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MATHEMATICS

Legendre Analysis, Thermodynamic Formalism, and Spectra of Perron–Frobenius Operators

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It is well known that, in classical equilibrium thermodynamic systems, some basic characteristics, such as complete energy, free energy, enthalpy, entropy, etc., are related to each other by (finite-dimensional) Legendre transforms with respect to certain variables determining these characteristics (see, e.g., [1] for details).

The first section of this paper considers mathematical objects naturally arising in relation to the general Fenchel–Legendre transform. In the second section, it is shown that, for these objects, thermodynamic characteristics such as internal energy, temperature, entropy, and heat transfer can be defined. In the framework of the formalism developed in this paper, the first and second principles of thermodynamics are valid.

In the third section, it is established that the logarithms of the spectral radii of weighted shift and Perron–Frobenius operators convexly depend on phase potentials (Theorem 1). In light of the results obtained in the second section, it is natural to treat these values as the corresponding thermodynamic potentials, which, in particular, deepens our understanding of the thermodynamic nature of the Perron–Frobenius operators (cf. [2]). For the potentials under examination, we specify conditions under which the corresponding equilibrium state is unique (Theorem 3) and describe the equilibrium states in terms of the action functional on the basis of the probabilistic ideology rather than of the Legendre transform (Theorem 4).

1. ELEMENTS OF LEGENDRE ANALYSIS

We start with reminding the reader of basic facts related to the Fenchel–Legendre transform. Consider an arbitrary topological vector space L and its dual space L^* consisting of all continuous linear functionals on L. We denote vectors from L by φ and linear functionals from L^* by μ. The inner product of a vector and a functional is defined naturally as $\langle\varphi, \mu\rangle = \mu(\varphi)$. Let $\lambda(\varphi)$ be a convex lower semicontinuous function on L. We define its dual function $S(\mu)$ on L^* by the formula

$$S(\mu) = \inf_{\varphi \in L}(\lambda(\varphi) - \langle\varphi, \mu\rangle). \qquad (1)$$

The dual function $S(\mu)$ differs from the Legendre transform of the function $\lambda(\varphi)$ only in its sign. Therefore, it is always concave and upper semicontinuous (with respect to the *-weak topology on L^*). Definition (1) implies the Young inequality

$$S(\mu) \le \lambda(\varphi) - \langle\varphi, \mu\rangle. \qquad (2)$$

Since the Legendre transform is involutive, the initial function $\lambda(\varphi)$ can be expressed in terms of its dual as

$$\lambda(\varphi) = \sup_{\mu \in L^*}(S(\mu) + \langle\varphi, \mu\rangle). \qquad (3)$$

Obviously, the Young inequality becomes an equality precisely for those vectors φ at which the infimum in (1) is attained and precisely for those functionals μ at which the supremum in (3) is attained. We define a Lagrangian manifold $\mathcal{L} \subset L \times L^*$ as the set of pairs (φ, μ) at which the Young inequality becomes an equality. In other words,

$$\mathcal{L} = \{(\varphi, \mu) |\ S(\mu) = \lambda(\varphi) - \langle\varphi, \mu\rangle\}. \qquad (4)$$

Statement 1. *The following three conditions are equivalent*:

(a) *a pair* (φ, μ) *belongs to* $\mathcal{L}$;

(b) *the linear functional* μ *is a subgradient of the function* λ *at the point* φ;

(c) *the vector* φ *is a subgradient of the function* $-S$ *at the point* μ.

Corollary. *The Lagrangian manifold* $\mathcal{L}$ *is the graph of the subdifferential of the function* $\lambda(\varphi)$.

It is useful to consider the Lagrangian manifold $\mathcal{L}$ as a natural domain of definition for the function $\lambda(\varphi)$. The point is that the subgradient of $\lambda(\varphi)$ may take many values, or it may not exist at all. Nevertheless, Statement 1 allows us to define it as a single-valued function on $\mathcal{L}$. Namely, we define the subgradient of a function $\lambda(\varphi)$ at the point $(\varphi, \mu) \in \mathcal{L}$ to be the linear functional $\lambda'(\varphi) = \mu$ and its differential to be $d\lambda = \langle\delta\varphi, \mu\rangle$. Similarly, the differential of a function $S(\mu)$ at the point

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$(\varphi, \mu) \in \mathcal{L}$ is defined as $dS = -\langle\varphi, \delta\mu\rangle$. These subgradients and differentials coincide with the usual derivatives and differentials at all points $(\varphi, \mu) \in \mathcal{L}$ at which the functions $\lambda(\varphi)$ and $S(\mu)$ are Gateaux differentiable. But even at the points where they are not differentiable, the formal equalities $d\lambda = \langle\delta\varphi, \mu\rangle$ and $dS = -\langle\varphi, \delta\mu\rangle$ have a meaning, which is clarified by the following assertion.

