Canonical structures and orthogonality of forces and currents in irreversible Markov chains

Large Deviation Theory in Statistical Physics, ICTS

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Joint work with Rob Jack (Cambridge) and Johannes Zimmer (Bath).

Motivation / Outline

Many non-equilibrium systems can be described by irreversible Markov chains (with persistent currents/broken detailed balance).

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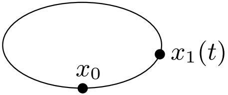
Application: These new insights can be useful to obtain a better understanding of physical/stochastic processes, which can e.g. be helpful for developing new sampling techniques.

I. Introductory example

Prior example: Independent diffusions

Consider N independently diffusing particles $x_1, x_2, \ldots, x_N$ on a ring with fixed initial condition $x_i(0) = x_0$ and dynamics

$$\dot{x}_i = \sqrt{2k_B T}\,\xi_i$$



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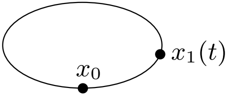

where ξ_i is white noise.

Denote with $\rho_t(x)$ the probability that x_i is in x at time t. ρ evolves by the **Fokker-Planck equation** (FPE)

$$\dot{\rho} = k_BT\Delta\rho = -\operatorname{div} J(\rho)$$

for the **probability current**

$$J(\rho) := -k_BT\nabla\rho.$$

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Similar, the **empirical current** j^N should satisfy

$$(j_t^N)_{t \in [0,\tau]} \approx (J(\rho_t^N))_{t \in [0,\tau]}.$$

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The probability to observe this path is asymptotically, as $N \to \infty$, given by

$$\mathrm{Prob}\Big((\rho_t^N, j_t^N)_{t\in[0,\tau]} \approx (\rho_t, j_t)_{t\in[0,\tau]}\Big) \asymp \exp\Big\{-N I_{[0,\tau]}\big((\rho_t, j_t)_{t\in[0,\tau]}\big)\Big\},$$

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for the **rate function**

$$I_{[0,\tau]}\big((\rho_t, j_t)_{t\in[0,\tau]}\big) = \frac{1}{4}\int_0^\tau \mathrm{d}t \int \mathrm{d}u\, (k_B T \rho_t)^{-1}\big(j_t - J(\rho_t)\big)^2.$$

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Note:
$I_{[0,\tau]}$ is uniquely minimised for the solution of the FPE $(\hat{\rho}_t, J(\hat{\rho}_t))_{t\in[0,\tau]}$.

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For diffusive systems, currents J are given by the linear flux-force relation

$$J(\rho) = \chi(\rho)F(\rho)$$

for a "force" $F(\rho)$ and a "mobility" $\chi(\rho)$ (as in MFT, see [Bertini et al., Reviews of Modern Physics 87.2 (2015): 593]).

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Example: For the diffusion from before

$$\dot{\rho} = k_B T \Delta\rho = -\operatorname{div} J(\rho),$$

where

$$J(\rho) = -k_B T \nabla\rho = (k_B T \rho)(-\nabla \log \rho),$$

such that

$$\chi(\rho) = k_B T \rho \quad \text{and} \quad F(\rho) = -\nabla \log \rho.$$

Ψ-$\Psi^\star$ formalism

The rate function is

$$I_{[0,\tau]}\big((\rho_t, j_t)_{t\in[0,\tau]}\big) = \frac{1}{2}\int_0^\tau \mathrm{d}t \; \Phi(\rho_t, j_t, F(\rho_t)),$$

where

$$\Phi(\rho, j, F) = \frac{1}{2}\int_\Lambda \big(j - J(\rho)\big)\cdot\chi(\rho)^{-1}\big(j - J(\rho)\big)\,\mathrm{d}u$$

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&= \frac{1}{2}\int_\Lambda j\cdot\chi(\rho)^{-1} j\,\mathrm{d}u - \int_\Lambda j\cdot F\,\mathrm{d}u + \frac{1}{2}\int_\Lambda F\cdot\chi(\rho)F\,\mathrm{d}u.
\end{aligned}$$

