Part II - Markov dynamics and large deviation functions: first steps

Lecture Stoch. process 2012 (2.1)

MOTIVATIONS:

- Classical thermodynamics provides a frame to understand the <u>mean-value</u> of macroscopic observables (energy, density, susceptibility, ...)
- Physical systems are composed of numerous but finite # of particles → one wants to understand <u>fluctuations</u> of those observables.
- In particular even at equilibrium, fluctuation of <u>time-integrated</u> observables are difficult to catch

  e.g: currents, # events

GENERIC SETUP:

- Set of <u>configurations</u> $\{\mathcal{C}\}$ (finite or discrete)

  e.g: occupation numbers $\{n_i\}$ on sites i of a network / lattice.

- Transition <u>rates</u> $W(\mathcal{C}\to\mathcal{C}')$ between configurations $(\mathcal{C}\neq\mathcal{C}')$ (continuous-time dynamics)
- Evolution of the probability $P(\mathcal{C},t)$ of being in $\mathcal{C}$ at time t:

Master Equation

$$\boxed{\begin{aligned}\partial_t P(\mathcal{C},t) &= \sum_{\mathcal{C}'} W(\mathcal{C}'\to\mathcal{C})P(\mathcal{C}',t) - r(\mathcal{C})P(\mathcal{C},t)\\ \text{with}\quad r(\mathcal{C}) &= \sum_{\mathcal{C}'} W(\mathcal{C}\to\mathcal{C}') \qquad \text{(escape rate from conf. } \mathcal{C})\end{aligned}}$$

one assumes $W(\mathcal{C}\to\mathcal{C})=0$

- Where does this come from? Come back to discrete time

$$P(\mathcal{C},t+dt) = \sum_{\mathcal{C}'} \underbrace{dt\, W(\mathcal{C}'\to\mathcal{C})}\, P(\mathcal{C}',t) - \underbrace{\Big(1 - dt \overbrace{\sum_{\mathcal{C}'} W(\mathcal{C}\to\mathcal{C}')}^{r(\mathcal{C})}\Big)}\, P(\mathcal{C},t)$$

This is also what we wrote $P(\mathcal{C},t+dt\,|\,\mathcal{C}',t)$ → probability to have jumped from $\mathcal{C}'$ to $\mathcal{C}$ between t and $t+dt$

probability to have remained in $\mathcal{C}$ btw t and $t+dt$

To understand / remember / recover the second term, one remarks that it ensures probability conservation:

$$\sum_{\mathcal{C}} P(\mathcal{C},t+dt) = \sum_{\mathcal{C}} P(\mathcal{C},t)$$

PROPERTIES :

- **Conservation of probability**: one has

$$\partial_t \sum_{\mathcal{C}} P(\mathcal{C},t) = 0$$ as directly checked. Since $\sum_{\mathcal{C}} P(\mathcal{C},0)=1$

indeed $= \sum_{\mathcal{C}\mathcal{C}'} \{W(\mathcal{C}'\to\mathcal{C})P(\mathcal{C}',t) - W(\mathcal{C}\to\mathcal{C}')P(\mathcal{C},t)\}$

this property remains valid at all times

- **Steady state**:

[This is the case if one can reach any state from any other through $\{W(\mathcal{C}\to\mathcal{C}')\}$, and if there are no recurrent states]

One assumes there exist a unique steady state $P_{st}(\mathcal{C})$ solution of $\partial_t P(\mathcal{C},t)=0$

i.e. verifying the ~~detailed~~ global balance condition

$$\sum_{\mathcal{C}'} W(\mathcal{C}\to\mathcal{C}')P_{st}(\mathcal{C}) = \sum_{\mathcal{C}'} W(\mathcal{C}'\to\mathcal{C})P_{st}(\mathcal{C}') \qquad \forall \mathcal{C}$$

- **"Equilibrium dynamics" : detailed balance condition**

$$W(\mathcal{C}\to\mathcal{C}')P_{eq}(\mathcal{C}) = W(\mathcal{C}'\to\mathcal{C})P_{eq}(\mathcal{C}') \qquad \forall \mathcal{C},\mathcal{C}'$$

. the steady state is then called "equilibrium state" $P_{st}=P_{eq}$

. this condition is much more restrictive

. interpretation 1: there is no current of probability in the steady state

$$0 = \sum_{\mathcal{C}'} \Big(\underbrace{W(\mathcal{C}'\to\mathcal{C})P_{eq}(\mathcal{C}') - W(\mathcal{C}\to\mathcal{C}')P_{eq}(\mathcal{C})}_{\text{current of probability in } \mathcal{C} \ (=0)} \Big)$$

. interpretation 2: the dynamics starting from P_{eq} is **reversible**

using detailed balance condition

$$\underbrace{P_{eq}(\mathcal{C}_0)W(\mathcal{C}_0\to\mathcal{C}_1)\dots W(\mathcal{C}_{K-1}\to\mathcal{C}_K)}_{\text{probability density of the history } \mathcal{C}_0\to\dots\to\mathcal{C}_K \text{ of the system}} = \underbrace{P_{eq}(\mathcal{C}_K)W(\mathcal{C}_K\to\mathcal{C}_{K-1})\dots W(\mathcal{C}_1\to\mathcal{C}_0)}_{\text{probability density of the time-reversed history } \mathcal{C}_K\to\dots\to\mathcal{C}_0 \text{ of the system}}$$

