A NEW APPROACH TO CONSTRAINED-MAXIMIZATION NONEQUILIBRIUM PROBLEMS

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ABSTRACT

Many nonequilibrium problems in thermodynamics, information theory, economics, control theory and other sciences require the description of a smooth constrained evolution towards an equilibrium state maximizing some function of the state variables. We present a novel mathematical formalism designed to model a wide class of such nonequilibrium problems. It is based on a type of nonlinear evolution equation with the following main relevant properties. Its solutions maintain invariant the value of each of the constraints like, for a typical thermodynamic nonequilibrium problem, the energy and the number of particles of each species. It maintains a positive-definite time rate of change of the function of the state variables to be maximized like, in the thermodynamic example, the entropy function. Its solutions converge towards an equilibrium state maximizing that function subject to the values of the constraints. A byproduct of the mathematical formalism is a numerical scheme for nonlinear optimization under nonlinear constraints similar to the well-known gradient-projection and steepest-ascent methods of nonlinear programming. However, the principal application of the formalism is to provide a tool for the time-dependent description of nonequilibrium states and their approach to equilibrium.

INTRODUCTION

We will consider the following constrained maximization problem

$$\max \quad F(x_1,\dots,x_k,\dots) \tag{1a}$$

$$\text{subject to} \quad G_i(x_1,\dots,x_k,\dots) = b_i \qquad i=1,\dots,n \tag{1b}$$

where $F, G_1,\dots,G_n$ are continuously partially differentiable functions of the variables $x_1,\dots,x_k,\dots$ We will denote the maximizing state by $x_1^*,\dots,x_k^*,\dots$

Problem (1) has a large number of applications in physics, engineering and social sciences [1], and many methods have been developed for its numerical solution [2]. In a later section, we discuss how a problem with inequality constraints can be transformed into Problem (1). A well-known example in the thermodynamics context or in the information-theory context is the maximum entropy problem [3]

$$\max \quad -\textstyle\sum_k p_k \ln p_k \tag{2a}$$

$$\text{subject to} \quad \textstyle\sum_k E_k p_k = \langle E\rangle \tag{2b}$$

$$\textstyle\sum_k N_{ik} p_k = \langle N_i\rangle \qquad i=1,\dots,r \tag{2c}$$

$$\textstyle\sum_k p_k = 1 \tag{2d}$$

$$p_k \geq 0 \qquad k=1,\dots \tag{2e}$$

the solution of which is

$$p_k^* = \frac{1}{Q}\exp\left(-\beta E_k + \sum_{i=1}^{r} \nu_i N_{ik}\right) \tag{3a}$$

$$Q = \textstyle\sum_k \exp\left(-\beta E_k + \sum_{i=1}^{r} \nu_i N_{ik}\right) \tag{3b}$$

where the values of $\beta, \nu_1,\dots,\nu_r$ are determined by the values $\langle E\rangle, \langle N_1\rangle,\dots,\langle N_r\rangle$ of the constraints.

Here, we discuss an extension of Problem (1) to the nonequilibrium domain. The nonequilibrium problem is to find functions $x_1(t),\dots,x_k(t),\dots$ with $x_1(0)=x_{10},\dots,x_k(0)=x_{k0},\dots$ (where $x_{10},\dots,x_{k0},\dots$ are arbitrarily given initial conditions) such that for all values of the variable t (with $0 \leq t < +\infty$)

$$\frac{d}{dt} F(x_1(t),\dots,x_k(t),\dots) > 0 \tag{4a}$$

and

$$G_i(x_1(t),\ldots,x_k(t),\ldots) = G_i(x_{10},\ldots,x_{k0},\ldots) \qquad i=1,\ldots,n \tag{4b}$$

Problem (4) can be viewed from slightly different perspectives. For example, in the context of Problem (2), the functions $x_1(t),\ldots,x_k(t),\ldots$ would represent the state of a system which evolves in time from an arbitrarily given nonequilibrium state $x_{10},\ldots,x_{k0},\ldots$ towards the state of maximum entropy while keeping invariant the values $\langle E\rangle,\langle N_1\rangle,\ldots,\langle N_n\rangle$ of the energy and the number of particles of each type. Again, functions $x_1(t),\ldots,x_k(t),\ldots$ could be thought of as parametric equations -- the variable t being the parameter -- of a smooth trajectory from the initial state $x_{10},\ldots,x_{k0},\ldots$ to the maximizing state $x_1^*,\ldots,x_k^*,\ldots$ along which functions G_i are invariant and function F is always increasing. Finally, for increasing values of the variable t, functions $x_1(t),\ldots,x_k(t),\ldots$ can be viewed as successive approximations to the solution of the constrained-maximization Problem (1).

