Fluctuations of the entropy production in nonequilibrium steady states

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Review paper with Jaksic and Pillet, Nonlin. 24 (2011) 699763

Contribution from many, many others:

T. Bodineau, E.G.D. Cohen, D. Evans, G. Gallavotti, J. Kurchan, J. Lebowitz, R. Lefevere, C. Maes and collaborators, D. Searle, H. Spohn, D. Ruelle, Schnakenberg, and

Basic questions

1. What is a nonequilibrium steady state?

2. How to define entropy production?

3. Fluctuations properties of the entropy production:

$\rightarrow$ Gallavotti-Cohen fluctuation theorem

$\rightarrow$ Kubo formula, Onsager relations

Main goals of the lectures: Expose the general theory (this is the soft part) plus provide realistic examples + proofs (some hard problems in ergodic theory/probability

Two complementary point of view

• Dynamical system theory (review paper by JPR, Ruelle, Gallavotti, Cohen, etc..)

→ Popular among people who like Gaussian thermostats or other

→ Models are easy to simulate and hard to analyze

• Markovian dynamics (Maes, Spohn-Lebowitz,...)

→ Traditional approach in physics to nonequilibrium using Markov process (Onsager, Lebowitz, etc...)

→ Models are harder to simulate and easier to analyze

The two approaches are deeply linked at the mathematical levels via Markov partition (probabilistic representation of dynamical systems...) and "dilation" of Markov processes but also by the use of same tools (spectral analysis, Perron-Frobenius, etc...).

2 basic examples from molecular dynamics (more later)

- Hamiltonian $H(p,q) = p^2 + V(q)$ with a confining potential V.
- External non-Hamiltonian force $F(q)$.
- A thermostat or heat bath

Ex 1 (Langevin equation): stochastic and canonical heat bath

$$\begin{aligned} dq &= p\, dt \\ dp &= (-\nabla V(q) + F(q) - \lambda p)\, dt + \sqrt{2\lambda T} dB \end{aligned}$$

T= reservoir temperature, λ=coupling, B=Brownian motion.

Ex 2 (Gaussian thermostat): deterministic and micocanonical heat bath (by construction the energy E is conserved)

$$\begin{aligned} \frac{dq}{dt} &= p \\ \frac{dp}{dt} &= -\nabla V(q) + F(q) - \frac{F \cdot p}{p \cdot p} p \end{aligned}$$

Part I: Entropy production in Markov chain

$\longrightarrow$ Schnakenberg, Qian & Qian, Kurchan, Spohn-Lebowitz, Maes et al., etc..

Goal of the section: Explain the ideas and concepts for the simplest possible example. Rich in concepts but no technical difficulties.

Assume: Irreducible Markov chain X_n with finite state space S, transition matrix $P(x, y)$ and stationary distribution $\pi(x)$.

Main ideas:

Non-equilibrium $\equiv$ lack of detailed balance (or time-reversibility)

Entropy production $\equiv$ measure of the irreversibility

Detailed balance

Detailed balance means $\pi(x)P(x,y) = \pi(y)P(y,x)$ for all x, y

This implies stationarity

$$\sum_x \pi(x)P(x,y) = \pi(y) = \sum_x \pi(y)P(y,x)$$

and is equivalent to the time-reversibility of the stationary Markov chain X_n.

$$\frac{\mathbf{P}_\pi(X_0 = x_n, \cdots X_n = x_0)}{\mathbf{P}_\pi(X_0 = x_0, \cdots X_n = x_n)} = \frac{\pi(x_n)P(x_n, x_{n-1})\cdots P(x_1, x_0)}{\pi(x_0)P(x_0, x_1)\cdots P(x_{n-1}, x_n)} = 1$$

or

$$\mathbf{P}_\pi = \mathbf{P}_\pi \circ \Theta, \quad \Theta(X_0, \cdots, X_n) = (X_n \cdots, X_0).$$

Any path and the time reversed path have the same probability.

Entropy production

If no detailed balance we assume the weak reversibility assumption

$$P(x,y) > 0 \Leftrightarrow P(y,x) > 0.$$

We interpret

$$\mu(x)P(x,y)$$

as the probability current from state x to state y if X_n is in state μ and define

$$F(x,y) = \log \frac{\pi(x)P(x,y)}{\pi(y)P(y,x)} \text{ (= entropy production observable)}$$

and $F \equiv 0$ iff detailed balance holds.

Path space interpretation

By construction we have

$$\frac{P_\pi(X_0 = x_n, \cdots X_n = x_0)}{P_\pi(X_0 = x_0, \cdots X_n = x_n)} = \exp\left(-\sum_{k=0}^{n-1} F(x_k, x_{k+1})\right)$$

Let us define the ergodic average

$$\underbrace{S_n(F) = S_n(F)(X_0, \cdots, X_n) = \sum_{k=0}^{n-1} F(X_i, X_{i+1})}$$

= Total entropy production along a path

In other words the Radon-Nikodym derivative

$$\frac{dP \circ \Theta}{dP}\Big|_{[0,n]} = \exp(-S_n(F)) \,.$$

Relation with relative entropy I

By the law of large numbers for the Markov chain $Z_n = (X_n, X_{n+1})$ with stationary distribution $\pi(x)P(x,y)$ and obtain that with probability 1

$$\begin{aligned}\lim_{n\to\infty} \frac{1}{n} \sum_{k=0}^{n-1} F(X_k, X_{k+1}) &= \sum_{x,y} \pi(x)P(x,y) \log \frac{\pi(x)P(x,y)}{\pi(y)P(y,x)} \\ &\equiv \mathrm{EP}(\pi, P) \text{ (Steady state entropy production)}\end{aligned}$$

Let $\mathcal{H}(\mu|\nu)$ denote the relative entropy of μ with respect to ν. Then

$$\mathrm{EP}(\pi, P) = \mathcal{H}(Z_n \,|\, Z_n \circ \Theta) \quad \text{for } Z_n \text{ stationary}$$

In particular we have $\mathrm{EP}(\pi, P) \geq 0$ (relative entropy is nonnegative) and

$$\boxed{\mathrm{EP}(\pi, P) > 0 \text{ iff no detailed balance}}$$

Relation with relative entropy II

• For Markov chains the relative entropy $\mathcal{H}(\mu|\pi)$ is always monotone decreasing under the evolution:

$$\mathcal{H}(\mu P|\pi) \leq \mathcal{H}(\mu|\pi)\,.$$

• This is **NOT** useful (to my knowledge) in nonequilibrium since in general π is unknown.

• For an arbitrary state μ of the MC X_n consider

$$\text{EP}(\mu, P) = \sum_{x,y} \mu(x)P(x,y) \log \frac{\mu(x)P(x,y)}{\mu(y)P(y,x)}$$

Fact: If detailed balance holds then

$$\text{EP}(\mu, P) = H(\mu P|\pi) - H(\mu|\pi)$$

Dependence on initial states

- For non-equilibrium steady states $\pi(x)$ is in general not explicitly known.
- Pick instead $\widetilde{F}(x,y) = \log \dfrac{P(x,y)}{P(y,x)}$ which does not involve π.
- $F(x,y)$ and $\widetilde{F}(x,y)$ have the same ergodic averages

$$S_n(F) = S_n(\widetilde{F}) + \log \pi(X_0) - \log \pi(X_n)$$

- For any initial distribution μ with $\mu(x) > 0$ we have

$$\frac{P_\mu(X_0 = i_n, \cdots X_n = i_0)}{P_\mu(X_0 = i_0, \cdots X_n = i_n)} \equiv \exp\left(-S_n(\widetilde{F}) + R(i_n) - R(i_0)\right)$$

The boundary terms $R(x)$ involving μ and π are negligible for large n.

Helmholtz decomposition of a Markov chain

We write

$$\frac{P(x,y)}{P(y,x)} = e^{H(y)-H(x)+\Delta(x,y)} \quad \text{with} \quad \Delta(x,y) = -\Delta(y,x)$$

There is a unique such decomposition if we think of it as an Helmoltz decomposition

Associate a graph $G = (V,E)$ to the Markov chain in the usual way:

$$V = S \qquad E = \{(x,y) \in S \times S\,;\, P(x,y) > 0\}$$

A flow on the graph G is a function $F : E \to \mathbb{R}$ such that

$$F(x,y) = -F(y,x)$$

.

Theorem: There exists a unique decomposition

$$F(x, y) = F_p(x, y) + F_c(x, y)$$

where

(a) $F_p(x, y)$ is a potential difference, i.e., there exists a function $H : V \to \mathbb{R}$ such that

$$F_p(x, y) = H(y) - H(x)$$

which we can write as $F_p = \nabla H$.

