

• Large deviation functions as maximal eigenvalues

Lecture on
Stoch. processes (2.10)

1. Cases of observables of type A₂

- * Time evolution for $P(\epsilon, A_2, t)$:

$$\partial_t P(\epsilon, A_2, t) = \sum_{\epsilon'} W(\epsilon' \rightarrow \epsilon) P(\epsilon', A_2 - a_2(\epsilon' \rightarrow \epsilon), t) - n(\epsilon) P(\epsilon, A_2, t)$$

This evolution is non-diagonal in the direction A_2 ,
the operator of evolution is very difficult to diagonalize.

- * Going to the s-state: Laplace transform

One introduces $\hat{P}(\epsilon, s, t) = \sum_{A_i} e^{-sA_i} P(\epsilon, A_i, t)$.

This quantity is more detailed than $\langle e^{-sA_i} \rangle$, but it obeys closed equation of evolution, as detailed now.

It verifies $\langle e^{-sA_i} \rangle = \sum_{\epsilon, A_i} e^{-sA_i} P(\epsilon, A_i, t) = \sum_{\epsilon} \hat{P}(\epsilon, s, t)$

- * Time evolution: from the time evolution of $P(\epsilon, A_i, t)$ one finds:

$$\partial_t \hat{P}(\epsilon, s, t) = \sum_{\epsilon'} e^{-s a_2(\epsilon' \rightarrow \epsilon)} W(\epsilon' \rightarrow \epsilon) \hat{P}(\epsilon', s, t) - n(\epsilon) \hat{P}(\epsilon, s, t)$$

This time, the operator is diagonal in direction s. Putting $| \hat{P}(s) \rangle = \sum_{\epsilon} \hat{P}(\epsilon, s, t) | \epsilon \rangle$

one has

$$\partial_t | \hat{P}(s) \rangle = W(s) | \hat{P}(s) \rangle$$

$$(W(s))_{\epsilon \epsilon'} = e^{-s a_2(\epsilon' \rightarrow \epsilon)} W(\epsilon' \rightarrow \epsilon) - n(\epsilon) \delta_{\epsilon \epsilon'}$$

here, only the non-diagonal part of the evolution operator is modified by s: it is the part describing jumps

- * Largest eigenvalue of W(s): one has $\langle e^{-sA_i} \rangle = \sum_{\epsilon} \hat{P}(\epsilon, s, t)$
 $| \hat{P}_0 \rangle = e^{tW(s)} | \hat{P}_0 \rangle \sim e^{\underbrace{t \max_{\epsilon} \text{Sp } W(s)}_{\text{max eigenvalue of } W(s)}} \Rightarrow \sim e^{t \max_{\epsilon} \text{Sp } W(s)}$

Hence $\langle e^{-sA_i} \rangle \sim e^{t \max_{\epsilon} \text{Sp } W(s)}$ and by definit.

$(\psi(s) = \max_{\epsilon} \text{Sp } W(s)$
it is the largest eigenvalue of $W(s)$)

2. Case of observable of type A_2

Lecture on
Stat. process (2.11)

$\partial_t P(\epsilon, A_2, t)$ is not as directly obtained as previously.

* first approach: time discretization ok up to order dt

$$P(\epsilon, A_2, t+dt) = \sum_{\epsilon'} dt W(\epsilon' \rightarrow \epsilon) P(\epsilon', A_2, t) + (1 - dt n(\epsilon)) P(\epsilon, A_2 - \frac{\int dt a_2(\epsilon')}{t})$$

$\approx dt a_2(\epsilon)$

Hence, in the $dt \rightarrow 0$ limit:

$$P(\epsilon, A_2, t) = dt \partial_{A_2} P(\epsilon, A_2, t) a_2(\epsilon)$$

$$\partial_t P(\epsilon, A_2, t) = \sum_{\epsilon'} W(\epsilon' \rightarrow \epsilon) P(\epsilon', A_2, t) - (n(\epsilon) P(\epsilon, A_2, t) + a_2(\epsilon) \partial_{A_2} P(\epsilon, A_2, t))$$

On, introducing $\hat{P}(\epsilon, s, t) = \int dA_2 e^{-sA_2} P(\epsilon, A_2, t)$

one again has $\langle e^{-sA_2} \rangle = \int dA_2 \{ P(\epsilon, A_2, t) = \sum_{\epsilon'} \hat{P}(\epsilon, s, t) \}$

) Thanks to
Laplace
transform, the
derivative ∂_{A_2}

The equation of evolution is thus (by integration by part) it becomes a single factor

$$\partial_t \hat{P}(\epsilon, s, t) = \sum_{\epsilon'} W(\epsilon' \rightarrow \epsilon) \hat{P}(\epsilon', s, t) - (n(\epsilon) + s a_2(\epsilon)) \hat{P}(\epsilon, s, t)$$

On, in vector notation:

$$\partial_t |\hat{P}(s, t)\rangle = |W(s)| \hat{P}(s, t)\rangle$$

$$(|W(s)|)_{pp'} = W(\epsilon' \rightarrow \epsilon) - (n(\epsilon) + s a_2(\epsilon)) \delta_{pp'}$$

this time, it is the
diagonal part of the operator of evolution
which is modified by s ,

This corresponds to the fact that $A_2 = \int_0^t d\tau a_2(\epsilon(\tau))$
is an observable which does not evolve at jumps.

