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SOME NOTES ON DYNAMIC PRINCIPLE FOR ENSEMBLE CONTROL TOOLS

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The purpose of these notes is a supplement of our recent findings [1] by theoretical constructions, which are important both for the theory of dynamic ensemble control tools and for derivation of new thermostats and their application. It is shown that the principle is applicable to dynamical systems that go beyond the Hamiltonian systems considered in the cited article. We pay special attention to gradient dynamical systems, for which we have obtained a new promising theoretical result.

Keywords: ensemble control tool, temperature expression, gradient system, invariant density

Introduction

In our paper [1], we presented a dynamic principle that was aimed to construction of ensemble control tools applied to Hamiltonian systems in contact with a thermostat and allowing deterministic and stochastic sampling schemes of the canonical ensemble. This new method was based on the fundamental laws of statistical physics, with reproduction of the known ones, as well as derivation of new dynamic thermostat equations.

Hamiltonian system consisting of N particles in d-dimensional space is described by the equations of motion $\dot{x} = \mathbf{J}\nabla H(x)$, where $H(x)$ is the Hamiltonian function, $x = (p, q) \in \mathbb{R}^{2dN}$, $\{p\}$ are momentum variables, $\{q\}$ are position variables, and $\mathbf{J}$ is the symplectic unit. In article [1], we have shown how these equations should be modified if the Hamiltonian system is in contact with the thermal bath. In these Notes, we extend this theory so that it allows construction of a wider range of thermostats, deterministic and stochastic, which can also be used for gradient systems (in addition to Hamiltonian). Since this paper is a supplement to [1], it would be wasteful to reproduce here the corresponding definitions. We simply refer to [1] for details of notations and definitions. In short, the definition of temperature expression and the dynamic principle scheme are the same as in [1].

Equations of motion

Key properties of Hamiltonian equations of motion allowing their modification according to the dynamic principle with the canonical density being invariant are

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$$\dot{H}(x) = \nabla H(x) \cdot \mathbf{J}\nabla H(x) = 0,$$

$$\nabla \cdot (\mathbf{J}\nabla H(x)) = 0,$$

that is, $H(x)$ is a first integral and $\mathbf{J}\nabla H(x)$ is an incompressible vector field.

To generalize the theoretical scheme of [1], we set the probability density $\sigma(x)$ in the form

$$\sigma(x) \propto \exp\left\{-\frac{1}{\vartheta}V(x)\right\},$$

$x \in M = \mathbb{R}^n$ (phase space is not necessarily even dimensional) so that $V(x): M \to \mathbb{R}$ is a coercive function, that is, $V(x) \to +\infty$ as $|x| \to +\infty$. It is also assumed that $V(x) \in C^2$. Alternatively, we can set the potential function, $V(x)$, in the form

$$V(x) = -\vartheta \ln \sigma(x),$$

where $\vartheta > 0$ is a parameter.

Consider a pair of vector fields, namely, a potential field $\nabla V(x)$, and an incompressible one $\mathbf{G}(x)$, that is, $\nabla \cdot \mathbf{G}(x) = 0$ for all $x \in M$, such that

$$\nabla V(x) \cdot \mathbf{G}(x) = 0$$

for all $x \in M$ (in other words, $\nabla V(x)$ and $\mathbf{G}(x)$ form a cosymmetric pair as defined in [2]). Then we relate to system S the unperturbed equations of motion

$$\dot{x} = \mathbf{G}(x).$$

Thus, we arrive at the following properties,

$$\dot{V} = \nabla V(x) \cdot \mathbf{G}(x) = 0,$$

$$\nabla \cdot \big(\mathbf{G}(x)\sigma(x)\big) = 0,$$

in other words, $V(x)$ is the first integral and density $\sigma(x)$ is invariant for the dynamics $\dot{x} = \mathbf{G}(x)$.

