

• Large deviation functions as maximal eigenvalues

Lecture on (2.10)
Stoch. processes

1. Cases of observables of type A_2

* Time evolution for $P(\mathcal{C}, A_2, t)$:

$$\partial_t P(\mathcal{C}, A_2, t) = \sum_{\mathcal{C}'} W(\mathcal{C}' \rightarrow \mathcal{C}) P(\mathcal{C}', A_2 - a_2(\mathcal{C}' \rightarrow \mathcal{C}), t) - r(\mathcal{C}) P(\mathcal{C}, A_2, t)$$

this evolution is non-diagonal in the direction A_1 ,
the operator of evolution is very difficult to diagonalize.

* Going to the s -state: Laplace transform This quantity is more detailed than $\langle e^{-sA_1} \rangle$, but it obeys

One introduces $\hat{P}(\mathcal{C}, s, t) = \sum_{A_1} e^{-sA_1} P(\mathcal{C}, A_1, t)$ closed equation of evolution, as detailed now.

It verifies $\langle e^{-sA_1} \rangle = \sum_{\mathcal{C}, A_1} e^{-sA_1} P(\mathcal{C}, A_1, t) = \sum_{\mathcal{C}} \hat{P}(\mathcal{C}, s, t)$

* Time evolution: from the time evolution of $P(\mathcal{C}, A_1, t)$ one finds:

$$\partial_t \hat{P}(\mathcal{C}, s, t) = \sum_{\mathcal{C}'} e^{-s a_1(\mathcal{C}' \rightarrow \mathcal{C})} W(\mathcal{C}' \rightarrow \mathcal{C}) \hat{P}(\mathcal{C}', s, t) - r(\mathcal{C}) \hat{P}(\mathcal{C}, s, t)$$

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

one has

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

$$(W(s))_{\mathcal{C}\mathcal{C}'} = e^{-s a_1(\mathcal{C}' \rightarrow \mathcal{C})} W(\mathcal{C}' \rightarrow \mathcal{C}) - r(\mathcal{C}) \delta_{\mathcal{C}\mathcal{C}'}$$

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 $\langle e^{-sA_1} \rangle \approx \sum_{\mathcal{C}} \hat{P}(\mathcal{C}, s, t)$
 but $|\hat{P}(s, t)\rangle = e^{t W(s)} |\hat{P}_0\rangle \sim e^{t \max Sp W(s)} \rightarrow \nu e^{t \max Sp W(s)}$
maximal eigenvalue of $W(s)$

Hence $\langle e^{-sA_1} \rangle \sim \nu e^{t \max Sp W(s)}$ and by definit°

$$\psi(s) = \max Sp W(s)$$

it is the largest eigenvalue of $W(s)$

2. Case of observable of type A_2

$\partial_t P(\mathcal{E}, A_2, t)$ is not as directly obtained as previously.

* first approach: time discretization OK up to order dt

$$P(\mathcal{E}, A_2, t+dt) = \sum_{\mathcal{E}'} \int dt W(\mathcal{E}' \rightarrow \mathcal{E}) P(\mathcal{E}', A_2, t) + (1 - dt n(\mathcal{E})) P(\mathcal{E}, A_2 - \int_t^{t+dt} da_2(\mathcal{E}(\tau))) \approx dt a_2(\mathcal{E})$$

Hence, in the $dt \rightarrow 0$ limit: $P(\mathcal{E}, A_2, t) - dt \partial_{A_2} P(\mathcal{E}, A_2, t) a_2(\mathcal{E})$

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

Or, introducing $\hat{P}(\mathcal{E}, s, t) = \int dA_2 e^{-sA_2} P(\mathcal{E}, A_2, t)$
 one again has $\langle e^{-sA_2} \rangle = \int dA_2 \langle P(\mathcal{E}, A_2, t) \rangle = \sum_{\mathcal{E}} \hat{P}(\mathcal{E}, s, t)$

