divide physics and mathematics. The consequences turned out to be catastrophic.” For example, in mathematical physics, the objectivity is directly related to some fundamental concepts and principles, such as geometrical nonlinearity, constitutive laws, and work-conjugate principle, etc. A function(al) can be called objective or free energy only if certain intrinsic constraints (physical laws) are satisfied (see [16]). Unfortunately, the objective function in mathematical optimization has been misused with other concepts such as cost function, energy function, and energy functional, which leads to some conceptual mistakes. This section will discuss some important

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4 It should be emphasized here that to find the largest local maximum of $f(x)$ is not simply equivalent to solve the problem $\min \{-f(x) | x \in X\}$.

5 See the web page at [http://en.wikipedia.org/wiki/Mathematical_optimization](http://en.wikipedia.org/wiki/Mathematical_optimization)
issues in classical Lagrangian mechanics/duality, mathematical optimization, and general systems theory.

6.1 Canonical systems

According to E. Tonti [39], in virtually every physical system there exists at least three types of variables:

(1) the configuration variable \( x \in X \), which describes the state or output of the system, such as the Lagrangian generalized coordinates (or displacements) in analytical mechanics [29], decision variable in game theory, etc.

(2) the source variable \( x^* = f \in X^* \), which represents the input of the system, such as the external force in mechanics and charge density in theory of electrical field, etc.

(3) a pair of internal (or intermediate) variables \((\varepsilon, \varepsilon^*) \in E \times E^*\), which describes certain interior (constitutive) properties of the system, such as strain and stress in elasticity, velocity and momentum in dynamics, etc.

By the facts that the constitutive laws should be objective (coordinates-free) and physical variables appear always in one-to-one pairs (i.e. the Hill work-conjugacy principle in continuum mechanics [9]), it is reasonable to assume that for a given natural system, there exists a certain objective measure \( \varepsilon = \bar{\Lambda}(x) : X_a \subset X \rightarrow E_a \subset E \) and a stored energy \( \bar{W} : E_a \rightarrow \mathbb{R} \) such that the constitutive duality relation \( \varepsilon^* = \nabla \bar{W}(\varepsilon) : E_a \rightarrow E^*_a \subset E^* \) is canonical (i.e., one-to-one on \( E_a \times E^*_a \)). Such a system is the so-called canonical system and is denoted as \( S_a = \{\langle X_a, X^*_a \rangle, \langle E_a ; E^*_a \rangle, \bar{\Lambda}, C\} \) (see Chapter 4, [9]), where \( C = \nabla \bar{W} : E_a \rightarrow E^*_a \) represents the constitutive mapping, \( \langle *, * \rangle \) and \( \langle *, * \rangle \) denote the bilinear forms on \( X \times X^* \) and \( E \times E^* \), respectively. The system is called geometrically nonlinear (resp. linear) if the geometrical operator \( \bar{\Lambda} \) is nonlinear (resp. linear); the system is called physically (or constitutively) nonlinear (resp. linear) if the constitutive operator \( C \) is nonlinear (resp. linear); the systems is called fully nonlinear (resp. linear) if it is both geometrically and physically nonlinear (resp. linear).

The most simple geometrically linear system is controlled by the quadratic function \( II(x) = \frac{1}{2}(x, Ax) - \langle x, f \rangle \), where \( A \in \mathbb{R}^{n \times n} \) is a symmetrical matrix. If \( A \) is positive (semi) definite, by Cholesky decomposition we know that there exists a matrix \( D : \mathbb{R}^n \rightarrow \mathbb{R}^m \) such that \( A = D^T D \). Therefore, we have \( \frac{1}{2}(x, Ax) = \frac{1}{2}(Dx, Dx) = T(Dx) \) and \( T(y) \) is an objective function of \( y = Dx \in \mathbb{R}^m \). By the fact that any symmetrical matrix can be written in difference of two positive definite matrices, it turns out that any given quadratic function can be written in the so-called d.c. (difference of convex functions) form.

