Controlled thermodynamic systems and stochastic variational principles

Michele Pavon

Dipartimento di Matematica Pura ed Applicata
Università di Padova, Italy

A Thermodynamics Day, Padova, June 11, 2010

A system of stochastic oscillators

Mechanical system in a force field coupled to a heat bath:

$$dx(t) = v(t)\,dt, \tag{1}$$

$$M dv(t) = -Bv(t)\,dt - \nabla V(x(t))dt + \Sigma dW(t). \tag{2}$$

1. $V \in C^1$ bounded below, tends to infinity for $|x| \to \infty$;

2. $W(t), t \geq 0$ standard n-dimensional Wiener process ($\dot{W}$ is Gaussian white noise, $(dW(t))^2 \approx dt$);

3. M, B and Σ are $n \times n$ matrices with $M = M^T > 0$. B and Σ need not be diagonal or even symmetric.

A system of stochastic oscillators (cont'd)

- Model (1)-(2) generalizes Ornstein-Uhlenbeck model of physical Brownian motion (equivalently, it generalizes the Nyquist-Johnson model (1928) of RLC network with noisy resistor and nonlinear capacitor);

- It can, for instance, describe a system of n oscillators with velocity coupling trough first neighbour interaction and different spatial arrangements (closed ring, linear array).

A system of stochastic oscillators (cont'd)

Equilibrium and Fluctuation-Dissipation relation

Gibbsian postulate of classical statistical mechanics: equilibrium state of microscopic system at absolute temperature T and with Hamiltonian function H given by Maxwell-Boltzmann distribution

$$\bar{\rho} = Z^{-1} \exp\left[-\frac{H}{kT}\right] \tag{3}$$

where Z is the *partition function*. In our case

$$H(x, v) = \frac{1}{2}\langle v, Mv\rangle + V(x).$$

Proposition 1 The Maxwell-Boltzmann distribution (3) is invariant for system of stochastic oscillators if and only if

$$\Sigma\Sigma^T = kT(B + B^T). \tag{4}$$

A system of stochastic oscillators (cont'd)

It has been shown that

1. System with Maxwell-Boltzmann distribution satisfies suitable Newton law if and only if $\boldsymbol{B}$ is symmetric;

2. Maxwell-Boltzmann distribution necessary for time-reversal invariance.

3. Connection between existence of an invariant measure and complete controllability of an associated deterministic system (pervasive damping).

A system of stochastic oscillators (cont'd)

H-Theorem

Let $\rho_0(x,v)$ be density of (x_0,v_0) and let $\rho_t(x,v)$ denote the corresponding solution of the Fokker Planck equation

$$\frac{\partial \rho}{\partial t} + v \cdot \nabla_x \rho - \nabla_v \cdot (Bv\rho) = \frac{1}{2}\sum_{i,j=1}^{n} a_{ij} \frac{\partial^2}{\partial v_i \partial v_j}\rho, \tag{5}$$

where

$$(a_{ij}) = \Sigma\Sigma^T.$$

Suppose Maxwell-Boltzmann density is stationary solution of (5)

A system of stochastic oscillators (cont'd)

Consider now the *free energy* functional

$$\boldsymbol{kT}\mathbb{D}(\boldsymbol{\rho_t}||\bar{\boldsymbol{\rho}}) = \boldsymbol{F}(\boldsymbol{\rho_t}) = \boldsymbol{kT}\int_{\mathbb{R}^n}\int_{\mathbb{R}^n}\log\frac{\boldsymbol{\rho_t}}{\bar{\boldsymbol{\rho}}}\boldsymbol{\rho_t}\,\boldsymbol{dxdv},$$

where $\bar{\boldsymbol{\rho}}$ is given by (3) . We have

$$\frac{\boldsymbol{d}}{\boldsymbol{dt}}\boldsymbol{F}(\boldsymbol{\rho_t}) = -\frac{\boldsymbol{kT}}{\mathbf{2}}\int_{\mathbb{R}^n}\int_{\mathbb{R}^n}\langle\boldsymbol{\Sigma\Sigma^T\nabla_v}\log\frac{\boldsymbol{\rho_t}}{\bar{\boldsymbol{\rho}}},\boldsymbol{\nabla_v}\log\frac{\boldsymbol{\rho_t}}{\bar{\boldsymbol{\rho}}}\rangle\boldsymbol{\rho_t}\,\boldsymbol{dxdv} \qquad (6)$$

This can be recognized as a form of the H-Theorem.

