

DUALITY AND TRIALITY: Unify Mathematical Physics and Global Optimization

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1 Introduction

The term *duality* used in our daily life means the sort of harmony of two opposite or *complementary* parts by which they integrate into a whole. Inner beauty in natural phenomena is bound up with duality, which has always been a rich source of inspiration in human knowledge through the centuries. Duality in mathematics, roughly speaking, is a fundamental concept that underlies many aspects of extremum principles in natural systems. Eigenvectors, geodesics, minimal surfaces, KKT conditions, Hamiltonian canonical equations and equilibrium states of many field equations are all critical points of certain functions on some appropriate constraint sets or manifolds. By using abstract languages, a common mathematical structure can be found in many physical theories. This structure is independent of the physical contents of the system and exists in wider classes of problems in engineering and sciences (see Strang [17]). Considerable attention has been attracted on this fascinating research subject during the last years. A comprehensive study on duality theory in general nonconvex systems was given D.Y. Gao [4]. Generally speaking, duality in mathematical physics falls principally into three categories: (1) the classical saddle Lagrange duality (i.e. mono-duality) in convex optimization and static systems, (2) the nice bi-duality in convex Hamilton systems or the d.c. programming (difference of convex functions) and (3) the interesting tri-duality in general nonconvex systems.

This paper presents a brief survey and some new developments on the duality and triality theories in general nonconvex and nonconservative systems. By using the *canonical dual transformation method* developed recently, certain NP-hard nonconvex problems in n-dimensional space can be converted into a one-dimensional algebraic system. The triality theory reveals some interesting extremality properties and intrinsic symmetry in nonconvex, nonconservative systems. Based on this theory, a primal-dual algorithms is proposed for solving general nonconvex problems. Application is illustrated by a semi-linear, nonconvex parametric variational problem. Complete solutions are obtained in n-dimensional space.

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2 Problems And Motivations

The problem in nonsmooth, nonconvex, and nonconservative systems is of significant practical importance and has attracted considerable attention during the last years. As it was shown in the author's recent work (see Gao, 1998-2001) that by introducing certain suitable bilinear forms, many nonlinear, nonconvex systems, either conservative or dissipative, can be written in the following stationary variational problem

$$(\mathcal{P}) : \quad \Pi(u) \rightarrow \text{sta} \quad \forall u \in \mathcal{U}_k, \quad (1)$$

where the feasible space \mathcal{U}_k is a convex, non-empty subset of the configuration (or state) space \mathcal{U} , in which, the essential boundary-initial conditions and certain constraints are prescribed; $\Pi : \mathcal{U}_k \rightarrow \mathbb{R}$ is the total action of the system; the notation $\Pi(u) \rightarrow \text{sta} \quad \forall u \in \mathcal{U}_k$ stands for finding the stationary (or critical) points of Π over the feasible space \mathcal{U}_k .

The general variational form of the problem (\mathcal{P}) covers a great variety of situations. Very often, we have $\Pi(u) = K(\partial_t u) - P(u)$, where $\partial_t : \mathcal{U}_k \rightarrow \mathcal{V}$ is a time-differential operator from \mathcal{U}_k to the space of velocity \mathcal{V} ; the functional $K(v)$ stands for the total kinetic energy of the system, and $P : \mathcal{U}_k \rightarrow \mathbb{R}$ is the total potential of the system. In Newtonian mechanics, the operator ∂_t is simply the time derivative $\partial/\partial t$, the kinetic energy $K(v)$ is usually a convex (quadratic) Gâteaux differentiable functional, and the velocity-momentum relation $p = DK(v)$ is invertible. The complementary kinetic energy $K^*(p)$ can be obtained easily by the classical *Legendre transformation* $K^*(p) = \langle v(p) \cdot p \rangle - K(v(p))$, where $\langle * \cdot * \rangle$ stands for the bilinear form between the velocity space \mathcal{V} and its dual space \mathcal{V}^* , i.e. the momentum space. Furthermore, we let $\langle *, * \rangle : \mathcal{U} \times \mathcal{U}^*$ be the bilinear form between \mathcal{U} and its dual space \mathcal{U}^* , i.e. the force space, then the adjoint operator $\partial_t^* : \mathcal{V}^* \rightarrow \mathcal{U}^*$ can be defined by

$$\langle \partial_t u \cdot p \rangle = \langle u, \partial_t^* p \rangle.$$

Thus, if the total potential $P : \mathcal{U}_k \rightarrow \mathbb{R}$ is Gâteaux differentiable, the stationary condition $D\Pi(u) = 0$ leads to the abstract Euler-Lagrange equation:

$$\partial_t^* DK(\partial_t u) - DP(u) = 0. \quad (2)$$

If the total potential $P(u)$ is convex, then the total action $\Pi(u)$ of the system is a so-called *d.c. functional*, i.e., the difference of convex functionals. In this case, the classical Hamiltonian $H(u, p) = K^c(p) + P(u)$ is a convex functional and the Euler-Lagrange equation (2) can be written in the generalized *canonical Hamiltonian forms* (see Gao, 2000):

$$\partial_t u = D_p H(u, p) = DK^c(p), \quad \partial_t^* p = D_u H(u, p) = DP(u).$$

