On Unified Modeling, Canonical Duality-Triality Theory, Challenges and Breakthrough in Optimization

David Yang Gao
Faculty of Science and Technology,
Federation University, Mt Helen, Victoria 3353, Australia

Abstract

A unified model is addressed for general optimization problems in multi-scale complex systems. Based on necessary conditions and basic principles in physics, the canonical duality-triality theory is presented in a precise way to include traditional duality theories and popular methods as special applications. Two conjectures on NP-hardness are discussed, which should play important roles for correctly understanding and efficiently solving challenging real-world problems. Applications are illustrated for both nonconvex continuous optimization and mixed integer nonlinear programming. Misunderstandings and confusion on some basic concepts, such as objectivity, nonlinearity, Lagrangian, and Lagrange multiplier method are discussed and classified. Breakthrough from recent false challenges by C. Zălinescu and his co-workers are addressed. This paper will bridge a significant gap between optimization and multi-disciplinary fields of applied math and computational sciences.

Keywords: Multi-scale modeling, Properly posed problem, Nonlinearity, Objectivity, Canonical duality, Triality, Gap function, Global optimization, NP-hardness.

1 Introduction and Motivation

General problems in mathematical optimization are usually formulated in the following form

$$\min f(x), \quad \text{s.t.} \quad g(x) \leq 0,$$

where the unknown $x \in \mathbb{R}^n$ is a vector, $f(x) : \mathbb{R}^n \to \mathbb{R}$ is the so-called “objective” function, and $g(x) = (g_j(x)) : \mathbb{R}^n \to \mathbb{R}^m$ is a vector-valued constraint function. It must be emphasized that, different from the basic concept of objectivity in continuum physics and nonlinear analysis, the objective function used extensively in optimization literature is allowed to be any arbitrarily given function, even the linear function. Therefore, this mathematical problem is artificial. Although it enables one to “model” a very wide range of problems, it comes at a price: many global optimization problems are considered to be NP-hard. Without detailed information on these arbitrarily given functions, it is impossible to have a powerful theory for solving the general nonconvex problem.

Canonical duality-triality is a newly developed and continuously improved methodological theory. This theory comprises mainly 1) a canonical transformation, which is a versatile methodology that can be used to model complex systems within a unified framework; 2) a complementary-dual principle, which can be used to formulate a perfect dual problem with a unified analytic solution; and 3) a triality theory, which can identify both global and local extrema and to develop effective canonical dual algorithms for solving real-world problems in both

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1This terminology is used mainly in English literature. The function $f(x)$ is called the target function in Chinese and Japanese literature.
continuous and discrete systems. This theory was developed from Gao and Strang’s original work on nonconvex variational/boundary value problems in large deformation mechanics [2]. It was shown in Gao’s book [1] and in the recent articles [5, 42] that both the (external) penalty and Lagrange multiplier methods are special applications of the canonical duality theory in convex optimization. It is now understood that this theory reveals an intrinsic multi-scale duality pattern in complex systems, many popular theories and powerful methods in nonconvex analysis, global optimization, and computational science can be unified within the framework of the canonical duality-triality theory. Indeed, it is easy to show that the popular semi-definite programming (SDP) methods in global optimization and the half-quadratic regularization in image processing are naturally covered by the canonical duality theory [41, 53, 71].

Mathematics and mechanics have been complementary partners since the Newton times. Many fundamental ideas, concepts, and mathematical methods extensively used in calculus of variations and optimization are originally developed from mechanics. It is known that the classical Lagrangian duality theory and the associated Lagrange multiplier method were developed by Lagrange in analytical mechanics [50]. The modern concepts of super-potential and sub-differential in convex analysis were proposed by J.J. Moreau from frictional mechanics [57]. However, as V.I. Arnold indicated [17]: “In the middle of the twentieth century it was attempted to divide physics and mathematics. The consequences turned out to be catastrophic”.

Indeed, the canonical duality theory was developed from some fundamental concepts of objectivity and work-conjugate principle in continuum physics. Due to the existing gap between nonlinear analysis/mechanics and optimization, this theory has been mistakenly challenged by M. Voisei, C. Zălinescu and his former student in a set of more than 12 papers. Although knowledgeable scholars can easily understand the conceptual mistakes in these challenges, the large number of so-called “counterexamples” and false conclusions generated negative impacts to the communities. Therefore, it is necessary to have a formal response to the recent paper by Zălinescu [69]. Instead of directly responding all these challenges one by one, this paper presents the canonical duality theory in a systematical way from a unified modeling, basic assumptions to the theory, method, and applications. The methodology, conjectures, and responses are important for understanding not only this unconventional theory, but also many challenging problems in complex systems. A hope to bridge the existing gap between the mathematical optimization and the interdisciplinary fields of mathematical physics is author’s main goal of this paper.

2 Multi-Scale Modeling and Properly Posed Problems

The canonical duality theory was developed from Gao and Strang’s work on minimum potential energy principle for solving the following variational problem in large deformation theory [2]:

\[
(P_0) : \min \{\Pi(u) = W(Du) + F(u) \mid u \in U_c\},
\]

where the unknown \(u(x)\) is a function in a differentiable manifold \(U\) over a field; \(F : U_c \subset U \to \mathbb{R}\) is an external energy; \(D : U_a \to \mathcal{W}\) is a linear differential operator which assigns each configuration \(u\) to an internal variable \(w = Du\) in different scale; the real-valued function \(W : W_a \subset \mathcal{W} \to \mathbb{R}\) is the so-called internal (or stored) energy. In \(U_a\) the geometrical constraints (such as boundary and initial conditions) are pre-described for each given problem; while \(W_a\)
contains certain physical (constitutive) constraints of the system. The feasible set \( \mathcal{U}_c = \{ u \in \mathcal{U}_a | Du \in W_a \} \) is known as the \textit{kinetically admissible space} in nonlinear field theory.

### 2.1 Objectivity, Subjectivity and Well-posed Problem

Objectivity is a basic concept in mathematical modeling and nonlinear analysis [1, 20, 21, 55]. Let \( \mathcal{R} \) be a special orthogonal group, i.e. \( R \in \mathcal{R} \) if and only if \( R^T = R^{-1} \) and \( \det R = 1 \). A mathematical definition was given in Gao’s book (Definition 6.1.2 [1]).

**Definition 1 (Objectivity)** A set \( W_a \) is said to be objective if \( Rw \in W_a \) \( \forall w \in W_a, \forall R \in \mathcal{R} \). A real-valued function \( W : W_a \rightarrow \mathbb{R} \) is said to be objective if \( W(Rw) = W(w) \) \( \forall w \in W_a, \forall R \in \mathcal{R} \).

**Lemma 1** A real-valued function \( W(w) \) is objective if and only if there exists a real-valued function \( \Phi(E) \) such that \( W(w) = \Phi(w^T w) \).

Geometrically speaking, an objective function is rotational symmetry, which should be a \( \text{SO}(n) \)-invariant in \( n \)-dimensional Euclidean space. Physically, an objective function doesn’t depend on observers. Because of Noether’s theorem, rotational symmetry of a physical system is equivalent to the angular momentum conservation law (see Section 6.1.2 [1]). Therefore, the objectivity is essential for any real-world mathematical models. It was emphasized by P. Ciarlet that the objectivity is not an assumption, but an axiom [20]. Indeed, the objectivity is also known as the \textit{axiom of frame-invariance} [18].

In Gao and Strang’s work, the internal energy \( W(w) \) must be an objective function such that its variation (Gâteaux derivative) \( \sigma = \partial W(w) \) is the so-called \textit{constitutive duality law}, which depends only on the intrinsic property of the system. Dually, the external energy \( F(u) \) can be called the \textit{subjective function} [32], which depends on each problem such that its variation is governed by the \textit{action-reaction duality law}: \( \bar{u}^* = -\partial F(u) \in U^* \). A system is conservative if the action is independent of the reaction. Therefore, the subjective function must be linear on its domain \( U_a \) and, by Riesz representation theorem, we should have \( F(u) = -\langle u, \bar{u}^* \rangle \), where the bilinear form \( \langle u, u^* \rangle : U \times U^* \rightarrow \mathbb{R} \) puts \( U \) and \( U^* \) in duality. Together, \( \Pi(u) = W(Du) + F(u) \) is called the total potential and the minimum potential energy principle leads to the general variational problem (2). From the point view of linguistics, if we consider \( F(u) \) as a subject, \( W(w) \) as an object, and the operation “+” as a predicate, then \( \Pi(u) \) forms a grammatically correct sentence. The criticality condition \( \partial \Pi(u) = 0 \) leads to the equilibrium equation

\[ A(u) = D^* \partial W(Du) = \bar{u}^* \]

where \( D^* : W^*_a \rightarrow U^* \) is an adjoint operator of \( D \) and \( A : \mathcal{U}_c \rightarrow U^* \) is called \textit{equilibrium operator}. The triality structure \( \mathcal{S}^e = \{ [U, U^*]; A \} \) forms an elementary system in Gao’s book (Chapter 4.3, [1]). This abstract form covers most well-known equilibrium problems in real-world applications ranging from mathematical physics in continuous analysis to mathematical programming in discrete systems (see the celebrate text by Gil Strang [66]). Particularly, if

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2i.e., every differentiable symmetry of the action of a physical system has a corresponding conservation law.

3By the facts that (object, subject) is a duality pair in a noun (or pronoun) space, which is dual to a verb space, the multi-level duality pattern \( \{ \text{object, subject}; \text{predicate} \} \) is called triality, which is essential for languages and sciences.
\(W(w)\) is quadratic such that \(\partial^2 W(w) = H\), then the operator \(A : X \rightarrow X^*\) is linear and can be written in the triality form: \(A = D^* H D\), which appears extensively in mathematical physics, optimization, and linear systems [1] [56]. Clearly, any convex quadratic function \(W(Du)\) is objective due to the Cholesky decomposition \(A = \Lambda^* \Lambda \succeq 0\).

In operations research, the decision variable is usually a vector \(u \in \mathbb{R}^n\). If it represents the products of a manufacture company, its dual variable \(\bar{u}^* \in \mathbb{R}^n\) can be considered as market price (or demands), so the external energy \(F(u) = -\langle u, \bar{u}^* \rangle = -u^T \bar{u}^*\) in this system is the total income of the company. The products are produced by workers \(w = D \chi \in \mathbb{R}^m\) and \(D \in \mathbb{R}^{m \times n}\) is a matrix due to the cooperation. Workers are paid by salary \(\sigma\) income of the company. The products are produced by workers \(w \in W\), therefore, the internal energy \(W(w)\) in this example is the cost, which could be an objective function (not necessary since the company is a man-made system). Thus, \(\Pi(u) = W(Du) + F(u)\) is the total cost or target and the minimization problem \(\min \Pi(\chi)\) leads to the equilibrium equation \(D^T \partial e W(Du) = \bar{u}^*\), which is an algebraic equation in \(\mathbb{R}^n\).

According to the action-reaction duality in physics, if there is no action or demand (i.e. \(\bar{u}^* = 0\)), the system has non reaction (i.e. \(u = 0\)). Dually, for any given non-trivial input a real-world problem should have at least one non-trivial solution.

**Definition 2 (Properly and Well-Posed Problems)** A problem is called properly posed if for any given non-trivial input it has at least one non-trivial solution. It is called well-posed if the solution is unique.

Clearly, this definition is more general than Hadamard’s well-posed problems in dynamical systems since the continuity condition is not required. Physically speaking, any real-world problems should be well-posed since all natural phenomena exist uniquely. But practically, it is difficult to model a real-world problem precisely. Therefore, properly posed problems are allowed for the canonical duality theory. This definition is important for understanding the triality theory and NP-hard problems.