Those probabilities are the same : reversibility $\Leftrightarrow$ equilibrium.

very similar to the case of Langevin dynamics (part I)

Operator notation :

- One considers a vector space of basis $|\mathcal{C}\rangle$, $\mathcal{C}$ in the set of all configs.
- The space is orthonormal, the scalar product denoted $\langle\cdot|\cdot\rangle$:

$$\langle \mathcal{C}' | \mathcal{C} \rangle = \delta_{\mathcal{C}\mathcal{C}'} \qquad \text{(Kronecker delta)}$$

- Traduction of the Markov evolution : (master equation)

Defining the vector $|P(t)\rangle = \sum_{\mathcal{C}} P(\mathcal{C},t)\,|\mathcal{C}\rangle$ of components $P(\mathcal{C},t)$:

$$\partial_t |P(t)\rangle = \mathbb{W}\,|P(t)\rangle \quad \text{with} \quad \boxed{\mathbb{W}_{\mathcal{C}\mathcal{C}'} = W(\mathcal{C}'\to\mathcal{C}) - r(\mathcal{C})\delta_{\mathcal{C}\mathcal{C}'}}$$

$\mathbb{W}_{\mathcal{C}\mathcal{C}'}$ is the element $\mathcal{C}\mathcal{C}'$ of the matrix (or 'operator') $\mathbb{W}$.
named 'evolution operator'

- Traduction of the conservation of probability :

This vector is termed "the total vector", or "Attila's vector" (car toutes ses composantes sont des uns)

$$\partial_t \sum_{\mathcal{C}} P(\mathcal{C},t) = 0 \iff \sum_{\mathcal{C}} \mathbb{W}_{\mathcal{C}\mathcal{C}'} \;\forall \mathcal{C}' \iff \boxed{\langle - | \,\mathbb{W} = 0 \quad \text{with } \langle - | = \sum_{\mathcal{C}} \langle \mathcal{C} |}$$

in other words, the vector $\langle -|$ is a left eigen vector of $\mathbb{W}$ of eigenvalue 0.

- Traduction of the steady state property :
  - The global balance condition rewrites $\boxed{\mathbb{W}|P_{st}\rangle = 0}$

    in other words the vector $|P_{st}\rangle$ is a right eigenvalue of $\mathbb{W}$ of e.v. 0.
  - It must exists if probability is conserved, since $\mathbb{W}$ and $\mathbb{W}^T$ have the same spectrum (and a left eigen vector of $\mathbb{W}$ corresponds to a right $\vec{ev}$ of $\mathbb{W}^T$)

→ We thus see how, using Algebra, conservation of probability ensures the existence of a steady state

- Remark: All other eigenvalues of $\mathbb{W}$ are of ~~modulus~~ real part < 0.

  This is the Perron-Frobenius theorem. It ensures that $e^{t\mathbb{W}}|P(0)\rangle = |P(t)\rangle \xrightarrow{t\to\infty} |P_{st}\rangle$.

- Translation of the detailed balance condition:

$$W(\mathcal{C}'\to\mathcal{C})\, P_{eq}(\mathcal{C}') = W(\mathcal{C}\to\mathcal{C}')\, P_{eq}(\mathcal{C}) \qquad \forall \mathcal{C}\,\mathcal{C}'$$

$$\Leftrightarrow \quad \mathbb{W}_{\mathcal{C}\mathcal{C}'}\, P_{eq}(\mathcal{C}') = \mathbb{W}_{\mathcal{C}'\mathcal{C}}\, P_{eq}(\mathcal{C})$$

$$\Leftrightarrow \quad P_{eq}^{-1/2}(\mathcal{C})\, \mathbb{W}_{\mathcal{C}\mathcal{C}'}\, P_{eq}(\mathcal{C}')^{1/2} = P_{eq}(\mathcal{C}')^{-1/2}\, \mathbb{W}_{\mathcal{C}'\mathcal{C}}\, P_{eq}(\mathcal{C})^{1/2}$$

Hence $\mathbb{W}^{sym}$ can be interpreted as a quantum Hamiltonian (see also Langevin case)

$$\Leftrightarrow \quad \boxed{\text{the 'symetrised operator' } \mathbb{W}^{sym} = \hat{P}_{eq}^{-1/2}\, \mathbb{W}\, \hat{P}_{eq}^{1/2} \text{ is symmetric}}$$

where $\hat{P}_{eq}$ is the diagonal operator of elements $P_{eq}(\mathcal{C})$.

In this case, $\mathbb{W}^{sym}$ (and hence $\mathbb{W}$) can be diagonalized in an orthonormal basis.

- Formal solution through matrix exponentiation:

× form 1 :
$$\begin{cases} \partial_t |P(t)\rangle = \mathbb{W}\,|P(t)\rangle \\ |P(0)\rangle = |P_0\rangle = \sum_{\mathcal{C}} P_0(\mathcal{C})|\mathcal{C}\rangle \end{cases}$$
has a solution
$$|P(\mathcal{C},t)\rangle = e^{t\mathbb{W}}|P_0\rangle = \sum_{n\geq 0} \frac{t^n}{n!}\mathbb{W}^n|P_0\rangle$$
but this form is not very useful.