In the next section, we present a nonlinear differential equation for the state variables $x_1,\ldots,x_k,\ldots$ the solutions of which are functions $x_1(t),\ldots,x_k(t),\ldots$ that indeed solve the general nonequilibrium problem just stated. When interpreted in the context of Problem (2), this nonlinear differential equation represents an evolution equation describing a constant-energy and constant-particle-number evolution or relaxation towards increasing entropy states. Indeed, the structure of the nonlinear equation has been developed by the author in the context of quantum thermodynamics [4] in response to a need for an extension of the Schroedinger equation of motion of quantum mechanics to the broader set of nonmechanical quantum states that allow a nonstatistical unification of mechanics and thermodynamics [5].

NONLINEAR EVOLUTION EQUATION

The solution of the following first-order nonlinear differential equation is also a solution of the nonequilibrium Problem (4)

$$\underline{\dot{x}} = \frac{1}{\tau}\,[\underline{f} - (\underline{f})_{L(\underline{g}_1,\ldots,\underline{g}_n)}] \tag{5}$$

where the symbols are defined and explained in the remainder of this section. The validity of our assertion is shown in the next section.

We have defined the following vectors

$$\underline{x} = \{x_1,\ldots,x_k,\ldots\} \tag{6}$$

$$\underline{f} = \{f_1,\ldots,f_k,\ldots\} \qquad \text{where } f_k = \partial F/\partial x_k \tag{7}$$

$$\underline{g}_i = \{g_{i1},\ldots,g_{ik},\ldots\} \qquad \text{where } g_{ik} = \partial G_i/\partial x_k \tag{8}$$

so that, for example, Problem (1) can be restated as follows

$$\max \qquad F(\underline{x}) \tag{1'a}$$

$$\text{subject to} \qquad G_i(\underline{x}) = b_i \qquad i=1,\ldots,n \tag{1'b}$$

The standard method to solve problem (1) is to associate a Lagrange multiplier $\lambda_1,\ldots,\lambda_n$ with each of the constraints, solve the necessary conditions

$$\frac{\partial F}{\partial x_k} - \sum_{i=1}^{n} \lambda_i \frac{\partial G_i}{\partial x_k} = 0 \qquad k=1,\ldots \tag{9}$$

to yield $x_k = x_k(\lambda_1,\ldots,\lambda_n)$, substitute this result in the constraints to yield the values of the Lagrange multipliers $\lambda_i^* = \lambda_i^*(b_1,\ldots,b_n)$ and, hence, the solution x_k^*. In terms of the notation just introduced, Conditions (9) can be rewritten as

$$\underline{f} - \sum_{i=1}^{n} \lambda_i \underline{g}_i = 0 \tag{10}$$

If the state vector $\underline{x}$ is a continuous function of time, i.e., we have a continuous one-parameter family $\underline{x}(t)$ of state vectors, then the time rates of change of the functions $F,G_1,\ldots,G_n$ are given by

$$\dot{F} = \underline{f}\cdot\underline{\dot{x}} \tag{11}$$

$$\dot{G}_i = \underline{g}_i\cdot\underline{\dot{x}} \qquad i=1,\ldots,n \tag{12}$$

where clearly

$$\underline{\dot{x}} = \{\dot{x}_1,\ldots,\dot{x}_k,\ldots\} \tag{13}$$

and the dot product has the obvious meaning (for example, $\underline{f}\cdot\underline{\dot{x}} = f_1\dot{x}_1+\ldots+f_k\dot{x}_k+\ldots$).

The symbol

$$L(\underline{g}_1,\ldots,\underline{g}_n) \tag{14}$$

denotes the linear span of vectors $\underline{g}_1,\ldots,\underline{g}_n$, i.e., the linear manifold formed by all the vectors that are linear combinations of $\underline{g}_1,\ldots,\underline{g}_n$.

In general, vectors $\underline{f},\underline{g}_1,\ldots,\underline{g}_n$ are all functions of $\underline{x}$. If, for a given $\underline{x}$, the vector $\underline{f}$ is an element of $L(\underline{g}_1,\ldots,\underline{g}_n)$ then there exist coefficients $\lambda_1,\ldots,\lambda_n$ such that $\underline{f} = \lambda_1\underline{g}_1+\ldots+\lambda_n\underline{g}_n$, i.e., Condition (10) is satisfied. This happens whenever $\underline{f},\underline{g}_1,\ldots,\underline{g}_n$ are evaluated at a maximizing state vector $\underline{x}^*$ which solves the constrained-maximization Problem (1) for some given values of $b_1,\ldots,b_n$.