(b) $F_c(x, y)$ is a circulation, i.e., for any $x \in V$ we have

$$\sum_{y:(x,y)\in V} F(x, y) = 0$$

which we write as $\text{div} F_C = 0$.

Physical Interpretation

Revisit once more $\mathsf{EP}(\mu, \mathsf{P})$.

Use the decomposition $\log \frac{P(y,x)}{P(x,y)} = \beta\,[H(x) - H(y) + \Delta(x,y)]$

Use now the entropy $\mathcal{H}(\mu) = -\sum_x \mu(x) \log \mu(x)$

Find

$$\mathsf{EP}(\mu, P) =$$

$$\underbrace{\sum_{x,y} \mu(x) P(x,y)\,[H(x) - H(y) + \Delta(x,y)]}_{\substack{\text{Physical entropy production} \\ = \beta \times \text{ dissipated heat}}} + \underbrace{[\mathcal{H}(\mu P) - \mathcal{H}(\mu)]}_{\substack{\text{Increase in} \\ \text{configurational entropy}}}$$

Large deviations : reminder

Theorem (Gärtner-Ellis Theorem)

- $\{\Gamma_n\}$ sequence of random variables taking values in $\mathbb{R}^d$.
- For all $\gamma \in \mathbb{R}^d$ the logarithmic moment generating function

$$e(\gamma) = \lim_{n\to\infty} \frac{1}{n} \log \mathbf{E}\left[\exp(-\gamma \cdot \Gamma_n)\right]$$

exists and is smooth (at least $\mathcal{C}^1$).

Then $\frac{\Gamma_n}{n}$ satisfy a large deviation principle with rate function

$$I(z) = -\inf_{\gamma} \left(z \cdot \gamma + e(\gamma)\right) \quad \text{Legendre transform.}$$

i.e. we have

$$\lim_{\epsilon\to 0} \lim_{n\to\infty} \frac{1}{n} \log P\left\{\frac{\Gamma_n}{n} \in B_\epsilon(z)\right\} = -I(z)\,.$$

Symbolically $\qquad P_\pi\left(\frac{\Gamma_n}{n} \approx z\right) \asymp \exp\left[-nI(z)\right]$

Large deviations for the entropy production

For an irreducible Markov chain Y_n with initial state $\mu(x)$ and transition matrix $Q(x, y)$ and an observable $f(x)$ the moment generating function can be written as

$$\mathbf{E}_\mu\left[\exp(-\alpha S_n(f))\right] = \langle \mu\,,\, Q_\alpha^n 1\rangle$$

with $Q_\alpha(x, y) \equiv Q(x, y)e^{-\alpha f(y)}$ and $1(x) = 1$.

Therefore the logarithmic moment generating function for the $S_n(F)$

$$e(\alpha) \equiv \lim_{n\to\infty} \frac{1}{n} \log E_\mu\left[\exp(-\alpha S_n(f))\right]$$

exists and is smooth by Perron-Frobenius theorem and analytic perturbation theory for eigenvalues.

So we have

$$P_\pi\left(\frac{S_n(f)}{n} \approx z\right) \asymp \exp\left[-nI(z)\right]$$

and the rate function $I(z)$ is nonnegative, (strictly convex), with a minimum at $z_0 = \mathbf{E}_\pi[P]$.

Gallavotti-Cohen fluctuation theorem I

Apply to the entropy production (use the Markov chain $Z_n = (X_n, X_{n+1})$)

Theorem: $e(\alpha) = e(1-\alpha)$.

Proof.

$$\begin{aligned}
&\mathbf{E}_\pi\left[e^{-\alpha S_N(F)}\right] \\
&= \sum_{x_0,\cdots,x_N} \frac{[(\pi(x_0)P(x_0,x_1)\cdots P(x_{N-1},x_N)]^{1-\alpha}}{[\pi(x_N)P(x_N,x_{N-1})\cdots P(x_1,x_0)]^{\alpha}} \\
&= \sum_{x_0,\cdots,x_N} \frac{[(\pi(x_N)P(x_N,x_{N-1})\cdots P(x_1,x_0)]^{1-\alpha}}{[\pi(x_0)P(x_0,x_1)\cdots P(x_{N-1},x_N)]^{\alpha}} \\
&= \sum_{x_0,\cdots,x_N} \pi(x_0)P(x_0,x_1)\cdots P(x_{n-1},x_n) \ \times \\
&= \times \left(\frac{\pi(x_0)P(x_0,x_1)}{\pi(x_1)P(x_1,x_0)}\right)^{-(1-\alpha)} \cdots \left(\frac{\pi(x_{N-1})P(x_{N-1},x_N)}{\pi(x_N)P(x_N,x_{N-1})}\right)^{-(1-\alpha)} \\
&= \mathbf{E}_\pi\left[e^{-(1-\alpha)S_N(F)}\right]
\end{aligned}$$

Gallavotti-Cohen fluctuation theorem II

Consequence 1: Since $e'(0) = -\text{EP}(\pi, P)$ the symmetry implies that

$$\text{EP}(\pi, P) > 0 \qquad \text{Positivity of entropy production}$$

Consequence 2: The symmetry implies the Gallavotti-Cohen fluctuation theorem

$$\boxed{I(z) - I(-z) = -z}$$

i.e., the odd part of I is linear with slope $-1/2$.

Or

$$\frac{P_\pi\left(\frac{S_n(F)}{n} \approx +z\right)}{P_\pi\left(\frac{S_n(F)}{n} \approx -z\right)} \asymp e^{nz}$$

The probability to observe a value of the entropy production and its negative value has a universal ratio.

- It is universal, no free parameters, etc...
- experimentally observable....

Green-Kubo formula and Onsager relations

If $\frac{P(x,y)}{P(y,x)} = e^{H(y)-H(x)+\Delta(x,y)}$ then assume that

$$\boxed{\Delta(x,y) = \sum_l \alpha_l J_l(x,y) = \alpha \cdot J}$$

$\alpha_l =$ thermodynamic forces: external forces, temperature differences

$J_l(x,y) =$ thermodynamic fluxes of energy, momenta, etc...

The transition probabilities $P(x,y) = P^{(\alpha)}(x,y)$ and the steady state $\pi = \pi^{(\alpha)}$ depends on the parameters α.

For $\alpha = 0$, π_0 corresponds thermodynamical equilibrium (detailed balance) with

$$\pi_0(x) \propto \exp(-H(x))$$

Logarithmic joint moment generating function for the fluxes $J_l(x,y)$

$$e(\alpha,\gamma) = \lim_{n\to\infty} \frac{1}{n} \log \mathbf{E}_{\pi^{(\alpha)}}^{(\alpha)} \left[\exp\left(-\gamma \cdot J(x,y)\right)\right]$$

By the same argument we now have the symmetry

$$e(\alpha,\gamma) = e(\alpha,\alpha-\gamma)$$

We have

$$\frac{\partial e}{\partial \gamma_l}(\alpha,0) = -\mathbf{E}_{\pi^{(\alpha)}}^{(\alpha)}[J_l]$$

and thus

$$\frac{\partial^2 e}{\partial \alpha_k \partial \gamma_l}(0,0) = -\frac{\partial}{\partial \alpha_k}\mathbf{E}_{\pi^{(\alpha)}}^{(\alpha)}[J_l]|_{\alpha=0} = -L_{kl}$$

i.e., $L_{kl} =$ are the linear response coefficients

$$\mathbf{E}_{\pi_\alpha}[J_l] = \sum_i L_{kl}\alpha_k + O(\alpha^2)$$

.

Since e is a moment generating function, we have using stationarity

$$\frac{\partial^2 e}{\partial \alpha_k \partial \alpha_l}(0,0) = \sum_{k=0}^{\infty} \mathbf{E}_{\pi_0}\left[J_k(X_0, X_1) J_l(X_k, X_{k+1})\right]$$

Integrated flux-flux correlation matrix

The symmetry $e(\alpha,\gamma) = e(\alpha,\alpha-\gamma)$ implies upon differentiation, that

$$\frac{\partial^2 e}{\partial \alpha_i \partial \gamma_j}(0,0) = -\frac{1}{2}\frac{\partial^2 e}{\partial \alpha_i \partial \alpha_j}(0,0)$$

and thus

$$\frac{\partial}{\partial \alpha_k}\mathbf{E}_{\pi_\alpha}(F_l)|_{\alpha=0} = L_{kl} = \sum_{k=-\infty}^{\infty} \mathbf{E}_{\pi_0}\left[J_k(X_0, X_1) J_l(X_k, X_{k+1})\right]$$

Kubo formula and Onsager relations $L_{kl} = L_{lk}$.