From traditional point view of Hamilton mechanics, the canonical Hamilton forms hold only for conservative systems. It was shown in author's book (Gao, 2000a) that as long as we can choose certain suitable weight function, the generalized canonical Hamilton also hold for dissipative systems. For example, let us consider the simplest second order, ordinary differential equation over the time domain $I = (0, t_c)$ with linear dissipation

$$u_{,tt} + \omega(t)u_{,t} + f(u) = 0, \quad (3)$$

where $p(t)$ is a given non-negative function on I , which describes the dissipation of the system; $f(u) = DP(u)$ is a potential field and P is a given potential. Introducing the

weight function $w(t) = \exp(\int \omega(t) dt)$, the bilinear forms $\langle *, * \rangle$ and $\langle * \cdot * \rangle$ can be defined as

$$\langle u, u^* \rangle = \int_I w(t) u u^* dt, \quad \langle v \cdot v^* \rangle = \int_I w(t) v p^* dt.$$

Then, by integration by parts, the formal adjoint operator of $\partial_t = \frac{d}{dt}$ is $\partial_t^* = -\partial_t - \omega(t)$. The kinetic energy for this dissipative system is a weighted quadratic functional $K(v) = \int_I \frac{1}{2} w(t) v^2 dt$. If the total potential P is also a quadratic functional, say $P(u) = \int_I \frac{1}{2} w(t) u^2 dt$, then (3) is a linear equation. In this case, the weight function $w(t)$ is nothing but the Wronskian of any two linearly independent solutions of the system.

For conservative systems, the weight function $w = 1$, and the canonical Hamilton forms take a traditional skew-symmetrical structure

$$u_{,t} = D_p H(u, p), \quad p_{,t} = -D_u H(u, p).$$

However, this nice symmetry is broken in nonsmooth, nonconvex systems.

Generally speaking, many efficient numerical methods in nonlinear variational analysis and mathematical programming are based on the (at least local) convexity of the cost function. Numerical results produced by these methods convergence only to certain local minimizers. In nonconvex systems with multi-minimizers, different step size and initial conditions might lead to different numerical results. In nonlinear dynamical systems, the so-called *chaotic phenomenon* of a nonlinear dynamical system is mainly due to the nonconvexity of the total potential of the system. Very small perturbations of the system's initial conditions and parameters may lead the system to different potential wells with significantly different performance characteristics. The numerical results vary with the methods used (cf. e.g., Gao, 2000a). This is the one of main reasons why the traditional perturbation analysis and the direct approaches cannot successfully be applied to chaotic systems.

Duality theory plays fundamental roles in natural phenomena. Actually, the concept of the subdifferential and associated Fenchel-Moreau transformation leads naturally to a beautiful duality theory in convex analysis (cf. e.g. Ekeland and Temam, 1976). During the last decade, the so-called *primal-dual interior point method* has emerged as the most important and efficient revolutionary technique in mathematical programming (cf. e.g., Wright, 1998). The advantage of the primal-dual approaches relying on a common mathematical structure that underlies many physical theories. Actually, the so-called *canonical dual transformation method* developed recently is based on this fundamental structure. The key idea of this potentially useful method is to choose a suitable geometrical mapping Λ from $\mathcal{U}_a \subset \mathcal{U}$ into an another canonical space \mathcal{W} such that the total action can be written in the difference of canonical functionals, i.e. $\Pi(u) = \Phi(\Lambda(u)) - \Psi(u)$. By the definition introduced in [Gao, 2000a], a real valued functional $\Psi : \mathcal{U}_a \subset \mathcal{U} \rightarrow \mathbb{R}$ is called the canonical functional on \mathcal{U}_a if it is Gâteaux differentiable, either convex or concave, and the duality relations

$$u^* = D\Psi(u) \Leftrightarrow u = D\Psi^*(u^*) \Leftrightarrow \Psi(u) + \Psi^*(u^*) = \langle u, u^* \rangle \quad (4)$$

hold on $\mathcal{U}_a \times \mathcal{U}_a^* \subset \mathcal{U} \times \mathcal{U}^*$; where $\Psi^* : \mathcal{U}_a^* \rightarrow \mathbb{R}$ is the *canonical conjugate functional* of Ψ , defined by the canonical Legendre transformation

$$\Psi^*(u^*) = \text{sta}_{u \in \mathcal{U}_a} \{ \langle u, u^* \rangle - \Psi(u) \}. \quad (5)$$

It was shown in the author's book (Gao, 2000a) that if the primal functionals $\Psi(u)$ and $\Phi(\xi)$ are nonsmooth, their canonical Legendre conjugates $\Psi^*(u^*)$ and $\Phi^*(\xi^*)$ might be smooth. Thus, by using this canonical dual transformation, many nonsmooth primal problems can be transformed into smooth dual problems. The system is called *geometrically linear (resp. nonlinear)* if $\Lambda : \mathcal{U} \rightarrow \mathcal{W}$ is a linear (resp. nonlinear) mapping. A self-contained comprehensive presentation of this canonical dual transformation method in general nonconvex, nonsmooth systems was given recently by Gao (2000a).

In this paper, we will show that the canonical dual transformation method can also be used in general nonsmooth, nonconvex and nonconservative systems, where Φ is usually a saddle-functional. The next section will discuss bi-duality and bi-polarity principles in geometrically linear systems; while the geometrically nonlinear systems will be discussed in Section 4. Based on the triality theory, discovered recently in nonlinear bifurcation and phase transitions, a potentially useful triality algorithm is proposed for solving general problems in nonsmooth/nonconvex dynamical systems. Application in semi-linear nonconvex systems is illustrated in the last section. Some new phenomena in chaotic systems are presented and a tri-duality theorem is obtained, which can be used for solving nonconvex problems in phase transitions and super-conductivity.

