Why do irreversible processes converge faster to equilibrium than reversible ones?

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joint work with R. L. Jack and J. Zimmer

Claim: **Irreversible systems converge faster to equilibrium** [Hwang et al. 2005][Pavliotis2013][ReyBellet-Spiliopoulos2015,2016] [Bierkens2015]

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- Understanding the physics of non-equilibrium systems
- Acceleration of sampling methods like MCMC

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We investigate the effect of **breaking detailed balance** on the convergence to the steady state.

We will consider (interacting) particle systems and their hydrodynamic scaling limits.

We consider systems on two scales:

(1) Microscopic systems

finite state, ergodic and irreducible continuous time Markov processes with unique steady state π and dynamics given by

$$\begin{aligned}\dot{\mu}_t(x) &= \sum_y \mu_t(y)c(y \to x) - \mu_t(x)c(x \to y) \\ &= \mathcal{L}^\dagger \mu_t(x).\end{aligned}$$

(2) Macroscopic systems

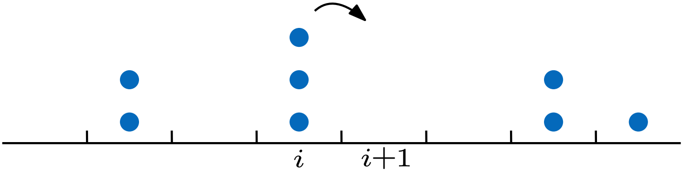
drift diffusive systems of the form

$$\partial_t \rho = \nabla \cdot \big(D(\rho)\nabla\rho\big) - \nabla \cdot \big(\chi(\rho)E\big).$$

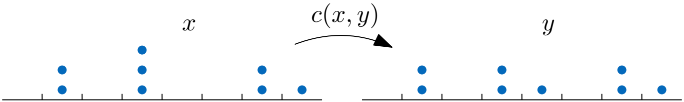
Microscopic systems

Microscopic systems = particle systems

We consider a system of indistinguishable particles which hop between sites



leading to a transition from state x to state y



Microscopic systems

Relations to physics: **Equilibrium systems** are characterised by 'detailed balance'

$$\pi(x)c(x \to y) = \pi(y)c(y \to x),$$

which correspond to vanishing currents in the steady state, whereas **non-equilibrium systems** are characterised by a non-zero current in the steady state. The microscopic current for a measure μ is given by

$$J^{x,y}(\mu) = \mu(x)c(x \to y) - \mu(y)c(y \to x).$$

$J^{x,y}(\pi) = 0$ (for all x, y) if and only if the system is an equilibrium system (i.e. satisfies detailed balance).

Microscopic systems

Alternative characterisation in terms of the generator $\mathcal{L}$:

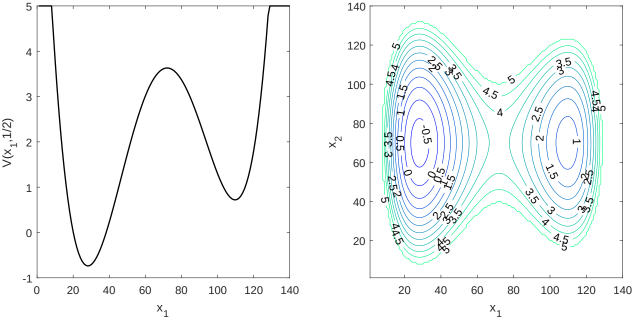
The process is reversible (satisfies detailed balance) if $\mathcal{L}$ is symmetric w.r.t. the inner product in $L^2(\pi)$.

In general, we can write any generator $\mathcal{L}$ as $\mathcal{L} = \mathcal{L}_S + \mathcal{L}_A$, where $\mathcal{L}_S$ is symmetric and $\mathcal{L}_A$ is anti-symmetric (w.r.t. $L^2(\pi)$).

$\mathcal{L}_S$ is again a generator with unique stationary measure π.