× form 2 : description in terms of a jump process. To eliminate the diagonal term in
$$\partial_t |P(t)\rangle_{\mathcal{C}} = \sum_{\mathcal{C}'} W(\mathcal{C}'\to\mathcal{C})\, |P(t)\rangle_{\mathcal{C}'} - r(\mathcal{C})|P(t)\rangle_{\mathcal{C}}$$
one sets $Q(\mathcal{C},t) = e^{-t r(\mathcal{C})}\, P(\mathcal{C},t)$ which verifies:

Remark: if rates depend on time, set $Q(\mathcal{C},t) = e^{-\int_0^t r(\mathcal{C}(\tau))d\tau} P(\mathcal{C},t)$

$$(*) \quad \underline{\partial_t |Q(t)\rangle = W(t)\,|Q(t)\rangle} \quad \text{with} \quad W(t)_{\mathcal{C}\mathcal{C}'} = W(\mathcal{C}'\to\mathcal{C})\, e^{t(r(\mathcal{C}')-r(\mathcal{C}))}$$

this is a linear evolution with time-dependent operator $W(t)$

The solution is $|Q(t)\rangle = \mathcal{T}exp\left(\int_0^t W\right)|Q(0)\rangle$ (∗∗)

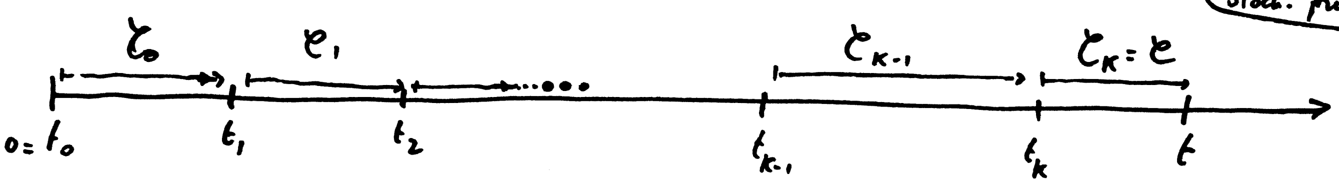
where the time-ordered exponential $\mathcal{T}exp$ writes

$$\mathcal{T}exp\left(\int_0^t W\right) = \sum_{K\geq 0} \mathcal{T}\left(\int_0^t W\right)^K = \sum_{K\geq 0} \int_0^t dt_K \int_0^{t_K} dt_{K-1} \cdots \int_0^{t_2} dt_1\, W(t_K)\ldots W(t_1) \qquad K\in\mathbb{N}$$

$$= \sum_{K\geq 0} \int_0^t dt_1 \int_{t_1}^t dt_2 \cdots \int_{t_{K-1}}^t dt_K\, W(t_K)\ldots W(t_1)$$

check that (∗∗) solves (∗) using this expression

Final form of the result: coming back to $P(\mathcal{C},t)$ from $Q(\mathcal{C},t)$:



sum over the number of jumps — sum over the histories of configurations — integrals over the time jump t_k's between $\mathcal{C}_{k-1}$ and $\mathcal{C}_k$

$$P(\mathcal{C},t) = \sum_{K\geq 0} \sum_{\mathcal{C}_0 \cdots \mathcal{C}_K} \int_{t_0}^{t} dt_1 \int_{t_1}^{t} dt_2 \cdots \int_{t_{K-1}}^{t} dt_K$$

$$Ⓐ \rightarrow \quad r(\mathcal{C}_0)\, e^{-(t_1-t_0)\, r(\mathcal{C}_0)} \times \cdots \times r(\mathcal{C}_{K-1})\, e^{-(t_K - t_{K-1})\, r(\mathcal{C}_{K-1})}\, e^{-(t-t_K)\, r(\mathcal{C}_K)}$$

$$Ⓑ \rightarrow \quad \times \frac{W(\mathcal{C}_0 \to \mathcal{C}_1)}{r(\mathcal{C}_0)} \times \cdots \times \frac{W(\mathcal{C}_{K-1} \to \mathcal{C})}{r(\mathcal{C}_{K-1})}$$

sampling of the initial condit° $\rightarrow \quad \times\, P_0(\mathcal{C}_0)$

- in Ⓐ: all the $r(\mathcal{C}_{k-1})\, e^{-(t_k - t_{k-1})\, r(\mathcal{C}_{k-1})}$ $(1 \leq k \leq K)$ represent the probability that the time t_k of jump between $\mathcal{C}_{k-1}$ and $\mathcal{C}_k$ is t_k.
- $e^{-(t-t_K)\, r(\mathcal{C}_K)}$ represents the probability not to jump between t_K and t

hence Ⓐ is the probability distribution of the times of jump $\{t_k\}$.

- in Ⓑ: $\dfrac{W(\mathcal{C}_{k-1} \to \mathcal{C}_k)}{r(\mathcal{C}_{k-1})}$ represents the (normalised) probability to jump to $\mathcal{C}_k$ starting from $\mathcal{C}_{k-1}$.