If, for a given $\underline{x}$, vector $\underline{f}$ is not an element of $L(\underline{g}_1,\ldots,\underline{g}_n)$ then we will see that the effect of Equation (5) is to change $\underline{x}$ as a function of time so that $\underline{f}$ approaches $L(\underline{g}_1,\ldots,\underline{g}_n)$ and, thus, if the functions $F,G_1,\ldots,G_n$ are such that Condition (10) is also sufficient to determine the maximizing solution $\underline{x}^*$, then $\underline{x}$ approaches $\underline{x}^*$.

The symbol

$$(\underline{f})_{L(\underline{g}_1,\ldots,\underline{g}_n)} \tag{15}$$

unique vector in $L(\underline{g}_1,\ldots,\underline{g}_n)$ such that its dot product with any vector $\underline{h}$ in $L(\underline{g}_1,\ldots,\underline{g}_n)$ is equal to the dot product of vector $\underline{f}$ with $\underline{h}$, i.e.,

$$\underline{h}\cdot(\underline{f})_{L(\underline{g}_1,\ldots,\underline{g}_n)} = \underline{h}\cdot\underline{f} \tag{16}$$

for every vector $\underline{h}$ in $L(\underline{g}_1,\ldots,\underline{g}_n)$.

In general, even if the constraints $G_1(\underline{x})=b_1,\ldots,G_n(\underline{x})=b_n$ are linearly independent, the vectors $\underline{g}_1(\underline{x}),\ldots,\underline{g}_n(\underline{x})$ need not be linearly independent for all state vectors $\underline{x}$. We will denote by $\underline{h}_1,\ldots,\underline{h}_m$ a set of vectors that are linearly independent and span $L(\underline{g}_1,\ldots,\underline{g}_n)$. A simple procedure to find such linearly independent vectors is as follows. First, let $\underline{h}_1 = \underline{g}_1$ and i = 2, and evaluate the Gram determinant

$$\begin{vmatrix} \underline{g}_i\cdot\underline{g}_i & \underline{g}_i\cdot\underline{h}_1 \\ \underline{h}_1\cdot\underline{g}_i & \underline{h}_1\cdot\underline{h}_1 \end{vmatrix} \tag{17}$$

If the determinant is equal to zero then $\underline{g}_i$ is linearly dependent on $\underline{h}_1$. Let i = i + 1 and repeat the step. If, instead, the determinant is strictly positive (Gram determinants are nonnegative) then let $\underline{h}_2 = \underline{g}_i$, because $\underline{g}_i$ is linearly independent of $\underline{h}_1$. Next, let i = i + 1 and evaluate the Gram determinant

$$\begin{vmatrix} \underline{g}_i\cdot\underline{g}_i & \underline{g}_i\cdot\underline{h}_1 & \underline{g}_i\cdot\underline{h}_2 \\ \underline{h}_1\cdot\underline{g}_i & \underline{h}_1\cdot\underline{h}_1 & \underline{h}_1\cdot\underline{h}_2 \\ \underline{h}_2\cdot\underline{g}_i & \underline{h}_2\cdot\underline{h}_1 & \underline{h}_2\cdot\underline{h}_2 \end{vmatrix} \tag{18}$$

Again, if this determinant is equal to zero then $\underline{g}_i$ is a linear combination of $\underline{h}_1$ and $\underline{h}_2$. Let i = i + 1 and repeat the step. If, instead, it is strictly positive then let $\underline{h}_3 = \underline{g}_i$, because $\underline{g}_i$ is linearly independent of $\underline{h}_1$ and $\underline{h}_2$. Continue in a similar way until i = n. Clearly, this procedure eliminates from the set $\underline{g}_1,\ldots,\underline{g}_n$ only those vectors that are linearly dependent on the others, so that the remaining set of linearly independent vectors $\underline{h}_1,\ldots,\underline{h}_m$ still spans the linear manifold $L(\underline{g}_1,\ldots,\underline{g}_n)$.