We obtain

$$\Phi(\rho, j, F) = \Psi(\rho, j) - \int_\Lambda j \cdot F \,\mathrm{d}u + \Psi^\star(\rho, F)$$

for

$$\Psi(\rho, j) := \frac{1}{2}\int_\Lambda j \cdot \chi(\rho)^{-1} j \,\mathrm{d}u, \quad \text{and} \quad \Psi^\star(\rho, F) := \frac{1}{2}\int_\Lambda F \cdot \chi(\rho) F \,\mathrm{d}u.$$

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Note that Ψ and $\Psi^\star$ are convex Legendre duals, which are **symmetric** in j, resp. F, as opposed to $j \cdot F$, which is **anti-symmetric** (in fact linear) in both arguments.

II. Markov chains

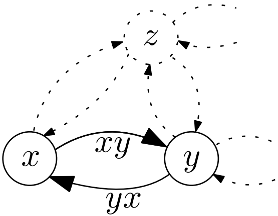
Questions

Why is the rate functional for diffusions quadratic?
$\rightarrow$ linear flux-force relation

What can we say about Markov chains?
$\rightarrow$ nonlinear flux-force relation, thus rate functional not quadratic

Rate functional for Markov chains

Consider an ergodic Markov chain with transition rates r_{xy} and unique steady state $\pi > 0$. We assume that $r_{xy} > 0 \Leftrightarrow r_{yx} > 0$. We interpret the Markov chain as a graph with states $x, y \in V$ and edges $xy \in E$ whenever $r_{xy} > 0$.



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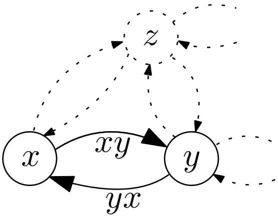

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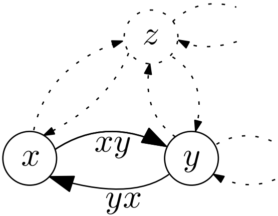

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The probability distribution of the Markov chain then evolves by

$$\dot{\rho}_t(x) = -\operatorname{div} J(\rho_t)(x) := -\sum_y J_{xy}(\rho_t).$$

Rate functional for Markov chains

The rate function for fluctuations of the density and the current is given by

$$I_{[0,\tau]}\big((\rho_t, j_t)_{t\in[0,\tau]}\big) = \frac{1}{2}\int_0^\tau \sum_{xy\in E} \Big[j_t\big(\operatorname{arcsinh}(j_t/a) - \operatorname{arcsinh}(j^F/a)\big) - \Big(\sqrt{a^2 + (j_t)^2} - \sqrt{a^2 + (j^F)^2}\,\Big)\Big] \mathrm{d}t,$$

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where $a = a(\rho_t)$ and $j^F = j^F(\rho_t)$ are discussed later, see [Maes and Netočný, EPL (Europhysics Letters) 82.3 (2008): 30003] and [Bertini et al., Stoch. Proc. and their Appl. 125.7 (2015): 2786-2819].

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This expression is not quadratic, but can be bounded above by a quadratic approximation, see e.g. [Gingrich et al., Physical Review Letters 116.12 (2016): 120601].

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More general, we define for generic forces F and currents j

$$j^F(\rho) := a(\rho) \sinh\big(\tfrac{1}{2} F\big) \quad \text{and} \quad F^j(\rho) := 2 \operatorname{arcsinh}\big(j/a(\rho)\big).$$

Recall: The rate functional is given in terms of

$$\begin{aligned}\Phi(\rho, j, F) = \sum_{xy \in E} & j\big(\operatorname{arcsinh}(j/a(\rho)) - \operatorname{arcsinh}(j^F/a(\rho))\big) \\ & - \left(\sqrt{a(\rho)^2 + j^2} - \sqrt{a(\rho)^2 + (j^F)^2}\,\right) \\ = & \\ = & \end{aligned}$$