Thanks to Laplace transform, the derivative ∂_{A_2} becomes a simple factor

The equation of evolution is thus (by integration by part)
 $\partial_t \hat{P}(\mathcal{E}, s, t) = \sum_{\mathcal{E}'} W(\mathcal{E}' \rightarrow \mathcal{E}) \hat{P}(\mathcal{E}', s, t) - (n(\mathcal{E}) + s a_2(\mathcal{E})) \hat{P}(\mathcal{E}, s, t)$

Or, in vector notation:

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

$$(W(s))_{\mathcal{E}\mathcal{E}'} = W(\mathcal{E}' \rightarrow \mathcal{E}) - (n(\mathcal{E}) + s a_2(\mathcal{E})) \delta_{\mathcal{E}\mathcal{E}'}$$

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

This corresponds to the fact that $A_2 = \int_0^t dt a_2(\mathcal{E}(\tau))$ is an observable which does not evolve at jumps.

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

jumps are described by the non-diagonal part of W

is an example of Feynman-Kac formula

Second derivation of the result:

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

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

$$\langle e^{-sA_2} \rangle = \sum_{K \geq 0} \sum_{\xi_0, \dots, \xi_K} \int_{t_0}^t dt_1 \dots \int_{t_{K-1}}^t dt_K e^{-\sum_{k=1}^K (t_k - t_{k-1}) (n(\xi_{k-1}) + s a_2(\xi_{k-1})) - (t - t_K) (n(\xi_K) + s a_2(\xi_K))} \times \prod_{k=1}^K W(\xi_{k-1} \rightarrow \xi_k) P_0(\xi_0)$$

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

$$\langle - | T \exp \underline{W}_s(t) | P_0 \rangle$$

time dependent operator of evolution corresponding precisely to $W(s)$ for s associated to A_2

which is compatible with $|\hat{P}(s, t)\rangle = T \exp \underline{W}_s(t) | P_0 \rangle$

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 max e.v. of

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

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]

Lecture on Stoch. processes (2.13)

Consider the observable $Q_{\epsilon_s} = \text{Log} \frac{W(\epsilon_0 \rightarrow \epsilon_1) \dots W(\epsilon_{N-1} \rightarrow \epsilon_N)}{W(\epsilon_N \rightarrow \epsilon_{N-1}) \dots W(\epsilon_1 \rightarrow \epsilon_0)}$ ("entropy current")

Upon a jump $\epsilon \rightarrow \epsilon'$ one has $Q_s \rightarrow Q_s + \text{Log} \frac{W(\epsilon \rightarrow \epsilon')}{W(\epsilon' \rightarrow \epsilon)}$

The modified operator of evolution for s associated to Q_s is

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

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

One thus has $(W(s))_{\epsilon\epsilon'} = (W(1-s))_{\epsilon'\epsilon}$
 $W(s)^T = W(1-s)$

Relates rare events ($s \neq 1$) to not 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: s conjugated to $A=A$

By writing $W_s(\epsilon \rightarrow \epsilon') = e^{-sA(\epsilon \rightarrow \epsilon')} W(\epsilon \rightarrow \epsilon')$; $r_s(\epsilon) = \sum_{\epsilon'} W_s(\epsilon \rightarrow \epsilon')$

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

(probability-conserving) evolution with modified rates $W_s(\epsilon \rightarrow \epsilon')$ for a population of copies of the system.

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

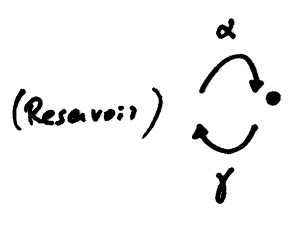
- evolution with rate $W_s(\epsilon \rightarrow \epsilon')$ of each copy
- cloning/pruning of copies with rate $r_s(\epsilon) - r(\epsilon)$

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.]