Remark: This formula, written as: $\partial_t |\hat{P}(s, t)\rangle = |W(s)| \hat{P}(s, t)\rangle - s \hat{a}_2 |\hat{P}(s, t)\rangle$ diagonal operator of
elements $a_2(\epsilon)$

jumps are described
by the non-diagonal
part of $|W(s)|$

is an example of Feynman-Kac formula

• Second derivation of the result:

$$\text{One has } A_2 = \sum_{k=1}^K (t_k - t_{k-1}) a_2(\epsilon_{k-1}) + (t - t_K) a_2(\epsilon_K)$$

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Lecture on
Stoch. processes

Thus, using the expression previously obtained for the probab. l.f. of an history,

$$\langle e^{-sA_2} \rangle = \sum_{K \geq 0} \sum_{\epsilon_0 \dots \epsilon_{K-1}, \epsilon_K} \int_{t_0}^t \dots \int_{t_{K-1}}^t e^{-\sum_{k=1}^K (t_k - t_{k-1})(a(\epsilon_{k-1}) + s a_2(\epsilon_{k-1})) - (t - t_K)(a(\epsilon_K) + s a_2(\epsilon_K))} \times \prod_{k=1}^K W(\epsilon_{k-1}, \epsilon_k) P_0(\epsilon_k)$$

Indeed the derivation of the time-ordered exp. formula does not involves the conservation of probability presented by NW.
And one recognizes precisely the expansion of: It thus also works for NW.

$$\langle - | T_{\text{exp}} \underbrace{W_s(t)}_{\text{time dependent operator of evolution}} | P_0 \rangle$$

corresponding precisely to $W(s)$ for s associated to A_2

$$\text{which is compatible with } |\hat{P}(s, t)\rangle = T_{\text{exp}} \underbrace{W_s(t)}_{\text{operator}} |P_0\rangle$$

• Remark: mixed observables:

The l.d.f. $\Psi(s_1, s_2) = \lim_{t \rightarrow \infty} \frac{1}{t} \log \langle e^{-s_1 A_1 - s_2 A_2} \rangle$ is the mix e.v. of

$$(W(s_1, s_2))_{\epsilon \epsilon'} = e^{-s_1 a_1(\epsilon \rightarrow \epsilon') - s_2 a_2(\epsilon \rightarrow \epsilon')} W(\epsilon \rightarrow \epsilon') - (n(\epsilon) + s_2 a_2(\epsilon)) \delta_{\epsilon \epsilon'}$$

both diagonal and non-diagonal parts of the operator of evolution are modified, respectively by s_2 and s_1 .

Example:

- Time reversal symmetry and fluctuation theorem:

(J. Stat. Phys. 95 333 (1999), Lebowitz & Spohn)

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Lecture
Stat. physics

Consider the observable $Q_{ss} = \log \frac{W(\epsilon_0 \rightarrow \epsilon_1) \dots W(\epsilon_{n-1} \rightarrow \epsilon_n)}{W(\epsilon_n \rightarrow \epsilon_{n-1}) \dots W(\epsilon_1 \rightarrow \epsilon_0)}$ ("entropy current")

Upon a jump $\epsilon \rightarrow \epsilon'$ one has $Q_{ss} \approx Q_{ss} + \log \frac{W(\epsilon \rightarrow \epsilon')}{W(\epsilon' \rightarrow \epsilon)}$

The modified operator of evolution for s associated to Q_{ss} is

$$\begin{aligned} (W(s))_{\epsilon \epsilon'} &= e^{-s \log \frac{W(\epsilon' \rightarrow \epsilon)}{W(\epsilon \rightarrow \epsilon')}} W(\epsilon' \rightarrow \epsilon) - n(\epsilon) \delta_{\epsilon \epsilon'} \\ &= W(\epsilon \rightarrow \epsilon')^{1-s} W(\epsilon \rightarrow \epsilon')^s - n(\epsilon) \delta_{\epsilon \epsilon'} \end{aligned}$$

Results of this class are among the few results valid in non-equilibrium steady states.

One thus has $(W(s))_{\epsilon \epsilon'} = (W(1-s))_{\epsilon' \epsilon}$

$$W(s)^T = W(1-s)$$

Relative movements ($s \neq 0$) are rare ones ($s = 0$). Implies Fluctuation-Dissipation Relation, and Onsager Relations.