The following are two equivalent explicit expressions for the projection (15) of vector $\underline{f}$ onto the linear manifold $L(\underline{g}_1,\ldots,\underline{g}_n)$. The first is

$$(\underline{f})_{L(\underline{g}_1,\ldots,\underline{g}_n)} = \sum_{i=1}^{m}\sum_{j=1}^{m} (\underline{f}\cdot\underline{h}_j)\,[M(\underline{h}_1,\ldots,\underline{h}_m)^{-1}]_{ji}\,\underline{h}_i \tag{19}$$

where $M(\underline{h}_1,\ldots,\underline{h}_m)^{-1}$ is the inverse of the Gram matrix

$$M(\underline{h}_1,\ldots,\underline{h}_m) = \begin{bmatrix} \underline{h}_1\cdot\underline{h}_1 & \cdots & \underline{h}_m\cdot\underline{h}_1 \\ \vdots & \ddots & \vdots \\ \underline{h}_1\cdot\underline{h}_m & \cdots & \underline{h}_m\cdot\underline{h}_m \end{bmatrix} \tag{20}$$

and $\underline{h}_1,\ldots,\underline{h}_m$ are linearly independent vectors spanning $L(\underline{g}_1,\ldots,\underline{g}_n)$. The second expression is a ratio of two determinants

$$(\underline{f})_{L(\underline{g}_1,\ldots,\underline{g}_n)} = - \frac{\begin{vmatrix} 0 & \underline{h}_1 & \cdots & \underline{h}_m \\ \underline{f}\cdot\underline{h}_1 & \underline{h}_1\cdot\underline{h}_1 & \cdots & \underline{h}_m\cdot\underline{h}_1 \\ \vdots & \vdots & \ddots & \vdots \\ \underline{f}\cdot\underline{h}_m & \underline{h}_1\cdot\underline{h}_m & \cdots & \underline{h}_m\cdot\underline{h}_m \end{vmatrix}}{\begin{vmatrix} \underline{h}_1\cdot\underline{h}_1 & \cdots & \underline{h}_m\cdot\underline{h}_1 \\ \vdots & \ddots & \vdots \\ \underline{h}_1\cdot\underline{h}_m & \cdots & \underline{h}_m\cdot\underline{h}_m \end{vmatrix}} \tag{21}$$

where the determinant at the denominator is always strictly positive because the vectors $\underline{h}_1,\ldots,\underline{h}_m$ are linearly independent.

We have so far defined all the symbols that appear in differential Equation (5), except for τ which is a characteristic time and may be a constant or any positive functional of the state vector.

Though the explicit definitions just given are relatively involved, they never require the solution of implicit nonlinear equations and can all be directly implemented in a numerical scheme to integrate Equation (5).

Using Relation (21) we may rewrite Equation (5) in the following useful form

$$\dot{\underline{x}} = \frac{1}{\tau}\frac{\begin{vmatrix} \underline{f} & \underline{h}_1 & \cdots & \underline{h}_m \\ \underline{f}\cdot\underline{h}_1 & \underline{h}_1\cdot\underline{h}_1 & \cdots & \underline{h}_m\cdot\underline{h}_1 \\ \vdots & \vdots & \ddots & \vdots \\ \underline{f}\cdot\underline{h}_m & \underline{h}_1\cdot\underline{h}_m & \cdots & \underline{h}_m\cdot\underline{h}_m \end{vmatrix}}{\begin{vmatrix} \underline{h}_1\cdot\underline{h}_1 & \cdots & \underline{h}_m\cdot\underline{h}_1 \\ \vdots & \ddots & \vdots \\ \underline{h}_1\cdot\underline{h}_m & \cdots & \underline{h}_m\cdot\underline{h}_m \end{vmatrix}} \qquad (22)$$

Before we proceed to the next section where we study the general properties of Equation (5), we consider a simplest example generated by the constrained maximization problem

$$\max \quad -(x^2 + y^2 + z^2) \qquad (23a)$$

$$\text{subject to} \quad z = b \qquad (23b)$$

so that, in our notation, we have

$x_1 = x,\ x_2 = y,\ x_3 = z$

$\underline{x} = \{x,y,z\}$

$F = -x^2 - y^2 - z^2$

$f_1 = \partial F/\partial x = -2x,\ f_2 = \partial F/\partial y = -2y,\ f_3 = \partial F/\partial z = -2z$

$\underline{f} = \{-2x,-2y,-2z\}$

$G = z$

$g_1 = \partial G/\partial x = 0,\ g_2 = \partial F/\partial y = 0,\ g_3 = \partial F/\partial z = 1$

$\underline{g} = \{0,0,1\}$

and, therefore, $m = 1$ and $\underline{h}_1 = \underline{g} = \{0,0,1\}$. Equation (22) becomes

$$\dot{\underline{x}} = \frac{1}{\tau}\frac{\begin{vmatrix} \underline{f} & \underline{h}_1 \\ \underline{f}\cdot\underline{h}_1 & \underline{h}_1\cdot\underline{h}_1 \end{vmatrix}}{\underline{h}_1\cdot\underline{h}_1} \qquad (24)$$