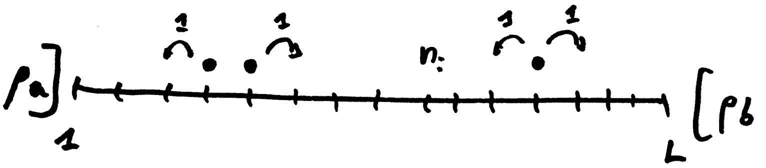
hence Ⓑ represents the probability of the history of configurations $\mathcal{C}_0 \ldots \mathcal{C}_K$

<u>Remark:</u> one can rewrite $Ⓐ = \prod_{k=0}^{K-1} r(\mathcal{C}_k) \cdot e^{-\int_0^t dt'\, r(\mathcal{C}_{t'})}$

check that this is the correct solution when rates depend on time and hence $r(\mathcal{C}) = r(\mathcal{C},t)$

LARGE DEVIATION FUNCTIONS

• Examples and motivation :



$n_i \in \{0,1\}$ occupation number

. total current on a time interval $[0,t]$: $Q = \#\left\{\begin{matrix}\text{jumps to}\\ \text{the right}\end{matrix}\right\} - \#\left\{\begin{matrix}\text{jumps to}\\ \text{the left}\end{matrix}\right\}$

in time : $Q \mapsto Q+1$ each time a particle jumps to the right
$Q \mapsto Q-1$ — — — left .

. total time and space integrated density :

$$\rho = \frac{1}{L} \int_0^t d\tau \sum_{i=1}^{L} n_i(t)$$

evolution in time : continuous (no jumps)

on each interval $[t_{k-1}, t_k[$ where the system does not change configurat°:

$$\rho \mapsto \rho + \frac{1}{L} \int_{t_{k-1}}^{t_k} d\tau \sum_{i=1}^{L} \overbrace{n_i(t_{k-1})}^{\text{constant}} = \rho + (t_k - t_{k-1}) \frac{1}{L} \sum_{i=1}^{L} n_i(t_{k-1})$$

• 'dynamical activity' K : on a time interval $[0,t]$, $K = \#\left\{\begin{matrix}\text{change}\\ \text{of configurat°}\end{matrix}\right\}$

in time : $K \mapsto K+1$ each time a configuration changes

• 'integrated escape rate' R : configuration at time τ, constant $\mathcal{C}_\tau = \mathcal{C}_{k-1}$ for $\tau \in [t_{k-1}, t_k[$

$$R = \int_0^t d\tau \, r(\mathcal{C}_\tau)$$

$$R = \sum_{k=1}^{K} (t_k - t_{k-1}) \, r(\mathcal{C}_{k-1}) + (t - t_K) \, r(\mathcal{C}_K)$$

→ What is the distribution of those history-dependent observables?
What can we learn from those distribution in terms of dynamical phase transitions?

lecture on Stoch. processes 2012

- Generic cases: A_1 A_2 observables depending on the history of the system on $[0,t]$

A_1 defined as: $\begin{cases} A_1\big|_{t=0}=0 \end{cases}$, $A_1 \mapsto A_1 + a_1(\mathcal{C}\to\mathcal{C}')$ at each jump $\mathcal{C}\to\mathcal{C}'$

(A_1 only changes at jump times)

A_2 defined as $A_2 = \int_0^t d\tau\, a_2(\mathcal{C}_\tau) = \sum_{k=1}^{K} (t_k - t_{k-1})\, a_2(\mathcal{C}_{k-1}) + (t-t_K)\, a_2(\mathcal{C}_K)$

(A_2 evolves continuously in time)

- Large deviation function:

× in direct space: for A an observable of type A_1 or A_2:

. the probability density of being in $\mathcal{C}$ at time t, having observed a value A of the observable, is denoted $P(\mathcal{C},A,t)$.

. the probability distribution of A at time t is

$$P(A,t) = \sum_{\mathcal{C}} P(\mathcal{C},A,t) \quad \text{and scales as}$$

$$\boxed{P(A,t) \sim \exp\left(+t\,\pi(A/t)\right)} \quad \text{as } t\to\infty$$

Other scalings are possible, but for finite systems, this is the most generic.

π is a dynamical equivalent of the entropy
$\pi(a)$ describes more than the mean and the variance of a → "large deviation function"

. π is difficult to determine in general ("microcanonical problem")
one prefers to go to the "canonical dynamical ensemble"

× in Laplace space: one has the $t\to\infty$ scaling

$$\boxed{\langle e^{-sA}\rangle \sim \exp\left(t\,\psi(s)\right)} \quad \text{as } t\to\infty$$

average taken on histories on time interval $[0,t]$

$\psi(s)$ is the cumulant generating function: (ψ is a "dynamical free energy")

$$\boxed{\partial_s^k \psi\big|_{s=0} = (-1)^k \frac{1}{t}\langle A^k\rangle_c}$$

$\langle A^k\rangle_c$ is the k^{th} cumulant of A.

• **Interpretation of s; link between $\psi(s)$ and $\pi(a)$:**

× Starting from $\langle e^{-sA}\rangle = \int dA\, P(A,t)\, e^{-sA}$ $A = at$

$$e^{+t\psi(s)} \sim \int da\; e^{\underbrace{t[\pi(a)-sa]}}$$

in the $t\to\infty$ limit, one may use the saddle point theorem

One has $$\boxed{\psi(s) = \max_a \left(\pi(a) - sa\right)}$$ ψ and π are legendre transformed.