Examples of cosymmetric pairs $\big(\mathbf{G}(x), \nabla V(x)\big)$ include, but are not limited to:

$$\mathbf{G}(x) = 0 \text{ (trivial case),}$$

$$\mathbf{G}(x) = \mathbf{\Lambda}\nabla V(x),$$

where $\mathbf{\Lambda}$ is an antisymmetric constant matrix; in particular $\mathbf{\Lambda} = \mathbf{J}$ (symplectic unit) in even-dimensional phase space,

$$\mathbf{G}(x) = \mathbf{\Lambda}(x)\nabla V(x),$$

where $\mathbf{\Lambda}(x)$ is a linear antisymmetric operator (matrix) depending on x, for example an antisymmetric operator $\mathbf{\Lambda}(x)$ satisfying the Jacobi identity (Poisson system).

Vector fields $\mathbf{G}(x)$ are incompressible in all these cases.

When S system (please refer to article [1] for designation details) is in contact with the environmental reservoir $\Sigma = S^* + \Sigma \setminus S^*$ then since we do not aim to use the most general temperature expressions (ϑ-expressions) and their properties, for the purpose of simplicity and clarity of presentation, we take the following particular ϑ-expression as a basis,

$$\Theta(x,\vartheta) = \varphi(x,\vartheta)\cdot\nabla_x V(x) - \vartheta\nabla_x \cdot \varphi(x,\vartheta)$$

(as defined in the article [1]) and modify the equations of motion according to the dynamic principle, that is,

$$\nabla_x V(x)\cdot \mathbf{G}(x) \propto \Theta(x,\vartheta),$$

assuming the validity of the ergodic hypothesis. Note that it is always possible to expand $\mathbf{G}(x)$ into two parts, first, $\mathbf{G}_1(x)$ associated with cosymmetry of the potential vector field $\nabla_x V(x)$, namely $\nabla_x V(x)\cdot \mathbf{G}_1(x) = 0$ for all $x \in M$, and second, $\nabla_x V(x)\cdot \mathbf{G}_2(x) = 0$, that is vanishing on average only. Explicitly,

$$\mathbf{G}(x) = \mathbf{G}_1(x) + \mathbf{G}_2(x).$$

Similarly, we relate to the system S^* the equations of motion,

$$\dot{y} = \mathbf{G}^*(y), \quad y \in M^*,$$

the equilibrium probability density,

$$\sigma^*(y) \propto \exp\left\{-\frac{1}{\vartheta}V^*(y)\right\},$$

and the ϑ-expression,

$$\Theta^*(y,\vartheta) = \varphi^*(y,\vartheta)\cdot\nabla_y V^*(y)\cdot\vartheta\nabla_y \cdot \varphi^*(y,\vartheta).$$

When the S^* system is involved in a joint motion with the system S and an influence of $\Sigma \setminus S^*$ on the dynamics is ignored (in the general case of an infinite reservoir, it has to be stochastic by necessity), then, following the procedure described in [1], we arrive at the particular case of the thermostatted stable deterministic dynamics among others,

$$\dot{x} = \mathbf{G}_1(x) + \sum_{(l)} \Theta_l^*\left(y,\vartheta\right)\varphi_l\left(x,\vartheta\right),$$

$$\dot{y} = \mathbf{G}_1^*(y) - \sum_{(k)} \Theta_k\left(x,\vartheta\right)\varphi_k^*\left(y,\vartheta\right),$$

under reasonable conditions on vector fields $\left\{\varphi_k\left(x,\vartheta\right)\right\}$ and $\left\{\varphi_l^*\left(y,\vartheta\right)\right\}$. One can verify that the density $\rho(x,y) = \sigma(x)\sigma^*(y)$ is invariant for the dynamics. This form of deterministic equations of motion, that is a deterministic thermostat, covers a wide range of thermostats we can find in the literature. It is also evident that the expression

$$\sum_{(l)} \Theta_l^*(y,\vartheta)\left[\varphi_l(x,\vartheta)\cdot\nabla_x V(x)\right] - \sum_{(k)} \Theta_k(x,\vartheta)\left[\varphi_k^*(y,\vartheta)\cdot\nabla_y V^*(y)\right]$$

is zero on average as required. The proof is by direct calculation.