### 2.2 Nonconvex Analysis and Boundary-Value Problems

For static systems, the unknown of a mixed boundary-value problem is a vector-valued function

\[ u(x) \in U_a = \{ u \in C[\Omega, \mathbb{R}^m] \mid u(x) = \bar{u} \ \forall x \in \Gamma_u \}, \quad \Omega \subset \mathbb{R}^d, \quad d \leq 3, \quad m \geq 1, \quad \partial \Omega = \Gamma_u \cup \Gamma_t, \]

and the input is \(\bar{u}^* = \{ f(x) \ \forall x \in \Omega, \ t(x) \ \forall x \in \Gamma_t \} [2]\). In this case, the external energy is \(F(u) = -\langle u, \bar{u}^* \rangle = -\int_\Omega u \cdot f \, d\Omega - \int_{\Gamma_t} u \cdot t \, d\Gamma\). In nonlinear analysis, \(D\) is a gradient-like partial differential operator and \(w = Du \in W_a \subset L^p[\Omega; \mathbb{R}^{m \times d}]\) is a two-point tensor field [1] over \(\Omega\). The internal energy \(W(w)\) is defined by

\[ W(w) = \int_\Omega U(x, w) \, d\Omega, \]  

where \(U(x, w) : \Omega \times W_a \rightarrow \mathbb{R}\) is the stored energy density. The system is (space) homogeneous if \(U = U(w)\). Thus, \(W(w)\) is objective if and only if \(U(x, w)\) is objective on an objective set \(W_a\). By the facts that \(w = Du\) is a two-point tensor, which is not considered as a strain measure; but the (right) Cauchy-Green tensor \(C = w^T w\) is an objective strain tensor, there must exists a function \(\Phi(C)\) such that \(W(w) = \Phi(C)\). In nonlinear elasticity, the function \(\Phi(C)\) is usually convex and the duality \(C^* = \partial \Phi(C)\) is invertible (i.e. Hill’s work-conjugate
principle \[\Pi\]). These basic truths in continuum physics laid a foundation for the canonical duality theory.

By finite element method, the domain \(\Omega\) is divided into \(m\)-elements \(\{\Omega^e\}\) such that the unknown function is piecewisely discretized by \(u(x) \simeq N_e(x)\chi_e\ \forall x \in \Omega^e\). Thus, the nonconvex variational problem \(2\) can be numerically reformulated in a global optimization problem

\[
\min \{\Pi(\chi) = W(D\chi) - \langle \chi, f \rangle \mid \chi \in \chi_e\},
\]

where \(\chi = \{\chi_e\}\) is the discretized unknown \(u(x)\), \(D\) is a generalized (high-order) matrix depending on the interpolation \(N_e(x)\) and \(\chi_e\) is a convex constraint set including the boundary conditions. The canonical dual finite element method was first proposed in 1996 \[22\]. Powerful applications have been given recently in engineering and sciences \[47, 62\].

2.3 Lagrangian Mechanics and Initial Value Problems

In Lagrange mechanics \[50, 51\], the unknown \(u(t) \in U \subset C^1[\Omega; \mathbb{R}^n]\) is a vector field over a time domain \(\Omega \subset \mathbb{R}\). Its components \(\{u_i(t)\} (i = 1, \ldots, n)\) are known as the Lagrangian coordinates. Its dual variable \(\bar{u}^*\) is the action vector function in \(\mathbb{R}^n\), denoted by \(f(t)\). The external energy \(F(u) = -\langle u, \bar{u}^* \rangle = -\int_\Omega u(t) \cdot f(t) \, dt\). While the internal energy \(W(Du)\) is the so-called action:

\[
W(Du) = \int_\Omega L(t, u, \dot{u}) \, dt, \quad L = T(\dot{u}) - U(t, u),
\]

where \(Du = \{1, \partial_t\}u = \{u, \dot{u}\}\) is a vector-valued mapping, \(T\) is the kinetic energy density, \(U\) is the potential density, and \(L = T - U\) is the Lagrangian density. Together, \(\Pi(u) = W(Du) + F(u)\) is called the total action. This standard form holds from the classical Newton mechanics to quantum field theory\[4\]. Its stationary condition leads to the well-known Euler-Lagrange equation:

\[
A(u) = D^*\partial W(Du) = \{1, -\partial_t\} \cdot \partial L(u, \dot{u}) = -\partial_t \partial_{\dot{u}} T(\dot{u}) - \partial_u U(t, u) = f.
\]

The system is called (time) homogeneous if \(L = L(u, \dot{u})\). In general, the kinetic energy \(T\) must be an objective function of the velocity \(\dot{x}_k = x_k(u)\) of each particle \(x_k = x_k(u) \in \mathbb{R}^3\ \forall k \in \{1, \ldots, K\}\), while the potential density \(U\) depends on each problem. For Newtonian mechanics, we have \(u(t) = x(t)\) and \(T(\dot{v}) = \frac{1}{2}m\|\dot{v}\|^2\) is quadratic. If \(U = 0\), the equilibrium equation \(A(u) = -m\ddot{x}(t) = f\) includes the Newton second law: \(F = m\ddot{x}\) and the third law: \(-F = f\). The first law \(v = \dot{x} = v_0\) holds only if \(f = 0\). In this case, the system has either a trivial solution \(x = 0\) or infinitely many solutions \(x(t) = v_0t + x_0\), depending on the initial conditions in \(U\). This simple fact in elementary physics plays a key role in understanding the canonical duality theory and NP-hard problems in global optimization.

By using the methods of finite difference and least squares \[51, 62\], the general nonlinear dynamical system \(3\) can also be formulated as the same global optimization problem \(4\), where \(\chi = \{u_i(t_k)\}\) is the Lagrangian coordinates \(u_i(i = 1, \ldots, n)\) at each discretized time \(t_k(k = 1, \ldots, m)\), \(D\) is a finite difference matrix and \(\chi_e\) is a convex constraint set including the initial condition \[52\]. By the canonical duality theory, an intrinsic relation between chaos in nonlinear dynamics and NP-hardness in global optimization was revealed recently in \[52\].

\[4\]See Wikipedia: https://en.wikipedia.org/wiki/Lagrangian_mechanics

\[5\]The objectivity of \(T(v)\) is also called the isotropy in Lagrange mechanics since \(v\) is a vector (see \[51\])
2.4 Mono-/Bi-Dualities and Duality Gap

Lagrangian duality was developed from Lagrange mechanics since 1788 [50], where the kinetic energy \( T(v) = \sum_k \frac{1}{2} m_k |v_k|^2 \) is a quadratic (objective) function. For convex static systems (or dynamical systems but \( U(u) = 0 \)), the stored energy \( W : \mathcal{W}_a \to \mathbb{R} \) is convex and its Legendre conjugate \( W^*(\sigma) = \{(w; \sigma) - W(w) : \sigma = \partial W(w)\} \) is uniquely defined on \( \mathcal{W}_a^* \). Thus, by \( W(Du) = \langle Du; \sigma \rangle - W^*(\sigma) \) the total potential \( \Pi(u) \) can be written in the Lagrangian form\(^6\):

\[
L(u, \sigma) = \langle Du, \sigma \rangle - W^*(\sigma) - \langle u, f \rangle = \langle u, D^*\sigma - f \rangle - W^*(\sigma),
\]

where \( u \in \mathcal{U}_a \) can be viewed as a Lagrange multiplier for the equilibrium equation \( D^*\sigma = f \in \mathcal{U}_a^* \). In linear elasticity, \( L(u, \sigma) \) is the well-known *Hellinger-Reissner complementary energy* \([\text{i}]\). Let \( \mathcal{S}_c = \{\sigma \in \mathcal{W}_a^* : D^*\sigma = f\} \) be the so-called *statically admissible space*. Then the Lagrangian dual of the general problem (\( P_0 \)) is given by \([\text{i}]\):

\[
(P_0^*): \quad \max \{\Pi^*(\sigma) = -W^*(\sigma) : \sigma \in \mathcal{S}_c\},
\]

and the saddle Lagrangian leads to a well-known min-max duality in convex (static) systems:

\[
\min \Pi(u) = \min_{u \in \mathcal{U}_c} \max_{\sigma \in \mathcal{W}_a^*} L(u, \sigma) = \max_{\sigma \in \mathcal{W}_a^*} \min_{u \in \mathcal{U}_a} L(u, \sigma) = \max_{\sigma \in \mathcal{S}_c} \Pi^*(\sigma).
\]

This one-to-one duality is the so-called the *mono-duality* in Chapter 1 [\text{i}], or the *complementary-dual variational principle* in continuum physics. In finite elasticity, the Lagrangian dual is also known as the *Levison-Zubov principle*. However, this principle holds only for convex problems.

For convex Hamiltonian systems the action \( W(Du) \) in [\text{i}] is a d.c. (difference of convex) functional and the Lagrangian has its standard form in Lagrangian mechanics (see Chapter 2.5.2 [\text{i}] with \( u = q(t) \) and \( \sigma = p \):

\[
L(q, p) = \langle \dot{q}, p \rangle - \int_{\Omega} [\mathcal{T}^*(p) + U(q)] \, dt - \langle q, f \rangle,
\]

where \( q \in \mathcal{U}_a \subset \mathcal{C}^1[\Omega, \mathbb{R}^n] \) is the Lagrange coordinate and \( p \in \mathcal{S}_a \subset \mathcal{C}[\Omega, \mathbb{R}^n] \) is the momentum. In this case, the Lagrangian is a bi-concave functional on \( \mathcal{U}_a \times \mathcal{S}_a \), but the Hamiltonian \( H(q, p) = \langle Dq; p \rangle - L(q, p) \) is convex\(^7\). The total action and its canonical dual are [\text{i}]

\[
\Pi(q) = \max \{L(q, p) : p \in \mathcal{V}_a^*\} = \int_{\Omega} [\mathcal{T}(\dot{q}) - U(q)] \, dt - \langle q, f \rangle \quad \forall q \in \mathcal{U}_c
\]

\[
\Pi^d(p) = \max \{L(q, p) : q \in \mathcal{U}_a\} = \int_{\Omega} [\mathcal{U}^*(\dot{p}) - \mathcal{T}^*(p)] \, dt \quad \forall p \in \mathcal{S}_c
\]

Although both of them are d.c. functionals, the duality between the kinetic energy \( T(\dot{q}) \) and the potential \( U(q) \) leads to a so-called *bi-duality* first presented in author’s book Chapter 2 [\text{i}]:

\[
\min \Pi(q) = \min \Pi^d(p), \quad \max \Pi(q) = \max \Pi^d(p).
\]

The mathematical proofs of this theory were given in Chapter 2.6 [\text{i}] for convex Hamiltonian systems and in Corollary 5.3.6 [\text{i}] for nonconvex programming problems. This bi-duality

\(^6\)In Physics literature, the same notation \( L \) is used for both action \( L(u, \dot{u}) \) and the Lagrangian \( L(u, p) \) since both represent the same physical quantity.

\(^7\)This is the reason that instead of the Lagrangian, the Hamiltonian is extensively used in dynamics.
revealed not only an interesting dynamical extremum principle in periodic motion, but also an important truth in convex Hamiltonian systems (see page 77 [1]): the least action principle is incorrect for any periodic motion, it holds only for linear potential \( U(q) \).

In real-world problems the stored energy \( W(w) \) is usually nonconvex in order to model complex phenomena. Its complementary energy can’t be determined uniquely by the Legendre transformation. Although its Fenchel conjugate \( W^\#: W^* \to \mathbb{R} \cup \{+\infty\} \) can be uniquely defined, the Fenchel-Moreau dual problem

\[
(P^\#_0) : \max\{\Pi^z(\sigma)| \sigma \in S_c\}
\]

is not considered as a complementary-dual problem due to Fenchel-Young inequality:

\[
\min\{\Pi(u)| u \in U_c\} \geq \max\{\Pi^z(\sigma)| \sigma \in S_c\},
\]

and \( \theta = \min \Pi(u) - \max \Pi^z(\sigma) \neq 0 \) is the well-known duality gap. This duality gap is intrinsic to all Lagrange-Fenchel-Moreau types duality problems since the linear operator \( D \) can’t change the nonconvexity of \( W(Du) \). It turns out that the existence of a pure stress based complementary-dual principle has been a well-known debate in nonlinear elasticity for more than fifty years [54].