3 Bi-Duality And Bi-Polarity Principles

Recall that a nonsmooth dynamical system is called a geometrically linear if there exists a linear operator $\Lambda : \mathcal{U}_a \subset \mathcal{U} \rightarrow \mathcal{W}_a \subset \mathcal{W}$ such that $\Psi : \mathcal{U}_a \rightarrow \mathbb{R}$ and $\Phi : \mathcal{W}_a \rightarrow \mathbb{R}$ are canonical functionals and the feasible space $\mathcal{U}_k = \{u \in \mathcal{U}_a \mid \Lambda u \in \mathcal{W}_a\}$, then the primal problem (\mathcal{P}) can be written in the following canonical form

$$(\Pi) : \quad \Pi(u) = \Phi(\Lambda u) - \Psi(u) \rightarrow \text{sta} \quad \forall u \in \mathcal{U}_k, \quad (6)$$

Let \mathcal{W}^* be the dual space of \mathcal{W} defined by the bilinear form $\langle *, * \rangle : \mathcal{W} \times \mathcal{W}^* \rightarrow \mathbb{R}$, and $\Lambda^* : \mathcal{W}^* \rightarrow \mathcal{U}^*$ the adjoint operator of $\Lambda : \mathcal{U} \rightarrow \mathcal{W}$ associated with this bilinear form. If Π is Gâteaux differentiable on \mathcal{U}_k , the stationary condition of Π leads to the canonical governing equation

$$\Lambda^* D\Phi(\Lambda u) - D\Psi(u) = 0. \quad (7)$$

It is known that if the canonical functional Φ is nonsmooth at $\xi = \Lambda(u)$, the Gâteaux derivative of Φ is not unique at ξ . So the traditional direct methods for solving this nonsmooth variational problem are difficult. By the fact that the canonical conjugate $\Phi^* : \mathcal{W}^* \rightarrow \mathbb{R}$ might be smooth on a subset $\mathcal{W}_a^* = \{\xi^* \in \mathcal{W}^* \mid \xi^* = D\Phi(\xi) \quad \forall \xi \in \mathcal{W}_a\}$, and the duality relations

$$\xi^* = D\Phi(\xi) \Leftrightarrow \xi = D\Phi^*(\xi^*) \Leftrightarrow \Phi(\xi) + \Phi^*(\xi^*) = \langle \xi; \xi^* \rangle \quad (8)$$

hold on $\mathcal{W}_a \times \mathcal{W}_a^*$, the Lagrangian $\Xi : \mathcal{Z}_a = \mathcal{U}_a \times \mathcal{W}_a^* \rightarrow \mathbb{R}$ associated with the canonical primal problem has the standard form:

$$\Xi(u^*, \xi^*) = \langle \Lambda u; \xi^* \rangle - \Phi^*(\xi^*) - \Psi(u). \quad (9)$$

Since $\Phi : \mathcal{W}_a \rightarrow \mathbb{R}$ is a canonical functional, by the duality relation (8) it is easy to check that for each fixed $u \in \mathcal{U}_k$

$$\Pi(u) = \text{sta}\{\Xi(u, \xi^*) \quad \forall \xi^* \in \mathcal{W}_a^*\}.$$

On the other hand, for each fixed $\xi^* \in \mathcal{W}_a^*$, the dual action $\Pi^d(\xi^*)$ associated with the primal problem (II) can be defined by

$$\Pi^d(\xi^*) = \text{sta}_{u \in \mathcal{U}_a} \Xi(u, \xi^*) = \Psi^*(\Lambda^* \xi^*) - \Phi^*(\xi^*), \quad (10)$$

where the conjugate functional $\Psi^*(u^*)$ is defined by

$$\Psi^*(\Lambda^* \xi^*) = \text{sta} \{ \langle u, \Lambda^* \xi^* \rangle - \Psi(u) \mid \forall u \in \mathcal{U}_a \}. \quad (11)$$

In the case that the canonical functional Ψ is either convex or concave, the criticality condition of this problem leads to the balance inclusion $\Lambda^* \xi^* \in \partial \Psi(\bar{u})$, where $\partial = \{\partial^-, \partial^+\}$ stands for either sub-differential ∂^- or super-differential ∂^+ . Let $\mathcal{U}_a^* = \{u^* \in \partial \Psi(u) \mid \forall u \in \mathcal{U}_a\}$, and

$$\mathcal{W}_k^* = \{\xi^* \in \mathcal{W}_a^* \mid \Lambda^* \xi^* \in \mathcal{U}_a^*\} \quad (12)$$

be the *dual feasible space*. Since $\Psi : \mathcal{U}_a \rightarrow \mathbb{R}$ is a canonical functional, the duality relation (4) holds on $\mathcal{U}_a \times \mathcal{U}_a^*$, and for each given $\xi^* \in \mathcal{W}_k^*$, the conjugate $\Psi^*(\Lambda^* \xi^*)$ is well defined. Thus, the canonical dual problem associated with (II) can be proposed as the following

$$(\Pi^d) : \quad \Pi^d(\xi^*) = \Psi(\Lambda^* \xi^*) - \Phi^*(\xi^*) \rightarrow \text{sta} \quad \forall \xi^* \in \mathcal{W}_k^*. \quad (13)$$