But

$\underline{f}\cdot\underline{h}_1 = \underline{f}\cdot\underline{g} = 0 + 0 - 2z = -2z$

$\underline{h}_1\cdot\underline{h}_1 = \underline{g}\cdot\underline{g} = 0 + 0 + 1 = 1$

and, therefore, Equation (24) yields

$$\dot{x} = \frac{1}{\tau}\begin{vmatrix} -2x & 0 \\ -2z & 1 \end{vmatrix} = -\frac{2}{\tau}x$$

$$\dot{y} = \frac{1}{\tau}\begin{vmatrix} -2y & 0 \\ -2z & 1 \end{vmatrix} = -\frac{2}{\tau}y \qquad (25)$$

$$\dot{z} = \frac{1}{\tau}\begin{vmatrix} -2z & 1 \\ -2z & 1 \end{vmatrix} = 0$$

and the rate of change of function F is

$$\dot{F} = \underline{f}\cdot\dot{\underline{x}} = -2x(-2x/\tau) - 2y(-2y/\tau) = \frac{4}{\tau}(x^2+y^2)$$

If τ is a positive constant, Equations (25) can be integrated to yield

$x(t) = x_0\exp(-2t/\tau)$

$y(t) = y_0\exp(-2t/\tau)$

$z(t) = z_0$

We see that choosing any initial state $\{x_0,y_0,z_0\}$ with $z_0 = b$ so that the constraint of Problem (23) is satisfied, yields a solution $\underline{x}(t)$ which as $t\to\infty$ tends to the maximizing point $\{0,0,b\}$. We also notice that the solution $\underline{x}(t)$ is a parametric equation of the most direct path compatible with the constraint $z = b$ connecting the initial state to the maximizing state. Indeed, eliminating the parameter t we obtain $x/y = x_0/y_0$, i.e., the equation of a line from $\{x_0,y_0,b\}$ to $\{0,0,b\}$.

PROPERTIES OF THE NONLINEAR EVOLUTION EQUATION

If $\underline{x}(t)$ is a solution of Equation (5) with initial condition $\underline{x}(0) = \underline{x}_0$ then the rates of change of the functions $G_1,\ldots,G_n$ are equal to zero, and, therefore, at all times t

$$G(\underline{x}(t)) = G(\underline{x}_0)$$

namely, the solution $\underline{x}(t)$ maintains invariant the values of the constraints. We may verify this, for example, by using the fact (Equation (16)) that

$$\underline{g}_i\cdot(\underline{f})_{L(\underline{g}_1,\ldots,\underline{g}_n)} = \underline{g}_i\cdot\underline{f}$$

because $\underline{g}_i$ clearly lies in $L(\underline{g}_1,\ldots,\underline{g}_n)$, and Equation (12) yields

$$\dot{G}_i = \underline{g}_i\cdot\dot{\underline{x}} = \frac{1}{\tau}[\underline{g}_i\cdot\underline{f} - \underline{g}_i\cdot(\underline{f})_{L(\underline{g}_1,\ldots,\underline{g}_n)}] = 0 \qquad (26)$$

The rate of change of the function F instead is always nonnegative. Specifically,

$$\dot{F} = \tau\, \dot{\underline{x}}\cdot\dot{\underline{x}} > 0 \quad \text{if} \quad \dot{\underline{x}} \neq 0 \tag{27}$$

and $\dot{F} = 0$ if and only if $\dot{\underline{x}} = 0$ (because only the zero vector has zero norm). To verify Relation (27), we first note that vector $\dot{\underline{x}}$ as given by Equation (5) is orthogonal to the linear manifold $L(\underline{g}_1,\ldots,\underline{g}_n)$ for it is the vector difference of $\underline{f}$ and its projection onto $L(\underline{g}_1,\ldots,\underline{g}_n)$. It follows that

$$\dot{\underline{x}}\cdot(\underline{f})_{L(\underline{g}_1,\ldots,\underline{g}_n)} = 0$$

and Equation (11) yields

$$\dot{F} = \underline{f}\cdot\dot{\underline{x}} = (\tau\dot{\underline{x}} + (\underline{f})_{L(\underline{g}_1,\ldots,\underline{g}_n)})\cdot\dot{\underline{x}} = \tau\, \dot{\underline{x}}\cdot\dot{\underline{x}} \tag{28}$$

where we solved Equation (5) for $\underline{f}$.