**Remark 1 (Lagrange Multiplier Law)** Strictly speaking, the Lagrange multiplier method can be used mainly for equilibrium constraint in \( S_c \) and the Lagrange multiplier must be the solution to the primal problem (see Section 1.5.2 [1]). The equilibrium equation \( D^*\sigma = f \) must be an invariant under certain coordinates transformation, say the law of angular momentum conservation, which is guaranteed by the objectivity of the stored energy \( W(Du) \) in continuum mechanics (see Definition 6.1.2, [1]), or by the isotropy of the kinetic energy \( T(\dot{u}) \) in Lagrangian mechanics [51]. Specifically, the equilibrium equation for Newtonian mechanics is an invariant under the Calilean transformation; while for Einstein’s special relativity theory, the equilibrium equation \( D^*\sigma = f \) is an invariant under the Lorentz transformation. For linear equilibrium equation, the quadratic \( W(w) \) is naturally an objective function for convex systems. Unfortunately, since the concept of the objectivity is misused in mathematical optimization and the notation of the Euclidian coordinate \( x = \{x_i\} \) is used as the unknown, the Lagrange multiplier method and augmented methods have been mistakenly used for solving general nonconvex optimization problems, which produces many artificial duality gaps [5].

### 3 Unified Problem and Canonical Duality-Triality Theory

In this section, we simply restrict our discussion in finite-dimensional space \( \mathcal{X} \). Its element \( \chi \in \mathcal{X} \) could be a vector, a matrix, or a tensor[9]. In this case, the linear operator \( D \) is a

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8 This truth is not known to many people in physics. Only in a footnote of the celebrated book (Section 1.2, [51]) Landau and Lifshitz pointed out that the least action principle holds only for a sufficient small of time interval, not for the whole trajectory of the system.

9 Tensor is a geometrical object in mathematics and physics, which is defined as a multi-dimensional array satisfying a transformation law, see [https://en.wikipedia.org/wiki/Tensor]. A tensor must be independent of a particular choice of coordinate system (frame-invariance). But this terminology has been also misused recent years in optimization literature such that any multi-dimensional array of data is called tensor.
generalized matrix $D : X \rightarrow W$ and $W$ is a generalized matrix space equipped with a natural norm $\|w\|$. Let $X_a \subset X$ be a convex subset and $X_a^*$ be its dual set such that for any given input $f \in X_a^*$ the subjective function $\langle \chi, f \rangle \geq 0 \ \forall \chi \in X_a$. Then the multi-scale optimization problem (6) can be re-proposed as

$$\begin{align*}
(P) : \quad \min \{ \Pi(\chi) = W(D\chi) - \langle \chi, f \rangle \mid \chi \in \mathcal{X}_c \},
\end{align*}$$

where $\mathcal{X}_c = \{ \chi \in X_a \mid D\chi \in W_a \}$. Although the objectivity is necessary for real-world modeling, the numerical discretization of $W(Du)$ could lead to a complicated function $W(D\chi)$, which may not be objective in $w = D\chi$. Also in operations research, many challenging problems are artificially proposed. Thus, the objectivity required in Gao and Strang’s work on nonlinear elasticity has been relaxed by the canonical duality since 2000 [26].

### 3.1 Canonical Transformation and Gap Function

In the canonical duality theory, a real-valued function $\Phi : \mathcal{E}_a \subset \mathcal{E} \rightarrow \mathbb{R}$ is said to be canonical if the duality relation $\varsigma = \partial \Phi(\xi) : \mathcal{E}_a \rightarrow \mathcal{E}^*_a \subset \mathcal{E}^*$ is bijective. The canonical duality is a fundamental principle in sciences and oriental philosophy, which underlies all natural phenomena. Therefore, instead of the objectivity in continuum physics, a generalized objective function $W(w)$ is used in the canonical duality theory under the following assumption.

**Assumption 1** For a given $W : \mathcal{W}_a \rightarrow \mathbb{R}$, there exists a canonical measure $\xi : \mathcal{W}_a \rightarrow \mathcal{E}_a$ and a canonical function $\Phi : \mathcal{E}_a \rightarrow \mathbb{R}$ such that the following conditions hold:

- (A1.1) Positivity: $W(w) \geq 0 \ \forall w \in \mathcal{W}_a$;
- (A1.2) Canonicality: $W(w) = \Phi(\xi(w)) \ \forall w \in \mathcal{W}_a$; And either
- (A1.3) Coercivity: $\lim W(w) = \infty$ as $\|w\| \rightarrow \infty$, or
- (A1.3*) Boundness: $\mathcal{W}_a$ is bounded.

Generally speaking, the conditions (A1.1) and (A1.2) are necessary for any real-world problems; while (A1.3) and (A1.3*) depend mainly on the magnitude of the input $f \in X_a^*$. Usually, the coercivity is for small $\|f\|$ (within the system’s capacity, such as elasticity) and the boundness is for big $\|f\|$ (beyond the system’s capacity, such as plasticity) [24].

Let $\Lambda = \xi \circ D : X_a \rightarrow \mathcal{E}_a$ be the so-called geometrically admissible operator. The canonicality $W(D\chi) = \Phi(\Lambda(\chi))$ is also called the canonical transformation in the canonical duality theory. Let $\langle \xi ; \varsigma \rangle : \mathcal{E} \times \mathcal{E}^* \rightarrow \mathbb{R}$ be the bilinear form which puts $\mathcal{E}$ and $\mathcal{E}^*$ in duality. By (A1.2), we have $\mathcal{X}_c = \{ \chi \in X_a \mid \Lambda(\chi) \in \mathcal{E}_a \}$ and the problem $(P)$ can be equivalently reformulated in the following canonical form

$$\begin{align*}
(P) : \quad \min \{ \Pi(\chi) = \Phi(\Lambda(\chi)) - \langle \chi, f \rangle \mid \chi \in \mathcal{X}_c \}. \tag{19}
\end{align*}$$

By the facts that the canonical duality is a universal principle in nature and the canonical measure $\Lambda(\chi)$ is not necessarily to be objective, the canonical transformation holds for general problems and the problem $(P)$ can be used to model general complex systems. The criticality condition of (P) is governed by the fundamental principle of virtual work:

$$\begin{align*}
\langle \Lambda(\chi) \delta \chi ; \varsigma \rangle = \langle \delta \chi , \Lambda^*_\Theta(\chi) \varsigma \rangle = \langle \delta \chi , f \rangle \ \forall \delta \chi \in \mathcal{X}_c, \quad \tag{20}
\end{align*}$$

A generalized matrix $D = \{ D_{i,j} \}$ is a multi-dimensional array but not necessary to satisfy a transformation law, so it is not a tensor. In order to avoid confusion, it can be called a tentrix.
where $\Lambda_t(\chi) = \partial \Lambda(\chi)$ represents a generalized Gâteaux (or directional) derivative of $\Lambda(\chi)$, its adjoint $\Lambda_t^*$ is called the balance operator, $\varsigma = C^*(\xi) = \partial \Phi(\xi)$ and $C^*: \mathcal{E}_a \to \mathcal{E}_a^*$ is a canonical dual (or constitutive) operator. The strong form of this virtual work principle is called the canonical equilibrium equation:

$$\Lambda(\chi) = \Lambda_t^*(\chi)C^*(\Lambda(\chi)) = f. \quad (21)$$

A system governed by this equation is called a canonical system and is denoted as (see Chapter 4, [1])

$$\mathcal{S}_a = \{(\mathcal{X}, \mathcal{X}^*), (\mathcal{E}, \mathcal{E}^*); (\Lambda, C^*)\}.$$ 

**Definition 3 (Classification of Nonlinearities)** The system $\mathcal{S}_a$ is called geometrically nonlinear (resp. linear) if the geometrical operator $\Lambda: \mathcal{X}_a \to \mathcal{E}_a$ is nonlinear (resp. linear); the system is called physically (or constitutively) nonlinear (resp. linear) if the canonical dual operator $C^*: \mathcal{E}_a \to \mathcal{E}_a^*$ is nonlinear (resp. linear); the systems is called fully nonlinear (resp. linear) if it is both geometrically and physically nonlinear (resp. linear).

Both geometrical and physics nonlinearities are basic concepts in nonlinear field theory. The mathematical definition was first given by the author in 2000 under the canonical transformation [26]. A diagrammatic representation of this canonical system is shown in Figure 1.

$$\chi \in \mathcal{X}_a \quad \xrightarrow{A} \quad \mathcal{X}_a^* \ni \chi^*$$

$$\xi \in \mathcal{E}_a \quad \xrightarrow{C^*} \quad \mathcal{E}_a^* \ni \varsigma$$

Figure 1: Diagrammatic representation for a canonical system

This diagram shows a symmetry broken in the canonical equilibrium equation, i.e., instead of $\Lambda^*$, the balance operator $\Lambda_t^*$ is adjoined with $\Lambda_t$. It was discovered by Gao and Strang [2] that by introducing a complementary operator $\Lambda_c(\chi) = \Lambda(\chi) - \Lambda_t(\chi)\chi$, this locally broken symmetry is recovered by a so-called complementary gap function

$$G_{ap}(\chi, \varsigma) = \langle -\Lambda_c(\chi); \varsigma \rangle, \quad (22)$$

which plays a key role in global optimization and the triality theory. Clearly, if $\Lambda = \mathbf{D}$ is linear, then $G_{ap} = 0$. Thus, the following statement is important to understand complexity:

*Only the geometrical nonlinearity leads to nonconvexity in optimization, bifurcation in analysis, chaos in dynamics, and NP-hard problems in complex systems.*

### 3.2 Complementary-Dual Principle and Analytical Solution

For a given canonical function $\Phi: \mathcal{E}_a \to \mathbb{R}$, its conjugate $\Phi^*: \mathcal{E}_a^* \to \mathbb{R}$ can be uniquely defined by the Legendre transformation
\[ \Phi^*(\zeta) = \text{sta}\{\langle \xi; \zeta \rangle - \Phi(\xi) | \xi \in \mathcal{E}_a \}, \quad (23) \]

where \(\text{sta}\{f(\chi) | \chi \in \mathcal{X}\}\) stands for finding the stationary value of \(f(\chi)\) on \(\mathcal{X}\), and the following canonical duality relations hold on \(\mathcal{E}_a \times \mathcal{E}_a^*\):

\[ \zeta = \partial \Phi(e) \iff e = \partial \Phi^*(\zeta) \iff \Phi(e) + \Phi^*(\zeta) = \langle e; \zeta \rangle. \quad (24) \]

If the canonical function is convex and lower semi-continuous, the Gâteaux derivative \(\partial\) should be replaced by the sub-differential and \(\Phi^*\) is replaced by the Fenchel conjugate \(\Phi^\ast(\zeta) = \sup\{\langle \xi; \zeta \rangle - \Phi(\xi) | \xi \in \mathcal{E}_a \}\). In this case, (24) is replaced by the generalized canonical duality

\[ \zeta \in \partial \Phi(e) \iff e \in \partial \Phi^*(\zeta) \iff \Phi(e) + \Phi^*(\zeta) = \langle e; \zeta \rangle \quad \forall (\xi, \zeta) \in \mathcal{E}_a \times \mathcal{E}_a^*. \quad (25) \]

If the convex set \(\mathcal{E}_a\) contains inequality constrains, then (25) includes all the internal KKT conditions [3, 24]. In this sense, a KKT point of the canonical form \(\Pi(\chi)\) is a generalized critical point of \(\Pi(\chi)\).