6.2 Geometrically linear systems and Lagrangian duality

In fact, the most popular Lagrangian in its original form is actually defined by

\[
II(x) = T(Dx) - U(x),
\]

The skew symmetric matrix \( A_s = \frac{1}{2}(A - A^T) \) does not store energy since \( x^T A_s x \equiv 0 \).
where the objective function $T(y) : \mathcal{Y}_a \subset \mathbb{R}^m \rightarrow \mathbb{R}$ is a kinetic energy, while $U : \mathcal{X}_a \subset \mathbb{R}^n \rightarrow \mathbb{R}$ is a potential energy of the system\footnote{The Lagrangian form was first introduced by W. Hamilton in classical mechanics and denoted by $L = T - U$, which is the standard notation extensively used from dynamical systems to quantum field theory (see \cite{22}).}, which could be linear or convex such that $II(x)$ is well-defined on the so-called \textit{kinetically admissible space} $\mathcal{X}_a = \{x \in \mathcal{X}_a | Dx \in \mathcal{Y}_a \}$ \cite{4}. For Newtonian mechanics, $T(y)$ is quadratic and the objectivity of this kinetic energy ensures the validity of Newton’s laws under the Galilean transformation; while for Einstein’s special relativity theory, the objective function $T(y)$ is strictly convex (see Chapter 2, \cite{9}), which is an invariant under the Lorentz transformation. In either case, the so-called \textit{complementary energy} $T^*(y^*)$ can be uniquely defined on $\mathcal{Y}_a^* \subset \mathbb{R}^m$ by the classical Legendre transformation $T^*(y^*) = \text{sta}\{\langle y; y^* \rangle - T(y) | y \in \mathcal{Y}_a \}$ such that the original Lagrangian $II(x)$ is equivalent to its mixed form

$$L(x, y^*) = \langle Dx; y^* \rangle - T^*(y^*) - U(x) : \mathcal{X}_a \times \mathcal{Y}_a^* \rightarrow \mathbb{R}$$

which is the standard form in mathematical optimization. For conservative systems to quantum field theory (see \cite{29}). Particularly, if $U(x) = \langle x, f \rangle$ is linear and $T(y) = \frac{1}{2} \langle y, C y \rangle$ is quadratic, where $C$ is a linear operator, the equilibrium equation takes a particular symmetrical form $D^*CDx = f$ which is repeated throughout the field equations of mathematical physics \cite{37}.

For geometrically linear static systems, both the input and the configuration variables are time independent. In this case, the convex objective function $T(y)$ is the so-called internal (or stored) energy and $U(x)$ is the external potential, which should be linear $U(x) = \langle x, f \rangle$ such that its derivative $\nabla U(x) = f$ is a given source of the system. Therefore, the Lagrangian form $II(x)$ represents the \textit{total potential} of the system, which is convex on $\mathcal{X}_a$ and its mixed form $L(x, y^*)$ is a saddle function on $\mathcal{X}_a \times \mathcal{Y}_a^*$. Therefore, the traditional saddle Lagrangian duality theory links the convex primal problem $\min\{II(x) | x \in \mathcal{X}_a\}$ to a unique dual problem

$$\max \left\{ T^*(y^*) - \langle y^*, f \rangle \right\} | y^* \in \mathcal{Y}_a^* \},$$

where $\mathcal{Y}_a^* = \{y^* \in \mathcal{Y}_a^* | D^*y^* = f \in \mathcal{X}_a^* \subset \mathbb{R}^n \}$ is the so-called \textit{statically admissible space}. The objectivity of this dual problem is guaranteed by the objectivity of $T(y)$.