If π is convex, one may perform the inverse legendre transform:

$$\boxed{\pi(a) = \min_s \left(\psi(s) + sa\right)}$$

× If $a^*(s)$ is the a where the $\max_a$ is reached
or if $s^*(a)$ — s —— $\min_s$ ——
one says that $a^*(s)$ and s / $s^*(a)$ and a are 'conjugated'

× ⚠ s plays a role similar to the inverse temperature β:
it fixes the average value of A (in the same way as β fixes the average value of the energy E)

× Indeed, in the large time limit: the mean value of an observable O in the 's-state' writes

$$\langle O(\mathcal{C})\rangle_s \equiv \frac{\langle O(\mathcal{C}(t))e^{-sA}\rangle}{\langle e^{-sA}\rangle} = \frac{1}{\langle e^{-sA}\rangle}\sum_{\mathcal{C},A} \overbrace{P(\mathcal{C},A,t)}^{\sim e^{t\pi(A/t)}\tilde{P}(\mathcal{C},A/t)}\, O(\mathcal{C})\, e^{-sA} \qquad A = at$$

$$\sim \frac{\int da \sum_{\mathcal{C}} \tilde{P}(\mathcal{C},a)\, O(\mathcal{C})\, e^{t(\pi(a)-sa)}}{\int da\; e^{t(\pi(a)-sa)}}$$

the saddle is reached at the same value $a = a^*(s)$

$$\langle O(\mathcal{C})\rangle_s \sim \sum_{\mathcal{C}} \tilde{P}(\mathcal{C}, a^*(s))\, O(\mathcal{C}) \quad \text{i.e.} \quad \boxed{\langle O(\mathcal{C})\rangle_s \overset{t\to\infty}{=} \langle O(\mathcal{C})\rangle\big|_{A=a^*(s)t}}$$

mean value in the s-state, of $O(\mathcal{C})$ at final time

Mean value of $O(\mathcal{C})$ at final time for histories with $A = a^*(s)\,t$

In the same way, if $\pi(a)$ is convex: by inverse Legendre transform

$$\boxed{\langle \mathcal{O}(\mathcal{C})\rangle\Big|_{A=at} \overset{t\to\infty}{=} \langle \mathcal{O}(\mathcal{C})\rangle_{s=s^*(a)}}$$

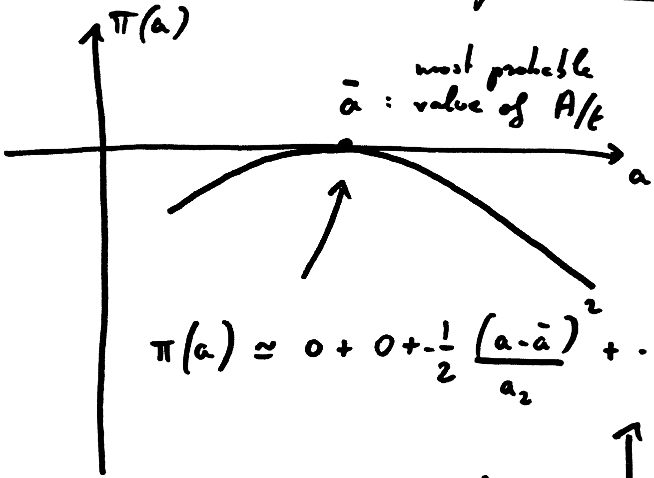
Mean value of $\mathcal{O}(\mathcal{C})$ at final time for histories with a value $A=at$ of the observable A

Mean value in the s-state of $\mathcal{O}(\mathcal{C})$ at final time:

$$\langle \mathcal{O}(\mathcal{C})\rangle_s = \frac{\langle \mathcal{O}(\mathcal{C}(t))\, e^{-sA}\rangle}{\langle e^{-sA}\rangle}$$

In other words, to characterize the value of the observable $\mathcal{O}$ in histories with a value $A\sim at$ of the observable A, one has to compute $\langle \mathcal{O}(\mathcal{C})\rangle_s$ at $s=s^*(a)$.

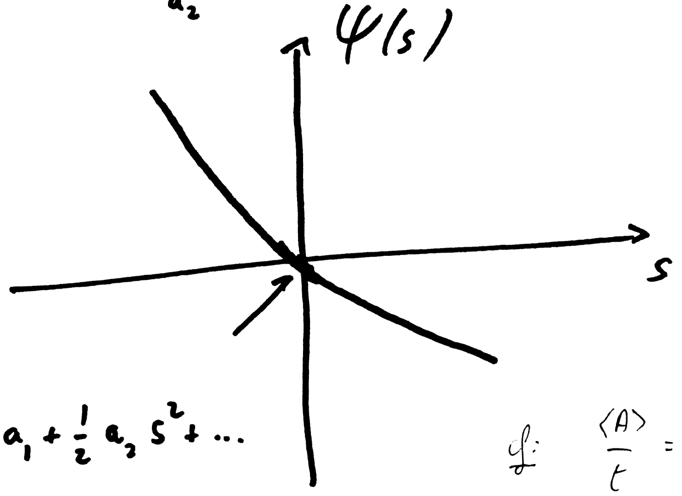
- Generic shape of the functions $\pi(a)$ and $\psi(s)$:



$\bar{a} = a_1 = \dfrac{\langle A\rangle}{t}$ mean value

$a_2 = \dfrac{\langle A^2\rangle_c}{t}$ second cumulant

$$\pi(a) \simeq 0 + 0 - \frac{1}{2}\frac{(a-\bar{a})^2}{a_2} + \dots \Big\} \to P(A=at,t) \sim e^{-\frac{1}{2}\frac{(a-\bar{a})^2}{a_2}t} \quad \text{[Gaussian distribution]}$$