By the complementarity \(\Phi(\Lambda(\chi)) = \langle \Lambda(\chi); \zeta \rangle - \Phi^*(\zeta)\), the canonical form of \(\Pi(\chi)\) can be equivalently written in Gao and Strang’s total complementary function \(\Xi : \mathcal{X}_a \times \mathcal{E}_a^* \to \mathbb{R}\) [2]

\[ \Xi(\chi, \zeta) = \langle \Lambda(\chi); \zeta \rangle - \Phi^*(\zeta) - \langle \chi, f \rangle. \quad (26) \]

Then, the canonical dual function \(\Pi^d : \mathcal{S}_c \to \mathbb{R}\) can be obtained by the canonical dual transformation:

\[ \Pi^d(\chi) = \text{sta}\{\Xi(\chi, \zeta) | \chi \in \mathcal{X}_a\} = G^\Lambda_{ap}(\zeta) - \Phi^*(\zeta), \quad (27) \]

where \(G^\Lambda_{ap}(\zeta) = \text{sta}\{\langle \Lambda(\chi); \zeta \rangle - \langle \chi, f \rangle | \chi \in \mathcal{X}_a\}\), which is defined on the canonical dual feasible space \(\mathcal{S}_c = \{\zeta \in \mathcal{E}_a^* | \Lambda^*_c(\chi)\zeta = f \quad \forall \chi \in \mathcal{X}_a\}\). Clearly, \(\mathcal{S}_c \neq \emptyset\) if \((P)\) is properly posed.

**Theorem 1 (Complementary-Dual Principle [1])** The pair \((\bar{\chi}, \bar{\zeta})\) is a critical point of \(\Xi(\chi, \zeta)\) if and only if \(\bar{\chi}\) is a critical point of \(\Pi(\chi)\) and \(\bar{\zeta}\) is a critical point of \(\Pi^d(\zeta)\). Moreover,

\[ \Pi(\bar{\chi}) = \Xi(\bar{\chi}, \bar{\zeta}) = \Pi^d(\bar{\zeta}). \quad (28) \]

**Proof.** The criticality condition \(\partial \Xi(\bar{\chi}, \bar{\zeta}) = 0\) leads to the following canonical equations

\[ \Lambda(\bar{\chi}) = \partial \Phi^*(\bar{\zeta}), \quad \Lambda^*_c(\bar{\chi})\bar{\zeta} = f. \quad (29) \]

The theorem is proved by the canonical duality [24] and the definition of \(\Pi^d\).

**Theorem 1** shows a one-to-one correspondence of the critical points between the primal function and its canonical dual. In large deformation theory, this theorem solved the fifty-year old open problem on complementary variational principle and is known as the Gao principle in literature [54].

In real-world applications, the geometrical operator \(\Lambda\) is usually quadratic homogeneous i.e. \(\Lambda(\alpha\chi) = \alpha^2\Lambda(\chi)\quad \forall \alpha \in \mathbb{R}\). In this case, we have [2]

\[ \Lambda_t(\chi)\chi = 2\Lambda(\chi), \quad \Lambda_c(\chi) = -\Lambda(\chi), \quad \text{and} \]

\[ \Xi(\chi, \zeta) = G_{ap}(\chi, \zeta) - \Phi^*(\zeta) - \langle \chi, f \rangle = \frac{1}{2}\langle \chi, G(\zeta)\chi \rangle - \Phi^*(\zeta) - \langle \chi, f \rangle, \quad (30) \]

where \(G(\zeta) = \partial^2_{\chi}G_{ap}(\chi, \zeta)\). Then, the canonical dual function \(\Pi^d(\zeta)\) can written explicitly as

\[ \Pi^d(\zeta) = \{\Xi(\chi, \zeta) | G(\zeta)\chi = f \quad \forall \chi \in \mathcal{X}_a\} = -\frac{1}{2}\langle [G(\zeta)]^+f, f \rangle - \Phi^*(\zeta), \quad (31) \]

where \(G^+\) represents a generalized inverse of \(G\).
Theorem 2 (Analytical Solution Form) If $\bar{\varsigma} \in S_c$ is a critical point of $\Pi^d(\varsigma)$, then

$$\bar{\chi} = [G(\bar{\varsigma})]^+ f$$

is a critical point of $\Pi(\chi)$ and $\Pi(\bar{\chi}) = \Xi(\bar{\chi}, \bar{\varsigma}) = \Pi^d(\bar{\varsigma})$. Dually, if $\bar{\chi} \in X_c$ is a critical point of $\Pi(\chi)$, it must be in the form of (32) for a critical point $\bar{\varsigma} \in S_c$ of $\Pi^d(\varsigma)$.

This unified analytical solution form holds not only for general global optimization problems in finite dimensional systems, but also for a large-class of nonlinear boundary/initial value problems in nonconvex analysis and dynamic systems [40].

3.3 Triality Theory and NP-Hard Criterion

Definition 4 (Degenerate and Non-Degenerate Critical Points, Morse Function) Let $\bar{\chi} \in X_c$ be a critical point of a real-valued function $\Pi : X_c \to \mathbb{R}$. $\bar{\chi}$ is called degenerate (res. non-degenerate) if the Hessian matrix of $\Pi(\chi)$ is singular (resp. non-singular) at $\bar{\chi}$. The function $\Pi : X_c \to \mathbb{R}$ is called a Morse function if it has no degenerate critical points.

Theorem 3 (Triality Theory [26]) Suppose that $\Phi : E_a \to \mathbb{R}$ is convex, $(\bar{\chi}, \bar{\varsigma})$ is a non-degenerate critical point of $\Xi(\chi, \varsigma)$ and $X_o \times S_o$ is a neighborhood $^{11}$ of $(\bar{\chi}, \bar{\varsigma})$.

If $\bar{\varsigma} \in S^+_c = \{\varsigma \in S_c | G(\varsigma) \succeq 0\}$, then

$$\Pi(\bar{\chi}) = \min_{\chi \in X_o} \Pi(\chi) = \max_{\varsigma \in S^+_c} \Pi^d(\varsigma) = \Pi^d(\bar{\varsigma}). \quad (33)$$

If $\bar{\varsigma} \in S^-_c = \{\varsigma \in S_c | G(\varsigma) \prec 0\}$, then we have either

$$\Pi(\bar{\chi}) = \max_{\chi \in X_o} \Pi(\chi) = \max_{\varsigma \in S^-_c} \Pi^d(\varsigma) = \Pi^d(\bar{\varsigma}), \quad (34)$$

or (if $\dim \Pi = \dim \Pi^d$)

$$\Pi(\bar{\chi}) = \min_{\chi \in X_o} \Pi(\chi) = \min_{\varsigma \in S^-_c} \Pi^d(\varsigma) = \Pi^d(\bar{\varsigma}). \quad (35)$$

The statement (33) is the so-called canonical min-max duality, which can be proved easily by Gao and Strang’s work in 1989 [2]. Clearly, $\varsigma \in S^+_c$ if and only if $G_{ap}(\chi, \varsigma) \geq 0 \ \forall \chi \in X$. This duality theory shows that the Gao-Strang gap function provides a global optimum criterion. The statements (33) and (35) are called the canonical double-max and double-min dualities, respectively, which can be used to find local extremum solutions.

The triality theory shows that the nonconvex minimization problem ($P$) is canonically dual to the following maximum stationary problem

$$(P^d) : \ \max \ \text{sta}\{\Pi^d(\varsigma) | \ \varsigma \in S^+_c\}. \quad (36)$$

$^{11}$The neighborhood $X_o$ of $\bar{\chi}$ means that on which, $\bar{\chi}$ is the only critical point (see page 140 [1]).
Theorem 4 (Existence and Uniqueness Criteria \[31\]) For a properly posed \((P)\), if the canonical function \(\Phi : E_a \to \mathbb{R}\) is convex, \(\int S^+_c \neq \emptyset\), and

\[
\lim_{\alpha \to 0^+} \Pi^d(\varsigma_0 + \alpha \varsigma) = -\infty \quad \forall \varsigma_0 \in \partial S^+_c, \quad \forall \varsigma \in S^+_c,
\]

then \((P^d)\) has at least one solution \(\varsigma \in S^+_c\) and \(\bar{\chi} = [G(\varsigma)]^+f\) is a solution to \((P)\). The solution is unique if \(H = \partial G(\xi) > 0\).

Proof. Under the required conditions \(-\Pi^d : S^+_c \to \mathbb{R}\) is convex and coercive and \(\int S^+_c \neq \emptyset\). Therefore, \((P^d)\) has at least one solution. If \(H > 0\), then \(\Pi^d : S^+_c \to \mathbb{R}\) is strictly concave and \((P^d)\) has a unique solution. \(\Box\)

This theorem shows that if \(\int S^+_c \neq \emptyset\) the nonconvex problem \((P)\) is canonically dual to \((P^d)\) which can be solved easily. Otherwise, the problem \((P)\) is canonically dual to the following minimal stationary problem, i.e. to find a global minimum stationary value of \(\Pi^d\) on \(S_c\):

\[
(P^s) : \min \{\Pi^d(\varsigma) | \varsigma \in S_c\},
\]

which could be really NP-hard since \(\Pi^d(\varsigma)\) is nonconvex on the nonconvex set \(S_c\). Therefore, a conjecture was proposed in \[30\].

Conjecture 1 (Criterion of NP-Hardness) A properly posed problem \((P)\) is NP-hard if and only if \(\int S^+_c = \emptyset\).

The triality theory was discovered by the author during his research on post-buckling of a large deformed elastic beam in 1996 \[23\], where the primal variable \(u(x)\) is a displacement vector in \(\mathbb{R}^2\) and \(\varsigma(x)\) is a canonical dual stress also in \(\mathbb{R}^2\). Therefore, the triality theory was correctly proposed in nonconvex analysis, which provides for the first time a complete set of solutions to the post-buckling problem. Physically, the global minimizer \(\bar{u}(x)\) represents a stable buckled beam configuration (happened naturally), the local minimizer is an unstable buckled state (happened occasionally), while the local maximizer is the unbuckled beam state. Mathematical proof of the triality theory was given in \[1\] for one-D nonconvex variational problems (Theorem 2.6.2) and for finite dimensional optimization problems (Theorem 5.3.6 and Corollary 5.3.1). In 2002, the author discovered some countexamples to the canonical double-min duality when \(\dim \Pi \neq \dim \Pi^d\) and this statement was removed from the triality theory (see Remark 1 in \[27\] and Remark for Theorem 3 in \[28\]). Recently, the author and his co-workers proved that the canonical double-min duality holds weakly when \(\dim \Pi \neq \dim \Pi^d\) \[4, 19, 59\]. It was also discovered by using the canonical dual finite element method that the local minimum solutions in nonconvex mechanics are very sensitive not only to the input and boundary conditions of a given system, but also to such artificial conditions as the numerical discretization and computational precision, etc. The triality theory provides a precise mathematical tool for studying and understanding complicated natural phenomena.

The canonical duality-triality theory has been successfully used for solving a wide class problems in both global optimization and nonconvex analysis \[41\], including certain challenging problems in nonlinear PDEs and large deformation mechanics \[33\].