Stochastic dynamics

Following procedure described in [1], we consider a particular ϑ-expression of the form

$$\Theta_L(x,\vartheta) = \sum_{l=0}^{L} \Theta_l(x,\vartheta)\vartheta^{2l}$$

for all $L \in \mathbb{R}_{\geq 0}$, where

$$\Theta_l(x,\vartheta) = \varphi_l(x)\cdot\nabla V(x) - \vartheta\nabla\cdot\varphi_l(x), \quad l = 0,1,\ldots,L,$$

and $\{\varphi_l(x)\}_{l=0}^{L}$ is a set of vector fields on M such that $\varphi_l(x)\sigma(x) \to 0$ as $|x| \to \infty$, then introduce the set of independent vectors of white noises, $\{\xi(l;t)\}_{l=0}^{L}$, $L \in \mathbb{R}_{\geq 0}$ such that

$$\langle \xi(l;t)\rangle = 0, \quad \langle \xi_i(l;t)\xi_j(l';t')\rangle = 2\lambda_l\vartheta\delta_{ij}\delta_{ll'}\delta(t-t'),$$

where $\{\lambda_l\}_{l=0}^{L}$ is a set of constant parameters, and also the set of vector fields, $\{\zeta(l;x)\}_{l-0}^{L}$, $L \in \mathbb{R}_{\geq 0}$ such that

$$\nabla \circ \zeta(l;x) = 0$$

for any $l \geq 0$, where «$\circ$» denotes the component-wise product of two vectors (the Hadamard product).

Starting with the relationship

$$\nabla V(x)\cdot\mathbf{G}_2(x,\lambda) = \sum_{l=0}^{L} \lambda_l\Theta_l(x,\vartheta)\vartheta^{2l},$$

and then strictly following the procedure outlined in [1], we arrive at the following stochastic dynamics:

$$\dot{x} = \mathbf{G}_1(x) - \sum_{l=0}^{L} \lambda_l\eta(l;x)\circ\nabla V(x)\vartheta^{2l} + \sum_{l=0}^{L} \zeta(l;x)\circ\xi(l;t)\vartheta^{l}, \tag{1}$$

where $\eta(x) \equiv \zeta(x)\circ\zeta(x)$. One can verify that the density $\sigma(x)$ is invariant for the dynamics as required. As for the stochastic dynamics, it is very likely that it is ergodic.

Deterministic dynamics

Utilizing the notations from [1], we consider the S^* system in the phase space M^* with the probability density function $\sigma^*(y) \propto \exp\left[-\vartheta^{-1}V^*(y)\right]$, $y \in M^*$, and the equations of motion, $\dot{y} = \mathbf{G}^*(y)$, where the vector field $\mathbf{G}^*(y)$ is cosymmetric to the potential vector field $\nabla_y V^*(y)$ on M^*. When the S^* system is involved in a joint motion with the S system and they are in a contact with the reservoir then, following the procedure described in article [1], we arrive, among other things, at the following deterministic dynamics

$$\begin{aligned} \dot{x} &= \mathbf{G}(x) + \sum_{l=0}^{L} \Theta_l^*\left(y,\vartheta\right)\vartheta^{2l}\varphi_l(x), \\ \dot{y} &= \mathbf{G}^*(y) - \sum_{l=0}^{L} \Theta_k\left(x,\vartheta\right)\vartheta^{2k}\varphi_k^*(y), \end{aligned} \tag{2}$$

where

$$\Theta_l^*\left(y,\vartheta\right) = \varphi_l^*(y)\cdot\nabla_y V^*(y) - \vartheta\nabla_y\cdot\varphi_l^*(y), \quad l = 0,1,...,L,$$

and $\left\{\varphi_l^*(y)\right\}_{l=0}^{L}$ is a set of vector fields on M such that $\varphi_l^*(y)\sigma^*(y) \to 0$ as $|y| \to +\infty$. One can verify that $\rho(x,y) = \sigma(x)\sigma^*(y)$ is invariant for the dynamics. However, the ergodicity of these equations of motion is generally unsolvable. For specific systems, the expected answer to the question of their ergodicity will be rather negative than positive. Nevertheless, numerical simulation of a system can demonstrates its ergodicity from a practical point of view. This last point underlies the use of deterministic thermostats in molecular dynamics.