There exists, however, a stronger form.

Differentials of Markov diffusion

For f defined on $[t_0, t_1]$ and $dt > 0$, let

$$d_+ f(t) := f(t + dt) - f(t), \quad d_- f(t) = f(t) - f(t - dt)$$

be *forward and backward increment* at time t, respectively. Consider a Markov diffusion process $\{X(t); t_0 \leq t \leq t_1\}$ with diffusion coefficient σ^2. Under mild assumptions, X admits both forward and backward drifts

$$b_+(X(t), t) = \lim_{dt \searrow 0} E\left\{\frac{d_+ X(t)}{dt} | X(\tau), t_0 \leq \tau \leq t\right\},$$
$$b_-(X(t), t) = \lim_{dt \searrow 0} E\left\{\frac{d_- X(t)}{dt} | X(\tau), t \leq \tau \leq t_1\right\}.$$

Differentials of Markov diffusion (cont'd)

Hence $\boldsymbol{X}$ possesses two differentials

$$\begin{aligned} d_+ \boldsymbol{X}(t) &= \boldsymbol{b}_+(\boldsymbol{X}(t), t)dt + \boldsymbol{\sigma} d\boldsymbol{W}_+(t), \\ d_- \boldsymbol{X}(t) &= \boldsymbol{b}_-(\boldsymbol{X}(t), t)dt + \boldsymbol{\sigma} d\boldsymbol{W}_-(t). \end{aligned}$$

Moreover,

$$\boldsymbol{b}_-(\boldsymbol{x}, t) = \boldsymbol{b}_+(\boldsymbol{x}, t) - \boldsymbol{\sigma}^2 \nabla \log \boldsymbol{\rho}(\boldsymbol{x}, t).$$

A stronger form of the H-Theorem

Suppose, for simplicity, that $\boldsymbol{\Sigma} = \boldsymbol{\sigma I}$ and $\boldsymbol{B} = \boldsymbol{\beta I}$ are diagonal satisfying Einstein's relation. Introduce the free energy density $\boldsymbol{\psi(x,v,t) = kT \log \frac{\rho_t}{\bar{\rho}}(x,v)}$, so that $\boldsymbol{F(\rho_t) = \mathbb{E}(\psi(x(t),v(t),t))}$. It can be shown that $-\boldsymbol{\psi}$ is the value function of the following reverse-time stochastic control problem

$$-\boldsymbol{\psi(x,v,t) = inf_{u \in \mathcal{U}} \mathbb{E}\left(\frac{kT\sigma^2}{2}\int_{t_0}^{t} \|u - \bar{b}_-\|^2 ds - \psi(x(0),v(0),0)\right)},$$

subject to

$$\begin{aligned} \boldsymbol{dx(t)} &= \boldsymbol{v(t)dt}, \quad \boldsymbol{x(t) = x} \\ \boldsymbol{Mdv(t)} &= \boldsymbol{u(x(t),v(t),t)dt + \sigma dW(t)}, \quad \boldsymbol{v(t) = v}, \end{aligned}$$

and $\boldsymbol{\bar{b}_- = \beta v - \nabla V(x)}$ may be seen as the equilibrium backward drift of $\boldsymbol{Mv}$.

A stronger form of the H-Theorem (cont'd)

The optimal feedback control law $u^*(x,v,t)$ is the backward drift of Mv of the evolution starting with $\rho_0(x,v)$, namely $b_- = -\beta v - \nabla V(x) - \sigma^2 \nabla_v \log \rho_t(x,v)$. The stochastic process $\psi(x(t),v(t),t)$ is consequently a reverse-time submartingale and the free energy decay follows simply taking expectations.

May be interpreted as a principle of minimum dissipation. Indeed, it can also be rephrased as follows: *The probability distribution induced on path space by the actual physical evolution is the one that minimizes relative entropy distance from the equilibrium path space measure among those having initial marginal* $\rho_0(x,v)$ (instance of theory of Schrödinger bridges).