Theorem 1 (Complementarity Theorem) *Suppose that \mathcal{U}_k and \mathcal{W}_k^* are not empty. If $(\bar{u}, \bar{\xi}^*) \in \mathcal{U}_a \times \mathcal{W}_a^*$ is a critical point of Ξ , then $(\bar{u}, \bar{\xi}^*) \in \mathcal{U}_k \times \mathcal{W}_k^*$, and \bar{u} is a critical point of Π , $\bar{\xi}^* \in \mathcal{W}_k^*$ is a critical point of Π^d , and*

$$\Pi(\bar{u}) = \Xi(\bar{u}, \bar{\xi}^*) = \Pi^d(\bar{\xi}^*). \quad (14)$$

This theorem shows that the canonical problems (II) and (Π^d) are equivalent and the complementarity condition (18) holds for all critical points of Ξ . Thus, for a given nonsmooth primal problem, if there exists a linear operator $\Lambda : \mathcal{U} \rightarrow \mathcal{W}$ such that the canonical conjugate functionals Φ^* and Ψ^* are smooth, the canonical dual problem is much easier than the primal one. It was shown in the author's book [Gao, 2000a] that in geometrically linear static systems, the Lagrangian $\Xi(u, \xi^*)$ is usually a saddle functional (say convex in u and concave in ξ^*). In this case, we have the traditional min-max (or mono-) duality theory, i.e.

$$\Pi(\bar{u}) = \inf_{u \in \mathcal{U}_a} \sup_{\xi^* \in \mathcal{W}_a^*} \Xi(u, \xi^*) = \sup_{\xi^* \in \mathcal{W}_a^*} \inf_{u \in \mathcal{U}_a} \Xi(u, \xi^*) = \Pi^d(\bar{\xi}^*).$$

However, in convex Hamilton systems, $\Xi(u, \xi^*)$ is the so-called *super-Lagrangian* (concave in both u and ξ^*), and its extremality conditions are controlled by the following theorem.

Theorem 2 (Bi-duality Theorem) *Suppose that both the canonical functionals $\Phi : \mathcal{W}_a \rightarrow \mathbb{R}$ and $\Psi : \mathcal{U}_a \rightarrow \mathbb{R}$ are convex. For each critical point $(\bar{u}, \bar{\xi}^*)$ of Ξ , we have either*

$$\Pi(\bar{u}) = \inf_{u \in \mathcal{U}_k} \Pi(u) = \inf_{\xi^* \in \mathcal{W}_k^*} \Pi^d(\xi^*) = \Pi^d(\bar{\xi}^*), \quad (15)$$

or

$$\Pi(\bar{u}) = \sup_{u \in \mathcal{U}_k} \Pi(u) = \sup_{\xi^* \in \mathcal{W}_k^*} \Pi^d(\xi^*) = \Pi^d(\bar{\xi}^*). \quad (16)$$

This bi-duality theorem shows that in periodic convex Hamilton systems, the least action principle is no longer true on the whole time domain. The extremality condition of the critical points are controlled by both double-min (15) and double-max (16) laws.

In many applications the functional $\Psi(u)$ is usually linear, i.e. $\Psi(u) = \langle u, u_0^* \rangle$, where $u_0^* \in \mathcal{U}^*$ is a given input. In this case, the dual feasible space is a linear manifold:

$$\mathcal{W}_k^* = \{\xi^* \in \mathcal{W}_a^* \mid \langle u, \Lambda^* \xi^* - u_0^* \rangle \quad \forall u \in \mathcal{U}_a\},$$

and the dual action takes a very simple form: $\Pi^d(\xi^*) = -\Phi(\xi^*)$. In order to relax the balance constraint $\Lambda^* \xi^* = u_0^*$ in the dual feasible space \mathcal{W}_k^* , we let

$$\xi^* = \xi_o^* + \xi_p^* \quad \text{such that} \quad \Lambda^* \xi_o^* = 0, \quad \Lambda^* \xi_p^* = u_0^*,$$

where ξ_o^* is a homogeneous solution of the balance equation; while ξ_p^* is a nonhomogeneous solution of the balance equation $\Lambda^* \xi_p^* = u_0^*$. Let \mathcal{U}^o be the so-called *polar configuration space*, placed in duality with \mathcal{U}^{o*} by the bilinear form $\langle *, * \rangle : \mathcal{U}^o \times \mathcal{U}^{o*} \rightarrow \mathbb{R}$. For the given geometrically linear system and $\Lambda : \mathcal{U} \rightarrow \mathcal{W}$, a linear mapping $\Lambda^o : \mathcal{U}^o \rightarrow \mathcal{W}^*$ is said to be a *null-source polar operator* of Λ if (see Gao, 2000a)

$$\langle \Lambda u; \Lambda^o u^o \rangle = \langle u, \Lambda^* \Lambda^o u^o \rangle = \langle {}^o \Lambda \Lambda u, u^o \rangle = 0, \quad (17)$$

where ${}^o \Lambda : \mathcal{W} \rightarrow {}^o \mathcal{U}$ is the adjoint operator of Λ^o . Clearly, if there exists a subset $\mathcal{U}_a^o \subset \mathcal{U}^o$ such that (17) holds for any given $u^o \in \mathcal{U}_a^o \subset \mathcal{U}^o$, then

$${}^o \Lambda \Lambda u = 0 \in {}^o \mathcal{U}, \quad (18)$$

which is the so-called *compatibility condition*. On the other hand, if (17) holds for any $u \in \mathcal{U}_a$, then the equation

$$\Lambda^* \Lambda^o u^o = 0 \in \mathcal{U}^* \quad (19)$$

is called *polar compatibility condition* (Gao, 2000a). For a given operator $\Lambda : \mathcal{U}_a \rightarrow \mathcal{W}$, the *null-source admissible polar configuration space* $\mathcal{U}_a^o \subset \mathcal{U}^o$ is defined by

$$\mathcal{U}_a^o = \{u^o \in \mathcal{U}^o \mid \langle \Lambda u; \Lambda^o u^o \rangle = 0 \quad \forall u \in \mathcal{U}_a\}. \quad (20)$$