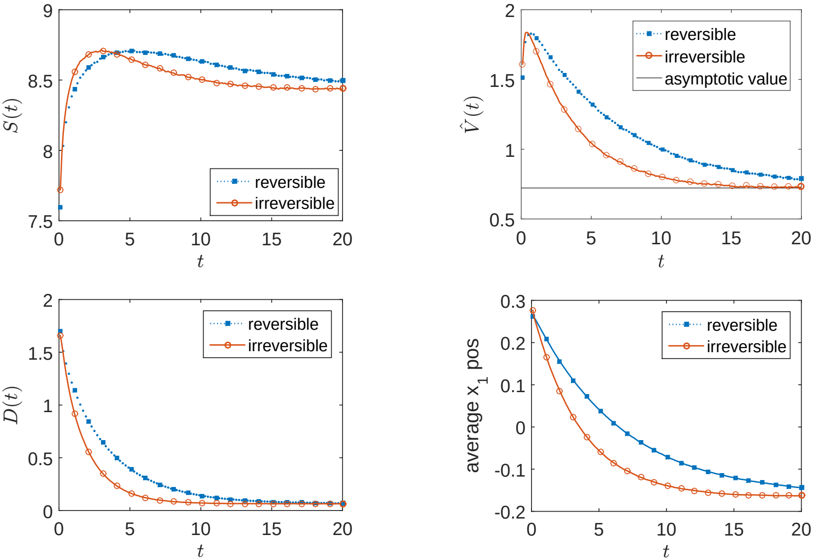
Example

We consider a system of independent particles in a potential U in 2d.



We can think here of a Monte Carlo sampling with many ($\approx 150\,000$) samples. Sampling from $\pi \propto \mathrm{e}^{-U}$. Lattice size $L^2 = 140 \times 140$.

Example - Test observable



[K., Jack, Zimmer, J Stat Phys 2017]

Acceleration of convergence

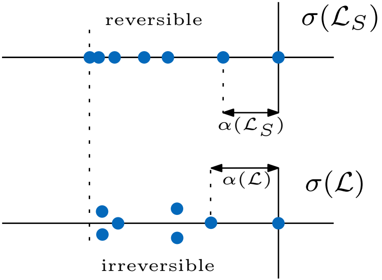
$\Rightarrow$ The Markov chain with generator $\mathcal{L} = \mathcal{L}_S + \mathcal{L}_A$ converges faster to π than the process with generator $\mathcal{L}_S$.

This convergence can be checked in different ways: (e.g.)

- The spectral gap of the generator
  (the largest non-zero eigenvalue of $\mathcal{L}$).
- The large deviation rate functional

Spectral gap

The spectrum $\sigma(\mathcal{L})$ is contained in $\mathbb{C}_- := \{z \in \mathbb{C} | \operatorname{Re}(z) \leq 0\}$ and $0 \in \sigma(\mathcal{L})$. We denote with $\alpha(\mathcal{L})$ the modulus of the real part of the non-zero eigenvalue with largest real part.



Spectral gap

We assume that $\mathcal{L}$ is diagonalisable such that we can write any distribution at time $t \in [0, \infty)$ as

$$\mu_t(x) = \pi(x) + \mathrm{e}^{-t\alpha(\mathcal{L})}\gamma(t, x)$$

for a (in t) bounded function $\gamma(t, x)$. Therefore

$$\|\mu_t - \pi\| \leq C\mathrm{e}^{-t\alpha(\mathcal{L})}.$$

(The initial distribution is here given by $\mu_0 = \pi + \gamma(0, \cdot)$)

Hence

Theorem (Spectral gap)

$$\alpha(\mathcal{L}) \geq \alpha(\mathcal{L}_S).$$

Large deviations

Large deviations characterise asymptotic probabilities (here as $t \to \infty$) in terms of a rate functional $I(\mu)$. In this case, we consider the empirical average $\Theta_t := \frac{1}{t}\int_0^t \delta_{X_u} du$, which satisfies

$$P[\Theta_t \approx \mu] \asymp \mathrm{e}^{-tI(\mu)}.$$

This notation stands for the following two inequalities: For all closed sets A and open sets O, we have

$$\limsup_{t\to\infty} \frac{1}{t} \log P[\Theta_t \in A] \leq - \inf_{\mu \in A} I(\mu)$$

and

$$\liminf_{t\to\infty} \frac{1}{t} \log P[\Theta_t \in O] \geq - \inf_{\mu \in O} I(\mu).$$

Large deviations

We compare

$$P[\Theta_t(\mathcal{L}_S) \approx \mu] \asymp \mathrm{e}^{-tI_S(\mu)} \qquad \text{and} \qquad P[\Theta_t(\mathcal{L}) \approx \mu] \asymp \mathrm{e}^{-tI(\mu)}.$$

Consistently with the above result, we have

Theorem (Rate functional)

$$I^S(\mu) \leq I(\mu)$$

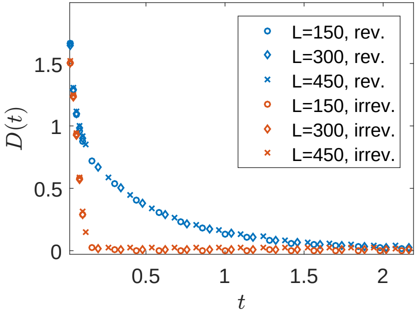
Informally this implies that asymptotically as $t \to \infty$

$$P[\Theta_t(\mathcal{L}_S) \approx \mu] \geq P[\Theta_t(\mathcal{L}) \approx \mu]$$

for $\mu \neq \pi$.