Thus, it is obvious that, following the dynamic principle presented in article [1], we obtain various stochastic as well as deterministic thermostat equations of motion. In the next section, we will expand the use of the dynamic principle by considering an important case of a gradient dynamical system.

Gradient dynamical systems

A gradient system on phase space $M = \mathbb{R}^n$ is described by the dynamical equations of the form

$$\dot{x} = -\nabla V(x), \tag{3}$$

where $x \in M = \mathbb{R}^n$, $V(x)$, is the potential function of the gradient system (it is assumed that $V(x)$ is twice continuously differentiable) such that $V(x) \to +\infty$ as $|x| \to +\infty$, or of the form

$$\dot{x} = -\mathbf{\Omega}(x)\nabla V(x),$$

where $\mathbf{\Omega}(x)$ is a symmetric positive definite operator (matrix) so that $\mathbf{\Omega}(x)$ can be regarded as a Riemannian metric, and the scalar product has the form $\left[\mathbf{A}(x),\mathbf{B}(x)\right] = \mathbf{A}(x)\cdot\mathbf{\Omega}(x)\mathbf{B}(x)$. In both cases, potential $V(x)$ is a Lyapunov function rather than a first integral, that is,

$$\dot{V}(x) = -\nabla V(x)\cdot\mathbf{\Omega}(x)\nabla V(x) \le 0,$$

and $\dot{V}(x)=0$ if and only if $\nabla V(x)=0$. The gradient system has the properties: (a) gradient flow is perpendicular to the level set $V(x)=v=\text{const}$; (b) the equation $\nabla V(x)=0$ defines the equilibrium points; (c) an isolated equilibrium point is asymptotically stable (for example, [3]).

It is worth noting that, if the dynamical equations have the form of the generalized gradient system,

$$\dot{x}=-\nabla V(x)+\mathbf{G}(x), \tag{4}$$

or $\dot{x}=-\mathbf{\Omega}(x)\nabla V(x)+\mathbf{G}(x)$, where $\mathbf{G}(x)$ and $\nabla V(x)$ form a cosymmetric pair, then $V(x)$ is still a Lyapunov function,

$$\dot{V}(x)=-\nabla V(x)\cdot\mathbf{G}(x)-\nabla V(x)\cdot\mathbf{\Omega}(x)\nabla V(x)=-\nabla V(x)\cdot\mathbf{\Omega}(x)\nabla V(x)\le 0.$$

The vector field $\mathbf{G}(x)$ is tangential to the level set $V(x)=v=\text{const}$.

An important property of the generalized gradient system concerns the equilibrium condition. Let us assume that

$$-\nabla V(x)+\mathbf{G}(x)=0. \tag{5}$$

Then it follows that

$$\nabla V(x)=0.$$

The proof is simple, multiplying equation (5) by the potential vector field $\nabla V(x)$ and taking into account that $\mathbf{G}(x)$ and $\nabla V(x)$ form a cosymmetric pair we arrive at the relationship

$$-\nabla V(x)\cdot\nabla V(x)=-\left|\nabla V(x)\right|^2=0,$$

which is the only possible if $\nabla V(x)=0$. The converse is not true, that is, from $\nabla V(x)=0$ does not follow equation (5).

It was shown [2] that the existence of a cosymmetry, that is, a vector field $\mathbf{G}(x)$ such that $\mathbf{F}(x)\cdot\mathbf{G}(x)=0$ for all $x\in M$, provided that x_0 is a non-cosymmetric critical point, that is, $\mathbf{F}(x_0)=0$, but $\mathbf{G}(x_0)\neq 0$, leads to the equilibrium point x_0 being an element of a one-parameter continuous family of solutions of the equation $\mathbf{F}(x)=0$ (see [2] for details). It can be expected that taking this fact into account in one way or another in the equations of motion can significantly affect the dynamic behavior of the gradient systems. However, as far as we know, there is no systematic method for finding a nontrivial cosymmetry.