Thus, for any given $u^o \in \mathcal{U}_a^o$, $\xi_o^* = \Lambda^o u^o$ is in the null space of the balance operator Λ^* . For a given particular solution $\xi_p^* \in \partial \Psi(u)$, replacing ξ^* by $\xi^* = \Lambda^o u^o + \xi_p^* \in \mathcal{W}_k^*$, and letting $\Phi^o(u^o) = \Phi^*(\Lambda^o u^o + \xi_p^*)$, the so-called *polar action* $\Pi^o(u^o)$ can be obtained as

$$\Pi^o(u^o) = \Pi^d(\Lambda^o u^o + \xi_p^*) = -\Phi^o(\Lambda^o u^o). \quad (21)$$

Let $\mathcal{U}_k^o \subset \mathcal{U}^o$ be the *polar feasible space* defined by

$$\mathcal{U}_k^o = \{u^o \in \mathcal{U}_a^o \mid \Lambda^o u^o \in \mathcal{W}_a^*\}. \quad (22)$$

Then the *polar variational problem* (\mathcal{P}^o) can be proposed as

$$(\mathcal{P}^o) : \quad \Pi^o(u^o) \rightarrow \text{sta} \quad \forall u^o \in \mathcal{U}_k^o. \quad (23)$$

The critical condition $D\Pi^o(u^o) = 0$ leads to the polar governing equation:

$${}^o \Lambda D\Phi^o(\Lambda^o u^o) = 0 \in {}^o \mathcal{U}, \quad (24)$$

which is the compatibility condition. Based on the bi-duality theorem, the so-called *Bi-Polarity Theorem* was proposed in general geometrically linear systems (see Gao, 2000a).

There are many choices for the null-source polar operator. In geometrically linear static systems, $\Lambda = \partial_x$ is usually a gradient-like operator, its adjoint $\Lambda = \partial_x^*$ is a divergence-like operator; while the polar operator Λ^o is a curl-like operator. In this case, the polar configuration variable u^o possesses certain beautiful geometrical meanings (see Gao, 2000a). In deformable dynamical systems such that $\Lambda = (\partial_t, -\partial_x)^T$ is a time-space differential operator, if $\partial_t \partial_x = \partial_x \partial_t$, we can simply let $\Lambda^o = (\partial_x^*, \partial_t^*)^T$ (see Gao, 2001a). Thus,

$$\langle \Lambda u; \Lambda^o u^o \rangle = \langle \partial_t u, \partial_x^* u^o \rangle - \langle \partial_x u; \partial_t^* u^o \rangle = \langle \partial_x \partial_t u - \partial_t \partial_x u, u^o \rangle = 0.$$

A diagrammatic representation for the geometrically linear system is shown in Fig. 1.

$$\begin{array}{ccc} u \in \mathcal{U} & \leftarrow \langle u, u^* \rangle & \rightarrow \mathcal{U}^* \ni u^* \\ \Lambda \downarrow & & \uparrow \Lambda^* \\ \xi \in \mathcal{W} & \leftarrow \langle \xi; \xi^* \rangle & \rightarrow \mathcal{W}^* \ni \xi^* \\ {}^o\Lambda \downarrow & & \uparrow \Lambda^o \\ {}^ou \in {}^o\mathcal{U} & \leftarrow \langle {}^ou, u^o \rangle & \rightarrow \mathcal{U}^o \ni u^o \end{array}$$

Figure 1: Structure of geometrically linear system and its polar

4 Triality Theory And Algorithm

For geometrically nonlinear systems, the canonical primal problem reads

$$(\text{II}) : \quad \Pi(u) = \Phi(\Lambda(u)) - \Psi(u) \rightarrow \text{sta} \quad \forall u \in \mathcal{U}_k, \quad (25)$$

where $\Lambda : \mathcal{U}_a \rightarrow \mathcal{W}$ is a nonlinear operator, and $\mathcal{U}_k = \{u \in \mathcal{U}_a \mid \Lambda(u) \in \mathcal{W}_a\}$. The Euler equation associated with this geometrically nonlinear variational problem is

$$\Lambda_t^*(\bar{u}) D_\Lambda \Phi(\Lambda(\bar{u})) - D\Psi(\bar{u}) = 0, \quad (26)$$

where $\Lambda_t^*(\bar{u})$ is the adjoint operator of $\Lambda_t(\bar{u})$, and $\Lambda_t(\bar{u})$ is the Gâteaux derivative of $\Lambda(u)$ at the critical point \bar{u} . By Gao-Strang (1989), we have the decomposition

$$\Lambda(u) = \Lambda_t(u)u + \Lambda_c(u),$$

where $\Lambda_c(u)$ is the complementary operator of $\Lambda_t(u)u$, which plays an important role in duality theory.