Macroscopic systems

With the appropriate rescaling of the rates, the systems becomes on large enough scales (for large L) 'independent' of the lattice size.



Plot of 1d system with $L = 150, 300, 450$.

The system then can be approximately described by a deterministic mass evolution.

Macroscopic systems

The macroscopic behaviour can be described in terms of a conservation law of the form

$$\partial_t \rho_t = -\nabla \cdot j_t \tag{1}$$

for some current j_t on a given domain Λ with a suitable boundary condition on $\partial\Lambda$.

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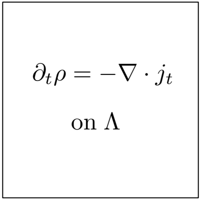

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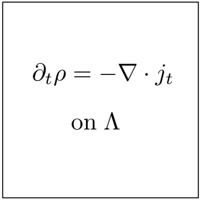

For the hydrodynamic limit, the associated hydrodynamic current $J(\rho_t)$ is given by

$$J(\rho_t) = -D(\rho_t)\nabla\rho_t + \chi(\rho_t)E. \tag{2}$$

We assume that equation (1) with $j_t = J(\rho_t)$ as in (2) has a unique steady state $\bar{\rho}$.

Splitting the current

A fundamental result from the Macroscopic Fluctuation Theory (MFT) is that one can split the current in the sum of a symmetric and an anti-symmetric term:

$$J = J_S + J_A$$

which satisfies an orthogonality condition

$$\langle J_S(\rho), J_A(\rho) \rangle_{\chi(\rho)^{-1}} := \int_\Lambda J_S(\rho) \cdot \chi(\rho)^{-1} J_A(\rho)\, dx = 0.$$

J_S and J_A can be obtained from the current of the adjoint process as $J_S = (J + J^*)/2$ and $J_A = (J - J^*)/2$.

Note: In general $J_S(\rho_t)$ is <u>not</u> $-D(\rho_t)\nabla\rho_t$.

Non-equilibrium systems

Non-equilibrium systems correspond to the case when J_A does not vanish, whereas equilibrium systems are characterised by $J = J_S$.

Similar to the microscopic case, where $\mathcal{L} = \mathcal{L}_S$ for reversible systems.

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In general, we can write the symmetric part of the current as

$$J_S(\rho_t) = -\chi(\rho_t)\nabla\frac{\delta\mathcal{V}}{\delta\rho_t}.$$

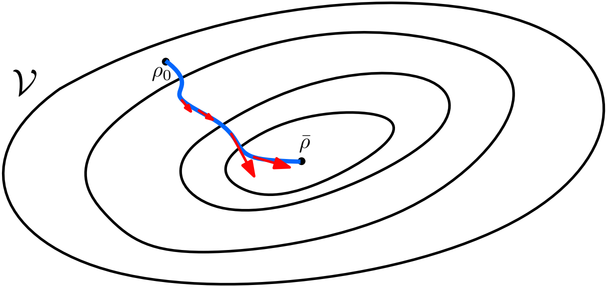
where $\mathcal{V}$ is the so called quasipotential.

- $\mathcal{V}(\rho) \geq 0$ with equality if and only if $\rho = \bar{\rho}$.
- $\mathcal{V}(\rho_t)$ is monotonic decreasing.
- $\mathcal{V}$ can be thought of as a (non-equilibrium) free energy that drives the system to the unique and globally attractive steady state $\bar{\rho}$.

Symmetric current

In the case that $J_A(\rho) = 0$, we can write the dynamics as the gradient flow (or **steepest descent**)

$$\partial_t \rho_t = \nabla \cdot \chi(\rho_t) \nabla \frac{\delta \mathcal{V}}{\delta \rho_t}.$$



Recall that a gradient flow consists of a metric M and an energy $\mathcal{V}$, such that $\partial_t \rho_t = -M(\rho_t) \frac{\delta \mathcal{V}}{\delta \rho_t}$.

(Here $M(\rho_t) = -\nabla \cdot \chi(\rho_t) \nabla$).