Statement 2. *If points* (φ, μ) *and* $(\varphi + \delta\varphi, \mu + \delta\mu)$ *belong to* $\mathcal{L}$, *then there exists a* $\theta \in [0, 1]$ *such that*

$$\lambda(\varphi + \delta\varphi) - \lambda(\varphi) = \langle\delta\varphi, \mu\rangle + \theta\langle\delta\varphi, \delta\mu\rangle, \quad (5)$$

$$S(\mu) - S(\mu + \delta\mu) = \langle\varphi, \delta\mu\rangle + (1-\theta)\langle\delta\varphi, \delta\mu\rangle. \quad (6)$$

Statement 3. *For any vector* $h \in L\backslash\{0\}$ *and a number* $U \in \mathbb{R}$,

(a) *the inequality*

$$\sup_{\langle h, \mu\rangle = U} S(\mu) \le \inf_{b \in \mathbb{R}} (\lambda(bh) - bU) \quad (7)$$

holds;

(b) *if the infimum on the right-hand side of* (7) *is attained at some* $b = b_0$ *and the function* $\lambda(\varphi)$ *is continuous at the point* b_0h, *then* (7) *becomes an equality, the supremum on the left-hand side of* (7) *is attained at some functional, and every such functional* $\mu_0 \in L^*$ *satisfies the condition* $(b_0h, \mu_0) \in \mathcal{L}$.

2. THERMODYNAMIC FORMALISM

In this section, we show that the nature of the objects considered above is similar to thermodynamic. In this connection, we introduce and use thermodynamic terminology.

We refer to the elements φ of the topological vector space L as phase potentials and to the elements $\mu \in L^*$ as states. The function $U(\varphi, \mu) = \langle\varphi, \mu\rangle$ is called internal energy. On the Cartesian product $L \times L^*$, there are two natural first-order differential forms, the heat form $\delta Q = \langle\varphi, \delta\mu\rangle$ and the work form $\delta W = -\langle\delta\varphi, \mu\rangle$. Obviously, $dU(\varphi, \mu) = \delta Q - \delta W$. This identity is usually called the energy preservation law, or the first principle of thermodynamics. The convex lower semicontinuous functional $\lambda(\varphi)$ is called the thermodynamic potential, and its dual functional $S(\mu)$ defined by formula (1) is the entropy. We call the subgradients of the thermodynamic potential $\lambda(\varphi)$ equilibrium states.

Let us fix a phase potential $h \in L$. The isolated thermodynamic system (TDS) with energy U is the set of pairs (h, μ) for which $\langle h, \mu\rangle = U$. An equilibrium TDS is a pair (h, μ) with energy U at with the entropy attains a conditional maximum.

Consider equilibrium TDSs with the same phase potential h but with different energy levels U. Let I denote the set of all numbers $b \in \mathbb{R}$ for which the function $\lambda(\varphi)$ is continuous at the point bh. It is known that the set of continuity points of any convex function is open and convex. Therefore, I is an interval. Suppose that it is nonempty. Consider the convex function $\lambda(bh)$ of the scalar argument $b \in I$. Let $U(b)$ denote an arbitrary subgradient of this function at the point b. Obviously, $U(b)$ is a (set-valued) nondecreasing function on I taking all values between $\inf_I U(b)$ and $\sup_I U(b)$. By virtue of Statement 3(b), for each energy level U between $\inf_I U(b)$ and $\sup_I U(b)$, there exists an equilibrium thermodynamic system (h, μ) with energy U. There must exist a number $b \in I$ such that the pair (bh, μ) belongs to the Lagrangian manifold $\mathcal{L}$. By Statement 1, μ is the equilibrium state corresponding to the potential bh. The number $T = -\dfrac{1}{b}$ is called the temperature of the equilibrium thermodynamic system (h, μ). The monotonicity of the function $U(b)$ implies that the energy of an equilibrium system does not decrease with increasing temperature. The multivalence points of $U(b)$ correspond to phase transitions of the first kind in physics (i.e., to the presence of equilibrium states with different energies at the same temperature, e.g., in ice melting).

We define the equilibrium manifold $\mathcal{E} \subset L \times L^* \times \mathbb{R}$ as the set of triples (h, μ, T) for which the pair (h, μ) is an equilibrium TDS with temperature T, or, equivalently, for which the pair $\left(-\dfrac{h}{T}, \mu\right)$ belongs to the Lagrangian manifold $\mathcal{L}$. Since $\mathcal{L}$ is specified by the equation $S(\mu) = \lambda(\varphi) - \langle\varphi, \mu\rangle$, the equilibrium manifold $\mathcal{E}$ is determined by the formula

$$\mathcal{E} = \left\{(h, \mu, T) \in L \times L^* \times \mathbb{R} \,|\, S(\mu) = \lambda\left(-\frac{h}{T}\right) + \left\langle\frac{h}{T}, \mu\right\rangle\right\}. \quad (8)$$

Statement 4 (the second principle of thermodynamics). *On the equilibrium manifold* $\mathcal{E}$, *the identity* $\delta Q = TdS$ *holds. More precisely, if points* (h, μ, T) *and* $(h + \delta h, \mu + \delta\mu, T + \delta T)$ *belong to* $\mathcal{E}$, *then, for some* $\Theta \in [0, 1]$,

$$\langle h, \delta\mu\rangle = T(S(\mu + \delta\mu) - S(\mu)) + \frac{\Theta}{T + \delta T}\langle h\,\delta T - T\,\delta h, \delta\mu\rangle. \quad (9)$$