Further ideas

• Nice (older) results from Schnakenberg and newer from Gaspard on the representation of EP(π, P) using cycles. This leads to a slightly different version of

$\rightarrow$ Kubo formula

$\rightarrow$ Fluctuation theorem

• Study the structure of the of the Donsker-Varadhan large deviation functional for the empirical measure.

$\rightarrow$ Maes and Netockny, Bodineau and Lefevere. See the diffusion case in next chapter..

$\rightarrow$ Explicit computations for the GC functional, Derrida et al.

• Go macroscopic (Jona-Lasino & al.)

Part II: Stochastic differential equation of molecular dynamics

Extending the previous theory to more general Markov processes is possible but this requires to prove strong ergodic properties.

In general for models of physical interests,

- Existence and to a less extent uniqueness of steady states

- Ergodicity and large deviations

are hard problems.

$\longrightarrow$ Consider concrete physically relevant problems

References:

- P. Cattiaux lecture here.
- M. Hairer: Various lectures notes (www.hairer.org)
- Rey-Bellet: Grenoble Summer School. Quantum Open Systems II. Springer LNM 1881 pp. 1–39. and pp. 41–78.

Notations

Stochastic differential equation: $x \in \mathbb{R}^d$ (or a manifold)

$$dx_t = b(x_t)dt + \sigma(x_t)dB_t$$

where

$b : \mathbb{R}^d \to \mathbb{R}^d$ is the drift

$\sigma : \mathbb{R}^d \to \mathcal{L}(\mathbb{R}^k, \mathbb{R}^d)$ is the diffusion matrix

B_t is a k-dimensional Brownian motion

We shall always assume that b and σ are sufficiently smooth, say C^∞.

However singular vector field, think Lenard-Jones or Coulomb, are interesting: many open problems!!

Generators and semigroup

If x_t is a solution of the SDE with initial condition $x_0 = x$ is and $f : \mathbb{R}^d \to \mathbb{R}$ is a (nice) function then

$$T_t f(x) = \mathbf{E}_x \left[f(x_t) \right]$$

is a semigroup (Markov property) with generator

$$L = \sum_{l=1}^{d} b_l(x) \partial_{x_l} + \sum_{k,l=1}^{d} \sigma(x) \left(\sigma(x)^T \partial_{x_k} \right)_{kl} \partial_{x_l}$$

The adjoint (on $L^2(\mathbb{R}^d)$) of L is denoted by L^T (Fokker-Planck operator)

$$L^T = - \sum_{l=1}^{d} \partial_{x_l} b_l(x) + \sum_{k,l=1}^{d} \partial_{x_k} \partial_{x_l} \left(\sigma(x) \sigma(x)^T \right)_{kl}$$

Analytical tool I : Hypoellipticity

In many physically relevant examples, noise does not act on all variables: the noise is degenerate.

$$\text{rank}\,\sigma\sigma^T(x) < d\,,$$

$$\text{Write } L = X_0 + \sum_{i=1} X_i^T X_i$$

Theorem (Hörmander Hypoelliptcity): If the Lie algebra generated by

$$\mathcal{A}_0 = \{X_i\}_{i\geq 1}\,, \mathcal{A}_1 = \{[X_i, Y]\}_{i\geq 0, Y\in\mathcal{A}_0}\,, \cdots, \mathcal{A}_k = \{[X_i\,,\,Y]\}_{i\geq 0\, Y\in\mathcal{A}_{k-1}}\,, \cdots$$

has full rank at every $x \in \mathbb{R}^d$ then

$$T^t f(x) = \int_{\mathbb{R}^d} p_t(x,y) f(y)\, dy, \qquad p_t(x,y) \text{ is } C^\infty \text{ in } (t,x,y)$$

In particular the semigroup is strong-Feller: (i.e. smoothing)

$$\text{If } f \in B(\mathbb{R}^d) \text{ then } T_f \in C_b(\mathbb{R}^d)$$

Analytical tool II : Irreducibility and controllability

If T_t is strong-Feller we say that the Markov process x_t is irreducible if for any $x \in \mathbb{R}^d$ and any open set A there exists t such that

$$P_t(x, A) > 0$$

• In general hypoellipticity (= local) does not imply irreducibility (= global)

Example: $X_0 = \sin(x)\partial_x$, $X_1 = \cos(x)\partial_x$

• Hypoellipticity + irreducibility implies at most one invariant measure π which has then a smooth density.

Associated ODE control system

$$\frac{dx_t}{dt} = b(x_t) + \sigma(x_t)u_t$$

where u_t is a (piecewise) smooth control (smoother than $\frac{dB_t}{dt}$!).

We say that y is accessible from x in time t if there exists a control u_s $0 \leq s \leq t$ such that $x_u(0) = x$ and $x_u(t) = y$.

Denote

$$A_{x,t} = \{y \in \mathbb{R}^d, y \text{ accessible from } x \text{ in time } t\}$$

Theorem (Stroock-Varadhan) We have

$$\text{supp} P_t(x, \cdot) = \overline{A_{x,t}}$$

Simple example

Take a generic smooth $F(p,q)$ and consider

$$dq = p\,dt, \quad dp = F(q,p)dt + dB$$

- Strong-Feller since

$$X_0 = F(p,q)\partial_p + p\partial_q\,, \quad X_1 = \partial_p\,, \quad [X_0, X_1] = \partial_q + \partial_p F(p,q)\partial_p$$

- Irreducible: Given initial p_0, q_0 and final p_1, q_1 pick an (arbitrary) time t and any smooth function $q(t)$ such that

$$q(0) = q_0\,,\ q(t) = q_1\,,\ \frac{dq}{dt}(0) = p_1\,,\ \frac{dq}{dt}(t) = p_1$$

and set

$$u(t) = \frac{dq}{dt}(t) - F\left(q(t), \frac{dq}{dt}(t)\right)$$

$\Rightarrow$ For any $t \geq 0$, supp $P_t(x,\cdot) = \mathbf{R}^n$ and some extra work shows that in fact $p_t(x,y) > 0$

Analytical tool III : Lyapunov function

A Lyapunov function is a function $V : \mathbb{R}^d \to \mathbb{R}$ such that

- V is smooth
- $V \geq 1$ V is bounded below.
- $\lim_{|x|\to\infty} V(x) = +\infty$ i.e. $\{V \leq \alpha\}$ is compact for any α.

Inequalities involving LV translate into ergodic properties for x_t

Standing assumptions: T_t is strong-Feller and irreducible

Notation: a, b are positive constants

K denote a compact subset of $\mathbb{R}^d$.

• (1) Existence of the dynamics

If there exists V such that

$$LV \leq aV + b$$

then the SDE has (pathwise) solutions for all $t > 0$ almost surely.

• (2) Existence of invariant measure and convergence

If there exists V such that

$$LV \leq -a + b\mathbf{1}_K$$

then the process x_t has a unique invariant measure π and $P_t(x, \cdot)$ converge to π in total variation for any initial x.

• (3) Exponential convergence to equilibrium

If there exists V such that

$$LV \le -aV + b\mathbf{1}_K$$

then there exists constants $c > 0$ and $\gamma > 0$ such that

$$\left| T_t f(x) - \int f d\pi \right| \le CV(x)e^{-\gamma t}$$

or equivalently the semigroup T_t has a spectral gap (i.e., quasi-compact) on the Banach space

$$B_V(\mathbb{R}^d) = \left\{ f : \mathbb{R}^d \to \mathbb{R}\,;\ \|f\|_V \equiv \sup_{x \in \mathbb{R}^d} \frac{|f|}{V} < \infty \right\}$$

Remark: Proof via coupling argument (Meyn-Tweedie or much simpler Hairer-Mattingly).
Proof via spectral argument (R-B., Grenoble lecture notes) via Nussbaum formula for the essential spectral radius ($= e^{-at}$)

• (4) Large deviations (cf Donsker-Varadhan, Wu, Kontayannis-Meyn)

Idea: For large deviations one needs some "super-exponential" convergence. (or hyper contractivity...)

If there exists $V = \exp(v)$ and a_n, b_n, K_n with $\boxed{\lim_{n\to\infty} a_n = \infty}$

$$LV \le -a_n V + b_n \mathbf{1}_{K_n}$$

then the semigroup T_t is compact on the Banach space B_V.

⇒ Large deviation principle for the ergodic average

$$\frac{1}{t}\int_0^t f(x_s)\,ds$$

for nice function f.