4 Applications in Complex Systems

Applications to nonconvex constrained global optimization have been discussed in \[5, 42\]. This section presents applications to two general global optimization problems.
4.1 Unconstrained Nonconvex Optimization Problem

\[ (P) : \min \left\{ \Pi(\chi) = \sum_{s=1}^{m} \Phi_s(\Lambda_s(\chi)) - \langle \chi, f \rangle \mid \chi \in \mathcal{X} \right\}, \]  \hspace{1cm} \text{(39)}

where the canonical measures \( \xi_s = \Lambda_s(\chi) \) could be either a scalar or a generalized matrix, \( \Phi_k(\xi_k) \) are any given canonical functions, such as polynomial, exponential, logarithm, and their compositions, etc. For example, if \( \chi \in \mathcal{X}_c \subset \mathbb{R}^n \) and

\[ W(\mathbf{D}\chi) = \sum_{i=1}^{n} \frac{1}{2} \alpha_i \chi^T Q_i \chi + \sum_{j \in J} \frac{1}{2} \alpha_j \left( \frac{1}{2} \chi^T Q_j \chi + \beta_j \right)^2 + \sum_{k \in K} \alpha_k \exp \left( \frac{1}{2} \chi^T Q_k \chi \right) + \sum_{\ell \in L} \frac{1}{2} \alpha_\ell \chi^T Q_\ell \chi \log \left( \frac{1}{2} \chi^T Q_\ell \chi \right), \]  \hspace{1cm} \text{(40)}

where \( \{Q_s\} \) are positive-definite matrices to allow the Cholesky decomposition \( Q_s = D_s^T D_s \) for all \( s \in \{I, J, K, L\} \) and \( \{\alpha_s, \beta_s\} \) are physical constants, which could be either positive or negative under Assumption 1. This general function includes naturally the so-called d.c. functions (i.e. difference of convex functions). By using the canonical measure

\[ \xi = \{\xi_s\} = \left\{ \frac{1}{2} \alpha_i \chi^T Q_i \chi, \frac{1}{2} \chi^T Q_r \chi \right\} \in \mathcal{E}_a = \mathbb{R}^p \times \mathbb{R}_+^q, \ p = \dim I, \ q = \dim J + \dim K + \dim L \]

where \( \mathbb{R}_+^q = \{ \chi \in \mathbb{R}^q \mid x_i \geq 0 \ \forall i = 1, \ldots, q \} \), \( W(\mathbf{w}) \) can be written in the canonical form

\[ \Phi(\xi) = \sum_{i \in I} \xi_i + \sum_{j \in J} \frac{1}{2} \alpha_j (\xi_j + \beta_j)^2 + \sum_{k \in K} \alpha_k \exp \xi_k + \sum_{\ell \in L} \alpha_\ell \xi_\ell \log \xi_\ell. \]

Thus, \( \partial \Phi(\xi) = \{1, \varsigma_\ell\} \) in which, \( \varsigma = \{\alpha_j (\xi_j + \beta_j), \alpha_k \exp \xi_k, \alpha_\ell (\log \xi_\ell - 1)\} \in \mathcal{E}_a^* \) and

\[ \mathcal{E}_a^* = \{\varsigma \in \mathbb{R}^q \mid \varsigma_j \geq -\alpha_j \beta_j \ \forall j \in J, \ \varsigma_k \geq \alpha_k \ \forall k \in K, \ \varsigma_\ell \in \mathbb{R} \ \forall \ell \in L\}. \]

The conjugate of \( \Phi \) can be easily obtained as

\[ \Phi^*(\varsigma) = \sum_{j \in J} \left( \frac{1}{2} \alpha_j \varsigma_j^2 + \beta_j \varsigma_j \right) + \sum_{k \in K} \varsigma_k (\ln (\alpha^{-1}_k \varsigma_k) - 1) + \sum_{\ell \in L} \alpha_\ell \exp (\alpha^{-1}_\ell \varsigma_\ell) - 1. \]  \hspace{1cm} \text{(41)}

Since \( \Lambda(\chi) \) is quadratic homogenous, the gap function \( G_{ap} \) and its \( \Lambda \)-conjugate \( G_{ap}^\Lambda \) in this case are

\[ G_{ap}(\chi, \varsigma) = \frac{1}{2} \chi^T G(\varsigma) \chi, \ G_{ap}^\Lambda (\varsigma) = \frac{1}{2} f^T [G(\varsigma)]^+ f, \ G(\varsigma) = \sum_{i \in I} \alpha_i Q_i + \sum_{s \in \{J, K, L\}} s_s Q_s. \]

Since \( \Pi^d(\varsigma) = -G_{ap}^\Lambda (\varsigma) - \Phi^*(\varsigma) \) is concave and \( S^+_c \) is a closed convex set, if for the given physical constants and the input \( f \) such that \( S^+_c \neq \emptyset \), the canonical dual problem \( (P^d) \) has at least one solution \( \varsigma \in S^+_c \subset \mathbb{R}^q \) and \( \bar{\chi} = [G(\varsigma)]^+ f \in \mathcal{X}_c \subset \mathbb{R}^n \) is a global minimum solution to \( (P) \). If \( n \gg q \), the problem \( (P^d) \) can be much easier than \( (P) \).
4.2 Mixed Integer Nonlinear Programming (MINLP)

The decision variable for (MINLP) is \( \chi = \{y, z\} \in \mathcal{Y}_a \times \mathbb{Z}_a \), where \( \mathcal{Y}_a \) is a continuous variable set and \( \mathbb{Z}_a \) is a set of integers. It was shown in \([30]\) that for any given integer set \( \mathbb{Z}_a \), there exists a linear transformation \( D_z : \mathbb{Z}_a \rightarrow \mathbb{Z} = \{\pm 1\}^n \). Thus, based on the unified model \([18]\), a general MINLP problem can be proposed as

\[
(P_{mi}) : \min \{ \Pi(y, z) = W(D_y y, D_z z) - \langle y, s \rangle - \langle z, t \rangle \mid (y, z) \in \mathcal{Y}_c \times \mathbb{Z}_c \}, \tag{42}
\]

where \( f = (s, t) \) is a given input, \( D \chi = (D_y y, D_z z) \in \mathcal{W}_y \times \mathbb{Z} \) is a multi-scale operator, and \( \mathcal{Y}_c = \{y \in \mathcal{Y}_a \mid D_y y \in \mathcal{W}_y\} \), \( \mathbb{Z}_c = \{z \in \mathbb{Z}_a \mid D_z z \in \mathbb{Z}\} \).

In \( \mathcal{Y}_a \) certain linear constraints are given. Since the set \( \mathbb{Z} \) is bounded, by Assumption 1 either \( W : \mathcal{W}_y \rightarrow \mathbb{R} \) is coercive or \( \mathcal{W}_y \) is bounded. This general problem \((P_{mi})\) covers many real-world applications, including the so-called fixed cost problem \([43]\). It must be emphasized that the integer constraint \( w_z = D_z z \in \mathbb{Z} \) is a constitutive condition governed by the physical property of the system, it must be relaxed by the canonicality. Let

\[
\epsilon = \Lambda_z(z) = (D_z z) \circ (D_z z) \in \mathcal{E}_z = \mathbb{R}_+^n, \tag{43}
\]

where \( x \circ y = \{x_i y_i\}^n \) is the Hadamard product in \( \mathbb{R}^n \), thus the integer constraint in \( \mathbb{Z} \) can be relaxed naturally by the canonical function \( \Psi(\epsilon) = \{0 \text{ if } \epsilon \leq e, \infty \text{ otherwise}\} \), where \( e = \{1\}^n \). Therefore, the canonical form of \((P_{mi})\) is

\[
\min \{ \Pi(y, z) = \Phi(\Lambda(y, z)) + \Psi(\Lambda_z(z)) - \langle y, s \rangle - \langle z, t \rangle \mid y \in \mathcal{Y}_c\}. \tag{44}
\]

Since the canonical function \( \Psi(\epsilon) \) is convex, semi-continuous, its Fenchel conjugate is

\[
\Psi^\star(\sigma) = \sup \{ \langle \epsilon; \sigma \rangle - \Psi(\epsilon) \mid \epsilon \in \mathbb{R}^n \} = \{ \langle \epsilon; \sigma \rangle \text{ if } \sigma \geq 0, \infty \text{ otherwise} \}.
\]

The generalized canonical duality relations \([25]\) are

\[
\sigma \geq 0 \iff \epsilon \leq e \iff \langle \epsilon - e; \sigma \rangle = 0. \tag{45}
\]

The complementarity shows that the canonical integer constraint \( \epsilon = e \) can be naturally relaxed by the \( \sigma > 0 \) in continuous space. Thus, if \( \xi = \Lambda(\chi) \) is a quadratic homogenous operator and the canonical function \( \Phi(\xi) \) is convex on \( \mathcal{E}_a \), the canonical dual to \((P_{mi})\) is

\[
(P_{mi}^d) : \max \left\{ \Pi^d(s, \sigma) = -\frac{1}{2} \left\| G(s, \sigma) \right\|^\top f - \Phi^d(s) - \langle e; \sigma \rangle \mid (s, \sigma) \in S_c^+ \right\}, \tag{46}
\]

where \( G(s, \sigma) \) depends on the quadratic operators \( \Lambda(\chi) \) and \( \Lambda_z(z) \), \( S_c^+ \) is a convex open set

\[
S_c^+ = \{(s, \sigma) \in \mathcal{E}_a^* \times \mathbb{R}_+^n \mid G(s, \sigma) \succeq 0, \sigma > 0\}. \tag{47}
\]

The canonical duality-triality theory has been used successfully for solving mixed integer programming problems \([39][43]\). Particularly, for the quadratic integer programming problem

\[
(P_{qi}) : \min \left\{ \Pi(x) = \frac{1}{2} x^T Q x - x^T f \mid x \in \{-1, 1\}^n \right\}, \tag{48}
\]

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we have $\mathcal{S}_c^+ = \{\sigma \in \mathbb{R}_+^n | \mathbf{G}(\sigma) = \mathbf{Q} + 2\text{Diag}(\sigma) \succeq 0, \sigma > 0\}$ and

$$(P_{qi}^d) : \max \left\{ \Pi^d(\sigma) = -\frac{1}{2} \mathbf{G}(\sigma)^T \mathbf{f} - \mathbf{e}^T \sigma | \sigma \in \mathcal{S}_c^+ \right\}$$

which can be solved easily if int$\mathcal{S}_c^+ \neq \emptyset$. Otherwise, $(P_{qi})$ could be NP-hard since $\mathcal{S}_c^+$ is an open set, which is a conjecture proposed in [30]. In this case, $(P_{qi})$ is canonically dual to an unconstrained nonsmooth/nonconvex minimization problem [31].

### 4.3 Relation with SDP Programming

Now let us show the relation between the canonical duality theory and the popular semi-definite programming relaxation.

**Theorem 5** Suppose that $\Phi : \mathcal{E}_a \to \mathbb{R}$ is convex and $\bar{\varsigma} \in \mathcal{E}_a^*$ is a solution of the problem

$$(P_{sd}^d) : \min \{ g + \Phi^*(\varsigma) \} \quad \text{s.t.} \quad \begin{pmatrix} \mathbf{G}(\varsigma) & \mathbf{f} \\ \mathbf{f}^T & 2g \end{pmatrix} \succeq 0 \quad \forall \varsigma \in \mathcal{E}_a^*, \ g \in \mathbb{R},$$

then $\chi = [\mathbf{G}(\varsigma)]^+ \mathbf{f}$ is a global minimum solution to the nonconvex problem $(P)$. 

**Proof.** The problem $(P_{sd}^d)$ can be equivalently written in the following problem (see [71])

$$\min \left\{ g + \Phi^*(\varsigma) | \ g \geq G^A_{ap}(\varsigma), \ \mathbf{G}(\varsigma) \succeq 0 \ \forall \varsigma \in \mathcal{E}_a^* \right\}. \quad (51)$$

Then, by using the Schur complement Lemma [70], this problem is equivalent to $(P_{sd}^d)$. The theorem is proved by the triality theory. \hfill \Box

It was proved [39] that for the same problem $(P_{qi})$, if we use different geometrical operator

$$\Lambda(\mathbf{x}) = \mathbf{x}\mathbf{x}^T \in \mathcal{E}_a = \{ \mathbf{\xi} \in \mathbb{R}^{n \times n} | \mathbf{\xi} = \mathbf{\xi}^T, \ \mathbf{\xi} \succeq 0, \ \text{rank} \ \mathbf{\xi} = 1, \ \xi_{ii} = 1 \ \forall i = 1, \ldots, n \},$$

and the associated canonical function $\Phi(\mathbf{\xi}) = \frac{1}{2} \langle \mathbf{\xi}; \mathbf{Q} \rangle + \{ 0 \text{ if } \mathbf{\xi} \in \mathcal{E}_a, +\infty \text{ otherwise} \}$, where $\langle \mathbf{\xi}; \varsigma \rangle = \text{tr}(\mathbf{\xi}^T \varsigma)$, we should obtain the same canonical dual problem $(P_{qi}^d)$. Particularly, if $\mathbf{f} = 0$, then $(P_{qi})$ is a typical linear semi-definite programming

$$\min \frac{1}{2} \langle \mathbf{\xi}; \mathbf{Q} \rangle \quad \text{s.t.} \ \mathbf{\xi} \in \mathcal{E}_a.$$

Since $\mathcal{E}_a$ is not bounded and there is no input, this problem is not properly posed, which could have either no solution or multiple solutions for a given indefinite $\mathbf{Q} = \mathbf{Q}^T$.