Example of a symmetric process

Consider the linear equation

$$\partial_t \rho_t = \Delta \rho_t + \nabla \cdot (\rho_t \nabla U).$$

This is the linear case (where $\chi(\rho_t) = \rho_t$) and the external force is of gradient type ($E = -\nabla U$).

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This is the linear case (where $\chi(\rho_t) = \rho_t$) and the external force is of gradient type ($E = -\nabla U$). It can be restated as

$$\partial_t \rho_t = \nabla \cdot \Big(\rho_t \nabla \log \Big(\frac{\rho_t}{\mathrm{e}^{-U}} \Big) \Big),$$

and thus $\mathcal{V}$ is

$$\frac{\delta \mathcal{V}}{\delta \rho_t} = \log \Big(\frac{\rho_t}{\mathrm{e}^{-U}} \Big).$$

Note that the steady state $\bar{\rho}$ is proportional to e^{-U}. The quantity $\nabla \frac{\delta \mathcal{V}}{\delta \rho_t}$ is the force which drives the process to the steady state $\bar{\rho}$.

Anti-symmetric current

We assume that the external field is given by $E = -\nabla U + \tilde{E}$ (where $\tilde{E}$ is not a gradient) and consider the Poisson equation

$$\nabla \cdot \big(\chi(\rho)\nabla\psi\big) = -\nabla \cdot \big(\chi(\rho)\tilde{E}\big),$$

which has (under some regularity assumptions on the rhs) a unique ρ dependent solution $\psi = \psi_\rho$.

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$$J(\rho_t) = -\chi(\rho)\nabla\frac{\delta\mathcal{V}}{\delta\rho} - \chi(\rho_t)\nabla\psi_\rho + J_F(\rho)$$

for the divergence free flux $J_F(\rho) := J_A(\rho) + \chi(\rho)\nabla\psi_\rho$.

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for the divergence free flux $J_F(\rho) := J_A(\rho) + \chi(\rho)\nabla\psi_\rho$. All of these three terms are orthogonal w.r.t. the inner product $\langle\cdot,\cdot\rangle_{\chi(\rho)^{-1}}$, and

$$\partial_t\rho_t = \nabla \cdot \chi(\rho_t)\nabla\frac{\delta\mathcal{V}}{\delta\rho_t} + \nabla\cdot\chi(\rho_t)\nabla\psi_{\rho_t}.$$

Large deviation rate functional

Under typical assumptions of no dynamical phase transition, the rate functional for the empirical density is given by

$$I_2(\rho) = \frac{1}{4}\int_\Lambda \nabla\frac{\delta\mathcal{V}}{\delta\rho}\cdot\chi(\rho)\nabla\frac{\delta\mathcal{V}}{\delta\rho}dx + \frac{1}{4}\int_\Lambda \nabla\psi_\rho\cdot\chi(\rho)\nabla\psi_\rho\,dx.$$

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Note that the first term corresponds to the contribution of the symmetric current and the second summand corresponds to the first part of the anti-symmetric current which is not divergence free. The divergence free part is not contributing to the rate functional.

Large deviation rate functional

The rate functional for the reversible process has $\nabla\psi = 0$, such that

Theorem (Rate functional)

$$I_2^S(\rho) \leq I_2(\rho).$$

This implies again that asymptotically, as $L \to \infty$, for $\rho \neq \bar{\rho}$

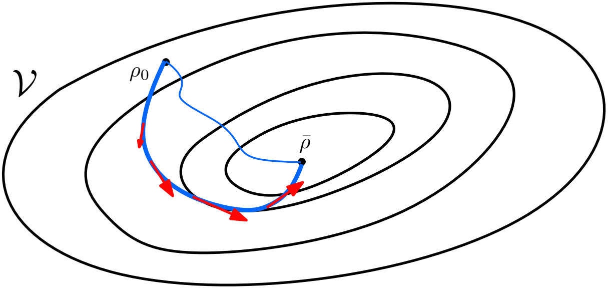
$$P[\Theta_t^L(J_S) \approx \rho] \geq P[\Theta_t^L(J) \approx \rho].$$

Intuition for the convergence

The orthogonality condition

$$0 = -\int_\Lambda J_S(\rho) \cdot \chi(\rho)^{-1} J_A(\rho)\, dx = \int_\Lambda \frac{\delta \mathcal{V}}{\delta \rho} \nabla \cdot J_A(\rho)\, dx$$

implies that J_A has no effect on the value of $\mathcal{V}$. That is, the current $J_A(\rho)$ **acts on the level sets of** $\mathcal{V}$.



Thanks