We say that f is dominated by v at infinity, write $f \ll v$

$$f \ll v \quad \text{if} \quad \lim_{R\to\infty} \sup_{|x|\geq R} \frac{|f|}{v} = 0 .$$

"Proof of LDP":

• Use Feynmann-Kac to write the moment generating function

$$\mathbf{E}_x \left[\exp\left(-\alpha \int_0^t f(x_s)\, ds \right) \right] = T_t^{(\alpha)} 1(x)$$

• Use compactness + assumption on f to show that $T_t^{(\alpha)}$ is compact too!

• Use perturbation theory and Perron-Frobenius and Gärtner-Ellis

• Use the Lyapunov bound to integrate x wrt to π $(\mathbf{E}_{\mathbf{x}} \to \mathbf{E}_\pi)$

Remark: In applications one need unbounded f!

A simple example: Overdamped Langevin equation

U is a smooth potential with compact level sets

$$dx = (-\nabla U(x) + F(x))dt + \sqrt{2T}dB$$

If $F = 0$ then $e^{-\frac{1}{T}U}dx$ is a stationary distribution. Liapunov function, try first U:

$$LU = T\Delta U - |\nabla U|^2 + F\nabla U$$

Exponential convergence if

$$\Delta U \ll |\nabla U|^2 \text{ and } F \ll |\nabla U|$$

for example if $k \geq 2$ and $U \sim q^k, \nabla U \sim q|q|^{k-2}, etc...$

Better try the Liapunov function $\exp(\theta U)$

$$L e^{\theta U} = \theta e^{\theta U} \left[T \Delta U + (T\theta - 1)|\nabla U|^2 + F \nabla U \right]$$

So for $\theta < \frac{1}{T}$ we have a super exponential Lyapunov function and thus a large deviation principle for any $f \ll U$ as long as $|F| \ll \nabla U|$ and $\Delta U \ll |\nabla U|^2$.

For more examples with stretched exponential, polynomial convergence etc...

• Bakry, Cattiaux, Guillin, and collaborators.

• Many cute examples in M. Hairer "How hot can a heat bath get?"

Entropy production for molecular dynamics

• Identify the entropy production: compute the Radon-Nikodym derivative of the Markov processes with respect to the time reversed process.

⟶ Use Feynmann-Kac & Girsanov formulas

⟶ Compare to a "nearby" reversible process, i.e. thermal equilibrium.

This is the "easy" part.

• Prove the fluctuation theorem

⟶ Prove a large deviation principle.

⟶ Technical difficulty: the flux and entropy production are unbounded and so are the boundary terms.

This is the hard part: construct a Liapunov function

Time reversal

- Markov process x_t with generator L and stationary distribution π, (i.e. we have $L^T\pi = 0$)

- The time-reversed process is the process with generator

$$L^* = \pi^{-1} L^T \pi$$

i.e. L^* is the adjoint of L on $L^2(\pi)$

Time-reversibility $\iff$ $L^* = L$

- For system with velocities generalize: consider an involution $J : \mathbb{R} \to \mathbb{R}^d$, that is, J is invertible and $J^2 = 1$

In all our examples $J(p,q) = (-p,q)$.

Time-reversibility $\iff$ $JL^*J = L$

Langevin equation and non-Hamiltonian forcing

- Hamiltonian system with $(p, q) \in \mathbb{R}^d \times \mathbb{R}^d$ and Hamiltonian $H(p, q) = \frac{p^2}{2} + V(q)$ with a smooth confining $V(q)$
- Heat reservoir at temperature T via a Langevin equation
- External force $F(q)$ which is not a gradient force

$$\begin{aligned} dq &= p\, dt \\ dp &= (-\nabla U(q) + F(q) - \lambda p)\, dt + \sqrt{2T} dB \end{aligned}$$

Generator $\quad L_F = (T\Delta_p - p\nabla_p) + (p\nabla_q - \nabla_q U(q)\nabla_p) + F(q)\nabla_p$

Fokker – Planck $\quad L_F^T = (T\Delta_p + \nabla_p p) - (p\nabla_q - (\nabla U(q)\nabla_p) - F(q)\nabla_p$

Entropy production for the Langevin equation

• If $F = 0$ then $\pi_0(x)dx = Z^{-1}e^{-\frac{1}{T}H(p,q)}dx$ is a stationary distribution and we have detailed balance

$$JL_0^* J = L_0$$

where $Jf(p,q) = f(-p,q)$.

• If $F \neq 0$, a simple computation shows that

$$J\pi_0^{-1} L_F^T \pi_0 J = L_F - \sigma \quad (\star)$$

with

$$\sigma = \frac{F(q) \cdot p}{T} = \frac{\text{power exerted by } F}{\text{Temperature}}$$

σ is the physical entropy production.

• Time-reversal on path

$$\Theta x_s = J x_{t-s} \quad 0 \le s \le t\,.$$

• Using Feynmann-Kac formula we obtain the path space interpretation

$$\frac{d\mathbf{P}|_{[0,t]} \circ \Theta}{d\mathbf{P}|_{[0,t]}} = \exp\left(- \int_0^t \sigma(x_s)\, ds + \frac{1}{T}(H(x_t) - H(x_0)) \right)$$

(Note here $P = P_{\pi_0}$ otherwise an extra boundary term...)

• Gallavotti-Cohen symmetry. From ($\star$) it follows immediately that since $J\sigma J = -\sigma$

$$J\pi_0^{-1} (L_F - \alpha\sigma)^T \pi_0 J = L_F - (1-\alpha)\sigma$$

This implies (formally) $e(\alpha) = e(1-\alpha)$ via a Perron Frobenius argument.

Entropy balance equation

Let $\mathcal{H}(\mu) = -\int \rho \log \rho \, dpdq$ denote the entropy of the measure $d\mu = \rho dpdq$.

If μ_t is the distribution of (p_t, q_t) then we have

$$\int \sigma(p,q) d\mu_t - \frac{d}{dt} \int \frac{1}{T} H(x) d\mu_t + \frac{d}{dt}\mathcal{H}(\mu_t) = \Sigma(\mu_t)$$

Physical entropy production $= \beta \times$ dissipated heat

Increase in entropy

where

$$\Sigma(\mu_t) = \int \sqrt{\frac{\lambda}{T}} \frac{1}{\rho_t} \left[\left(\frac{1}{T} \nabla_v + v \right) \rho_t \right]^2 dpdq \geq 0$$

From this we get

Theorem: If a stationary measure π_F exists then $\int \sigma d\pi_F \geq 0$ and

$$\int \sigma d\pi > 0 \text{ iff } F \neq \nabla W$$

Proof: • If $\mu_t = \pi$ we obtain

$$\int \sigma d\pi = \Sigma(\pi) \geq 0$$

• If $\Sigma(\pi) = 0$ then $\pi = \exp(-\frac{1}{T}\frac{p^2}{2})G(q)$. Use then Fokker-Planck.

Remark: The entropy balance equation is old...

Remark: In older literature what we call entropy production is the entropy flow. The entropy production is $\Sigma(\mu)$.....

Entropy balance and Donsker-Varadhan

Very nice recent work from Maes &Netockny and Bodineau & Lefevere

Large deviations for the empirical measure: if x_t is a Markov process let

$$\nu_t = \frac{1}{t}\int_0^t \delta_{x_s}\, ds$$

Note that $\int f(x) d\nu_t = \frac{1}{t}\int_0^t f(x_s) ds$ and $\lim_{t\to\infty} \nu_t = \pi$ almost surely by ergodicity

By a slight improvement of Donsker-Varadhan one has a LDP (work in the natural topology induced by the Banach space $\mathcal{B}_V$!)

$$P_\pi \{v_t \approx \mu\} \asymp \exp(-tI(\mu))$$

• Fact: one has from Donsker-Varadhan $I(\mu) = \sup_{g \geq 1} \left(-\int \frac{Lg}{g} \right)$

• Relation: $J\pi_0^{-1} \left(L_F - \alpha\sigma \right)^T \pi_0 J = L_F - (1 - \alpha)\sigma$

Theorem(Bodineau and Lefevere) The rate function $I(\mu)$ has the form

$$I(\mu) = \frac{1}{4} \underbrace{\Sigma(\mu)}_{\substack{\text{Entropy} \\ \text{production}}} + \underbrace{K(\mu)}_{\text{activity}} - \frac{1}{2} \underbrace{\int \sigma d\mu}_{\substack{\text{Entropy} \\ \text{flow}}}$$

• The first two terms are even under J while the entropy flow is odd under J

• The rate function for the large deviations for σ is given by the contraction principle $I(z) = \inf\{I(\mu)\,;\, \int \sigma d\mu = z\}$.

Consequence: The symmetry under time-reversal for $I(\mu)$ implies the symmetry of $I(z)$: $I(z) - I(-z) = -z$.