Property (27) implies that $\dot{F} = 0$ if and only if $\dot{x} = 0$, but Equation (5) implies that $\dot{\underline{x}} = 0$ if and only if vector $\underline{f}$ is a linear combination of vectors $\underline{g}_1,\ldots,\underline{g}_n$, i.e., Condition (10) is satisfied. It follows that if Condition (10) is also sufficient to determine the maximizing vector $\underline{x}^*$, then the condition $\dot{\underline{x}} = 0$ is equivalent to such condition, though it has the interesting feature that it does not involve additional variables such as the Lagrange multipliers. This proves that if we follow any one of such solutions that is initially compatible with the constraints we will eventually approach the maximizing state $\underline{x}^*$.

Moreover, the set of nonlinear equations $\dot{\underline{x}} = 0$ (where $\dot{\underline{x}}$ is given by Equation (5) or any of its equivalent forms such as Equation (22)) together with the constraint equations yield an alternative way to determine the maximizing vector $\underline{x}^*$. In the example at the end of the last section, the condition $\dot{\underline{x}} = 0$ requires $x^* = 0$ and $y^* = 0$, and the constraint requires $z^* = b$. It is noteworthy that the equation $\dot{F} = 0$, which is not independent of the equations generated by $\dot{\underline{x}} = 0$, often yields useful insights towards the solution of the set of generally nonlinear equations.

We finally remark that the numerical integration of Equation (5) starting from a feasible initial condition (i.e., a state compatible with the values of the constraints) would constitute an algorithm to converge towards the maximizing state. Such a numerical algorithm would bear a very close relation to the gradient-projection and steepest-ascent methods of nonlinear programming [6].

INEQUALITY CONSTRAINTS

The following constrained maximization problem with inequality constraints

$$\max \qquad \Phi(p_1,\ldots,p_r,p_{r+1},\ldots,p_k,\ldots) \tag{29a}$$

$$\text{subject to} \quad \Gamma_i(\underline{p}) \le \beta_i \qquad i=1,\ldots,u \tag{29b}$$

$$\Gamma_i(\underline{p}) \ge \beta_i \qquad i=u+1,\ldots,v \tag{29c}$$

$$\Gamma_i(\underline{p}) = \beta_i \qquad i=v,\ldots,n \tag{29d}$$

$$p_j \ge 0 \qquad j=1,\ldots,r \tag{29e}$$

can be transformed into a problem with equality constraints by defining the new auxiliary state variables $x_1,\ldots,x_r,x_{r+1},\ldots,x_{r+v},\ x_{v+r+1},\ldots,x_{v+k},\ldots$ such that the old variables can be calculated from the new using the relations

$$p_j = x_j^2 \qquad j = 1,\ldots,r \tag{30a}$$

$$p_j = x_{j+v} \qquad j = r+1,\ldots,k,\ldots \tag{30b}$$

and the new problem is Problem (1) with

$$F(\underline{x}) = \Phi(x_1^2,\ldots,x_r^2,x_{v+r+1},\ldots,x_{v+k},\ldots)$$

$$G_i(\underline{x}) = -\Gamma_i(x_1^2,\ldots,x_r^2,x_{v+r+1},\ldots,x_{v+k},\ldots) + x_{r+i}^2$$
$$b_i = -\beta_i \qquad i = 1,\ldots,u$$

$$G_i(\underline{x}) = \Gamma_i(x_1^2,\ldots,x_r^2,x_{v+r+1},\ldots,x_{v+k},\ldots) + x_{r+i}^2$$
$$b_i = \beta_i \qquad i = u+1,\ldots,v$$

$$G_i(\underline{x}) = \Gamma_i(x_1^2,\ldots,x_r^2,x_{v+r+1},\ldots,x_{v+k},\ldots)$$
$$b_i = \beta_i \qquad i = v,\ldots,n$$

SMOOTH CONSTRAINED APPROACH TO MAXIMUM ENTROPY

For example, Problem (2) can be transformed into Problem (1) by defining the auxiliary variables $x_1,\ldots,x_k,\ldots$ such that the original variables $p_k = x_k^2$. The new problem is Problem (1) with

$$F(\underline{x}) = -\textstyle\sum_k x_k^2 \ln x_k^2$$

$$G_1(\underline{x}) = \textstyle\sum_k E_k x_k^2 \quad \text{with } b_1 = \langle E\rangle$$

$$G_{i+1}(\underline{x}) = \textstyle\sum_k N_{ik} x_k^2 \quad \text{with } b_{i+1} = \langle N_i\rangle \quad \text{for } i=1,\ldots,r$$

$$G_{r+2}(\underline{x}) = \textstyle\sum_k x_k^2 \quad \text{with } b_{r+2} = 1$$