Large Deviations

Consider a large number N of i.i.d. Brownian particles X_i in equilibrium. Let $\bar{P}(t_0, t_1)$ be their distribution of $C(t_0, t_1)$. Consider the empirical distribution

$$\mu_N = \frac{1}{N}\sum_{i=1}^{N} \delta_{X^i}, \quad N = 1, 2, \ldots .$$

By the law of large numbers, the probability of observing μ_N with marginal density $\rho_0 \neq \bar{\rho}$ tends to zero. Nevertheless, for a fixed large N, since we have observed ρ_0 at time t_0, we know that $\mu_N \in \mathcal{D}(\rho_0)$. We ask, which one is its most probable form? Answer is provided by Sanov' theorem. Probability of observing $\mu_N \in \mathcal{D}(\rho_0)$ decays as

$$\exp\left[-N \inf\{\mathbb{D}(P(t_0, t_1)\|\bar{P}(t_0, t_1)); P(t_0, t_1) \in \mathcal{D}(\rho_0)\}\right]. \tag{7}$$

Hence, the path-space distribution corresponding to the initial density ρ_0 has most probable form!

Details in:

- M.Pavon, Critical Ornstein-Uhlenbeck processes, *Appl. Math. Opt.* **14** (1986), 265-276.

- F.Guerra and M.Pavon, Stochastic variational principles and free energy for dissipative processes, Proc. *MTNS-87 Conf.*, Phoenix,AZ,1988, 571-578.

- M.Pavon, Stochastic control and nonequilibrium thermodynamical systems, *Appl. Math. Opt.* **19** (1989), 187-202.

- P.Dai Pra and M.Pavon, Variational path-integral representations for the density of a diffusion process, *Stochastics* **26** (1989), 205-226.

- D.B.Hernandez and M.Pavon, Equilibrium description of a particle system in a heat bath, *Acta Applicandae Mathematicae* **14** (1989), 239-256.

- P.Dai Pra, A stochastic control approach to reciprocal diffusion processes, *Appl. Math. Opt.*, **23**, 313-329, 1991.

- M.Pavon and A.Wakolbinger, On free energy, stochastic control, and Schrödinger processes, *Modeling, Estimation and Control of Systems with Uncertainty*, A.G, Birkäuser, 1991, 334-348.

- M. Pavon and F. Ticozzi, Discrete-time classical and quantum Markovian evolutions: Maximum entropy problems on path space, *J. Math. Phys.*, **51**, (2010) 3372725.. Preprint arXiv:math-ph/0811.0933v2

- F. Ticozzi and M. Pavon, On Time-reversal and space-time harmonic processes for Markovian quantum channels, *Quantum Information Processing*, to appear. Preprint arXiv:quant-ph/0811.0929v2

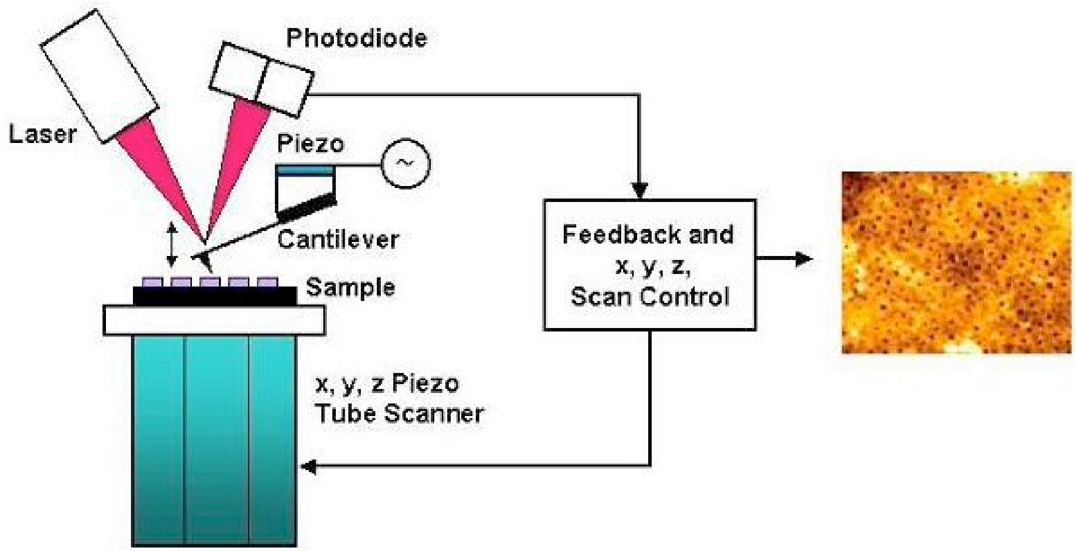
Feedback control of stochastic oscillators