Ergodic properties of the Langevin equation

See papers by Mattingly& Stuart, L. Wu and R.B.-Thomas and P. Carmona. See also the book by Kashminskii

- Assumption on U: U is smooth C^∞ and for large q

$$U(q) \sim |q|^k, \nabla U(q) \sim q|q|^{k-2}, \quad \text{with} \quad k \geq 2$$

- Assumption on $F(q)$: $|F(q)| \ll |\nabla U|$ and $|F| \ll U^{1/2}$

$\rightarrow$ Note the two assumptions are only for large q

Theorem: Pick a time $\tau > 0$ and $\theta < \frac{1}{T}$ then $W = e^{\theta H}$ is a super exponential Liapunov function:

$$T_\tau e^{\theta H} \leq \alpha_E e^{\theta H} + \beta_E \mathbf{1}_{\{H \leq E\}}$$

and $\lim_{E\to\infty} \alpha_E = 0$.

Remark: We do not use L but $e^{\tau L}$...

Some ideas of one possible proof

• Uniqueness and smoothness of the measure: already done!

• Try first the energy as a Lyapunov function:

$$LH = T - p^2 + p \cdot F(q)$$

. This does not have a sign but not as bad as it looks....

• Main idea: prove that if the system starts at energy $H(p(0), q(0)) = E$ then

$$\int_0^1 p^2(s)ds \geq cE$$

uniformly in $E \geq E_0$ (with very high probability).

• If we such bound then we have $H(x) = E \geq E_0$

$$T_1 H(x) - H(x) \leq cE$$

since the term $p \cdot F(q)$is negligible compared to $p^2 \simeq E$.

• To close the deal use that $Le^{\theta H} = \theta e^{\theta H}\left[T - (1-\theta T)p^2 + F(q)p\right]$ and the same estimate plus exponential martingale + Hólder inequality to construct the Lyapunov function.

We "morally" have $LH \leq -aH + b$

which we lift to $Le^{\theta H} \leq -aHe^{\theta H} + b$

• Rescaling argument: Natural time scale at energy E if $U \sim q^k$ is $E^{1/k-1/2}$. This is the time for "one period".

Rescale $\widetilde{p}(t) \equiv E^{-1/2}q(E^{1/k-1/2}t)$ $\qquad \widetilde{q}(t) \equiv E^{-1/k}q(E^{1/k-1/2}t)$

which gives

$$\frac{d\tilde{q}}{dt} = \tilde{p} \qquad \frac{d\tilde{p}}{dt} = -\tilde{q}|\tilde{q}|^{k-2} + O(E^{-\alpha})$$

$\rightarrow$ Control errors + noise...

Another (harder) example : Anharmonic chains

Hamiltonian system $p = (p_1, \cdots, p_N)$, $q = (q_1, \cdots, q_N)$

$$H(p,q) = \sum_{l=1}^{n} \frac{p_l^2}{2} + \sum_{l=1}^{n} V(q_l) + \sum_{l=1}^{N-1} U(q_l - q_{l-1}) \,.$$

Assume $V(q) \sim q^{k_1}$ $\quad U(q) \sim q^{k_2}$ $\quad$ and $\quad k_2 \geq k_1$

$$\begin{aligned}
dq_1 &= p_1 \, dt \\
dp_1 &= (-\nabla_{q_1} H(q) - \lambda p_1) \, dt + \lambda \sqrt{2 T_L} dB_L \\
dq_j &= p_j \, dt \\
dp_j &= -\nabla_{q_j} H(q) \qquad\qquad j = 2, \cdots, n-1 \\
dq_n &= p_n \, dt \\
dp_n &= (-\nabla_{q_n} H(q) - \lambda p_n) \, dt + \lambda \sqrt{2 T_R} dB_R
\end{aligned}$$

Entropy production for heat conduction

Choose a good reference measure (there are several options because you can measure energy flows in several ways!).

Define the energy of the particle i by

$$H_i = \frac{p_i^2}{2} + V(q_i) + \frac{1}{2}U(q_{i-1} - q_i) + \frac{1}{2}U(q_i - q_{i+1})$$

so that

$$H = \sum_i H_i$$

Writing a balance equation $\frac{d}{dt}H_i = \Phi_{i-1} - \Phi_i$ we have

$$\Phi_i = \frac{p_i + p_{i+1}}{2}\nabla V(q_i - q_{i+1}) \quad \text{heat flow from } i-1 \text{ to } i$$

We pick the reference state $\pi_0 \sim e^{-R_i}$ where

$$R_i = \frac{1}{T_L}\sum_{k\leq i} T_k + \frac{1}{T_R}\sum_{k>i} T_k$$

and after computing we find

$$J\pi_0^{-1} L^T \pi_0 = L - \sigma_i$$

where

$$\sigma_i = \left(\frac{1}{T_r} - \frac{1}{T_l}\right)\Phi_i$$

and again

$$J\pi_0^{-1}(L - \alpha\sigma_i)^T \pi_0 = L - (1-\alpha)\sigma_i$$

Ergodic properties

• Assume the coupling U is nice in the sense that U does not have a "flat piece" nor there are infinitely degenerate critical points for ∇U. This means the oscillators are really coupled.

$\rightarrow$ Hypoellipticity and controllability: "by induction over the chain".....

• Dissipation

$$LH = (T_L - p_1^2) + (T_R - p_n^2)$$

$\rightarrow$ Lyapunov function $W = e^{\theta H}$ if $\theta < \min\{\frac{1}{T_L}, \frac{1}{T_R}\}$.

$$T_\tau e^{\theta H} \leq \alpha_E e^{\theta H} + \beta_E \mathbf{1}_{\{H \leq E\}}$$

- Existence and uniqueness of the steady state.

- Spectral gap and compactness of the semigroup on $\mathcal{B}(W)$.

- Gallavotti-Cohen fluctuation Theorem

"Technical" issue σ is not relatively bounded by H!

$\rightarrow$ Write $\sigma_i = \sigma^* + LR_i$ where $\sigma^* \leq CH$ and $R_i \leq CH$

$\rightarrow$ Show the existence of $e(\alpha)$ only in a neighborhood of $[0, 1]$

$\rightarrow$ Control the boundary terms and show a LDP restricted to a neighborhood of the origin.

More examples

- More general heat conduction networks

- Molecular motors...

- Models of heat conduction by Lefevere (cf. Bodineau & Lefevere, Carmona)

- Models of heat conduction by Olla, Stolz & al. (microcanonical thermostats).

- Shear flows (Joubaud & Stolz)

- Other thermostats.....

Loose ends

• Villani (Hypocercivity) and Helffer-Nier have better estimates on the dynamics but (?) it works only at equilibrium. Does it?

• Hairer and Mattingly construct Lyapunov functions via "averaging".

• Bodineau and Lefevere (and Maes and Netockny) have a variational principle for the steady state based on Donsker-Vardahan large deviation functional.

• Large systems, Hydrodynamic limits and fluctuations, Jona-Lasino & al. (Macroscopic theory)

PART III: Deterministic dynamics

Basic questions

• What is nonequilibrium in this context?

→ Time reversibility symmetry breaking again but with a slightly different twist.

• A deterministic dynamics almost always has very many invariant measures. Which one to pick?

→ Pick a reference measure (encode the physics) and define a NESS as an SRB-measure

• Relations between stochastic and deterministic systems?

→ Extract stochastic process out of a deterministic one via Markov partition.

→ Stochastic process as reduced description of a (large deterministic) system.

Abstract definition of a NESS

Dynamical system with reference measure

• State space M (maybe a Polish space)

• Dynamics: a (invertible) map $F : M \to M$ (discrete-time) or a flow $\Phi_t : M \to M$ (continuous time).

• Reference measure μ_0. In general not invariant under the dynamics.

In applications μ_0 will encode thermodynamical parameters (Energy, temperature, ...).

NESS = SRB measures

Definition: A SRB measure μ_+ is an invariant measure for the dynamics, i.e. $\mu_+(F^{-1}A) = \mu_+(A)$ such that for $f \in \mathcal{C}_b(\mathbb{R}^d)$

1. μ_+ is ergodic: $\frac{1}{n}\sum_{k=0}^{n-1} f \circ F^k(x) \to \mu_+(f)$, $\boxed{\mu_+ \text{ almost surely}}$.

2. SRB measure: $\frac{1}{n}\sum_{k=0}^{n-1} f \circ F^k(x) \to \mu_+(f)$, $\boxed{\mu_0 \text{ almost surely}}$.

Think of nontrivial nonequilibrium occurs when $\mu_+ \perp \mu_0$.

The SRB measure μ_+ is also called the physical measure: it describe the statistics of μ_0 almost every point and is selected among all the (typically very many) invariant measures.