By introducing a Lagrange multiplier $x$, which must be a solution to the primal problem (see Lagrange multiplier’s law in Section 1.5 \cite{9}), to relax the equilibrium constraint $D^*y^* = f$ in $\mathcal{Y}_a^*$, the Lagrangian is exactly the mixed form $L(x, y^*)$ and the one-to-one Lagrangian saddle min-max duality

$$\min II(x) = \min_{x \in \mathcal{X}_a} \max_{y^* \in \mathcal{Y}_a^*} L(x, y^*) = \max_{y^* \in \mathcal{Y}_a^*} \min_{x \in \mathcal{X}_a} L(x, y^*) = \max_{y^* \in \mathcal{Y}_a^*} II^*(y^*)$$

where

$$D^*y^* = \nabla U(x), \quad Dx = \nabla T^*(y^*),$$

which is repeated throughout the field equations of mathematical physics \cite{37}.

For geometrically linear static systems, both the input and the configuration variables are time independent. In this case, the convex objective function $T(y)$ is the so-called internal (or stored) energy and $U(x)$ is the external potential, which should be linear $U(x) = \langle x, f \rangle$ such that its derivative $\nabla U(x) = f$ is a given source of the system. Therefore, the Lagrangian form $II(x)$ represents the \textit{total potential} of the system, which is convex on $\mathcal{X}_a$ and its mixed form $L(x, y^*)$ is a saddle function on $\mathcal{X}_a \times \mathcal{Y}_a^*$. Therefore, the traditional saddle Lagrangian duality theory links the convex primal problem $\min\{II(x) | x \in \mathcal{X}_a\}$ to a unique dual problem

$$\max \left\{ T^*(y^*) - \langle y^*, f \rangle \right\} | y^* \in \mathcal{Y}_a^* \},$$

where $\mathcal{Y}_a^* = \{y^* \in \mathcal{Y}_a^* | D^*y^* = f \in \mathcal{X}_a^* \subset \mathbb{R}^n \}$ is the so-called \textit{statically admissible space}. The objectivity of this dual problem is guaranteed by the objectivity of $T(y)$.

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$$\min II(x) = \min_{x \in \mathcal{X}_a} \max_{y^* \in \mathcal{Y}_a^*} L(x, y^*) = \max_{y^* \in \mathcal{Y}_a^*} \min_{x \in \mathcal{X}_a} L(x, y^*) = \max_{y^* \in \mathcal{Y}_a^*} II^*(y^*)$$

where

$$D^*y^* = \nabla U(x), \quad Dx = \nabla T^*(y^*),$$

which is repeated throughout the field equations of mathematical physics \cite{37}.
is called the mono-duality in canonical systems theory [9]. In mathematical economics, where the objective function $T(Dx)$ is corresponding to the revenue, denoted by $R(x)$, and the potential $U(x)$ is the cost function, denoted by $C(x)$, then $\Pi(x) = R(x) - C(x)$ is the so-called total profit. For geometrically linear static problems, the cost function $C(x)$ is usually linear, while the revenue $R(x)$ is a concave objective function of certain measure (norm) of $x$ in order to have maximum total profit $\Pi(x)$.

In geometrically linear dynamical systems, the convex function $T(y)$ is the kinetic energy and $U(x)$ represents the total potential of the system. In this case, the Lagrangian form $\Pi(x) = T(Dx) - U(x)$ is the so-called total action, which is a d.c. (difference of convex) function. Since the mixed Lagrangian form $L(x, y^*)$ is no longer a saddle function, the well-known Hamiltonian

$$H(x, y^*) = \langle Dx; y^* \rangle - L(x, y^*) = T^*(y^*) + U(x)$$

was introduced, which is convex and has been extensively used in dynamical systems. The Euler-Lagrange equations (55) is equivalent to the well-known canonical Hamiltonian equations

$$Dx = \nabla_y H(x, y^*), \quad D^*y^* = \nabla_x H(x, y^*).$$

Actually, although the Lagrangian is not a saddle function in convex Hamiltonian systems, it is a so-called super-critical function [9], and if the total potential $U(x)$ is strictly convex on $X_n \subset \mathbb{R}^n$ such that its Legendre conjugate $U^*(x^*)$ can be uniquely defined on $X_n^*$, then the canonical dual action of $\Pi(x)$ can still be defined by

$$\Pi^*(y^*) = \max\{L(x, y^*)| \ x \in X_n\} = U^*(D^*y^*) - T^*(y^*)$$

on $\mathcal{Y}_n^* = \{y^* \in \mathcal{Y}_n^* | D^*y^* \in X_n^*\}$, which is also a d.c. function. Therefore, instead of mono-duality in static systems, the convex Hamiltonian system is controlled by the so-called bi-duality theory.