• An example: death and birth process on one site



$n=0$ site empty $W(0 \rightarrow 1) = \alpha$ (birth)
 $n=1$ site occupied $W(1 \rightarrow 0) = \gamma$ (death)

$$\partial_t P(0,t) = \gamma P(1,t) - \alpha P(0,t)$$

$$\partial_t P(1,t) = \alpha P(0,t) - \gamma P(1,t)$$

$\alpha > 0$
 $\gamma > 0$

$$\partial_t \begin{pmatrix} P(0,t) \\ P(1,t) \end{pmatrix} = \underbrace{\begin{pmatrix} -\alpha & \gamma \\ \alpha & -\gamma \end{pmatrix}}_W \underbrace{\begin{pmatrix} P(0,t) \\ P(1,t) \end{pmatrix}}_{|P(t)\rangle}$$

indeed
 $W_{01} = W(1 \rightarrow 0) = \gamma$
 $W_{10} = W(0 \rightarrow 1) = \alpha$
 $W_{00} = -\alpha(0) = -W(0 \rightarrow 1) = -\alpha$
 $W_{11} = -\alpha(1) = -W(1 \rightarrow 0) = -\gamma$

* search for a steady-state: one even has an equilibrium state (detailed balance ok)

"Grand-canonical" form
 St. st. eq:

$$P(n) = \frac{1}{Z} e^{\mu n}$$

$\mu =$ "chemical potential"

$$\begin{cases} 0 = \gamma e^{\mu} - \alpha \\ 0 = \alpha - \gamma e^{\mu} \end{cases}$$

$$e^{\mu} = \frac{\alpha}{\gamma}$$

$$Z = e^{0\mu} + e^{1\mu} = 1 + \frac{\alpha}{\gamma}$$

$$P(n) = \frac{\left(\frac{\alpha}{\gamma}\right)^n}{1 + \frac{\alpha}{\gamma}} \quad (\text{unnormalized})$$

In vector form: $|P_{eq}\rangle = \frac{1}{\alpha + \gamma} \begin{pmatrix} \gamma \\ \alpha \end{pmatrix}$ is indeed a right eigen-vector of W of ev. 0.

* mean occupation number:

$$\langle n \rangle = \sum_n n P(n) = \frac{\alpha/\gamma}{1 + \alpha/\gamma} = \frac{\alpha}{\alpha + \gamma}$$

In details: one rewrites
 $\partial_t |P(t)\rangle = (\alpha + \gamma) \begin{pmatrix} -\frac{\alpha}{\alpha + \gamma} & \frac{\gamma}{\alpha + \gamma} \\ \frac{\alpha}{\alpha + \gamma} & -\frac{\gamma}{\alpha + \gamma} \end{pmatrix} |P(t)\rangle$
 and one changes time so as to absorb $(\alpha + \gamma)$

* reparametrization: one sets $\alpha = c$ | $\gamma = 1 - c$ which fixes the unit of time $0 < c < 1$

$$P_{eq}(n) = c^n (1-c)^{1-n}$$

$$\langle n \rangle = c$$

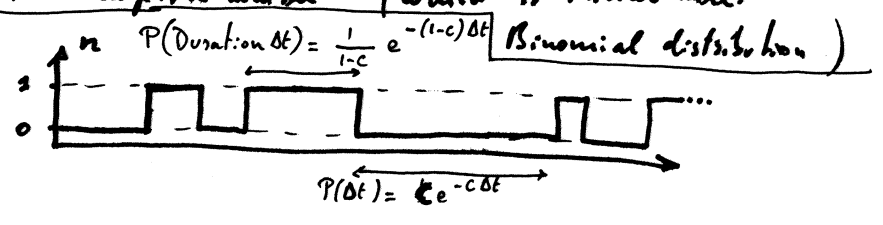
Binomial law • In vector form $|P_{eq}\rangle = \begin{pmatrix} c \\ 1-c \end{pmatrix} = (1-c)|0\rangle + c|1\rangle$
 $W = \begin{pmatrix} c & 1-c \\ c & -(1-c) \end{pmatrix}$

* generating function of the cumulant of the occupation number: $\langle e^{-sn} \rangle_{eq} = e^{\psi_{occ}(s)}$

$$\psi_{occ}(s) \equiv \log \langle e^{-sn} \rangle_{eq} = \log \{ 1 - c + c e^{-s} \}$$

Describes all the statistics of the occupation number (which is trivial here:

* remark: typical history:



x Large deviations of the time-averaged density $\rho(t) = \int_0^t dt n(t)$:

This is an observable of type 2 (time-integrated)

Mean value: one expects $\langle \rho \rangle = \int_0^t dt \langle n(t) \rangle \sim ct$
 $\approx c$ at large times

Variance: $\langle \rho(t)^2 \rangle = \langle (\int_0^t dt n(t))^2 \rangle = \int_0^t dt_1 \int_0^t dt_2 \langle n(t_1) n(t_2) \rangle$
difficult to determine since we don't know the 2-time correlation function

We thus go to the generating functional of the cumulants of ρ c.g.f.

$$\langle e^{-s\rho(t)} \rangle \underset{t \rightarrow \infty}{\sim} e^{t \Psi_\rho(s)}$$

The index ρ is there to remind us of which observable $\Psi_\rho(s)$ is the c.g.f.

We have seen that spectrum

$$\Psi_\rho(s) = \text{Max}_{\rho'} S_\rho W_\rho(s), \quad (W_\rho(s))_{\rho\rho'} = W(\rho \rightarrow \rho') - (n(\rho) + s n(\rho)) \delta_{\rho\rho'}$$

In our case:

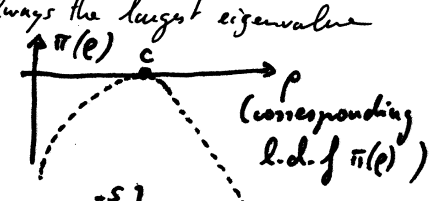
$$W_\rho(s) = \begin{pmatrix} c & 1-c \\ c & -[(1-c)+s] \end{pmatrix}$$

Eigenvalues are solutions in λ of $\det \begin{pmatrix} c-\lambda & 1-c \\ c & -\lambda-[(1-c)+s] \end{pmatrix} = 0$

One finds $S_\rho W_\rho(s) = \left\{ -\frac{1+s}{2} - \frac{1}{2} \sqrt{(1+s)^2 - 4cs}, -\frac{1+s}{2} + \frac{1}{2} \sqrt{(1+s)^2 - 4cs} \right\}$

$$\Psi_\rho(s) = -\frac{1+s}{2} + \frac{1}{2} \sqrt{(1+s)^2 - 4cs}$$

always the largest eigenvalue



Which is very different from $\Psi_{occ.}(s) = \log \{ 1-c + c e^{-s} \}$

One can compare the successive cumulants from $(i) \langle n^k \rangle_c = \frac{\partial^k}{\partial s^k} \Psi_{occ.}(s) \Big|_{s=0}$; $(ii) \frac{1}{t} \langle \rho^k \rangle_c = \frac{\partial^k}{\partial s^k} \Psi_\rho(s) \Big|_{s=0}$

- | | |
|---|--|
| $\langle n \rangle = c$ | $\frac{1}{t} \langle \rho \rangle = c$ |
| $\langle n^2 \rangle_c = c(1-c)$ | $\frac{1}{t} \langle \rho^2 \rangle_c = 2c(1-c)$ |
| $\langle n^3 \rangle_c = c(1-c)(1-2c)$ | $\frac{1}{t} \langle \rho^3 \rangle_c = 6c(1-c)(1-2c)$ |
| $\langle n^4 \rangle_c = c(1-c)(1-6c(1-c))$ | $\frac{1}{t} \langle \rho^4 \rangle_c = 24c(1-c)(1-5c(1-c))$ |
| ... | ... |

* Large deviations of the activity $K = \# \{ \text{configuration changes} \} :$ (2.16)

The mean value only depends on the equilibrium state, in the large time limit :