In addition we will often require that the dynamics is time-reversal invariant

Time reversal: Involution of phase space $J : M \to M$ so that

$$J^2 = J$$

Typical: $x = (q, p) \in M$ then $i(x) = (q, -p)$, i.e., i change signs of the velocities.

The dynamics is time-reversal invariant if

$$J \circ F = F^{-1} \circ J \qquad \text{or} \qquad J \circ \Phi_t = \Phi_{-t} \circ J$$

.

It is convenient to assume that the reference measure is time reversal invariant (but not really necessary...)

Example 1 : "Micro-canonical" NESS: Gaussian thermostats

- Hamiltonian: $H(q,p) = \frac{p^2}{2} + V(q)$

- External force: $F(q)$ non Hamiltonian external force (driving the system out of equilibrium).

- Reference measure: $\mu_0 = \mu_{0,E}$ Lebesgue (microcanonical) measure on the energy surface $\{H = E\}$

- Gaussian thermostat: $\alpha(p,q)$ thermostatting force (non-holonomic constraint) which constrains the system to stay on the energy surface $\{H = E\}$

- Time-reversal: $J(p,q) = (-p,q)$, $H \circ J = H$, and $\mu_0 \circ J = \mu_0$.

Equations of motion:

$$\begin{aligned} \dot{q} &= p \\ \dot{p} &= -\nabla V(q) + F(q) - \alpha(p,q) \end{aligned}$$

$$\alpha(p,q) = \frac{F(q) \cdot p}{p \cdot p} p$$

Dynamics is dissipative, yet energy conserving, and time-reversible.

Example 2 : "Canonical" NESS: Heat reservoirs

• Small system: (finitely many degrees of freedom) Hamiltonian

$$H_S(q,p) = \tfrac{p^2}{2} + V(q)$$

• K heat reservoirs: Hamiltonian systems, extended systems, ∞ many degrees of freedom. For example for $k = 1, \cdots, K$

$$H_k(\varphi_k, \pi_k) = \frac{1}{2}\int_{\mathbf{R}^d} |\nabla\varphi_k|^2 + |\pi_k|^2 \, dx \qquad \text{(Linear wave equation)}$$

with Gibbs measure

$$d\nu_{\beta_k}(\varphi_k, \pi_k) = Z^{-1} \exp(-\beta_k H_k(\varphi_k, \pi_k)) \prod_{x\in\mathbf{R}^d} d\varphi_x d\pi_k(x)$$

This is a Wiener measure (φ_k) times a white noise measure (π_k)

• Total Hamiltonian: Coupling V_k between the small system and reservoir k. Total Hamiltonian

$$H = H_S(p,q) + \sum_{k=1}^{K} H_k(\pi_k, \varphi_k) + \sum_{k=1} V_k(p,q,\pi_k,\varphi_k)$$

• Reference measure: Choose inverse temperatures $\beta_1, \cdots \beta_K$ and (arbitrary) measure ν_S on small system

$$\mu_0 = \nu_S \times \mu_{\beta_1} \times \cdots \times \mu_{\beta_K}$$

• Time-reversal: $J(p,q,\pi,\varphi) = (-p,q,-\pi,\varphi)$ and $H \circ J = H$ and $\mu_0 \circ J = \mu_0$.

Dynamics:

Hamiltonian flow on infinite dimensional phase space

Definition of entropy production

Reference measure evolved under the dynamics $\mu_t \equiv \mu_0 \circ \Phi_{-t}$

Radon-Nikodym derivative (Jacobian) $J_t = \frac{d\mu_t}{d\mu_0}$

Chain rule $J_{t+s} = J_t J_s \circ \Phi_{-t}$ implies that

$$J_t = \exp \left[\int_0^t \sigma \circ \Phi_{-s} \, ds \right] ,$$

where

$$\sigma = \frac{dJ_t}{dt}\Big|_{t=0} \equiv \text{Entropy production observable}$$

Examples

Example 1: Assume M is a compact manifold and $\mu_0 =$ is Lebesgue measure on M. Then

$$\sigma = \text{phase space contraction rate}$$

If the dynamics is $\dot{x} = G(x)$ then $\sigma(x) = \text{div}(G)(x)$

Example 2: Small system coupled to heat reservoirs. Then a computation shows that

$$\sigma = \sum_{k=1}^{K} \beta_k J_k = \text{"Physical entropy production"}$$

where

$$J_k = \text{Energy flow from small system into reservoir } k$$

Relative entropy and positivity of entropy production

Relative entropy: $\mathcal{H}(\mu|\nu) = \int \log\left(\frac{d\mu}{d\nu}\right) d\mu$. Then

$$H(\mu_t|\mu_0) = \int_0^t \mu_s(\sigma)\, ds$$

Since $H(\mu|\nu) \geq 0$ and if $t^{-1}\int_0^t \mu_s \to \mu$ (by the SRB-property) then

$$0 \leq \lim_{t\to\infty} \frac{1}{t} H(\mu_t|\mu_0) = \lim_{t\to\infty} \frac{1}{t} \int_0^t \mu_s(\sigma)\, ds = \mu_+(\sigma)$$

The entropy production in the steady state is non-negative

Under mild conditions one can prove

$$\mu_+(\sigma) > 0 \quad \text{iff} \quad \mu_+ \perp \mu_0$$

i.e. the entropy production is positive iff the NESS μ_+ is singular with respect to the reference measure μ_0.

Time reversal, Evans-Searle, Gallavotti-Cohen

Assume now TIME REVERSAL INVARIANCE

• We have $\sigma \circ J = -\sigma$ (i.e. the entropy production is odd under time-reversal).

• Time reversal on paths

$$\Theta : \{\Phi_t(x)\}_{0 \le s \le t} \mapsto \{\Phi_{t-s} \circ i(x)\}_{0 \le s \le t}$$

• Path space measure: The reference measure μ_0 on M induces a probability distribution P_{μ_0} on the path space $M^{[0,t]}$.

We have

$$\frac{dP_{\mu_0} \circ \Theta}{dP_{\mu_0}}\Big|_{[0,t]} = \exp\left[-\int_0^t \sigma \circ \Phi_s(x)\, ds \right] (\star)$$

(Looks familiar?)

Evans-Searle Symmetry

Moment generating function

$$g_t(\alpha) = \mu_0 \left(\exp \left[-\alpha \int_0^t \sigma \circ \Phi_s \, ds \right] \right)$$

Then $(\star)$ is equivalent that $g_t(\alpha) = g_t(1-\alpha)$.

Let $Q_{\mu_0,t}$ denote the probability distribution of $\frac{1}{t}\int_0^t \sigma(x_s)\, ds$ with initial distribution μ_0 and let $\tau(z) = -z$.

We obtain

$$\frac{dQ_{\mu_0,t} \circ \tau}{dQ_{\mu_0,t}}(z) = \exp(-tz). \qquad \text{Evans} - \text{Searle}$$

$\rightarrow$ True for all times t but it depends crucially on picking the reference measure μ_0.

$\rightarrow$ True even without any good ergodic properties!

From Evans-Searle to Gallavotti-Cohen

Assume that

$$e(\alpha) = \lim_{t\to\infty} \frac{1}{t} \log g_t(\alpha) = \lim_{t\to\infty} \frac{1}{t} \log \mu_0 \left(\exp \left[-\alpha \int_0^t \sigma \circ \Phi_s \, ds \right] \right)$$

exists and is C^1 then $e(\alpha) = e(1-\alpha)$ and we obtain a large deviation principle

$$\mu_0 \left(\frac{1}{t} \int_0^t \sigma \circ \Phi_s \, ds \approx z \right) \sim e^{-nI(z)}$$

where

$$I(z) - I(-z) = -z \quad \text{Gallavotti} - \text{Cohen symmetry}$$

Remark: The large deviations is with respect to the initial measure μ_0 not the NESS μ_+ which is singular to μ_0. Large deviations with respect to μ_+ is extra work (highly nontrivial exchange of limit!).

Gibbsian approach to non equilibrium

Another road to the fluctuation theorem (advocated by Maes) use the thermodynamic formalism of Ruelle.

It works best for a compact metric space M, and a continuous map $F : M \to M$.

Variational principle: For $\varphi : M \to \mathbb{R}$

$$P(\varphi) = \sup_{v \text{ invarariant}} \left\{ h_\nu(F) + \int \varphi d\nu \right\} .$$

where $h_\nu(F)$ is the Kolmogorov-Sinai entropy and $P(\varphi)$ is the topological pressure.