For a reference on large deviations, Laplace & Legendre transforms, see Hugo Touchette
The large deviation approach to statistical mechanics
Physics Reports 478 1 (2009)

$$\psi(s) \simeq -s\,a_1 + \frac{1}{2} a_2 s^2 + \dots$$

cf: $\dfrac{\langle A\rangle}{t} = -\dfrac{\partial \psi}{\partial s}\Big|_{s=0}$

$\dfrac{\langle A^2\rangle_c}{t} = \dfrac{\partial^2 \psi}{\partial s^2}\Big|_{s=0}$

Lecture on Stoch. processes

2012

• Large deviation functions as maximal eigenvalues

1 – Cases of observables of type A_1

× Time evolution for $P(\mathcal{C},A_1,t)$:

$$\partial_t P(\mathcal{C},A_1,t) = \sum_{\mathcal{C}'} W(\mathcal{C}'\to\mathcal{C})\, P(\mathcal{C}', A_1 - a_1(\mathcal{C}'\to\mathcal{C}), t) - r(\mathcal{C}) P(\mathcal{C}, A_1, t)$$

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

One introduces $\hat{P}(\mathcal{C},s,t) = \underbrace{\sum_{A_1} e^{-sA_1} P(\mathcal{C},A_1,t)}$

This quantity is more detailed than $\langle e^{-sA_1}\rangle$, but it obeys a closed equation of evolution, as detailed.

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

$$\partial_t \hat{P}(\mathcal{C},s,t) = \sum_{\mathcal{C}'} e^{-sa_1(\mathcal{C}'\to\mathcal{C})} W(\mathcal{C}'\to\mathcal{C})\, \hat{P}(\mathcal{C}',s,t) - r(\mathcal{C})\hat{P}(\mathcal{C},s,t)$$

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
$$\boxed{\begin{aligned} &\partial_t |\hat{P}(s,t)\rangle = \mathbb{W}(s)\, |\hat{P}(s,t)\rangle \\ &\big(\mathbb{W}(s)\big)_{\mathcal{C}\mathcal{C}'} = \underbrace{e^{-sa_1(\mathcal{C}'\to\mathcal{C})} W(\mathcal{C}'\to\mathcal{C})} - r(\mathcal{C})\,\delta_{\mathcal{C}\mathcal{C}'} \end{aligned}}$$

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

× Largest eigenvalue of $\mathbb{W}(s)$: one has $\langle e^{-sA_1}\rangle = \sum_{\mathcal{C}} \underbrace{\hat{P}(\mathcal{C},s,t)}$

but $|\hat{P}(s,t)\rangle = e^{t\mathbb{W}(s)}|\hat{P}_0\rangle \underset{t\to\infty}{\sim} e^{t \underbrace{\max \mathrm{Sp}\, \mathbb{W}(s)}_{\text{maximal eigenvalue of } \mathbb{W}(s)}} \Rightarrow \sim e^{t\max \mathrm{Sp}\,\mathbb{W}_s}$

Hence $\langle e^{-sA_1}\rangle \sim e^{t\max \mathrm{Sp}\,\mathbb{W}(s)}$ and by definit° $\boxed{\psi(s) = \max \mathrm{Sp}\, \mathbb{W}(s)}$

it is the largest eigenvalue of $\mathbb{W}(s)$

2. Case of observable of type A_2

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

* first approach: time discretization

OK up to order dt

$$P(\mathcal{C}, A_2, t+dt) = \sum_{\mathcal{C}'} dt\, W(\mathcal{C}' \to \mathcal{C})\, P(\mathcal{C}', A_2, t) + (1 - dt\, r(\mathcal{C}))\, \underbrace{P\Big(\mathcal{C},\ A_2 - \overbrace{\int_t^{dt+t} d\tau\, a_2(\mathcal{C}(\tau))}^{\simeq dt\, a_2(\mathcal{C})}\Big)}$$

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

$$\boxed{\partial_t P(\mathcal{C}, A_2, t) = \sum_{\mathcal{C}'} W(\mathcal{C}' \to \mathcal{C}) P(\mathcal{C}', A_2, t) - \Big(r(\mathcal{C}) P(\mathcal{C}, A_2, t) + a_2(\mathcal{C}) \partial_{A_2} P(\mathcal{C}, A_2, t)\Big)}$$

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

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

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

The equation of evolution is thus (by integration by part)

$$\partial_t \hat{P}(\mathcal{C}, s, t) = \sum_{\mathcal{C}'} W(\mathcal{C}' \to \mathcal{C}) \hat{P}(\mathcal{C}', s, t) - \big(r(\mathcal{C}) + s\, a_2(\mathcal{C})\big) \hat{P}(\mathcal{C}, s, t)$$

Or, in vector notation:

$$\boxed{\begin{aligned} \partial_t |\hat{P}(s,t)\rangle &= \mathbb{W}(s)\, |\hat{P}(s,t)\rangle \\ \big(\mathbb{W}(s)\big)_{\mathcal{C}\mathcal{C}'} &= W(\mathcal{C}' \to \mathcal{C}) - \big(r(\mathcal{C}) + s\, a_2(\mathcal{C})\big)\, \delta_{\mathcal{C}\mathcal{C}'} \end{aligned}}$$