Lecture on
Stoch. processes

multiply by K
and sum
over K and n

$$\partial_t P(n, K, t) = c P(0, K-1, t) \delta_{n1} + (1-c) P(1, K-1, t) \delta_{n0} - [c P(0, K, t) + (1-c) P(1, K, t)]$$

for those terms of the sum, one does $K \rightarrow K+1$

$$\partial_t \sum_{n, K} K P(n, K, t) = \sum_K \left\{ c K P(0, K-1, t) + K(1-c) P(1, K-1, t) - c K P(0, K, t) - (1-c) K P(1, K, t) \right\}$$

by definit^o: $\langle K \rangle$

averages over histories on $[0, t]$

$$\partial_t \langle K \rangle = \sum_K \left\{ c \underbrace{[K+1-K]}_{=1} P(0, K, t) + (1-c) \underbrace{[K+1-K]}_{=1} P(1, K, t) \right\}$$

$$\partial_t \langle K \rangle = c P(0, t) + (1-c) P(1, t) \quad \left\{ \begin{array}{l} \sum_K P(0, K, t) = P(0, t) \\ \sum_K P(1, K, t) = P(1, t) \end{array} \right.$$

for $t \rightarrow \infty$: $\partial_t \langle K \rangle = \underbrace{\langle c(1-n) + (1-c)n \rangle}_{\text{average over histories}} = \underbrace{\langle r(n) \rangle}_{\text{average in the equilibrium steady state}} = \langle r(n) \rangle_{\text{eq}}$

this relation is
generic
Check it!

$r(n) = c(1-n) + (1-c)n$
is the escape rate from
configuration n .

In our case: $\frac{1}{t} \langle K \rangle = 2c(1-c)$ $t \rightarrow \infty$

There is no generic way to extend this result for higher cumulants $\frac{1}{t} \langle K^k \rangle_c$ $k \geq 2$

Generating function: $\Psi_K(s) = \frac{1}{t} \log \langle e^{-sK} \rangle = \text{Max}_p S_p W_K(s)$

$(W_K(s))_{\text{ep}}$ = $e^{-s} W(e' \rightarrow e) - r(e) \delta_{ee'}$, hence

$$W_K(s) = \begin{pmatrix} -c & e^{-s}(1-c) \\ e^{-s}c & -(1-c) \end{pmatrix}$$

One finds $\Psi_K(s) = -\frac{1}{2} + \frac{1}{2} \sqrt{1 - 4c(1-c)(1 - e^{-2s})}$

No surprise here:
everything is analytic

from which one gets for instance

$$\frac{1}{t} \langle K \rangle = 2c(1-c)$$

$$(t \rightarrow \infty) \quad \frac{1}{t} \langle K^2 \rangle_c = 4c(1-c)(1 - 2c(1-c))$$

⋮

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

$$\partial_t \hat{P}(n, s, t) = \underbrace{e^{-s} [c n + (r+c)n]}_{\substack{\text{death \& birth process with} \\ \text{rates} \begin{matrix} \xrightarrow{e^{-s}c} \bullet \\ \bullet \xrightarrow{e^{-s}(r+c)} \end{matrix}}} \hat{P}(t-n, s, t) - e^{-s} \underbrace{(c+n)}_{r(n)} \hat{P}(n, s, t) + \underbrace{(e^{-s}-1) (c+n + n(r+c))}_{\text{cloning at rate } (e^{-s}-1)r(n)} \hat{P}(n, s, t)$$

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 $e^{-s} > 1$).

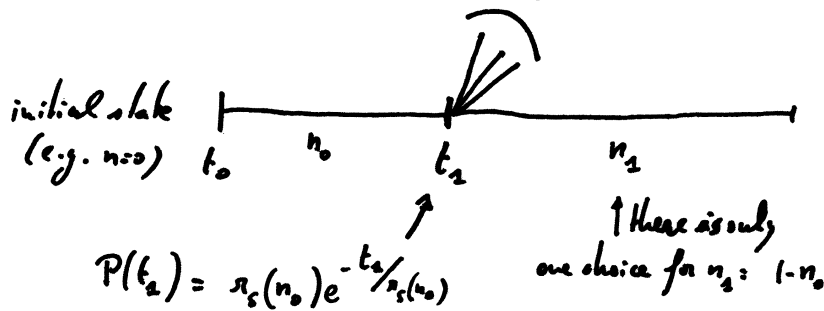
Each copy of the system evolves as follow:

lower integer

give rise to p offsprings:

$$p+1 = \lfloor (e^{-s}-1)r(n_0) \rfloor$$

this is



and so on

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

Each of the offsprings evolves independently afterwards.

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