If the dynamical system is "sufficiently chaotic" and φ is Hölder continuous then we the supremum is attained and is attained at a unique $\nu = \nu_\varphi$ which is called the equilbrium measure for the potential φ

Large deviations for ergodic averages $S_n(\psi)$

Large deviations: (Kiefer) If $\nu = \nu_\phi$ and $\psi : M \to \mathbb{R}$ is Hölder continuous then we have for "sufficiently chaotic map"

$$\epsilon_\psi(\alpha) = \lim_{n\to\infty} \frac{1}{n} \log \nu(e^{\alpha S_n(\psi)}) = P(\varphi + \alpha\psi)$$

and $e(\alpha)$ is smooth.

Examples: Anosov maps, Markov subshifts, one-dimensional Gibbs measure (space=time).

Assume now that there is time reversal $J : M \to M$ and assume that the potential φ is not time reversal invariant

$$\sigma = \sigma_\varphi = \varphi - \varphi \circ J$$

Canonical example and connection with SRB: M smooth manifold, F smooth uniformly hyperbolic map.

$$\varphi = -\log JDF^u , \quad \sigma = -\log DF$$

Theorem: We have $e(\alpha) = e(1-\alpha)$

Proof:

$$
\begin{aligned}
P(\varphi - \alpha\sigma_\varphi) &= \sup_\nu \left\{ h_\nu(F) + \int [\varphi - \alpha\sigma_\varphi]\, d\nu \right\} \\
&= \sup_\nu \left\{ h_\nu \circ J(F) + \int [(1-\alpha)\varphi - \alpha\varphi \circ J]\, d\nu \circ J \right\} \\
&= \sup_\nu \left\{ h_\nu(F^{-1}) + \int [(1-\alpha)\varphi - \alpha\sigma \circ J]\, d\nu \circ J \right\} \\
&= \sup_\nu \left\{ h_\nu(F) + \int [(1-\alpha)\varphi \circ J - \alpha\sigma]\, d\nu \right\} \\
&= P(\varphi - (1-\alpha)\sigma_\varphi)
\end{aligned}
$$

Examples

Two examples:

1) Anharmonic chain coupled to two heat reservoirs

Joint work with J.-P. Eckmann, C.-A. Pillet and L.E. Thomas.

2) Hyperbolic billiard under external electric field and Gaussian thermostat:

Joint work with L.-S. Young.

Based on results of

- Sinai, Bunimovich, and Chernov 1980's
- Chernov, Eyink, Lebowitz, and Sinai 1995
- Chernov 2002
- L.-S. Young 1995
- Wojtkowski

New results: Large deviation principle for billards!

Example 1 : Anharmonic chains

Small system $p = (p_1, \cdots, p_N)$, $q = (q_1, \cdots, q_N)$

$$H_S(p,q) = \sum_{l=1}^{n} \frac{p_l^2}{2} + \sum_{l=1}^{n} V(q_l) + \sum_{l=1}^{N-1} U(q_l - q_{l-1}) \,.$$

Assume $V(q) \sim q^{k_1}$ $\quad U(q) \sim q^{k_2}$ $\quad$ and $\quad k_2 \geq k_1$

Two reservoirs: Linear wave equations at inverse temperature β_L and β_R. Initial configurations of the reservoir distributed according to Gibbs measures μ_{β_L} and μ_{β_R}.

Coupling: $q_1 \cdot \int \phi_L \rho_L \, dx + q_N \cdot \int \phi_R \rho_R \, dx$

Special couplings: $|\widehat{\rho}_i(k)|^2 \sim \frac{1}{P_i(k^2)}$, P=polynomial

Extract a stochastic process

Integrate the (linear) equation for the bath yields generalized Langevin equation

$$\begin{aligned}
\frac{d^2 q_1}{dt^2} &= -\nabla_{q_1} H(p,q) - \int_0^t D(t-s)p(s)\,ds + \xi(t) \\
\frac{d^2 q_2}{dt^2} &= -\nabla_{q_1} H(p,q) \\
\cdots & \quad \cdots
\end{aligned}$$

where $\xi(t)$ is a Gaussian random process with covariance $TC(t)$ and $D(t) = \frac{d}{dt}C(t)$ (fluctuation-dissipation Thm).

If $|\widehat{\rho}_i(k)|^2 \sim \frac{1}{k^2+\gamma^2}$ then one finds a SDE

$$\begin{aligned}
\frac{d^2 q_1}{dt^2} &= -\nabla_{q_1} H(p,q) + r \\
dr &= -\gamma r + \lambda p + \sqrt{2T\lambda}dB
\end{aligned} \tag{1}$$

and we are in business again.

Example 2: Hyperbolic billiards

Single particle moving freely and colliding elastically on a periodic array of strictly convex smooth obstacles in $\mathbf{R^2}$. Periodicity reduces to a system on with phase space $(\mathbf{T^2} \setminus \cup_{\mathbf{i}} \mathbf{\Gamma_i}) \times \mathbf{R^2}$.

Assume: Finite horizon: every trajectory meets an obstacle.

Equations of motions: equilibrium

$$\begin{aligned} \dot{q} &= p \\ \dot{p} &= 0 \quad + \text{ elastic reflections} \end{aligned}$$

Energy is conserved $\rightarrow$ the phase space reduces to $(\mathbf{T^2} \setminus \cup_{\mathbf{i}} \mathbf{\Gamma_i}) \times \mathbf{S^1}$

The Lebesgue measure μ_0 on each energy surface is invariant, ergodic, and mixing (Sinai, Bunimovich, Chernov).

Equations of motions: non-equilibrium.

We add an External electric field E and Gaussian thermostat

$$\begin{aligned}\dot{q} &= p \\ \dot{p} &= E - \frac{E \cdot p}{p \cdot p} p \quad + \text{ elastic reflections}\end{aligned}$$

The system is time reversible, $i(p, q) = (-p, q)$.

If E is small enough there exists a SRB measure $\mu_+^{(E)}$ on each energy surface which is invariant, ergodic, and mixing (Chernov, Eyink, Lebowitz, Sinai; Chernov; Wojtkowski).

Linear response is treated in Chernov, Eyink, Lebowitz, Sinai;

We analyze the system in terms of the collision map:

$$F_E \,:\, (\theta, x) \mapsto (\theta', x')$$

where (θ, x) is the position of a collision on the boundary of the obstacles and θ is the angle of the incoming velocity with respect to the normal.

Discrete-dynamical system on the 2-dimensional phase space

$$M = \cup_i \partial \Gamma_i \times \left(-\frac{\pi}{2}, \frac{\pi}{2} \right)$$

If $E = 0$ (equilibrium) F_0 preserves the measure

$$\mu_0 = \text{const} \cos(\theta)\, d\theta\, dr$$

If $E \neq 0$ (non-equilibrium) F_E has an SRB measure (μ_0=reference measure)

$$\mu_+^{(E)} \quad \text{with} \quad \mu_+^{(E)} \perp \mu_0$$

.

Large deviations for billiards

Suppose g is Hölder continuous on M (or piecewise Hölder continuous; singularities). For convenience assume $\mu_+^{(E)}(g) = 0$.

Ergodic sum $S_n(g) = \sum_{k=0}^{n-1} g \circ F^{(E)}$

Autocorrelation function

$$\sigma^2(g) = \lim_{n\to\infty} \frac{1}{n} \mathrm{Var}(S_n(g)^2) = \mu_+^{(E)}(g^2) + 2 \sum_{n=1}^{\infty} \mu_+^{(E)}(g(g \circ F_E^n))$$

Fact:

$$0 < \sigma^2 < \infty\,, \quad \sigma^2(g) = 0 \text{ iff } g = C + h \circ F_E - h$$

Theorem (L.-S. Young, L. R.-B.) Assume $\sigma^2(g) > 0$.

• Large deviations: There exists an interval (z_-, z_+) which contains $\mu_+(g) = 0$ such that for $a \in (z_-, z_+)$ we have

$$\mu_+ \left\{ \frac{S_n(g)}{n} \approx a \right\} \sim \exp\left[-nI(a)\right].$$

Moreover $I(z)$ strictly convex and real-analytic with $I''(0) = \dfrac{1}{\sigma^2}$

• Moderate deviations: Let $1/2 < \beta < 1$. Then

$$\nu \left\{ \frac{S_n(g)}{n^\beta} \approx a \right\} \sim \exp\left[-n^{2\beta-1}\frac{a^2}{2\sigma^2}\right].$$

• Central Limit Theorem: Already known: Sinai & al, Liverani, Young...

$$\nu \left\{ a \leq \frac{S_n(g)}{n^{1/2}} \leq b \right\} \to \frac{1}{\sqrt{2\pi}\sigma} \int_a^b \exp\left[-\frac{z^2}{2\sigma^2}\right] dz\,.$$

Young towers

Our theorem is proved using Young towers introduced by Lai-Sang Young in 1995. The towers are a symbolic representation of non-uniformly hyperbolic dynamical systems.