Replacing the canonical functional $\Phi(\xi)$ by the inverse Legendre transformation, the extended Lagrangian

$$\Xi(u, \xi^*) = \langle \Lambda(u); \xi^* \rangle - \Phi^*(\xi^*) - \Psi(u) \quad (27)$$

is well defined on $\mathcal{U}_a \times \mathcal{W}_a^*$. It is easy to prove that the primal problem is equivalent to the following mixed variational problem

$$(\Xi) : \Xi(u, \xi^*) = \langle \Lambda(u); \xi^* \rangle - \Phi^*(\xi^*) - \Psi(u) \rightarrow \text{sta} \quad \forall (u, \xi^*) \in \mathcal{U}_a \times \mathcal{W}_a^*. \quad (28)$$

For a given $\xi^* \in \mathcal{W}_a^*$, the canonical dual action is

$$\Pi^d(\xi^*) = \text{sta}_{u \in \mathcal{U}_a} \Xi(u, \xi^*) = \Psi^\Lambda(\xi^*) - \Phi^*(\xi^*), \quad (29)$$

where $\Psi^\Lambda(\xi^*)$ is the so-called Λ -dual functional of Ψ (see Gao, 2000a), defined by

$$\Psi^\Lambda(\xi^*) = \text{sta}\{\langle \Lambda(u); \xi^* \rangle - \Psi(u) \quad \forall u \in \mathcal{U}_a\}. \quad (30)$$

Since $\Psi : \mathcal{U}_a \rightarrow \mathbb{R}$ is a canonical functional, the criticality condition of this Λ -dual transformation leads to the balance relation

$$\Lambda_t^*(\bar{u})\xi^* \in \partial\Psi(\bar{u}). \quad (31)$$

If for each given $\xi^* \in \mathcal{W}_k^* \subset \mathcal{W}_a^*$ such that the critical point \bar{u} can be well defined by solving this balance relation, then the canonical dual action has an explicit form (see Gao, 2000a). By the duality relation (4), it easy to prove that the complementarity theorem also holds for this geometrically nonlinear problem.

Particularly, if $\Psi(u) = \langle u, u_0^* \rangle$ is a linear functional and (31) holds, we have $\Psi^\Lambda(\xi^*) = \langle \Lambda_c(\bar{u}); \xi^* \rangle$, and $G(u, \xi^*) = \langle -\Lambda_c(\bar{u}); \xi^* \rangle$ is the so-called *complementary gap functional* (see Gao-Strang, 1989). The following extended triality theory is important in nonconvex analysis.

Theorem 3 (Triality Theorem) *Suppose that the canonical functional $\Phi : \mathcal{W}_a \rightarrow \mathbb{R}$ is convex and $\Psi : \mathcal{U}_a \rightarrow \mathbb{R}$ is linear. For each critical point $(\bar{u}, \bar{\xi}^*)$ of Ξ , let $\mathcal{U}_t \times \mathcal{W}_r^*$ be a neighborhood of $(\bar{u}, \bar{\xi}^*)$ such that on which the pair $(\bar{u}, \bar{\xi}^*)$ is the only critical point of Ξ .*

If the gap functional $G(u, \bar{\xi}^)$ is convex on \mathcal{U}_r , then*

$$\min_{u \in \mathcal{U}_a} \max_{\xi^* \in \mathcal{W}_a^*} \Xi(u, \xi^*) = \Xi(\bar{u}, \bar{\xi}^*) = \max_{\xi^* \in \mathcal{W}_a^*} \min_{u \in \mathcal{U}_a} \Xi(u, \xi^*) \quad (32)$$

However, if the gap functional $G(u, \bar{\xi}^)$ is concave in \mathcal{U}_r , then either*

$$\Pi(\bar{u}) = \min_{u \in \mathcal{U}_a} \max_{\xi^* \in \mathcal{W}_a^*} \Xi(u, \xi^*) = \Xi(\bar{u}, \bar{\xi}^*) = \min_{\xi^* \in \mathcal{W}_a^*} \max_{u \in \mathcal{U}_a} \Xi(u, \xi^*) = \Pi^d(\bar{\xi}^*), \quad (33)$$

or

$$\Pi(\bar{u}) = \max_{u \in \mathcal{U}_a} \max_{\xi^* \in \mathcal{W}_a^*} \Xi(u, \xi^*) = \Xi(\bar{u}, \bar{\xi}^*) = \max_{\xi^* \in \mathcal{W}_a^*} \max_{u \in \mathcal{U}_a} \Xi(u, \xi^*) = \Pi^d(\bar{\xi}^*). \quad (34)$$

Generally speaking, if $\Lambda(u)$ is a quadratic operator and $\Phi(\xi)$ is quadratic functional, then the saddle critical point of Ξ leads to a global minimizer of Π (see Gao, 2000a). Based on this theorem, a general alternative algorithm can be proposed for finding the global minimizer of the nonconvex variational problem (\mathcal{P}) (see Gao, 2002).

Primal-Dual Algorithm for Global Minimizer.

- (1) Choose $\xi_k^* \in \mathcal{W}_k^*$ such that the gap function $G(u, \xi_k^*) = \langle -\Lambda_c(u); \xi_k^* \rangle$ is a convex functional of $u \in \mathcal{U}_a$, finding u_k such that

$$\Xi(u_k, \xi_k^*) = \min_{u \in \mathcal{U}_a} \Xi(u, \xi_k^*). \quad (35)$$

- (2) For the given $u_k \in \mathcal{U}_a$, determining the dual feasible space $\mathcal{W}_k^* = \{\xi^* \in \mathcal{W}_a^* \mid \Lambda_t^*(u_k)\xi^* = D\Psi(u_k)\}$ and finding ξ_{k+1}^* by solving the dual problem

$$\Pi^d(\xi_{k+1}^*) = \max_{\xi^* \in \mathcal{W}_k^*} \Pi^d(\xi^*). \quad (36)$$

- (3) If $|\Pi^d(\xi_{k+1}^*) - \Pi^d(\xi_k^*)| \leq \epsilon$ ($\epsilon > 0$ is a previously given very small number), then ξ_{k+1}^* is a global maximizer of Π^d and the associated u_{k+1} is the global minimizer of Π . Otherwise, let $k = k + 1$ and go back to (1).

