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TIME REVERSAL OF MARKOV PROCESSES

A DONEV
COURANT

Consider a Markov jump process among a discrete set of states $\{i_1, i_2, \ldots, i_N\}$

Assume the initial point i_1 is chosen based on the equilibrium or stationary measure $\pi(i)$, and consider a **forward** path:

$$i_1 \to i_2 \to i_3 \cdots\cdots \to i_N$$

The probability of observing (2)
this sequence (path) is

$$P_f = \Pi(i_1)\, p(i_1 \to i_2)\, p(i_2 \to i_3) \ldots\ldots p(i_{N-1} \to i_N)$$

transition
probability
(time-independent)

Now consider the time reversed process (reading trajectories backward)

$$i_N \to i_{N-1} \to \ldots\ldots \to i_2 \to i_1$$

This trajectory is consistent with a Markov jump process with transition probability $p'(i_x \to i_y)$:

$$P_f = \pi(i_N) \left(\frac{\pi(i_{N-1})\, p(i_{N-1} \to i_N)}{\pi(i_N)} \right) \cdots \left(\frac{\pi(i_1)\, p(i_1 \to i_2)}{\pi(i_2)} \right)$$

$$= \pi(i_N)\, p'(i_N \to i_{N-1}) \cdots p'(i_2 \to i_1)$$

where

$$\boxed{p'(i_x \to i_y) = p(i_y \to i_x) \frac{\pi(i_y)}{\pi(i_x)}}$$

This is general and gives the time-reversed Markov process (generator).

A process is time-reversible if $p' = P$, i.e., the time-reversed process is the process itself. (so one cannot ~~tell~~ the "arrow" or direction of time by reading equilibrium trajectories).

this means that time reversibility $\equiv$

detailed balance

$$\boxed{p(i_x \to i_y)\,\Pi(i_x) = p(i_y \to i_x)\,\Pi(i_y)}$$

How to generalize to more types of Markov processes? (5)

Consider the matrix $P_{i_x, i_y} = p(i_x \to i_y)$

Define a dot product weighted by the equilibrium distribution:

$$(f, g)_\pi = \sum_i f_i g_i \pi_i$$

What is the adjoint of the generator P (matrix of transition probabilities) w.r.t. this dot product?

Note! $P_{i_x, i_x} = -\sum_{i_y} p(i_x \to i_y)$

$$(P f, g)_\pi = (f, P^* g)_\pi$$

Take $\begin{cases} f_{i'} = \delta_{i,i'} \\ g_{j'} = \delta_{j,j'} \end{cases}$

$$P_{j,i} \pi_j = P^*_{i,j} \pi_i$$

$$p(j \to i) \pi(j) = p^*(i \to j) \pi(i)$$

$$p^*(i \to j) = p(j \to i) \frac{\pi(j)}{\pi(i)} = p'(i \to j)$$

So <u>the generator of the time reversed process is the adjoint of the forward</u>

$$\boxed{\text{Time reversibility} \equiv \mathcal{L}_\pi^* = \mathcal{L}}$$

generator is <u>self-adjoint</u> in eq. inner product

These two results are general and apply to other Markov processes, notably, diffusion ones.

Recall $dx = a(x)dt + b(x)\,dW$

$$\mathcal{L} = a \cdot \frac{\partial}{\partial x} + \frac{1}{2}(bb^*) : \frac{\partial^2}{\partial x^2}$$

$\mathcal{L}_\pi^* = \,?$ (earlier we used L_2 inner product and not new one)

$$(f, \mathcal{L} g)_\pi = \int f(x)\, \pi(x)\, a(x) \cdot \frac{\partial g(x)}{\partial x}\, dx \qquad (8)$$

$$+ \frac{1}{2} \int f(x)\, \pi(x)\, (b b^*)(x) : \frac{\partial^2 g}{\partial x^2}\, dx$$

Let's write in component form and use integration by parts (boundary terms drop out under suitable assump.)

$$\text{term } 1 = \int f \pi\, a_i \frac{\partial g}{\partial x_i}\, dx_1 dx_2 \ldots dx_N$$

$$= - \int g \frac{\partial}{\partial x_i} (\pi f a_i)\, dx$$

$$= \int \pi g (\mathcal{L}_1^* f)\, dx \qquad \Longrightarrow$$

$$\Rightarrow \mathcal{L}_1^* f = -\frac{1}{\pi}\frac{\partial}{\partial x_i}(\pi f a_i)$$