Special type of Markov partition with countably many states, based on ideas of renewal theory: choose a set $\Lambda \subset M$ and construct a partition of $\Lambda \approx \cup_i \Lambda_i$ where Λ_i is a stable subset which "returns" ($\equiv$ full intersection) after time R_i. This gives a Markov extension. Finally quotient out the stable manifolds.

Consequence: our large deviation results apply to

- Billiards
- Quadratic maps
- Piecewise hyperbolic maps
- Hénon-type maps
- Rank-one chaos (Qiudong Wang and L.S. Young) Some periodically kicked limit cycles and certain periodically forced non-linear oscillators with friction.

Tower Ingredients

- Measure space (Δ_0, m) and a map $f : \Delta_0 \to \Delta_0$ (noninvertible)

- Return time $R : \Delta_0 :\to \mathbf{N}$.

  Assume exponential tail: $m\{R \geq n\} \leq De^{-\gamma n}$

  Assume aperiodicity: g.c.d.$\{R(x)\} = 1$

- Tower = suspension of f under the return time R

$$\underbrace{\Delta_l \equiv \{x \in \Delta_0\,;\, R(x) \geq l+1\}}_{\text{l-th floor}} \text{ and } \underbrace{\Delta \equiv \sqcup_{l\geq 0}\Delta_l}_{\text{tower}} \text{ (disjoint union)}$$

Dynamics $F : \Delta \to \Delta$ $\qquad F(x,l) = \begin{cases} (x, l+1) & R(x) > l+1 \\ (f(x), 0) & R(x) = l+1 \end{cases}$

• Markov partition $\Delta_l = \Delta_{l,1} \cup \cdots \Delta_{l,j_l}$ with $j_l < \infty$.

F maps Δ_{lj} onto a collection of $\Delta_{l+1,k}$'s plus possibly Δ_0.

The Markov partition is generating (i.e. each point has a unique coding).

• Dynamical distance:

$s(x,y) = \inf\{n, F^i(x)$ and $F^i(y)$ belong to the same $\Delta_{l,k}$, $0 \leq i \leq n\}$

For $\beta < 1$ let $d_\beta(x,y) = \beta^{s(x,y)}$

• Distortion estimates: Let JF the Jacobian of F with respect to m.

$$\left| \frac{JF(x)}{JF(y)} - 1 \right| \leq C d_\beta(x,y)$$

Remark: If $JF = $ const on each Δ_{lj} then we have a Markov chain on a countable state space

Transfer operators and large deviations

Think of m as the (image of) Lebesgue measure on unstable manifolds. The (image of the) SRB measure has then the form

$$\nu = hdm \,, \quad h \in L^1(m) \,.$$

The transfer operator $\mathcal{L}_0$ is the adjoint of $U\psi = \psi \circ F$

$$\int \varphi \, \psi \circ F \, dm = \int \mathcal{L}_0(\varphi)\psi \, dm$$

$$\mathcal{L}_0\varphi(x) = \sum_{y \,:\, F(y)=x} \frac{1}{JF(y)} \varphi(y)$$

$\nu = hdm$ F-invariant iff $\mathcal{L}_0 h = h$

Moment generating function and large deviations

Consider the moment generating function

$$\mu_+ \left(\exp\left[\theta S_n(g)\right]\right)$$

for the random variable $S_n(g) = g + g \circ F + \cdots + g \circ F^{n-1}$.

If

$$e(\theta) \equiv \lim_{n\to\infty} \frac{1}{n} \log \mu_+ \left(\exp\left[\theta S_n(g)\right]\right)$$

exists and is smooth (at least C^1) then we have large deviations with

$$I(z) = \sup_{\theta}(\theta z - e(\theta)), \qquad \text{Legendre Transform}.$$

(Gartner-Ellis Theorem)

Moment generating functions and transfer operators

To study the large deviations for $S_n(g)$ consider the generalized transfer operator

$$\mathcal{L}_g \varphi(x) = \sum_{y\,:\,F(y)=x} \frac{e^{g(y)}}{JF(y)} \varphi(y)$$

Then we have

$$\begin{aligned} \mu_+ \left(\exp\left[\theta S_n(g)\right]\right) &= m\left(\exp\left[\theta S_n(g)\right] h\right) \\ &= m\left(\mathcal{L}_0^n \left[\exp\left[\theta S_n(g)\right] h\right]\right) \\ &= m\left(\mathcal{L}_{\theta g}^n (h)\right) \end{aligned}$$

$\Rightarrow$ Large deviations follow from spectral properties of $\mathcal{L}_{\theta g}$

Spectral properties of transfer operators

Suppose $\mathcal{L}_{\theta g}$ is quasi-compact on some Banach space $X \ni h$, i.e. the essential spectral radius strictly smaller than the spectral radius.

By a Perron-Frobenius argument $\mathcal{L}_{\theta g}$ a maximal eigenvalue $\exp[e(\theta)]$ and a spectral gap (aperiodicity) and thus

$$e(\theta) = \lim_{n\to\infty} \frac{1}{n} \log \nu \left(\exp\left[\theta S_n(g)\right]\right)$$

By analytic perturbation theory $e(\theta)$ is real-analytic and then standard probabilistic techniques implies

$$\mu_+ \left\{ x\,;\, \frac{S_n(g)}{n} \approx z \right\} \sim e^{-nI(z)}$$

$$I(z) = \text{Legendre transform of } e(\theta)$$

as well as moderate deviations, central limit theorem, and so on...

Choice of Banach space

Recall $m\{R \geq n\} \leq De^{-\gamma n}$. Choose $\gamma_1 < \gamma$ and set

$$v(x) = e^{\gamma_1 l} \quad x \in \Delta_l$$

Banach space

$$X = \{\varphi : X \to \mathbf{C} ; \|\varphi\|_v \equiv \|\varphi\|_{v,\mathrm{sup}} + \|\varphi\|_{v,Lip} < \infty\}$$

with

$$\varphi_{v,\mathrm{sup}} = \sup_{l,j} \sup_{x \in \Delta_{l,j}} |\varphi(x)| e^{\gamma_1 l}$$

$$\varphi_{v,Lip} = \sup_{l,j} \sup_{x,y \in \Delta_{lj}} \frac{|\varphi(x) - \varphi(y)|}{d_\beta(x,y)} e^{\gamma_1 l}$$

Banach space of weigthed Lipschitz functions

Spectral analysis

Lasota York estimate: For g bounded Lipschitz

$$\|\mathcal{L}_g^n(\varphi)\|_v \leq \|\mathcal{L}_g^n(1)\|_{v,\text{sup}} \left(\beta^n \|\varphi\|_v + C\|\varphi\|_{v,\text{sup}}\right)$$

Pressure

$$P(g) = \lim_{n\to\infty} \frac{1}{n} \log \|\mathcal{L}_g^n(1)\|_{v,\text{sup}} .$$

Pressure at infinity: Control on the high floors of the towers!

$$P_*(g) = \lim_{n\to\infty} \frac{1}{n} \log \| \inf_{k\geq 0} \mathcal{L}_g^n(1)^{>k} \|_{v,\text{sup}} .$$

($\varphi^{>k} = \varphi$ for $x \in \Delta_l$ with $l > k$ and 0 otherwise)

Theorem:

The spectral radius of $\mathcal{L}_g$ is $e^{P(g)}$.

The essential spectral radius of $\mathcal{L}_g$ is $\max\{e^{P_*(g)}, \beta e^{P(g)}\}$

$\Rightarrow \mathcal{L}_g$ is quasicompact if $P_*(g) < P(g)$.

Theorem: $P_*(g) < P(g)$ if $(\max g - \min g) < \gamma$.

Theorem: If $P_*(g) < P(g)$ then $\exp(P(g))$ is a (simple) eigenvalue and no other eigenvalue on the circle $\{|z| = \exp(P(g))\}$.

Conclusion: The moment generating function

$$e(\theta) = \lim_{n\to\infty} \frac{1}{n} \log \nu\left(\exp\left[\theta S_n(g)\right]\right)$$

exists and is analytic if $|\theta| \leq \gamma/(\max g - \min g)$.

$\square$

Fluctuation theorem

Combine

- Time-reversal i, $i(p,q) = (-p,q)$
- Entropy production =phase space contraction

$$\Sigma = -\log JF^s - \log JF^u$$

- The SRB measure is "the equilibrium state" for the potential $-\log JF^u$ (use the Markov extension).
- The large deviation principle.