The components of vectors $\underline{f}$ and $\underline{g}_i$ become

$$f_k = \partial F/\partial x_k = -2x_k - 2x_k \ln x_k^2$$

$$g_{1k} = \partial G_1/\partial x_k = 2E_k x_k$$

$$g_{(i+1)} = \partial G_{i+1}/\partial x_k = 2N_{ik} x_k \qquad i=1,\ldots,r$$

$$g_{(r+2)k} = \partial G_{r+2}/\partial x_k = 2x_k$$

Thus, to set up Equation (5) or its equivalent form given by Equation (22) we must calculate the following dot products

$\underline{f} \cdot \underline{g}_1 = -4\sum_k E_k x_k^2 - 4\sum_k E_k x_k^2 \ln x_k^2$

$\underline{f} \cdot \underline{g}_{i+1} = -4\sum_k N_{ik} x_k^2 - 4\sum_k N_{ik} x_k^2 \ln x_k^2 \qquad i=1,..,r$

$\underline{f} \cdot \underline{g}_{r+2} = -4\sum_k x_k^2 - 4\sum_k x_k^2 \ln x_k^2$

$\underline{g}_1 \cdot \underline{g}_1 = 4\sum_k E_k^2 x_k^2$

$\underline{g}_1 \cdot \underline{g}_{i+1} = 4\sum_k E_k N_{ik} x_k^2 \qquad i=1,...,r$

$\underline{g}_1 \cdot \underline{g}_{r+2} = 4\sum_k E_k x_k^2$

$\underline{g}_{i+1} \cdot \underline{g}_{j+1} = 4\sum_k N_{ik} N_{jk} x_k^2 \qquad i=1,...,r;\ j=1,...,r$

$\underline{g}_{r+2} \cdot \underline{g}_{r+2} = 4\sum_k x_k^2$

For this particular problem, the original state vector $\underline{p}$ is related to the new state vector $\underline{x}$ by $p_k = x_k^2$, therefore, $\dot{p}_k = 2x_k\dot{x}_k$ where $\dot{x}_k$ is given by Equation (22). Substituting in this equation all the expressions just derived, we notice that the resulting equation for $\dot{p}_k$ contains only the square of the new variables, i.e., x_k^2. Hence, the resulting equation can be seen as an evolution equation for the original variables p_k which are guaranteed to satisfy the nonnegativity condition.

It is also noteworthy that the resulting evolution equation for the original state vector $\underline{p}$ maintains the initially zero components equal to zero at all times. Therefore, the convergence to the actual maximum entropy state is guaranteed only if the initial state vector $\underline{p}_0$ has no zero components. In other words, for the problem considered in this section, Condition (10), which is satisfied by the maximizing state $\underline{p}$* given by Equations (3), is not sufficient to determine $\underline{p}$* unless we further require that each p_k be strictly nonzero.

CONCLUSIONS

We presented a special nonlinear differential equation for the description of a smooth constrained evolution from an arbitrary initial nonequilibrium state compatible with the constraints, towards a state maximizing a given function of the state variables.

The nonlinear differential equation can be applied to a broad range of nonequilibrium problems in physics, engineering, and other sciences. We emphasized here its application in the context of thermodynamics and information theory.

REFERENCES

1. See, for example, P. Whittle, Optimization under Constraints, Wiley, London, 1971; M.I. Kamien and N.L. Schwartz, Dynamic Optimization, North-Holland, New York, 1981; M. Athans and P.L. Falb, Optimal Control, McGraw-Hill, New York, 1966; G. Hadley, Nonlinear and Dynamic Programming, Addision-Wesley, Reading, Mass., 1964.

2. See, for example, F.A. Lootsma, Editor, Numerical Methods for Nonlinear Optimization, Academic Press, London, 1972.

3. See, for example, R.D. Levine and M. Tribus, Editors, The Maximum Entropy Formalism, The M.I.T. Press, Cambridge, Mass., 1979.

4. See, for example, G.P. Beretta, E.P. Gyftopoulos, J.L. Park and G.N. Hatsopoulos, "Quantum Thermodynamics. A New Equation of Motion for a Single Constituent of Matter," Nuovo Cimento B, Vol. 82, 169 (1984); G.P. Beretta, articles in Frontiers of Nonequilibrium Statistical Physics, G.T. Moore and M.O. Scully, Editors, Plenum Press, New York, 1986.

5. G.N. Hatsopoulos and E.P. Gyftopoulos, "A Unified Quantum Theory of Mechanics and Thermodynamics," Foundations of Physics, Vol. 6, 15, 127, 436, 561 (1976).