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

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

Remark: This formula, written as:

diagonal operator of elements $a_2(\mathcal{C})$

$$\partial_t |\hat{P}(s,t)\rangle = \mathbb{W} |\hat{P}(s,t)\rangle - s\, \hat{a}_2 |\hat{P}(s,t)\rangle$$

is an example of <u>FEYNMAN-KAC</u> formula

jumps are described by the non-diagonal part of $\mathbb{W}$

× second derivation of the result:

One has $A_2 = \sum_{k=1}^{K} (t_k - t_{k-1})\, a_2(\mathcal{C}_{k-1}) + (t - t_K)\, a_2(\mathcal{C}_K)$

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

$$\left\langle e^{-sA_2} \right\rangle = \sum_{K\geq 0} \sum_{\mathcal{C}_0 \cdots \mathcal{C}_K} \int_{t_0}^{t} dt_1 \cdots \int_{t_{K-1}}^{t} dt_K \; e^{-\sum_{k=1}^{K} (t_k - t_{k-1})\left(r(\mathcal{C}_{k-1}) + s a_2(\mathcal{C}_{k-1})\right) - (t - t_K)\left(r(\mathcal{C}_K) + s a_2(\mathcal{C}_K)\right)} \times \prod_{k=1}^{K} W(\mathcal{C}_{k-1} \to \mathcal{C}_k) \quad P_0(\mathcal{C}_K)$$

Indeed the derivation of the time-ordered exp. formula does not involve the conservation of probability presented by $\mathbb{W}$. It thus also works for $\mathbb{W}(s)$

And one recognizes precisely the expression of:

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

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

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

• Remark: mixed observables:

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

$$\boxed{\left(\mathbb{W}(s_1,s_2)\right)_{\mathcal{C}\mathcal{C}'} = e^{-s_1 a_1(\mathcal{C}' \to \mathcal{C})} W(\mathcal{C}' \to \mathcal{C}) - \left(r(\mathcal{C}) + s_2 a_2(\mathcal{C})\right) \delta_{\mathcal{C}\mathcal{C}'}}$$

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]

Consider the observable $Q_{cs} = \log \dfrac{W(\mathcal{C}_0\to\mathcal{C}_1)\cdots W(\mathcal{C}_{K-1}\to\mathcal{C}_K)}{W(\mathcal{C}_K\to\mathcal{C}_{K-1})\cdots W(\mathcal{C}_1\to\mathcal{C}_0)}$ ("entropy current")

Upon a jump $\mathcal{C}\to\mathcal{C}'$ one has $Q_{cs} \to Q_{cs} + \log \dfrac{W(\mathcal{C}\to\mathcal{C}')}{W(\mathcal{C}'\to\mathcal{C})}$

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

$$\big(\mathbb{W}(s)\big)_{\mathcal{C}\mathcal{C}'} = e^{-s\log\frac{W(\mathcal{C}'\to\mathcal{C})}{W(\mathcal{C}\to\mathcal{C}')}}\, W(\mathcal{C}'\to\mathcal{C}) - r(\mathcal{C})\,\delta_{\mathcal{C}\mathcal{C}'}$$

$$= W(\mathcal{C}'\to\mathcal{C})^{1-s}\, W(\mathcal{C}\to\mathcal{C}')^{s} - r(\mathcal{C})\,\delta_{\mathcal{C}\mathcal{C}'}$$

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

One thus has $\big(\mathbb{W}(s)\big)_{\mathcal{C}\mathcal{C}'} = \big(\mathbb{W}(1-s)\big)_{\mathcal{C}'\mathcal{C}}$

$$\mathbb{W}(s)^T = \mathbb{W}(1-s)$$

Relates rare events ($s\simeq 1$) to not rare ones ($s=0$). Implies Fluctuation-Dissipation Relation, and Onsager Relations.

Since those to operators have the same spectrum, one has $\boxed{\psi(s) = \psi(1-s)}$

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 $A = A_1$

By writing $W_s(\mathcal{C}\to\mathcal{C}') = e^{-s\,a(\mathcal{C}\to\mathcal{C}')}\,W(\mathcal{C}\to\mathcal{C}')$; $r_s(\mathcal{C}) = \sum_{\mathcal{C}'} W_s(\mathcal{C}\to\mathcal{C}')$

$$\big(\mathbb{W}(s)\big)_{\mathcal{C}\mathcal{C}'} = \underbrace{W_s(\mathcal{C}'\to\mathcal{C}) - r_s(\mathcal{C})\,\delta_{\mathcal{C}\mathcal{C}'}} + \underbrace{\big(r_s(\mathcal{C}) - r(\mathcal{C})\big)\,\delta_{\mathcal{C}\mathcal{C}'}}$$

(probability-conserving) evolution with modified rates $W_s(\mathcal{C}\to\mathcal{C}')$ — cloning with rate $r_s(\mathcal{C}) - r(\mathcal{C})$

for a population of <u>copies</u> of the system.

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

- evolution with rate $W_s(\mathcal{C}\to\mathcal{C}')$ of each copy
- cloning/pruning of copies with rate $r_s(\mathcal{C}) - r(\mathcal{C})$

] favoring configurat. with an atypical value of A.

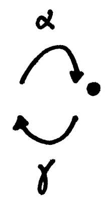
then the global increase/decrease rate of the population is $\psi(s)$

[There are tricks to keep the population size constant – see Refs.]