### 4.4 Relation to Reformulation-Linearization/Convexification Technique

The Reformulation-Linearization/Convexification Technique (RLT) proposed by H. Sherali and C.H. Tuncbilek [64] is one well-known novel approach for efficiently solving general polynomial programming problems. The key idea of this technique is also to introduce a geometrically nonlinear operator $\mathbf{\xi} = \Lambda(\mathbf{x})$ such that the higher-order polynomial object $W(\mathbf{x})$ can be reduced to a lower-order polynomial $\Phi(\mathbf{\xi})$. Particularly, for the quadratic minimization problems with linear inequality constraints in $\mathcal{X}_a$:

$$(P) : \min \left\{ \Pi(\mathbf{x}) = \frac{1}{2} \mathbf{x}^T \mathbf{Q} \mathbf{x} - \mathbf{x}^T \mathbf{f} | \ \mathbf{x} \in \mathcal{X}_a \right\}, \quad (52)$$
by choosing the quadratic transformation
\[ \xi = \Lambda(x) = x \bigotimes x \in \mathcal{E}_a \subseteq \mathbb{R}^{n \times n}, \] i.e., \( \xi = \{ \xi_{ij} \} = \{ x_i x_j \}, \ \forall 1 \leq i \leq j \leq n, \] (53)
where \( \bigotimes \) represents the Kronecker product (avoiding symmetric terms, i.e. \( \xi_{ij} = \xi_{ji} \)), the quadratic object \( W(w) \) can be reformulated as the following first-level RLT linear relaxation:
\[ W(x) = \frac{1}{2} x^T Q x = \frac{1}{2} \sum_{k=1}^{n} q_{kk} \xi_{kk} + \sum_{k=1}^{n-1} \sum_{l=k+1}^{n} q_{kl} \xi_{kl} = \Phi(\xi). \] (54)
The linear \( \Phi(\xi) \) can be considered as a special canonical function since \( \varsigma = \partial \Phi(\xi) \) is a constant and \( \Phi^*(\varsigma) = \langle \xi; \varsigma \rangle - \Phi(\xi) \equiv 0 \) is uniquely defined. Thus, using \( \Phi(\xi) = \langle \xi; \varsigma \rangle \) to replace \( W(x) \) and considering \( \xi \) as an independent variable, the problem \((P_q)\) can be relaxed by the following RLT linear program
\[ (P_{RLT}) : \min \{ \Phi(\xi) - \langle x, f \rangle \} \ | \ x \in \mathcal{X}_a, \ \xi \in \mathcal{E}_a \}. \] (55)
Based on this RLT linear program, a branch and bound algorithm was designed. It is proved that if \((\bar{x}, \bar{\xi})\) solves \((P_{RLT})\), then its objective value yields a lower bound of \((P_q)\) and \( \bar{x} \) provides an upper bound for \((P_q)\). Moreover, if \( \xi = \Lambda(\bar{x}) = \bar{x} \bigotimes \bar{x} \), then \( \bar{x} \) solves \((P_q)\).

This technique has been significantly adapted along with supporting approximation procedures to solve a variety of more general nonconvex constrained optimization problems having polynomial or more general factorable objective and constraint functions.

By the fact that for any symmetric \( Q \), there exists \( D \in \mathbb{R}^{n \times m} \) such that \( Q = D^T H D \) with \( H = \{ h_{kk} = \pm 1, \ h_{kl} = 0 \ \forall k \neq l \} \in \mathbb{R}^{m \times m} \), the canonicality condition can be simplified as
\[ W(Dx) = \frac{1}{2} (Dx)^T H (Dx) = \frac{1}{2} \sum_{k=1}^{m} h_{kk} \xi_{kk} = \Phi(\xi), \ \xi = \Lambda(x) = (Dx) \bigotimes (Dx) \in \mathbb{R}^{m \times m}. \] (56)
Clearly, if the scale \( m \ll n \), the problem \((P_{RLT})\) will be much easier than the problems using the geometrically nonlinear operator \( \xi = x \bigotimes x \). Moreover, if we using the Lagrange multiplier \( \varsigma \in \mathcal{E}_a^* = \{ \varsigma \in \mathbb{R}^{m \times m} \mid \langle \Lambda(x); \varsigma \rangle \geq 0 \ \forall x \in \mathbb{R}^n \} \) to relax the ignored geometrical condition \( \xi = \Lambda(x) \) in \((P_{RLT})\), the problem \((P_q)\) can be equivalently relaxed as
\[ (P_T) : \min \max \{ T(x, \xi, \varsigma) = \Phi(\xi) + \langle \Lambda(x) - \xi, \varsigma \rangle - \langle x, f \rangle \} \ | \ x \in \mathcal{X}_a, \ \xi \in \mathcal{E}_a, \ \varsigma \in \mathcal{E}_a^* } \}. \] (57)
Thus, if \((\bar{x}, \bar{\xi}, \bar{\varsigma})\) is a solution to \((P_T)\), then \( \bar{x} \) should be a solution to \((P_q)\). By using the sequential canonical quadratic transformation \( \Lambda(x) = \Lambda_p(\ldots (\Lambda_1(x) \ldots) \) (see Chapter 4, [11]), this technique can be used for solving general global optimization problems.

5 Symmetry, NP-Hardness and Perturbation Methods

The concept of symmetry is closely related to the duality and, in certain sense, can be viewed as a geometric duality. Mathematically, symmetry means invariance under transformation. By the canonicality, the object \( W(w) \) possesses naturally certain symmetry. If the subject \( F(\chi) = 0 \), then \( \Pi(\chi) = W(D\chi) = \Phi(\Lambda(\chi)) \) and \( (P) \) should have either a trivial solution or
multiple solutions due to the symmetry. In this case \( \Pi^d(\varsigma) = -\Phi^*(\varsigma) \) is concave and, by the triality theory, its critical point \( \tilde{\varsigma} \in \mathcal{S}_c^- \) is a global maximizer, \( \tilde{\chi} = [G(\tilde{\varsigma})]^f = 0 \) is the biggest local maximizer of \( \Pi(\chi) \), while the global minimizers must be \( \varsigma \in \partial \mathcal{S}_c^+ \) such that \( \Pi^d(\varsigma) = \min\{ -\Phi^*(\varsigma) \} \) for all edges. Strictly speaking, this is not a real-world problem but only a geometrical model. Without sufficient geometrical constraints in \( \mathcal{X}_n \), the graph is not physically fixed and any rigid motion is possible. However, by adding a linear perturbation \( \mathbf{f} \neq 0 \), this problem can be solved efficiently by the canonical duality theory \([67]\). Also it was proved by the author \([31, 39]\) that the general quadratic integer programming problem \((\mathcal{P}_{q_i})\) has a unique solution as long as the input \( \mathbf{f} \neq 0 \) is big enough. These results show that the subjective function plays an essential role for symmetry breaking to leads a well-posed problem. To explain the theory and understand the NP-hard problems, let us consider a simple problem in \( \mathbb{R}^n \):

\[
\min \left\{ \Pi(\mathbf{x}) = \frac{1}{2} \alpha (\frac{1}{2} \| \mathbf{x} \|^2 - \lambda)^2 - \mathbf{x}^T \mathbf{f} \quad \forall \mathbf{x} \in \mathbb{R}^n \right\},
\]

where \( \alpha, \lambda > 0 \) are given parameters. Let \( \Lambda(\mathbf{x}) = \frac{1}{2} \| \mathbf{x} \|^2 \in \mathbb{R} \), the canonical dual function is

\[
\Pi^d(\varsigma) = -\frac{1}{2} \varsigma^{-1} \| \mathbf{f} \|^2 - \lambda \varsigma - \frac{1}{2} \alpha^{-1} \varsigma^2,
\]

which is defined on \( \mathcal{S}_c = \{ \varsigma \in \mathbb{R} \mid \varsigma \neq -\lambda, \quad \varsigma = 0 \text{ iff } \mathbf{f} = 0 \} \). The criticality condition \( \partial \Pi^d(\varsigma) = 0 \) leads to a canonical dual equation

\[
(\alpha^{-1} \varsigma + \lambda) \varsigma^2 = \frac{1}{2} \| \mathbf{f} \|^2.
\]

This cubic equation has at most three real solutions satisfying \( \varsigma_1 \geq 0 \geq \varsigma_2 \geq \varsigma_3 \), and, correspondingly, \( \{x_i = f/\varsigma_i\} \) are three critical points of \( \Pi(\mathbf{x}) \). By the fact that \( \varsigma_1 \in \mathcal{S}_a^+ = \{ \varsigma \in \mathbb{R} \mid \varsigma \geq 0 \} \), \( \mathbf{x}_1 \) is a global minimizer of \( P(\mathbf{x}) \). While for \( \varsigma_2, \varsigma_3 \in \mathcal{S}_a^- = \{ \varsigma \in \mathbb{R} \mid \varsigma < 0 \} \), \( \mathbf{x}_2 \) and \( \mathbf{x}_3 \) are local min (for \( n = 1 \) and local max of \( \Pi(\mathbf{x}) \), respectively (see Fig. 2(a)).

![Graphs of \( \Pi(\mathbf{x}) \) (solid) and \( \Pi^d(\varsigma) \) (dashed) (\( \alpha = 1, \lambda = 2 \))]  

If we let \( \mathbf{f} = 0 \), the graph of \( \Pi(\mathbf{x}) \) is symmetric (i.e. the so-called double-well potential or the Mexican hat for \( n = 2 \) \([28]\)) with infinite number of global minimizers satisfying \( \| \mathbf{x} \|^2 = 2\lambda \).
In this case, the canonical dual \( \Pi^d(\varsigma) = -\frac{1}{2} \alpha^{-1} \varsigma^2 - \lambda \varsigma \) is strictly concave with only one critical point (local maximizer) \( \varsigma_3 = -\alpha \lambda < 0 \). The corresponding solution \( x_3 = f / \varsigma_3 = 0 \) is a local maximizer. By the canonical dual equation (60) we have \( \varsigma_1 = \varsigma_2 = 0 \) located on the boundary of \( S_\alpha^+ \), which corresponding to the two global minimizers \( x_{1,2} = \pm \sqrt{2 \lambda} \) for \( n = 1 \), see Fig. 1 (b). If we let \( f = -2 \), then the graph of \( \Pi(x) \) is quasi-convex with only one critical point. In this case, (60) has only one solution \( \varsigma_1 \in S_\alpha^+ \) (see Fig.1 (c)).

**Conjecture 2** For any given properly posed problem \((P)\) under the Assumption 1, there exists a constant \( f_c > 0 \) such that \((P^d)\) has a unique solution in \( S_\alpha^+ \) as long as \( \|f\| \geq f_c \).

This conjecture shows that any properly posed problems are not NP-hard if the input \( \|f\| \) is big enough. Generally speaking, most NP-hard problems have multiple solutions located either on the boundary or the outside of \( S_\alpha^+ \). Therefore, a quadratic perturbation method can be suggested as

\[
\Xi_{\delta_k}(\chi, \varsigma) = \Xi(\chi, \varsigma) + \frac{1}{2} \delta_k \| \chi - \chi_k \|^2 = \frac{1}{2} \langle \chi, G_{\delta_k}(\varsigma) \chi \rangle - \Phi^*(\varsigma) - \langle \chi, f_{\delta_k} \rangle + \frac{1}{2} \delta_k \langle \chi_k, \chi_k \rangle,
\]

where \( \delta_k > 0 \), \( \chi_k \ (k = 1, 2, \ldots) \) are perturbation parameters, \( G_{\delta_k}(\varsigma) = G(\varsigma) + \delta_k I \), and \( f_{\delta_k} = f + \delta_k \chi_k \). Thus, the original canonical dual feasible space \( S_\alpha^+ \) can be enlarged to \( S_{\delta_k}^+ = \{ \varsigma \in S_c | G_{\delta_k}(\varsigma) \succ 0 \} \) such that a perturbed canonical dual problem can be proposed as

\[
(P_{\delta_k}^d) : \max \left\{ \min \{ \Xi_{\delta_k}(\chi, \varsigma) \mid \chi \in X_a \} \mid \varsigma \in S_{\delta_k}^+ \right\}.
\]

Based on this problem, a canonical primal-dual algorithm has been developed with successful applications for solving sensor network optimization problems [61] and chaotic dynamics [52].