5 Applications in Semi-Linear, Nonconvex Systems

Now let us consider a nonconvex system controlled by the following stationary variational problem

$$(\mathcal{P}_\lambda) : \Pi(u) = \int_{\Omega} w \left[\frac{1}{2} \rho |Lu|^2 - W(u; \lambda) \right] d\Omega \rightarrow \text{sta} \quad \forall u \in \mathcal{U}_k, \quad (37)$$

where w is a given weight function, $\rho > 0$ is a given constant; $L : \mathcal{U} \rightarrow \mathcal{V}$ is a linear differential operator, \mathcal{V} is a linear space with Euclidean norm $|\cdot| : \mathcal{V} \rightarrow \mathcal{L}^2(\Omega; \mathbb{R})$. For a given parameter $\lambda > 0$ and an input function f , $W(u; \lambda) = \frac{1}{2} \alpha (\frac{1}{2} u^2 - \lambda)^2 + fu$ is a nonconvex functional, which is a double-well potential if the constant $\alpha > 0$. The Euler equation for this nonconvex variational problem is a semi-linear equation:

$$\rho L^* Lu - DW(u; \lambda) = 0 \quad \text{in } \Omega. \quad (38)$$

This equation arises in many applications. In phase transitions, the potential wells of W define the phases. Particularly, if L is a gradient operator over a space domain $\Omega \subset \mathbb{R}^n$ and $w = 1$, then (38) leads to the Landau-Ginzburg equation in superconductivity. Detailed study for this case was given recently in [Gao *et al*, 2002b].

In dynamical systems, if $L = \partial_t$ is a time derivative over a time domain $\Omega = I = (0, t_c) \in \mathbb{R}$ and $w = \exp[\int_{\Omega} \nu t dt]$, then (38) is the well-known Duffing equation with linear dissipation:

$$\rho(u'' + \nu u') + \alpha u \left(\frac{1}{2} u^2 - \lambda \right) = f(t), \quad \forall t \in \Omega = (0, t_c). \quad (39)$$

The system is extremely sensitive to the parameters $\lambda, \nu > 0$, input $f(t)$ and initial data in \mathcal{U}_k . It is discovered recently that for certain given periodic force $f(t) = f_o \cos(\omega t)$ and a linearly increasing the axial load $\lambda = kt + \lambda_0 > 0$, the system may experience three chaotic bifurcation before the system crushed. Based on the canonical dual transformation and triality, a bifurcation criterion and associated dual feed-back control against chaos were proposed recently (see Gao, 2001, 2002a).

The numerical approximation of the nonconvex variational problem (37) usually leads to the following nonconvex optimization problem in \mathbb{R}^n :

$$\Pi(\mathbf{x}) = \frac{1}{2} \mathbf{x}^T A \mathbf{x} + \frac{1}{2} \left(\frac{1}{2} |B \mathbf{x}|^2 - \lambda \right)^2 - \mathbf{c}^T \mathbf{x} \rightarrow \min \quad \forall \mathbf{x} \in \mathbb{R}^n, \quad (40)$$

where $A = A^T \in \mathbb{R}^{n \times n}$ and $B \in \mathbb{R}^{m \times n}$ are two given matrices; $\mathbf{c} \in \mathbb{R}^n$ is a given vector. It is known that if A is indefinite, even the quadratic programming

$$\frac{1}{2} \mathbf{x}^T A \mathbf{x} - \mathbf{c}^T \mathbf{x} \rightarrow \min \quad \forall \mathbf{x} \in \mathbb{R}^n$$

is a *NP-Hard* problem in global optimization. In this paper, we will show how to use the canonical dual transformation method to solve this problem.

To set up the nonconvex problem (40) in the framework of canonical system, we introduce a canonical geometrical measure $y = \Lambda(\mathbf{x}) = \frac{1}{2}|B\mathbf{x}|^2$. Clearly, $\Lambda : \mathbb{R}^n \rightarrow \mathbb{R}$ is a real-valued nonlinear mapping. In terms of y , the nonconvex function $W(\mathbf{x}) = \frac{1}{2}(\frac{1}{2}|B\mathbf{x}|^2 - \lambda)^2$ can be written as

$$\bar{W}(y) = \frac{1}{2}(y - \lambda)^2$$

which is a convex (canonical) function. Thus, the canonical dual variable of y can be simply defined by $y^* = D\bar{W}(y) = y - \lambda$. By the Legendre transformation, the canonical dual function of \bar{W} is

$$\bar{W}^*(y^*) = y(y^*)y^* - \bar{W}(y(y^*)) = \frac{1}{2}y^{*2} + \lambda y^*.$$

The extended Lagrangian Ξ associated with this geometrically nonlinear operator Λ is

$$\Xi(\mathbf{x}, y^*) = \Lambda(\mathbf{x})y^* - \bar{W}^*(y^*) + \frac{1}{2}\mathbf{x}^T A \mathbf{x} - \mathbf{c}^T \mathbf{x}. \quad (41)$$