Classical thermodynamics considers families of phase potentials $h = h(a)$ differentiably depending on a finite-dimensional parameter $a = (a_1, a_2, \ldots, a_n)$. The components a_i are called external parameters. For thermodynamic systems of the form $(h(a), \mu)$, the numbers $A_i = -\dfrac{\partial U(h(a), \mu)}{\partial a_i}$ are called thermodynamic forces, or internal parameters. In this notation, the work form has the standard thermodynamic expression $\delta W = -\langle \delta h(a), \mu \rangle = \sum_i A_i\, da_i$. For equilibrium TDSs with potentials $h(a)$, it is desirable to represent all quantities as functions of external parameters and temperature. For instance, a dependence $U = U(a, T)$ is called a caloric equation, and dependences $A_i = A_i(a, T)$ are thermal equations.

3. EQUILIBRIUM STATES OF DYNAMICAL SYSTEMS AND THE ACTION FUNCTIONAL

Consider a discrete-time dynamical system generated by a continuous mapping $\alpha: X \to X$ of a metric compact space X to itself. For any function $\varphi \in C(X)$, a weighted shift operator is, by definition, an operator $A_\varphi: C(X) \to C(X)$ of the form

$$A_\varphi f = e^{\varphi}(f \circ \alpha). \tag{10}$$

Suppose that an α-invariant Borel probability measure m is defined on X. Then, the operator A_φ acts also on the space $L^1(X, m)$. If the mapping α is locally expanding, then, in addition, we define the Perron–Frobenius operator E_φ on $C(X)$ by the formula

$$E_\varphi f(x) = \sum_{y \in \alpha^{-1}(x)} e^{\varphi(y)} f(y). \tag{11}$$

We denote the logarithm of the spectral radius of the operator A_φ on $C(X)$ by $\lambda_0(\varphi)$, the logarithm of the spectral radius of the operator A_φ on $L^1(X, m)$ by $\lambda_1(\varphi)$, and the logarithm of the spectral radius of E_φ by $\lambda_2(\varphi)$.

Theorem 1. *The functionals* $\lambda_0(\varphi)$, $\lambda_1(\varphi)$, *and* $\lambda_2(\varphi)$ *convexly depend on* $\varphi \in C(X)$. *Each of their subgradients is an* α*-invariant Borel probability measure on* X.

Thus, the functions $\lambda_i(\varphi)$ can be treated as thermodynamic potentials. For each of them, formula (1) defines the corresponding entropy $S_i(\mu)$ as a function on the space $C(X)^*$ dual to $C(X)$.

Theorem 2. *If a linear functional* $\mu \in C(X)^*$ *is not an* α*-invariant probability measure on* X, *then* $S_i(\mu) = -\infty$ *for* $i = 0, 1, 2$.

Theorem 3. *If the mapping* α *is locally expanding and topologically mixing and the function* $\varphi \in C(X)$ *satisfies the Hölder* (*Lipschitz*) *condition, then the Gateaux derivative* $\lambda_2'(\varphi)$ *exists. It is the only equilibrium state corresponding to the potential* φ.

Take a point $x \in X$ and consider its trajectory $\{\alpha^n(x)\}$. The term empirical measures is conventionally used for the functionals $\delta_{x,n}(f) = n^{-1}(f(x) + f(\alpha(x)) + \dots + f(\alpha^{n-1}(x)))$. Let $\tau_\varphi(\mu)$ denote the discrepancy in the Young inequality $\tau_\varphi(\mu) = S_2(\mu) + \mu(\varphi) - \lambda_2(\varphi)$.

Theorem 4. *Suppose that the mapping* α *is locally expanding and topologically mixing and a* $\mu_\varphi = \lambda_2'(\varphi)$ *is the equilibrium state corresponding to the Hölder potential* φ.

Then, for any functional $m \in C(X)^*$ *and any* $\varepsilon > 0$, *there exists a small neighborhood* $O(m) \subset C(X)^*$ *such that*

$$\limsup_{n \to \infty} \frac{1}{n} \ln \mu_\varphi \{x \in X \mid \delta_{x,n} \in O(m)\} < \tau_\varphi(m) + \varepsilon. \tag{12}$$

If, in addition, $m = \lambda_2'(\psi)$ *is the equilibrium state corresponding to a Hölder potential* ψ, *then, for any neighborhood* $O(m) \subset C(X)^*$,

$$\liminf_{n \to \infty} \frac{1}{n} \ln \mu_\varphi \{x \in X \mid \delta_{x,n} \in O(m)\} \ge \tau_\varphi(m). \tag{13}$$

A functional $\tau_\varphi(m)$ satisfying conditions (12) and (13) is called an action functional for empirical measures (on the set of equilibrium states). It is easy to see that, if $m = \lambda_2'(\psi)$, then $\tau_\varphi(m) = \lambda_2(\psi) - \lambda_2(\varphi) - \lambda_2'(\psi)(\psi - \varphi)$.

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