Consider now the same system of stochastic oscillators subject to an external force :

$$\begin{aligned} dx(t) &= v(t)\,dt, \\ M dv(t) &= -Bv(t)\,dt - \nabla V(x(t))dt + u(t, x(t), v(t)) + \Sigma dW(t). \end{aligned}$$

Here u is to be designed by the controller in order to achieve a certain desired evolution of the system.

AFM Experiment



Velocity-dependent feedback control (VFC) to reduce thermal noise of a cantilever in Atomic Force Microscopy (AFM)

AFM Experiment (cont'd)

In the AFM experiment:

- $\boldsymbol{V(x) = \frac{k}{2}\|x\|^2}$, where $\boldsymbol{k}$ is a spring constant of the AFM cantilever;
- Sensor provided by electric circuit detecting motion of the cantilever;
- Control force $\boldsymbol{u}$ is changed proportional to velocity in order to reduce thermal noise.

AFM Experiment (cont'd)

In the AFM experiment, $\boldsymbol{M} = \boldsymbol{m}\boldsymbol{I}_3$, $\boldsymbol{B} = \boldsymbol{\beta}\boldsymbol{I}_3$, $\boldsymbol{\beta} > \mathbf{0}$, $\boldsymbol{\Sigma} = \boldsymbol{\sigma}\boldsymbol{I}_3$. Einstein's relation reads

$$\boldsymbol{\sigma}^2 = \mathbf{2}\boldsymbol{kT\beta}. \tag{8}$$

The controlling feedback force is given by

$$\boldsymbol{u(t,x,v) = -\alpha v}, \quad \boldsymbol{\alpha} > \mathbf{0}.$$

The control then acts as a frictional force on the macromolecule. Since the frictional coefficient is now $\boldsymbol{\beta + \alpha}$, we can rewrite (8) as

$$\boldsymbol{\sigma}^2 = \mathbf{2}\boldsymbol{kT}_{\text{eff}}(\boldsymbol{\beta + \alpha}), \tag{9}$$

where the effective temperature $\boldsymbol{T}_{\text{eff}}$ is given by

$$\boldsymbol{T}_{\text{eff}} = \frac{\boldsymbol{\beta}}{\boldsymbol{\beta + \alpha}}\boldsymbol{T} < \boldsymbol{T}.$$

Shannon's entropy

My greatest concern was what to call it. I thought of calling it 'information', but the word was overly used, so I decided to call it 'uncertainty'. John von Neumann had a better idea, he told me, 'You should call it entropy, for two reasons. In the first place your uncertainty function goes by that name in statistical mechanics. In the second place, and more important, nobody knows what entropy really is, so in a debate you will always have the advantage.(C. E. Shannon as quoted in M. Tribus, E.C. McIrvine, Energy and information, Scientific American, 224 (September 1971), 178-184.)

Relative Entropy

For $\rho \geq 0$ and $\sigma \geq 0$ on $\mathbb{R}^n$, define the (*information*) *relative entropy* (*divergence*, *Kullback-Leibler index*, etc.)

$$\mathbb{D}(\rho||\sigma) = \begin{cases} \int_{\mathbb{R}^n} \log \frac{\rho}{\sigma} \rho \, dx, & Supp(\rho) \subseteq Supp(\sigma), \\ +\infty, & Supp(\rho) \not\subseteq Supp(\sigma). \end{cases} .$$

When ρ and σ satisfy

$$\int_{\mathbb{R}^n} \rho(x) dx = \int_{\mathbb{R}^n} \sigma(x) dx < \infty,$$

1. $\mathbb{D}(\rho||\sigma) \geq 0$,
2. $\mathbb{D}(\rho||\sigma) = 0$ if and only if $\rho = \sigma$.

For $\sigma \equiv 1$, $-\mathbb{D}(\rho||\sigma) = S(\rho)$ the entropy.