**Theorem 5 (Bi-Duality Theorem)** If $(\bar{x}, \bar{y}^*)$ is a critical point of the Lagrangian $L(x, y^*)$, then $\bar{x}$ is a critical point of $\Pi(x)$, $\bar{y}^*$ is a critical point of $\Pi^*(y^*)$ and $\Pi(\bar{x}) = L(\bar{x}, \bar{y}^*) = \Pi^*(\bar{y}^*)$. Moreover, if $n = m$, we have either

$$\Pi(\bar{x}) = \max_{x \in X_n} \Pi(x) \iff \max_{y^* \in \mathcal{Y}_n^*} \Pi^*(y^*) = \Pi^*(\bar{y}^*)$$

(56)

or

$$\Pi(\bar{x}) = \min_{x \in X_n} \Pi(x) \iff \min_{y^* \in \mathcal{Y}_n^*} \Pi^*(y^*) = \Pi^*(\bar{y}^*).$$

(57)

This bi-duality is actually a special case of the triality theory in geometrically linear systems, which was originally presented in Chapter 2 [9] for one-dimensional dynamical systems with a simple proof. This bi-duality reveals a stable periodical property in convex Hamiltonian systems.
6.3 Geometrically nonlinear systems and canonical duality

Problems in geometrically nonlinear systems are usually nonconvex. Due to the fact that the geometrically linear operator $D : \mathbb{R}^n \to \mathbb{R}^m$ can not change the convexity of the objective function, if $W(x)$ is nonconvex and $W(x) = T(Dx)$, the function $T(y)$ is still nonconvex and its Legendre conjugate $T^*(y^*)$ can not be uniquely defined. It turns out that traditional Lagrangian duality theory can not be applied directly in this case. Although the Fenchel conjugate $T^*(y^*) = \sup \{ \langle y, y^* \rangle - T(y) | y \in \mathcal{Y}_a \}$ can be uniquely defined, the function

$$L(x, y^*) = \langle Dx; y^* \rangle - T^*(y^*) - U(x)$$

(58)

is not the traditional Lagrangian form and the associate saddle min-max duality theory will produce the so-called duality gap in nonconvex optimization.

Actually, in terms of $U(x) = \langle x, f \rangle - \frac{1}{2} \langle x, Ax \rangle$, the total complementary function $\Xi(x, \varsigma)$ defined by (59) can be written as

$$\Xi(x, \varsigma) = \langle A(x); \varsigma \rangle - V^*(\varsigma) - U(x).$$

(59)

Comparing this $\Xi(x, \varsigma)$ with either $L(x, y^*)$ or the mixed Lagrangian form $L(x, y^*)$ we can see that the fundamental difference between the canonical duality theory and other methods is the canonical transformation $W(x) = V(A(x))$ instead of the linear transformation $W(x) = T(Dx)$ used in many other duality theories, including the Fenchel-Moreau-Rockafellar duality. In real applications, if the quadratic function $U(x)$ is nonconvex, the mixed Lagrangian form $L(x, y^*)$ is nonconvex in $x$ since $D$ is linear. However, the total complementary function $\Xi(x, \varsigma) : \mathcal{X} \subset \mathbb{R}^n \to \mathbb{R}$ is always convex for $\varsigma \in \mathcal{S}_a^+$ and concave for $\varsigma \in \mathcal{S}_a^-$ due to the geometrically nonlinear operator $A(x)$ and its canonical dual variable $\varsigma$. Therefore, $\Xi(x, \varsigma)$ was also called the nonlinear Lagrangian in [9] and the extended Lagrangian in [11]. If the geometrical operator $A(x)$ is quadratic and objective, the so-called $A$-transformation [11]

$$U^A(\varsigma) = \text{sta} \{ \langle A(x); \varsigma \rangle - U(x) | x \in \mathcal{X} \}$$

(60)

is actually the pure complementary gap function which is obtained from the complementary gap function $G_{ap}(x, \varsigma) = \frac{1}{2} \langle x, G(\varsigma)x \rangle$ by using the analytical solution form $x = [G(\varsigma)]^{-1} F(\varsigma)$.