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$$= \sum_{xy\in E} \left(\tfrac{1}{2} jF^j - \sqrt{a(\rho)^2 + j^2}\right) - \frac{1}{2} \sum_{xy\in E} jF + \sum_{xy\in E} \sqrt{a(\rho)^2 + (j^F)^2}$$
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where

$$j\cdot F = \frac{1}{2}\sum_{xy\in E} j_{xy}F_{xy},$$

$$\Psi^\star(\rho, F) = \sum_{xy\in E} a_{xy}(\rho)\big(\cosh\big(\tfrac{1}{2}F_{xy}\big) - 1\big),$$

and Ψ is the Legendre transformation

$$\Psi(\rho, j) = \sup_F \big(j\cdot F - \Psi^\star(\rho, F)\big).$$

Quick recap

For a large family of models (diffusions, Markov chains, MFT, ...(?)) with dynamics

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we can define a dual pairing $j \cdot F$ and Legendre duals $\Psi(j)$, $\Psi^\star(F)$.

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For a particular choice $\hat{F}$, we can describe the fluctuations in the system in terms of

$$\Phi(j, \hat{F}) := \Psi(j) - j \cdot \hat{F} + \Psi^\star(\hat{F}).$$

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Moreover Φ is minimised for $j = \partial_{\hat{F}} \Psi^\star$. The minimiser is given by J, such that $J = \partial_{\hat{F}} \Psi^\star$. In particular, $J = \chi \hat{F}$ if and only if

$$\Psi^\star(\hat{F}) = \frac{1}{2} \int \chi \hat{F}^2.$$

III. Splitting forces and currents

Adjoint process and splitting of forces

Given a process with force $F(\rho)$, we assume the existence of a time-reversed (or adjoint) process with force $F^*(\rho)$, the same stationary distribution π, and rate function

$$I^*_{[0,\tau]}\big((\rho_t, j_t)_{t\in[0,\tau]}\big) = \frac{1}{2}\int_0^\tau \mathrm{d}t\ \Phi(\rho_t, j_t, F^*(\rho_t)),$$

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such that

$$I_0(\rho_\tau) + I^*_{[0,\tau]}\big((\rho_{\tau-t}, -j_{\tau-t})_{t\in[0,\tau]}\big) = I_0(\rho_0) + I_{[0,\tau]}\big((\rho_t, j_t)_{t\in[0,\tau]}\big),$$

where I_0 is the rate function corresponding to sampling the initial condition from the stationary distribution π.

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Reversible (equilibrium) processes are characterised by $F(\rho) = F^*(\rho)$.

Splitting of forces for Markov chains

In general, we define the **reversible (equilibrium) part**

$$F^S(\rho) := \tfrac{1}{2}\big(F(\rho) + F^*(\rho)\big),$$

and an **irreversible (non-equilibrium) part**

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$$F^S_{xy}(\rho) = -\nabla^{x,y} \log \frac{\rho}{\pi} \quad \text{and} \quad F^A_{xy} = \log \frac{\pi(x) r_{xy}}{\pi(y) r_{yx}},$$

where $\nabla^{x,y} f = f(y) - f(x)$.

Splitting of forces for Markov chains

In general, we define the **reversible (equilibrium) part**

$$F^S(\rho) := \tfrac{1}{2}\big(F(\rho) + F^*(\rho)\big),$$

and an **irreversible (non-equilibrium) part**

$$F^A(\rho) := \tfrac{1}{2}\big(F(\rho) - F^*(\rho)\big).$$

For a Markov chain with steady state π, the force

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Note that F^A is independent of ρ.

IV. Justification for the splitting

Note that $F^S_{xy}(\rho) = -\nabla^{x,y}[\partial_\rho \mathcal{F}(\rho)]$ for the free energy

$$\mathcal{F}(\rho) = \sum_{x \in V} \rho(x) \log \frac{\rho(x)}{\pi(x)}.$$

Consequently, for a path $\dot{\rho}_t = -\operatorname{div} j_t$ the **change of free energy** is given by

$$\frac{d}{dt}\mathcal{F}(\rho_t) = -j_t \cdot F^S(\rho_t).$$

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$$j_t \cdot F^A$$

corresponds to the rate of flow of **housekeeping heat** into the environment.

Orthogonality of forces

In the case of diffusions (or MFT using local Einstein relation), we have

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In terms of $\Psi^\star$, we can rewrite this as

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We may interpret this as as generalised orthogonality.