Relative Entropy (cont'd)

- Originates from statistical mechanics (Boltzmann, Gibbs);
- Maximun entropy problems promoted to general inference method (Kullback, Jaynes);
- Concept plays central role in Information Theory (Shannon), Mathematical Statistics, Probability Theory (Sanov, Barron), Signal Processing (Burg,Byrnes, Georgiou, Lindquist,...);
- Umegaki-von Neumann relative entropy in Quantum Information Theory.

Thermodynamic systems

Consider open thermodynamical system. Macroscopic evolution $\sim$ n-dimensional Markov diffusion process $\{\boldsymbol{x}(\boldsymbol{t}); \boldsymbol{t}_0 \leq \boldsymbol{t}\}$

Let $\bar{\boldsymbol{\rho}}(\boldsymbol{x})$ be the Maxwell-Boltzmann probability density corresponding to thermodynamic equilibrium

$$\bar{\boldsymbol{\rho}}(\boldsymbol{x}) = \boldsymbol{Z}^{-1} \exp[-\frac{\boldsymbol{H}(\boldsymbol{x})}{\boldsymbol{kT}}],$$

where $\boldsymbol{H}$ is Hamiltonian function.

The Ito differential of $\boldsymbol{x}$ is

$$\boldsymbol{dx}(\boldsymbol{t}) = -\frac{\boldsymbol{\sigma}^2}{\boldsymbol{2kT}} \nabla \boldsymbol{H}(\boldsymbol{x}(\boldsymbol{t}))\boldsymbol{dt} + \boldsymbol{\sigma dW},$$

$\boldsymbol{W}$ is a standard $\boldsymbol{n}$-dimensional Wiener process.

Thermodynamic systems (cont'd)

Probability density ρ_t of $x(t)$ satisfies *Fokker-Planck equation*

$$\frac{\partial \rho}{\partial t} - \nabla \cdot (\frac{\sigma^2}{2kT} \nabla H \rho) = \frac{\sigma^2}{2} \Delta \rho.$$

Let us introduce the *fluxes* $J(x,t)$ and *forces* $\Phi(x,t)$ by

$$J(x,t) = -\frac{1}{2}\sigma^2 \nabla \rho_t(x) - \frac{1}{2kT}\sigma^2 \nabla H(x) \rho_t(x), \quad \Phi(x,t) = -\nabla \mu(x,t).$$

$\mu = H + kT \log \rho_t$ is *electrochemical potential*. Notice:

- Fokker-Plank equation may be rewritten as a continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot J = 0, \quad J = v\rho, \quad v = -\frac{\sigma^2}{2kT} \nabla H - \frac{\sigma^2}{2} \nabla \log \rho.$$

Thermodynamic systems (cont'd)

- Both fluxes and forces are zero in equilibrium. Moreover,

$$\boldsymbol{J(x,t) = \frac{\sigma^2}{2kT}\Phi(x,t)\rho_t(x)},$$

which plays the role of *constitutive relations*.

- Define *free energy* functional

$$\boldsymbol{F(\rho_t) = kT \int_{\mathbb{R}^n}\int_{\mathbb{R}^n} \log\frac{\rho_t}{\bar\rho}\rho_t\,dx = kT\mathbb{D}(\rho_t||\bar\rho)}.$$

The free energy decay may now be expressed as

$$\boldsymbol{\frac{d}{dt}F(\rho_t) = -\frac{\sigma^2 kT}{2}\int_{\mathbb{R}^n}|\nabla\log\frac{\rho_t}{\bar\rho}|^2\rho_t\,dx = -\int J(x,t)\Phi(x,t)dx}.$$

Controlling the Relative Entropy Evolution

Consider previous system subject to feedback control

$$dx^u(t) = \left(-\frac{\sigma^2}{2kT}\nabla H(x^u(t)) + u(x^u(t), t)\right) dt + \sigma dw.$$

$u(x, t)$ is *feedback control law* designed to alter natural evolution toward equilibrium. The density ρ_t^u of x_t^u satisfies the controlled Fokker-Planck equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left((-\frac{\sigma^2}{2kT}\nabla H + u)\rho\right) = \frac{\sigma^2}{2}\Delta\rho.$$

We are interested in the evolution of $\mathbb{D}(\rho_t^u || \rho_t)$. We need a simple but useful result.