### 6 Challenges and Breakthrough

Now let us turn our attention to the most recent challenges from C. Zălinescu, who claimed in the beginning of his new paper [69]:

“We believe one of the main aims of [5] is to question our counter-examples in [7], [6], [8], [9], [10], [11], [12], [15], [16], [13], [14].”

Readers can easily verify this false assertion by checking the first version\(^{12}\) of [5]. Although the canonical duality-triality theory has been repeatedly challenged by Zălinescu with two co-workers in the 11 papers [6-14] and the author has been invited by journal editors to write responses, he didn’t do it as the mistakes in these papers are so basic and should be easily understood by experts in the communities. Also the author believes that the truth needs no defending. The only half paragraph of comments on these false challenges added in the revision of [5] was based on the reviewers’ comments. However, even these added comments are considered by Zălinescu as one of main aims of [5]. Indeed, Zălinescu has been fully alarmed on all author’s recent papers and anxious to against any comments on his basic mistakes (see [68]). Unfortunately, without correct motivation and necessary knowledge for understanding the canonical duality theory, more mistakes have been produced both ethically and mathematically.

\(^{12}\)posted at [http://arxiv.org/abs/1310.2014](http://arxiv.org/abs/1310.2014)
6.1 Mathematical Mistakes

Zălinescu’s first aim in [69] is to point out “a false assertion, a not convincing proof, a non adequate application of a result of the paper, several inconsistencies”.

The so-called “false assertion” discovered by Zălinescu is only a sentence in author’s paper [5], i.e. any convex quadratic function is objective. By using a “counterexample” $W(u,v) = u^2 + 2v^2$, Zălinescu proved that this assertion is false. However, it was written clearly in [2] (equation (2) on page 3) that the objective function must be in the form of $W(Du)$. If we simply let $D = \text{Diag}(1, \sqrt{2})$ and $w = D(u,v)^T = (u, \sqrt{2}v)^T$, then $W(w) = \|w\|^2$ is truly an objective function in $\mathbb{R}^2$. This basic mistake shows that Zălinescu works only on the one-scale artificial optimization problem (1) and does not understand the multi-scale modeling of [2], a foundation not only for the canonical duality theory, but also for entitle applied mathematics beautifully presented in G. Strang’s textbook [66] from the first chapter of linear algebra to the last content on optimization [13].

In the same section, Zălinescu complained that the Definition 6.1.2 of objective function in [1] is not clear at least because $\Omega \times W_0$ does not seem to be an “objective set”. This complain shows that Zălinescu is confused about the difference between optimization in $X_0 \subset \mathbb{R}^n$ and nonlinear analysis in continuous space $W_0 \subset \mathbb{L}^p(\Omega; \mathbb{R}^d)$, where $x \in \Omega$ is not an unknown and, as discussed in Section 2.3 of this paper, the stored energy $W(w) = \int_{\Omega} U(x,w) d\Omega$ is objective iff the stored energy density $U(x,w)$ is an objective function of $w \in W_0$. By any numerical approximation, $x$ will be disappeared such that $U(x,w) \simeq U_k(w)$ and $W(w) = \sum_k U_k(w)$.

Regarding the so-called “not convincing proof”, serious researcher should provide either a convincing proof or a disproof, rather than a complaint. Note that the canonical dual variables $\sigma_0$ and $\sigma_1$ are in two different levers (scales) with totally different physical units [14], it is completely wrong to consider $(\sigma_0, \sigma_1)$ as one vector and to discuss the concavity of $\Xi_1(x, (\cdot, \cdot))$ on $S_0^+$. The condition “$S_0^+$ is convex” in Theorem 2 [5] should be understood in the way that $S_0^+$ is convex in $\sigma_0$ and $\sigma_1$, respectively, as emphasized in Remark 1 [5]. Thus, the proof of Theorem 2 given in [5] is indeed convincing by simply using the classical saddle min-max duality for $(x, \sigma_0)$ and $(x, \sigma_1)$, respectively.

Regarding the non adequate application, it is easy to check $x_1$ is a global minimizer since $(\mu_1, \sigma_1) \in S_0^+$ and $S_0^+ = \{ (\mu, \sigma) \in \mathbb{R}^2 \mid \mu > 0, q + \mu \sigma > 0 \}$ is convex in $\mu$ and $\sigma$ for any given $q \in \mathbb{R}$. Thus, Example 1 is indeed an adequate application of Theorem 2 in [5]. Dually, Zălinescu’s modified stored energy function $W(Dx) = -\frac{1}{2} x^2$ in [69] is totally artificial (against the basic law in current physics and Assumption A1.1, A1.3), it is not surprise to have $\text{int} S_0^+ = \emptyset$, which is the case for many artificially produced NP-hard problems.

The several inconsistencies discovered by Zălinescu proved the triality in the mathematical modeling $(P_0)$, i.e. the subjective function $F(u) = -\langle u, \hat{u}^* \rangle$ is necessary for any real-world problems, including the paper writing. In physics, the input $\hat{u}^*$ could be defects, white noise, or random dislocation and charges, etc (see [34]). Although there are many such “inconsistencies” and even mistakes in his publications including [11][2], the author never write any erratum as he has been busy in search natural beauty but realized that nothing is perfect in this real world.

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13 MIT’s online teaching project was started from Gil Strang’s this textbook

14 Let us consider Example 1 in [5]. If the unit for $x$ is the meter $(m)$ and for $q$ is $Kg/m$, then the units for the Lagrange multiplier $\mu$ (dual to the constraint $g(x) = \frac{1}{2}(\frac{x^2}{2} - d^2 - e)$ should be $Kg/m^3$ and for $\sigma$ (canonical dual to $\Lambda(x) = \frac{1}{2} x^2$) should be $Kg/m$, respectively, so that each terms in $\Xi_1(x, \mu, \sigma)$ make physical sense.
Indeed, readers can easily find many typos and inconsistencies in Zălinescu’s papers, especially in his current short paper [69].

6.2 Non-Mathematical Mistakes

Zălinescu’s second aim in [69] is quibbling about the basic mistakes in their false challenges published in [6-14]. The author believes that by now serious researchers should have a clear understanding on the canonical duality-triality theory, its history and unified applications to multidisciplinary fields, so he has no intention to argue with Zălinescu on tedious issues but to point out some hidden truths in the arguments and ethical mistakes made in [69].

a*). In Section 2 a), Zălinescu wrote: “it is not possible to find a word containing ‘objeective’ in Gao-Strangs paper [2]. So we have not any reason to guess that W has to be ‘objective’ and F to be ‘subjective’. In fact D.Y. Gao introduced 11 years later the notion objective function in his book [1], and also refers to a book by P.G. Ciarlet published in 2013”.

Objectivity is a basic concept in continuum physics and is usually discussed in the beginning of textbooks, say page 8 in [55] (published in 1983). Any one who ever took a graduate course of nonlinear field theory should know that the stored energy \( W \) must be objective, therefore, most research papers don’t mention this basic requirement except some review/survey articles on interdisciplinary topics, say [18]. P.G. Ciarlet’s new book (2013) on nonlinear analysis [21] is based on his well-known book on nonlinear elasticity published in 1988, in which, this basic requirement is called the **axiom of objectivity** (see page 101 [20]). The mathematical definition of the objectivity given in author’s book (Definition 6.1.2 [1]) is based on Axiom 3.3-1 in [20], which is correct and clear for any mathematicians who know the difference between the coordinates \( t, x \in \Omega \) and the Lagrangian coordinates \( u(t, x) \). In Gao-Strang’s paper, the geometrical constraint in \( U_a \) is relaxed by the indicator \( \Psi_{U_a}(u) = \{0 \text{ if } u \in U_a, \infty \text{ if } u \notin U_a \} \) such that the “subjective function” is written as the **external super-potential** \( F(u) = -\langle u, \bar{u}^* \rangle + \Psi_{U_a}(u) \) (see equation (85) in [2]). It is a common sense that the minimum potential energy principle holds only for the so-called dead loading systems, i.e. the input \( \bar{u}^* = \partial F(u) \) is independent of the output \( u \). Thus the external energy \( F(u) \) must be linear on its effective domain. Otherwise, the system is not conservative and the traditional variational method can’t be applied. In order to solve such problems, a so-called rate-variational method was proposed by Gao and Onat in 1990 [38]. However, M.D. Voisei and C. Zălinescu oppositely choose piecewise linear function \( W \) and quadratic function \( F \) as counterexamples to against Gao and Strang’s paper with six conclusions including [10] “About the (complementary) gap function one can conclude that it is useless at least in the current context. The hope for reading an optimization theory with diverse applications is ruined . . . ” Clearly, this is a duality mistake.

Zălinescu continues in a) with: “we didn’t find any mention about ‘objective function’ with the meaning from [1, Definition 6.1.2] until 2010 in Gao’s articles, that is before submitting all our papers on Gao’s works”. However, in his open letter to the author [14], Zălinescu wrote: “In 2006 I proposed my former student R. Strugarui to study your theory. . . . Z2G 27 May 2008: Some time ago I bought your book mentioned below and I began to read it”. Clearly, Zălinescu indeed read the book [1] before 2010, where the objective function is mathematically defined. This contradiction proves that Zălinescu does not tell the truth in the arguments.

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15Zălinescu (2012): “Open letter to David Yang Gao” (version 1) posted on his university web page
Zălinescu wrote in b): “Indeed, we proved that practically all statements called ‘triality theorem’ in Gao’s papers published before 2010 are false”.

As discussed in Section 3.3, the triality theorem was correctly proposed in 1997 from a post-buckling problem, where \( \dim \Pi = \dim \Pi^d \) \[23\]. Mathematical proof was given in 2000 \[25\] for nonconvex variational problems. Generalization to global optimization was made in 2000. Sooner in 2002 \[27, 28\] the author discovered that the double-min duality does not hold in its strong form if \( \dim \Pi \neq \dim \Pi^d \). But the triality theorem was still presented correctly in the “either-or” form since the double-max duality is always true. Careful readers can find immediately that instead of the original paper \[25\], its applications \[36, 37\] were challenged and the three key papers \[23, 27, 28\] were never cited by Zălinescu and his co-workers in [6-14].

It is now necessary to examine how they proved the “false” of the triality theorem.

Among the 11 papers [6-14], seven of them against the triality theorem in global optimization. The so-called proof is mainly a set of “counterexamples” in [7,8,11,14-16] with \( \dim \Pi \neq \dim \Pi^d \), which is exactly the “additional condition” discovered by the author in [27, 28]. This should be the only reason why [27, 28] were not cited by these people. One counterexample in [9] is the case that \( \varsigma \in \partial S^+_c \), so Voisei and Zălinescu concluded: “The consideration of the function \( \Xi \) is useless, at least for the problem studied in [46].” However, it was proved in [58] that by simply using a line perturbation \( f \neq 0 \), this so-called “counterexample” can be solved nicely by the triality theorem to obtain all global optimal solutions.