First, let us consider modified dynamical equations with trivial cosymmetry, $\mathbf{G}_1(x)\equiv 0$, and, for simplicity, but without prejudice to the content, we take $L=0$. Then, for example, as a direct consequence of equation (1), we arrive at a modified gradient system which is given by the stochastic equation

$$\dot{x}=-\lambda\eta(x)\circ\nabla V(x)+\zeta(x)\circ\xi(t), \tag{6}$$

Which is none other than the Smoluchowski stochastic equation (in a slightly generalized form). Probability density $\sigma(x) \propto \exp\left\{-\vartheta^{-1}V(x)\right\}$ is invariant for dynamics (6), the proof is by direct calculation, as well as the ergodicity property is very likely expected. It should be noted that equation (6) is a stochastic equation with additive noise so that its appearance should not be misleading.

In the case of deterministic dynamics, we get a diverse thermostatted equations of motion in depends on the form of configuration temperature expression. For example, assume that

$$\varphi(x) = -\nabla V(x),$$

then we get equations of motion

$$\begin{aligned} \dot{x} &= -\Theta^*\left(y,\vartheta\right)\nabla V(x), \\ \dot{y} &= -\Theta\left(x,\vartheta\right)\varphi^*(y), \end{aligned} \tag{7}$$

which the vector field $\varphi^*(y)$ and the temperature expressions $\Theta(x,\vartheta)$ and $\Theta^*(y,\vartheta)$ are as defined above. Probability density $\rho(x,y) = \sigma(x)\sigma^*(y)$ is invariant for the dynamics. However, if we attempt to sample the probability density with dynamical equations (7), then we immediately arrive at a wrong result. The reason is simple, dynamics (7) is not ergodic. Indeed, at an equilibrium point $\nabla V(x) = 0$, the evolution comes to halt and no longer fluctuates, irrespective to time dependence of $\Theta^*\left(y,\vartheta\right)$. For initial conditions with $\nabla V(x) \neq 0$, equations (7) define a gradient flow and all trajectories move along paths in x with equilibrium point at either end. That is to say, the dynamics (7) is not ergodic.

Note that when the expression $\Theta^*\left(y,\vartheta\right)$ is defined by the functions $\varphi^*(y) = Q^{-1} = \text{const}$ and $V^*(y) = \frac{1}{2}Qy^2$, $y \in \mathbb{R}$, that is, $\Theta^*\left(y,\vartheta\right) = y$, then we arrive at a very special case considered in [4,5]. The case of the potential function $V^*(y) = \frac{1}{2}\left(y,\mathbf{Q}y\right)$, $y \in \mathbb{R}^n$, where $\mathbf{Q}$ is a symmetric, positive definite matrix, can be considered in the same way.

If now we try to generate the required statistics by replacing the equations for y-variable with stochastic ones, that is,

$$\begin{aligned} \dot{x} &= -\Theta^*\left(y,\vartheta\right)\nabla V(x), \\ \dot{y} &= -\Theta\left(x,\vartheta\right)\varphi^*(y) - \lambda\eta(y)\circ\nabla V^*(y) + \zeta(y)\circ\xi(t), \end{aligned} \tag{8}$$

where $\nabla_y \circ \zeta(y) = 0$ and $\eta(y) \equiv \zeta(y)\circ\zeta(y)$, then we come to the same conclusion regarding ergodicity.

Now, it has to be expected that addition of cosymmetry of the potential vector field $\nabla V(x)$ to the equations of motion can significantly change the dynamic scenario, provided that the probability density $\rho(x,y) = \sigma(x)\sigma^*(y)$ remains invariant for the modified dynamics. It is also evident that a cosymmetry with cosymmetric critical points is insufficient for our purposes. A way to overcome this difficulty is to supplement the system with constrain on forces as it described in [4]. However, that way appears as an *ad hoc* trick even if we can give physical meaning to such kind of constrain in some cases.