Controlling the Relative Entropy Evolution (Cont'd)

Consider two families of nonnegative functions on $\mathbb{R}^n$:
$\{\rho_t; t_0 \leq t \leq t_1\}$ and $\{\tilde{\rho}_t; t_0 \leq t \leq t_1\}$.

Assumptions:

- **A1** There exist measurable functions $f(x,t)$ and $\tilde{f}(x,t)$ such that $\{\rho_t; t_0 \leq t \leq t_1\}$ and $\{\tilde{\rho}_t; t_0 \leq t \leq t_1\}$ are everywhere positive C^1 solutions of

$$\frac{\partial \rho_t}{\partial t} + \nabla \cdot (f \rho_t) = 0,$$
$$\frac{\partial \tilde{\rho}_t}{\partial t} + \nabla \cdot (\tilde{f} \tilde{\rho}_t) = 0.$$

Controlling the Relative Entropy Evolution (Cont'd)

- **A2**

  For every $t \in [t_0, t_1]$

$$\lim_{|x|\to\infty} f(x,t)\tilde{\rho}_t(x) = 0,$$
$$\lim_{|x|\to\infty} \tilde{f}(x,t)\tilde{\rho}_t(x) = 0,$$
$$\lim_{|x|\to\infty} \tilde{f}(x,t)\tilde{\rho}_t(x)\log\frac{\tilde{\rho}_t}{\rho_t}(x) = 0.$$

Lemma 1 *Suppose* $\mathbb{D}(\tilde{\rho}_t||\rho_t) < \infty, \forall t \geq 0$. *Assume moreover A1 and A2 above. Then*

$$\frac{d}{dt}\mathbb{D}(\tilde{\rho}_t||\rho_t) = \int_{\mathbb{R}^n}\left[\nabla \log\frac{\tilde{\rho}_t}{\rho_t}\cdot(\tilde{f}-f)\right]\tilde{\rho}_t\,dx.$$

Controlling the Relative Entropy Evolution (Cont'd)

Consider again the controlled evolution

$$dx^u(t) = \left(-\frac{\sigma^2}{2kT}\nabla H(x^u(t)) + u(x^u(t),t)\right)dt + \sigma dw.$$

By Lemma 1 , we have

$$\frac{d}{dt}\mathbb{D}(\rho_t^u||\rho_t) = \int_{\mathbb{R}^n}\left(\nabla \log \frac{\rho_t^u}{\rho_t}\cdot(u - \frac{\sigma^2}{2}\nabla \log \frac{\rho_t^u}{\rho_t})\right)\rho_t^u dx.$$

Suppose $\rho_t \equiv \bar{\rho}$ Maxwell-Boltzmann distribution. We get

Theorem 1 *Under assumptions A1 and A2,*

$$\frac{d}{dt}\mathbb{D}(\rho_t^u||\bar{\rho}) = -\frac{\sigma^2}{2}\int_{\mathbb{R}^n}\|\nabla \log \frac{\rho_t^u}{\bar{\rho}}\|^2\rho_t^u dx + \int_{\mathbb{R}^n}\nabla \log \frac{\rho_t^u}{\bar{\rho}}\cdot u\rho_t^u dx$$

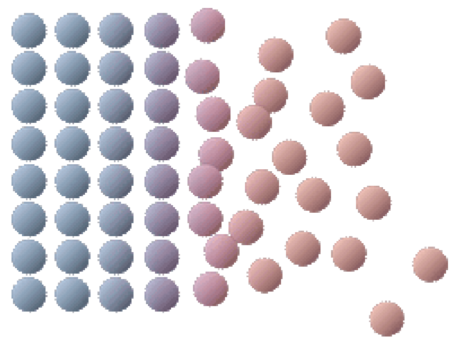
Applications

- Driving system to desired nonequilibrium steady state
  (ex.: cooling for AFM or macroscopic resonant-bar gravitational wave detectors).

- Modifying rate at which $\boldsymbol{\rho}_t^u$ tends to $\bar{\boldsymbol{\rho}}$.

Details in:

M. Pavon and F. Ticozzi,
On entropy production for controlled Markovian evolution, *J. Math. Phys.*, **47**, 063301 (2006).



(Thanks to Nino Trainito)