The rest papers [6,10,12,13] challenged the triality theory in nonconvex analysis. As discussed above, “counterexamples” in [6] are simply using linear \( W \) and nonlinear \( F \) to against Gao-Strang’s paper [2]. It is very interesting to point out that, instead of arguing the mathematical proof given in [25], Voisei and Zălinescu challenged Gao and Ogden’s papers [36, 37], which are applications of [25]. By using “a thorough analysis” and a convention \( 0/0 := 0 \) in measure theory, they proved in [12,13] that the main result in triality theory is false and if \( \beta \neq 0 \) (i.e. \( f \neq 0 \)) the canonical dual \( \Pi^d(\varsigma) \) is not well-defined. Unfortunately, they don’t know a basic truth guaranteed by the canonical duality theory, i.e. if \( f \neq 0 \), then \( \varsigma \to 0 \) can never happen (see Equation (60)), otherwise, Newton’s third law will be violated. Therefore, \( \Pi^d(\varsigma) \) is indeed well-defined. Also, the constitutive law \( \varsigma = \partial \Phi(\xi) \) for phase transitions in continuum mechanics holds only at the scale about \( \varsigma \sim 10^{-3} \text{m} \). Even the quantum mechanics can’t reach the scale of zero measure. Therefore, their papers [12,13] were rejected. However, Voisei and Zălinescu couldn’t understand their basic mistakes and had serious arguments with editors of these two decent mathematical physics journals.

The most funny mistake ever made by Zălinescu and his co-workers could be the one in their paper [6] published in a dynamical systems journal. As it is known that the bi-duality was first proposed and proved by the author for convex Hamiltonian systems [11], where the Lagrangian must be in its standard form \( L(q, p) \), i.e. Equation (12) in Lagrangian mechanics. Instead of finding any possible mistakes in author’s proof, Strugariu, Voisei and Zălinescu created an artificial “Lagrangian”:

\[
L(x, y) := -\frac{1}{2} \alpha \|x\|^2 - \frac{1}{2} \beta \|y\|^2 + \langle a, x \rangle \langle b, y \rangle,
\]

(Equation (1) in [6])

\[16\]The reference [16] is [3] in [9]
\[17\]see comments and links posted on http://arxiv.org/abs/1202.3515 and http://arxiv.org/abs/1101.3534
By using this “Lagrangian” as well as the associated “total action” and its Legendre dual

\[
f(x) = \max\{L(x, y) | y \in Y\} = -\frac{1}{2}\alpha\|x\|^2 + \frac{1}{2}\beta^{-1}(a, x)^2\|b\|^2 \quad \forall x \in X
\]

\[
g(y) = \max\{L(x, y) | x \in X\} = -\frac{1}{2}\beta\|y\|^2 + \frac{1}{2}\alpha^{-1}(b, y)^2\|a\|^2 \quad \forall y \in Y
\]

they produced a series of very strange counterexamples to against the bi-duality theory in convex Hamiltonian systems and the triality theory in geometrically nonlinear systems presented respectively by the author in Chapters 2 and 3 [1]. They claimed: “Because our counterexamples 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.”

Clearly, the quadratic function \(L(x, y)\) is totally irrelevant to the Lagrangian \(L(q, p)\) in Lagrangian mechanics and Gao’s book [1]. Without the differential operator \(D = \partial_t\), the quadratic d.c. function \(f(x)\) (or \(g(y)\)) is defined on one-scale space \(X\) (or \(Y\)) and is unbounded. Therefore, it’s critical point does not produce any motion. This basic mistake shows that these people don’t have basic knowledge not only in Lagrangian mechanics (vibration produced by the duality between the kinetic energy \(T(\partial_t u)\) and the potential energy \(U(u)\)), but also in d.c. programming (unconstrained quadratic d.c. programming does not make any sense [49]). It also shows that these people even don’t know what the Lagrangian coordinate is, otherwise, they would never use a time-independent vector \(x \in \mathbb{R}^n\) as an unknown in dynamical systems and Zălinescu wouldn’t complain the definition of the objectivity given in [1].

Moreover, the triality theory was developed from geometrically nonlinear systems, where the geometrical operator \(\Lambda(u)\) must be nonlinear in order to have canonicality condition (A1.2) and the triality theory (see [26]). By the fact that only the geometrical nonlinearity can produce multiple local minimizers, this is the reason why this terminology was emphasized in the title of Gao-Strang’s paper [2]. However, in [6] Strugariu, Voisei and Zălinescu choose either a null \(\Lambda(u) = 0\) (Example 3.4) or a linear \(\Lambda(u) = \langle a, u \rangle b\) (Example 3.5) as counterexamples to prove the false of the triality. These mistakes show that these people really don’t understand both the geometrical nonlinearity and the triality theorem.

Even more, since there is neither input in \(L(x, y)\) nor initial/boundary conditions in \(X\), all counterexamples they produced are simply not problems but only artificial “models”. Since they don’t follow the basic roles in mathematical modeling, such as the objectivity, symmetry, conservation and constitutive laws, etc, these artificial “models” are very strange and even ugly (see Examples 3.3, 4.2, 4.4 [6]).

All these conceptual mistakes show that Zălinescu and his two co-workers don’t know what they are doing: without understanding the title (geometrical nonlinearity) of [2] and the basic contents (objectivity, stored energy and external energy) in nonlinear analysis, they published the paper [10] in Applicable Analysis to against Gao-Strang’s work in nonlinear analysis; without necessary knowledge of Lagrangian mechanics they published the paper [6] in Discrete & Continuous Dynamical Systems-A to challenge Gao’s book on convex Hamiltonian systems. Readers are suggested to check the special issues of these two journals to understand why these papers can be published.

c*) Zălinescu wrote in c): “I ask the authors of [5] to give precise references where our counter-examples can be found in Gao’s works (or elsewhere); otherwise the statement “these so-called counterexamples are not new, which were first discovered by Gao” is a calumny.”
All these counter-examples are simply using the condition $\dim \Pi \neq \dim \Pi^d$ to against the double-min duality. Indeed, such a type of counter-examples is too simple, i.e. the double-well problem \cite{58} with $n \geq 2$, which can be found easily in author’s book \cite{1} and many articles, say \cite{25,26,27,29}. Precisely, Example 5.1 in \cite{27} and Example (2.14) in \cite{28} are the counter-examples first discovered by the author in 2003. So it was written clearly in Remark 1 on page 481 \cite{27} and Remark of Theorem 3 on page 288 \cite{28} that the double-min duality \cite{35} holds “under certain additional conditions”. It has been proved either in author’s book \cite{1} or in recent papers \cite{3,4,19,45} that $\dim \Pi = \dim \Pi^d$ is the only condition for the double-min duality. Anyone who knows the logic will surely understand the counterexamples discovered by Gao in 2003 must be the same type as those listed in \cite{6-14} by Zălinescu et al. The only reason why the author didn’t write down specifically the condition $\dim \Pi \neq \dim \Pi^d$ in \cite{27,28} is that he was not sure if there is any other conditions, so he was prefer to leave this uncertainty as an open problem to readers, which is author’s philosophy as the old saying;“hidden harmony is stronger than the explicit one”. Serious researchers may ask why such simple duplicated “counter-examples” can be published repeatedly in the international journals without citing \cite{27,28}?

As Zălinescu indicated in his open letter, the author is indeed one of three reviewers for his paper \cite{11} and Gao’s papers \cite{27,28} were pointed out in all the three reviewers’ reports\cite{18}. Unfortunately, Voice and Zălinescu still refuse to cite these two key papers in their revision \cite{11} but simply deleted the similar sentence “a correction of this theory is impossible without falling into trivia” as they conclude in \cite{6}. Since 2012 the author and his co-workers proved that even if $\dim \Pi \neq \dim \Pi^d$, the double-min duality still holds weakly in a beautiful symmetrical form \cite{19,45,59}. Zălinescu knows these progress, at least the paper \cite{4}, so his own statement in \cite{69} “Indeed, we proved that practically all statements called ‘triality theorem’ in Gao’s papers published before 2010 are false” is truly a calumny.

d*). In d) Zălinescu wrote: “Indeed, we never cited Gao’s papers \cite{6,7}\cite{19}. The simple reason is that we learned about the so called open problem from Gao’s paper \cite{6} (see footnote 4) from 2 reports on our paper \cite{11}, received on 06.05.2010; at that moment (06.05.2010) all the 11 papers were already submitted.”

As we know that Zălinescu has begun interesting in the canonical duality theory at least from 2006. At that time, the author published a very few papers in optimization journals. It is difficult to believe that Zălinescu didn’t read \cite{27} before to criticize this theory. Indeed, any people, if they simply check \cite{14}, should know immediately that this paper by Voisei and Zălinescu was submitted to the journal on 27.4.2011, i.e. almost one year after “that moment (06.05.2010)” (also the author is a reviewer, both \cite{27,28} were mentioned in the report), but neither \cite{27} nor \cite{28} was cited by these people. This contradiction shows again that Zălinescu does not tell the truth in \cite{69}. So there is no need to continue this discussion.

All the conceptual and mathematical mistakes in this set of published/rejected papers \cite{6-14} by Zălinescu and his two co-workers show a significant gap between their “thorough mathematics” and the applicable mathematics that the canonical duality-triality is based on.

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\textsuperscript{18}The author thanks these two reviewers for forwarding their reports. The second reviewer indicated specifically the Remark 1 in Gao’s paper \cite{27} and he recommended these people to “present their ‘counter-examples’ more as ‘examples ... ’”. The third reviewer wrote clearly “but counterexamples had already been discovered by Gao in his earlier paper”.

\textsuperscript{19}i.e. Gao’s paper \cite{27,28}
As V.I. Arnold concluded in his address \[17\]: “A teacher of mathematics, who has not got to grips with at least some of the volumes of the course by Landau and Lifshitz, will then become a relict like the one nowadays who does not know the difference between an open and a closed set.”

7 Conclusions

Based on necessary conditions and basic laws in physics, a unified multi-scale global optimization problem is proposed in the canonical form:

\[
\Pi(\chi) = W(D\chi) + F(\chi) = \Phi(\Lambda(\chi)) - \langle \chi, f \rangle.
\]

(62)

The object \( W \) depends only on the model and \( W(w) \geq 0 \forall w \in W_a \) is necessary; \( W \) should be an objective function for physical systems, but it is not necessary for artificial systems (such as management/manufacturing processes and numerical simulations, etc). The subject \( F \) depends on each properly posed problem and must satisfy \( F(\chi) \leq 0 \) together with necessary geometrical constraints for the output \( \chi \in X_a \) and equilibrium conditions for the input \( f \in X^* \).

The geometrical nonlinearity of \( \Lambda(\chi) \) is necessary for nonconvexity in global optimization, bifurcation in nonlinear analysis, chaos in dynamics, and NP-hardness in computer science.

Developed from large deformation nonconvex analysis/mechanics, the canonical duality-triality is a precise mathematical theory with solid foundation in physics and natural root in philosophy, so it is naturally related to the traditional theories and powerful methods in global optimization and nonlinear analysis. By the fact that the canonical duality is a universal law of nature, this theory can be used not only to model real-world problems, but also for solving a wide class of challenging problems in multi-scale complex systems. The conjectures proposed in this paper can be used for understanding and clarifying NP-hard problems.

Both the linear operator \( D \) and the geometrical admissible operator \( \Lambda \) can be generalized to the composition forms

\[
D = D_n \circ \cdots \circ D_1, \quad \Lambda(\chi) = \Lambda_m(\Lambda_{m-1}(\cdots(\Lambda_1(\chi))\cdots))
\]

(63)

in order to model high-order multi-scale problems (see Chapter 4 \[1\] and \[29, 47, 48\]).

In the set of 12 (= \([6-14] + [69]\)) papers, M.D. Voisei, C. Zălinescu and his former student R. Strugariu have made either mathematical mistakes (failed to correctly understand the canonical duality-triality theory and basic concepts in physics and nonlinear analysis), or ethic mistakes (repeatedly using the same condition \( \dim \Pi \neq \dim \Pi_d \) as “counter-examples” to against the double-min duality without citing author’s original papers \[27, 28\], wherein this condition was first discovered). The mathematical mistakes show a huge gap between mathematical optimization and nonlinear analysis/mechanics. It is author’s hope that by reading this paper, the readers can have a clear understanding not only on the canonical duality-triality theory and its potential applications in multidisciplinary fields, but also on the generalized duality-triality principle and its role in modeling/understanding real-world problems.

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