6. J.B. Rosen, "The Gradient Projection Method for Nonlinear Programming," Journal of the Society for Industrial and Applied Mathematics, Vol. 9, 514 (1961); R. Fletcher and M.J.D. Powell, "A Rapidly Convergent Descent Method for Minimization," Computational Journal, Vol. 6, 163 (1963).

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$$\underline{f} \cdot \underline{g}_1 = -4\sum_k E_k x_k^2 - 4\sum_k E_k x_k^2 \ln x_k^2$$

$$\underline{f} \cdot \underline{g}_{i+1} = -4\sum_k N_{ik} x_k^2 - 4\sum_k N_{ik} x_k^2 \ln x_k^2 \qquad i=1,..,r$$

$$\underline{f} \cdot \underline{g}_{r+2} = -4\sum_k x_k^2 - 4\sum_k x_k^2 \ln x_k^2$$

$$\underline{g}_1 \cdot \underline{g}_1 = 4\sum_k E_k^2 x_k^2$$

$$\underline{g}_1 \cdot \underline{g}_{i+1} = 4\sum_k E_k N_{ik} x_k^2 \qquad i=1,\ldots,r$$

$$\underline{g}_1 \cdot \underline{g}_{r+2} = 4\sum_k E_k x_k^2$$

$$\underline{g}_{i+1} \cdot \underline{g}_{j+1} = 4\sum_k N_{ik} N_{jk} x_k^2 \qquad i=1,\ldots,r;\ j=1,\ldots,r$$

$$\underline{g}_{r+2} \cdot \underline{g}_{r+2} = 4\sum_k x_k^2$$

For this particular problem, the original state vector $\underline{p}$ is related to the new state vector $\underline{x}$ by $p_k = x_k^2$, therefore, $\dot{p}_k = 2x_k\dot{x}_k$ where $\dot{x}_k$ is given by Equation (22). Substituting in this equation all the expressions just derived, we notice that the resulting equation for $\dot{p}_k$ contains only the square of the new variables, i.e., x_k^2. Hence, the resulting equation can be seen as an evolution equation for the original variables p_k which are guaranteed to satisfy the nonnegativity condition.

It is also noteworthy that the resulting evolution equation for the original state vector $\underline{p}$ maintains the initially zero components equal to zero at all times. Therefore, the convergence to the actual maximum entropy state is guaranteed only if the initial state vector $\underline{p}_0$ has no zero components. In other words, for the problem considered in this section, Condition (10), which is satisfied by the maximizing state $\underline{p}^*$ given by Equations (3), is not sufficient to determine $\underline{p}^*$ unless we further require that each p_k be strictly nonzero.

CONCLUSIONS

We presented a special nonlinear differential equation for the description of a smooth constrained evolution from an arbitrary initial nonequilibrium state compatible with the constraints, towards a state maximizing a given function of the state variables.

The nonlinear differential equation can be applied to a broad range of nonequilibrium problems in physics, engineering, and other sciences. We emphasized here its application in the context of thermodynamics and information theory.

REFERENCES

1. See, for example, P. Whittle, Optimization under Constraints, Wiley, London, 1971; M.I. Kamien and N.L. Schwartz, Dynamic Optimization, North-Holland, New York, 1981; M. Athans and P.L. Falb, Optimal Control, McGraw-Hill, New York, 1966; G. Hadley, Nonlinear and Dynamic Programming, Addision-Wesley, Reading, Mass., 1964.

2. See, for example, F.A. Lootsma, Editor, Numerical Methods for Nonlinear Optimization, Academic Press, London, 1972.

3. See, for example, R.D. Levine and M. Tribus, Editors, The Maximum Entropy Formalism, The M.I.T. Press, Cambridge, Mass., 1979.

4. See, for example, G.P. Beretta, E.P. Gyftopoulos, J.L. Park and G.N. Hatsopoulos, "Quantum Thermodynamics. A New Equation of Motion for a Single Constituent of Matter," Nuovo Cimento B, Vol. 82, 169 (1984); G.P. Beretta, articles in Frontiers of Nonequilibrium Statistical Physics, G.T. Moore and M.O. Scully, Editors, Plenum Press, New York, 1986.

5. G.N. Hatsopoulos and E.P. Gyftopoulos, "A Unified Quantum Theory of Mechanics and Thermodynamics," Foundations of Physics, Vol. 6, 15, 127, 436, 561 (1976).

6. J.B. Rosen, "The Gradient Projection Method for Nonlinear Programming," Journal of the Society for Industrial and Applied Mathematics, Vol. 9, 514 (1961); R. Fletcher and M.J.D. Powell, "A Rapidly Convergent Descent Method for Minimization," Computational Journal, Vol. 6, 163 (1963).

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