Since there is no method for finding a nontrivial cosymmetry in its classical sense, in order to consider an appropriate analogue of the equations of motion in the form,

$$\begin{aligned} \dot{x} &= -\Theta^{*}\left(y,\vartheta\right)\nabla V(x) + \mathbf{G}(x), \\ \dot{y} &= -\Theta\left(x,\vartheta\right)\varphi^{*}(y), \end{aligned} \qquad (9)$$

when an extra dynamic variable (phase-space vector) $z \in M^{n}$ is added to equations of motion instead of vector field $\mathbf{G}(x)$, and then the concept of cosymmetry on average is introduced. In other words, we propose an algorithmic method to generate the vector field orthogonal a given potential vector field in a wider sense.

In order to explicitly implement this kind of algorithm in the form of dynamic equations, we will use an analogue of the well-proven dynamic principle [1]. For the sake of clarity, as for the statistical properties of the dynamical variable *z*, we restrict ourselves to the Gaussian equilibrium density. In a generalized form, this theoretical construction will be considered separately. Thus, we assume that the equilibrium density of the dynamic variable $z \in M$ is Gaussian with zero mean,

$$\sigma_{z} \propto \exp\left\{-\frac{1}{\vartheta}b(z)\right\} \equiv \exp\left\{-\frac{1}{\vartheta}\frac{1}{2}\left(z\cdot\mathbf{Q}z\right)\right\},$$

where **Q** is a symmetric, positive definite operator (matrix), and then we require that

$$\nabla b(z)\cdot\dot{z} + \psi(z)\cdot\nabla V(x) \,\mathbb{R}\, 0,$$

provided that $\mathrm{E}\left\{\nabla b(z)\cdot\dot{z} + \psi(z)\cdot\nabla V(x)\right\} = 0$, as described in [1]. A solution of the above functional equation is as follows. Let the vector field $\psi(z)$ be $\psi(z) = \nabla b(z) = \mathbf{Q}z$, then

$$\dot{z} = -\nabla V(x)\,.$$

Thus, we arrive at the following equations of motion in the extended phase space,

$$\dot{x} = -\Theta^{*}\left(y,\vartheta\right)\nabla V(x) + \mathbf{Q}z\,,$$

$$\dot{y} = -\Theta\left(x,\vartheta\right)\varphi^{*}(y)\,,$$

$$\dot{z} = -\nabla V(x)\,.$$

It is easy to prove by direct calculation that the density

$$\rho \propto \exp\left\{-\frac{1}{\vartheta}V(x)\right\}\exp\left\{-\frac{1}{\vartheta}V^{*}(y)\right\}\exp\left\{-\frac{1}{\vartheta}\frac{1}{2}\left(z\cdot\mathbf{Q}z\right)\right\}$$

is invariant for the deterministic dynamics above.

Stochastic extension of these deterministic equations can be made in accordance with the procedure described above, e.g., in the form of following stochastic equations of motion:

$$\dot{x} = -\Theta^*(y, \vartheta)\nabla V(x) + \mathbf{Q}z\,,$$

$$\dot{y} = -\Theta(x, \vartheta)\varphi^*(y) - \lambda\eta(y)\circ\nabla V^*(y) + \zeta(y)\circ\xi(t)\,,$$

$$\dot{z} = -\nabla V(x)\,.$$

This and other forms of stochastic equations of motion will be considered separately.

Summary

We have shown that the dynamic principle [1] allows using cosymmetric vector pairs to construct stochastic and deterministic temperature control tools. We have also shown that the dynamic principle is applicable to several systems that go beyond the Hamiltonian ones considered in [1]. Special attention is paid to gradient systems for which new thermostat schemes were obtained.

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НЕСКОЛЬКО ЗАМЕЧАНИЙ О ДИНАМИЧЕСКОМ ПРИНЦИПЕ КОНТРОЛЯ СТАТИСТИЧЕСКОГО АНСАМБЛЯ

Цель настоящих заметок – дополнить наши недавние результаты [1] теоретическими конструкциями, важными как для теории инструментов динамического контроля статистического ансамбля, так и для получения новых термостатов и их практического использования. Показано, что динамический принцип применим к системам, выходящим за пределы ранее рассмотренных гамильтоновых систем. Специальное внимание уделено градиентным динамическим системам, для которых получен новый перспективный теоретический результат.

Ключевые слова: инструмент контроля ансамбля, выражение температуры, градиентная система, инвариантная плотность