The geometrical nonlinearity in continuum physics means large deformation (far from equilibrium states), which usually leads to bifurcation in static systems [33] and chaos in dynamical systems [12]. Therefore, geometrically nonlinear systems are usually nonconvex. This is the reason why the geometrical nonlinearity was emphasized in the title of Gao and Strang’s original work [21], although the system they studied is fully nonlinear and governed by a nonconvex/nonsmooth total (super) potential functional

$$\Pi(u) = \bar{W}(\bar{A}(u)) + \bar{F}(u),$$

(61)

where $\bar{W}(e)$ is called the stored energy, which is a canonical function(al) such that the constitutive law $e^* = \partial \bar{W}(e)$ is invertible on its effective domain; while $\bar{F}(u)$ is an external energy, which must be linear on the statically admissible space such that its Gâteaux derivative $\partial \bar{F}(u) = - \bar{u}^*$ leads to the external force (source) field
under the sign convention). The geometrically nonlinear operator \( e = \bar{\Lambda}(u) \) in Gao and Strang’s work should be an objective measure in order to satisfy certain well-known deformation laws (see Chapter 6, [31]). Therefore, the complementary gap function \( G_{op}(u, e^*) \) was naturally introduced. This objective function lays a foundation for the triality theory.

Oppositely, in a recent paper entitled “Some remarks concerning Gao-Strang’s complementary gap function” by Voisei and Zalinescu [40], they choose quadratic functions as the external energy \( \bar{F}(u) \) (see Examples 2, 4 and 5 in [40]), and piecewise linear function (see Example 1 in [40]) as the stored energy, they concluded: “About the (complementary) gap function one can conclude that it is useless at least in the current context”. Clearly, the piecewise linear function is not objective and cannot store energy; while for those quadratic functions \( \bar{F}(u) \) they listed, the dual variable \( u^* = \partial \bar{F}(u) \) depend on the configuration \( u \). Such force field is called follower force. In this case, the system is not conservative and traditional variational methods do not apply. Unfortunately, similar counter-examples and conclusions are repeatedly presented in many other papers (see [38] and references cited therein).

Actually, in order to study nonconvex variational problems in dissipative systems subjected to follower force field, a so-called rate variational method and the associated dual extremum principle were proposed in 1990 [17]. Also, Gao and Strang’s work has been extended to general nonconvex dynamical systems to allow \( \bar{F}(u) \) as a quadratic function, but notations were changed (see [11,12]). In fact, if we let \( \bar{\Lambda}(x) = \{ \Lambda(x), \frac{1}{2}\langle x, A x \rangle \} \) and \( \bar{W}(\bar{\Lambda}(x)) = V(\Lambda(x)) + \frac{1}{2}\langle x, A x \rangle \), the general nonconvex problem \( \bar{F} \) studied in this paper is simply a finite dimensional version of the Gao and Strang’s general work in large deformation theory. This method has been repeatedly used in many Gao’s papers (see [16,43]). Particularly, if \( \bar{\Lambda}(u) \) is a Cauchy-Riemann strain measure, then

\[
\Xi(u, e^*) = \langle \bar{\Lambda}(u); e^* \rangle - \bar{W}^*(e^*) + \bar{F}(u) \tag{62}
\]

is the well-known Hellinger-Reissner complementary energy in finite deformation theory. Furthermore, if the complementary energy \( \bar{W}^*(e^*) \) is replaced by \( \langle e; e^* \rangle - \bar{W}(e) \), the total complementary energy \( \Xi(u, e^*) \) can be written in the so-called pseudo-Lagrangian (it was denoted as \( L_p(u, e^*, e) \) in [21])

\[
\Xi_{hw}(u, e^*, e) = W(e) + \langle \bar{\Lambda}(u) - e; e^* \rangle + \bar{F}(u), \tag{63}
\]

and we have

\[
\Xi(u, e^*) = \text{sta}\{\Xi_{hw}(u, e^*, e) | e \in \mathcal{E}_a\}.
\]