For second part $D \equiv b b^*$

$$\text{term } 2 = \frac{1}{2}\int f \pi D_{ij} \frac{\partial^2 g}{\partial x_i \partial x_j}\, dx =$$

$$= -\frac{1}{2}\int \frac{\partial}{\partial x_i}(f \pi D_{ij}) \frac{\partial g}{\partial x_j}\, dx =$$

$$= +\frac{1}{2}\int \frac{\partial^2}{\partial x_i \partial x_j}(f \pi D_{ij})\, g\, dx$$

$$= \int \pi g (\mathcal{L}_2^* f)\, dx \quad \Rightarrow$$

$$\mathcal{L}_2^{*} f = \frac{1}{\pi} \frac{\partial^2}{\partial x_i \partial x_j} (f \pi D_{ij})$$

$$\boxed{\text{Note : } D_{ij} = D_{ji}}$$

$$\mathcal{L}_\pi^{*} = \mathcal{L}_1^{*} + \mathcal{L}_2^{*} =$$

$$= -\frac{1}{\pi} \frac{\partial}{\partial x_i} (\pi f a_i) + \frac{1}{\pi} \frac{\partial^2}{\partial x_i \partial x_j} (f \pi D_{ij})$$

$$= -a_i \frac{\partial f}{\partial x_i} - \frac{1}{\pi} \left[\frac{\partial}{\partial x_i} (a_i \pi) \right] f$$

$$+ \frac{1}{2} D_{ij} : \frac{\partial^2 f}{\partial x_i \partial x_j} + \frac{1}{2} \frac{1}{\pi} \frac{\partial^2}{\partial x_i \partial x_j} (\pi D_{ij})$$

$$+ \frac{1}{\pi} \frac{\partial}{\partial x_i} (\pi D_{ij}) \frac{\partial f}{\partial x_j}$$

Combine the two terms on the right:

$$\left[- \frac{\partial}{\partial x} \cdot (a \pi) + \frac{1}{2} \frac{\partial^2}{\partial x^2} : (D \pi) \right] \frac{f}{\pi} = 0 \, !$$

since π is the equilibrium distribution and thus the solution to the FPE

$$\mathcal{L}^* \pi = \left[- \frac{\partial}{\partial x} \cdot a + \frac{1}{2} \frac{\partial^2}{\partial x^2} : D \right] \pi = 0$$

Giving

$$\mathcal{L}^*_\pi = \mathcal{L}_{\text{reverse}} = -a \cdot \frac{\partial}{\partial x} + \frac{1}{\pi} \frac{\partial}{\partial x} \cdot (\pi D) \cdot \frac{\partial}{\partial x} + \frac{1}{2} D : \frac{\partial^2}{\partial x^2}$$

We see that

$$\mathcal{L}^*_\pi = a' \cdot \frac{\partial}{\partial x} + \frac{1}{2} D' : \frac{\partial^2}{\partial x^2}$$

where

$$\begin{cases} a' = -a + \frac{1}{\pi} \frac{\partial}{\partial x} \cdot (\pi D) \\ D' = b'(b')^* = D = b b^* \end{cases}$$

Therefore the time-reversed SDE is

$$\boxed{dx = -a\,dt + \frac{1}{\pi} \frac{\partial}{\partial x} \cdot (\pi D)\,dt + b\,dw}$$

stochastic "drift" term

The SDE is time-reversible if

$$\frac{2}{\Pi}\left[-a\Pi + \frac{1}{2}\frac{\partial}{\partial x}\cdot(\Pi D)\right] = 0$$

Now go back to the FPE at equilibrium:

$$\frac{\partial \Pi}{\partial t} = 0 = \frac{\partial}{\partial x}\cdot\left[\underbrace{\left(-a + \frac{1}{2}\frac{\partial}{\partial x}\cdot D\right)\Pi}_{\text{\underline{flux} in prob. space}}\right]$$

Therefore

$$\boxed{\text{time reversibility} \equiv \text{detailed balance } \mathcal{X}=\mathcal{X}^* \equiv \text{no flux in phase space at equilibrium}}$$