Since these two operators have the same spectrum, one has $(\Psi(s)) = \Psi(1-s)$

This symmetry is an instance of 'Gallavotti-Cohen relation' [J. Stat. Phys. 80: 931 (1995)] (or 'Fluctuation Theorem')

- Numerical algorithm for large deviation function: conjugated to $A = A_s$

By writing $W_s(\epsilon \rightarrow \epsilon') = e^{-s a(\epsilon \rightarrow \epsilon')} W(\epsilon \rightarrow \epsilon')$; $n_s(\epsilon) = \sum_p W_s(\epsilon \rightarrow p)$

$$(W(s))_{\epsilon \epsilon'} = \underbrace{W_s(\epsilon' \rightarrow \epsilon)}_{\text{(probability-conserving) evolution with modified rates } W_s(\epsilon \rightarrow \epsilon')} - \underbrace{n_s(\epsilon) \delta_{\epsilon \epsilon'}}_{\text{cloning with rate } n_s(\epsilon) - n(\epsilon)} + \underbrace{(n_s(\epsilon) - n(\epsilon)) \delta_{\epsilon \epsilon'}}_{\text{cloning with rate } n_s(\epsilon) - n(\epsilon)}$$

(probability-conserving) evolution with modified rates $W_s(\epsilon \rightarrow \epsilon')$ cloning with rate $n_s(\epsilon) - n(\epsilon)$

for a population of copies of the system.

One can devise an algorithm to measure $\Psi(s)$ numerically:

- evolution with rate $W_s(\epsilon \rightarrow \epsilon')$ of each copy

- cloning (pruning of copies with rate $n_s(\epsilon) - n(\epsilon)$)

favoring configurations with an atypical value of A .

then the global increase/decrease rate of the population is $\Psi(s)$
(There are tricks to keep the population size constant - see Refs.)

Population algorithm to measure $\Psi(s)$: for $s \rightarrow K$

Lecture 2.17
Stoch. Process

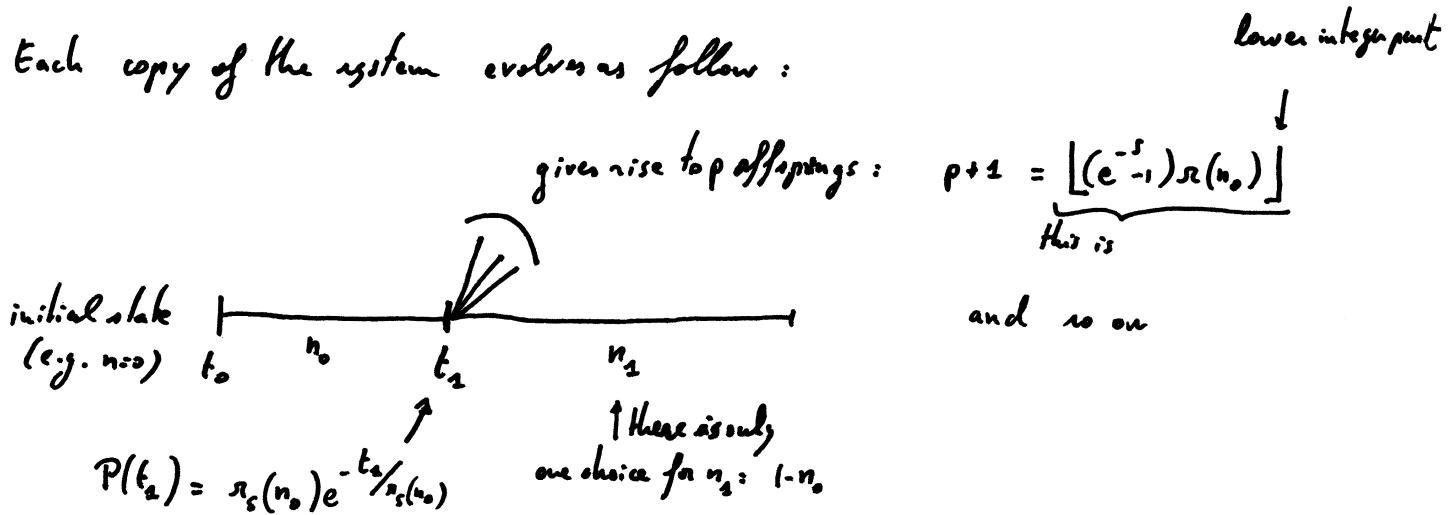
$$\partial_t \hat{P}(n, s, t) = \underbrace{e^{-s} [cn + (rc)n]}_{\text{death \& birth process with rates}} \hat{P}(t-n, s, t) - \underbrace{e^{-s} \left(c(cn) + n \right)}_{\frac{e^{-s}c}{rc}} \hat{P}(n, s, t) + (e^{-s}) \underbrace{\left(c(t-n) + n(rc) \right)}_{n(n)} \hat{P}(n, s, t) \underbrace{(e^{-s})}_{\text{cloning at rate } (e^{-s})n(n)}$$

For this simple example, we keep total population $N(t)$ non-constant.

Start with N_0 copies of the system ($N_0 \gg 1$, typically $10^2 - 10^3$)

Take $s < 0$ (so that $e^{-s} > 1$).

Each copy of the system evolves as follows:



Remark: it is better to take $\rho+1 = \lfloor (e^{-s})n_0 \rfloor + \varepsilon$ where ε is uniformly distributed on $[0, 1]$.

Each of the offsprings evolves independently afterwards.

In the large time limit: $N(t) \sim e^{t\Psi(s)}$