In large deformation mechanics, \( \Xi_{hw}(u, e^*, e) \) is called the Hu-Washizu generalized potential energy, proposed independently by Hai-Chang Hu in 1954 and

\[8\] The Hellinger-Reissner energy was first proposed by Hellinger in 1914. After the external energy \( \bar{F}(u) \) and the boundary conditions in the statically admissible space \( U_k = \{ u \in U_a | e = \bar{\Lambda}(u) \in \mathcal{E}_a \} \) were fixed by Reissner in 1953, the associated variational statement has been known as the Hellinger-Reissner principle. However, the extremality condition of this principle was an open problem, and also the existence of pure complementary variational principles has been a well-known debate existing for over several decades in large deformation mechanics (see [39]). This open problem was partially solved by Gao and Strang’s work and completely solve by the triality theory. While the pure complementary energy principle was formulated by Gao in 1999 [8].
K. Washizu in 1955. The associated variational statement is the well-known Hu-Washizu principle, which has important applications in computational mechanics of thin-walled structures, where the geometrical equation $e = \Lambda(u)$ is usually proposed by certain geometrical hypothesis [15,20].

It has been emphasized in many papers that the key step in the canonical duality theory is to choose a geometrically reasonable measure $\xi = \Lambda(x)$. It was shown in [25] that for a given nonconvex variational problem, the choice of $\Lambda(x)$ may not be unique and different geometrically admissible operators could lead to different canonical dual problems. But all these canonical dual problems must be equivalent in the sense that they have the same set of solutions. Also for complex systems, two type of sequential canonical transformations were proposed (see Chapter 4, [9]). By the fact that the objectivity and canonical duality are fundamental to all natural systems, for any given real problem, as long as the geometrical operator $\Lambda(x)$ can be chosen correctly such that the nonconvex objective function can be recast by adopting a canonical form $W(x) = V(\Lambda(x))$, the canonical duality theory can be used to establish elegant theoretical results and to develop efficient algorithms for robust computations. The triality theory reveals an intrinsic duality pattern in nonconvex systems and should play important roles not only for solving a large class of challenging problems in nonconvex analysis and global optimization, but also for understanding, modeling, and simulation of complex systems.

7 Conclusion Remarks

Motivated by an open problem on the double-min duality in the triality theory that was left unaddressed since 2003, we have presented a mathematically rigorous proof for this theory based on the elementary linear algebra. Our results show that the triality theory holds strongly in the tri-duality form if the primal and its dual problems have the same dimension. Otherwise, both the canonical min-max and double-max duality statements hold strongly, but double-min duality statement holds weakly in a super-symmetric form. Additionally, a weak saddle-duality theory is proposed, which shows that when the complementary gap function $G_{\text{ap}}(x, \xi)$ is negative, either the primal problem ($P$) (only if $m < n$) or its canonical dual ($P_d$) (only if $m > n$) could have saddle critical solutions. Therefore, this seven years old open problem is now solved completely and the triality theory is presented in an elegant form as expected.

The method adopted in this paper can be generalized for more general constrained global optimization problems. As it is mentioned in Remark 3 that the primal problem ($P$) could be NP-hard if its canonical dual has no critical point in $S_+^a$. Also, the extremality conditions for those critical points ($\bar{x}, \bar{\xi}$) are still unknown if the Hessian matrix $G(\bar{\xi})$ of the gap function is indefinite. Although a general theorem on the existence and uniqueness of the canonical dual solution in $S_+^a$ was proposed in [14], and some perturbation methods were discussed in [18], detailed quantitative study on these topics is fundamentally important and critical for understanding and solving NP-hard problems.

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