The criticality condition for Ξ leads to the canonical primal-dual equations:

$$(A + y^* B^T B)\mathbf{x} = \mathbf{c}, \quad (42)$$

$$\Lambda(\mathbf{x}) = y^* + \lambda. \quad (43)$$

Let the dual feasible space $\mathcal{W}_a^* = \{y^* \in \mathbb{R} \mid \det(A + y^* B^T B) \neq 0\}$. Then for any given $y^* \in \mathcal{W}_a^*$, substituting $\mathbf{x} = (A + y^* B^T B)^{-1}\mathbf{c}$ into Ξ , the canonical dual function of (\mathcal{P}) can be obtained as

$$\Pi^d(y^*) = \text{sta}\{\Xi(\mathbf{x}, y^*) \mid \forall \mathbf{x} \in \mathbb{R}\} = -\frac{1}{2}\mathbf{c}^T (A + y^* B^T B)^{-1}\mathbf{c} - \frac{1}{2}y^{*2} - \lambda y^*. \quad (44)$$

The criticality condition of Π^d leads to the canonical dual equation:

$$\frac{1}{2}\mathbf{c}^T (A + y^* B^T B)^{-1} B^T B (A + y^* B^T B)^{-1} \mathbf{c} + y^* + \lambda = 0. \quad (45)$$

This is an algebraic equation with only one unknown. Each root \bar{y}^* leads to a critical point of $\Pi(\mathbf{x})$, i.e.

$$\bar{\mathbf{x}} = (A + \bar{y}^* B^T B)^{-1}\mathbf{c}. \quad (46)$$

The following theorem shows the extremality of this critical point.

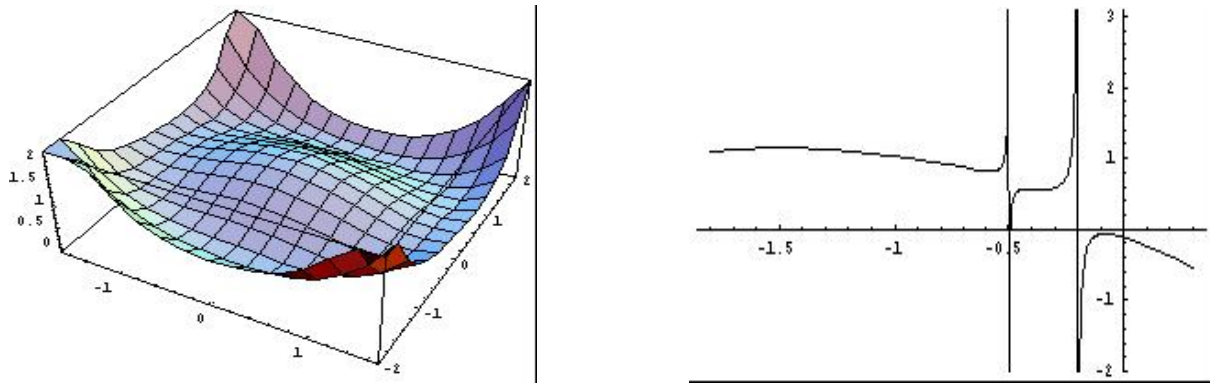
Theorem 4 *Suppose that $(\bar{\mathbf{x}}, \bar{y}^*)$ is a critical point of $\Xi(\mathbf{x}, y^*)$, then*

$$\Pi(\bar{\mathbf{x}}) = \Pi^d(\bar{y}^*). \quad (47)$$

If $(A + \bar{y}^ B^T B)$ is positive-definite, then $\bar{\mathbf{x}}$ is a local minimizer of Π and \bar{y}^* is a local maximizer of Π^d . If $(A + \bar{y}^* B^T B)$ is negative-definite, then $\bar{\mathbf{x}}$ and \bar{y}^* are either local minimizers or local maximizers of Π and Π^d , respectively.*

The equality (47) indicates that there is no duality gap between the primal and canonical dual functionals. This theorem shows that by the canonical dual transformation, the original n -dimensional nonconvex problem (\mathcal{P}) can be converted to solve an one-dimensional algebraic equation.

Example For two dimensional problem $n = 2$, we simply choose $A = \{a_{ij}\}$ with $a_{11} = 0.5$, $a_{22} = 0.2$, $a_{12} = a_{21} = 0$, $\mathbf{c} = \{c_1, c_2\}$ with $f_1 = 0.1$, $f_2 = 0.2$. For a given parameter $\lambda = 1.5$, the graph of $\Pi(\mathbf{x})$ is a nonconvex surface (see Fig. 2a) with four potential wells and one local minimizer. The graph of the canonical dual function $\Pi^d(y^*)$ is a two-dimensional curve (see Fig. 2b). The dual canonical dual algebraic equation (45) has total five real roots: $y_5^* = -1.48 < y_4^* = -0.58 < y_3^* = -0.41 < y_2^* = -0.35 < y_1^* = -0.08$. Since $(A + y_1^*I)$ is positive-definite, by theorem we know that $\mathbf{x}_1 = (A + y_1^*I)^{-1}\mathbf{c} = \{0.238, 1.67\}$ is a global minimizer of $\Pi(\mathbf{x})$.



(a) Graph of $\Pi(\mathbf{x})$.

(b) Graph of $\Pi^d(y^*)$

Figure 2: Graphs of the primal function $\Pi(\mathbf{x})$ and its canonical dual.

Detailed study on the canonical dual transformation for solving this nonconvex problem in n -dimensional space will be given in Gao (2003).

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