V. Applications

Monotonicity of the free energy

The generalised orthogonality can be shown to imply that

$$\Phi(\rho, j, F(\rho)) = -j \cdot F^S(\rho) + \Phi_S(\rho, 0, F^S(\rho)) + \Phi(\rho, j, F^A(\rho)),$$

(where for Markov chains Φ_S is Φ with $a_{xy}(\rho) = 2\sqrt{\rho(x) r^S_{xy} \rho(y) r^S_{yx}}$ and for diffusions $\Phi_S = \Phi$).

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We can use this to recover the well known fact that the free energy is decreasing along the dynamics of the Markov chain: For $\dot{\rho}_t = -\operatorname{div} J(\rho_t)$, we have $\Phi(\rho_t, J(\rho_t), F(\rho_t)) = 0$, and therefore

$$\frac{d}{dt}\mathcal{F}(\rho_t) = -\Phi_S(\rho_t, 0, F^S(\rho_t)) - \Phi(\rho_t, J(\rho_t), F^A(\rho_t)).$$

Level 2 and 2.5

For the 'level-2.5' large deviation one considers a single copy of the system and observes the fluctuations of the time average

$$\left(\frac{1}{T} \int_0^T \rho_t^1 \, \mathrm{d}t, \frac{1}{T} \int_0^T j_t^1 \, \mathrm{d}t \right) \approx (\rho, j)$$

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$$I_{2.5}(\rho, j) = \frac{1}{2}\Phi(\rho, j, F(\rho)) = \frac{1}{2}\Big[\Phi_S(\rho, 0, F^S(\rho)) + \Phi(\rho, j, F^A(\rho))\Big].$$

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From here, one can contract to 'level-2'

$$I_2(\rho) = \inf_{j:\operatorname{div} j=0} \frac{1}{2}\Phi(\rho, j, F(\rho)) = \frac{1}{2}\Big[\Phi_S(\rho, 0, F^S(\rho)) + \Phi(\rho, J^{\mathrm{ss}}, F^A(\rho))\Big].$$

Finite time Gallavotti-Cohen type symmetry

When we sample the initial data from π, the process has the rate function (note that $\mathcal{F}$ and I_0 from before coincide)

$$I_{[0,\tau]}\big((\rho_t, j_t)_{t\in[0,\tau]}\big) = \mathcal{F}(\rho_0) + \frac{1}{2}\int_0^\tau \mathrm{d}t\ \Phi(\rho_t, j_t, F(\rho_t)).$$

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In this case we obtain the following version of a finite time Gallavotti-Cohen type symmetry

$$-\frac{1}{N}\log\frac{\mathrm{Prob}\big[(\rho_t^N, j_t^N)_{t\in[0,\tau]} \approx (\rho_t, j_t)_{t\in[0,\tau]}\big]}{\mathrm{Prob}\big[(\rho_t^N, j_t^N)_{t\in[0,\tau]} \approx (\rho_{\tau-t}, -j_{\tau-t})_{t\in[0,\tau]}\big]}$$

$$\asymp \mathcal{F}(\rho_0) - \mathcal{F}(\rho_T) + \frac{1}{2}\int_0^\tau \mathrm{d}t\ \Big[\Phi(\rho_t, j_t, F(\rho_t)) - \Phi(\rho_t, -j_t, F(\rho_t))\Big]$$

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&\asymp \mathcal{F}(\rho_0) - \mathcal{F}(\rho_T) + \frac{1}{2}\int_0^\tau \mathrm{d}t\ \Big[\Phi(\rho_t, j_t, F(\rho_t)) - \Phi(\rho_t, -j_t, F(\rho_t))\Big] \\
&= \mathcal{F}(\rho_0) - \mathcal{F}(\rho_T) - \int_0^\tau \mathrm{d}t\ j_t\cdot F(\rho_t) = -\int_0^\tau \mathrm{d}t\ j_t\cdot F^A(\rho_t).
\end{aligned}$$

Conclusion

Ψ-$\Psi^\star$ can be seen as an universal structure for dynamical fluctuations of a large class of systems.

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This structure also allows to identify thermodynamic quantities on the scale of Markov chains, such as free energy, housekeeping heat, and entropy production.

Thank you!