- **An example:** death and birth process on one site

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

(Reservoir)



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

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

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

indeed
$\mathbb{W}_{01} = W(1\to 0) = \gamma$
$\mathbb{W}_{10} = W(0\to 1) = \alpha$
$\mathbb{W}_{00} = -r(0) = -W(0\to 1) = -\alpha$
$\mathbb{W}_{11} = -r(1) = -W(1\to 0) = -\gamma$

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

"Grand-canonical" form $\quad P(n) \stackrel{?}{=} \frac{1}{Z} e^{\mu n} \quad \mu =$ "chemical potential"

St. st. eq:
$$\left.\begin{array}{l} 0 = \gamma e^{\mu} - \alpha \\ 0 = \alpha - \gamma e^{\mu} \end{array}\right\} \quad e^{\mu} = \frac{\alpha}{\gamma}$$
$$Z = e^{0\mu} + e^{\mu} = 1 + \frac{\alpha}{\gamma}$$

$$\boxed{P_{eq}(n) = \frac{\left(\frac{\alpha}{\gamma}\right)^n}{1+\frac{\alpha}{\gamma}}} \quad \text{(normalized)}$$

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

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 $(\alpha+\gamma)$

× mean occupation number:
$$\langle n \rangle = \sum_n n P_{eq}(n) = \frac{\alpha/\gamma}{1+\alpha/\gamma} = \frac{\alpha}{\alpha+\gamma}$$

× reparametrization: one sets $\boxed{\alpha = c \mid \gamma = 1-c}$ $\quad 0<c<1$ which fixes the unit of time

Then:
$$\boxed{\begin{array}{l} P_{eq}(n) = c^n (1-c)^{1-n} \\ \hline \langle n \rangle = c \end{array}}$$
Binomial law

- In vector form $|P_{eq}\rangle = \begin{pmatrix} 1-c \\ c \end{pmatrix} = (1-c)|0\rangle + c\,|1\rangle$

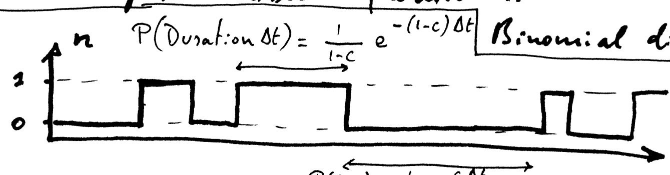
$$\mathbb{W} = \begin{pmatrix} c & 1-c \\ c & -(1-c) \end{pmatrix}$$

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

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

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

× remark: typical history:



× <u>Large deviations of the time-averaged density</u> $\rho(t) = \int_0^t d\tau\, n(\tau)$:

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

<u>Mean value</u>: one expects $\langle \rho \rangle = \int_0^t d\tau \underbrace{\langle n(\tau) \rangle}_{\simeq\, c \text{ at large times}} \underset{t\to\infty}{\sim} ct$

<u>Variance</u>: $\langle \rho(t)^2 \rangle = \left\langle \left(\int_0^t d\tau\, n(\tau) \right)^2 \right\rangle = \int_0^t d\tau_1 \int_0^t d\tau_2 \underbrace{\langle n(\tau_1) n(\tau_2) \rangle}_{=\,?}$

difficult to determine since we don't know the 2-time correlation function

We thus go to the <u>generating functional of the cumulants</u> of ρ (c.g.f.)

$$\langle e^{-s\rho(t)} \rangle \underset{t\to\infty}{\sim} e^{t\,\psi_\rho(s)}$$

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

We have seen that

$$\boxed{\psi_\rho(s) = \mathrm{Max}\ \underset{\text{spectrum}}{S_p}\ \mathbb{W}_\rho(s)}\ ,\quad \big(\mathbb{W}_\rho(s)\big)_{\mathcal{C}\mathcal{C}'} = W(\mathcal{C}' \to \mathcal{C}) - \big(r(\mathcal{C}) + s\,\overset{\rho(t) = \int_0^t d\tau\, n(\tau)}{n(\mathcal{C})}\big)\delta_{\mathcal{C}\mathcal{C}'}$$

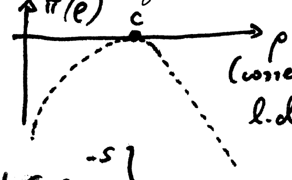
In our case:

$$\boxed{\mathbb{W}_\rho(s) = \begin{pmatrix} c & 1-c \\ c & -[(1-c)+s] \end{pmatrix}}$$

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

One finds $S_p\, \mathbb{W}_\rho(s) = \left\{ -\frac{1+s}{2} - \frac{1}{2}\sqrt{(1+s)^2 - 4cs}\ ,\ \underbrace{-\frac{1+s}{2} + \frac{1}{2}\sqrt{(1+s)^2 - 4cs}}_{\text{always the largest eigenvalue}} \right\}$

$$\boxed{\psi_\rho(s) = -\frac{1+s}{2} + \frac{1}{2}\sqrt{(1+s)^2 - 4cs}} \quad \rightarrow$$



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

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

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

× Large deviations of the activity $K = \#\{\text{configuration changes}\}$:

(2.16

lecture on Stoch. processes 2012

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

Indeed:

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

multiply by K and sum over K and n

for these terms of the sum, one does $K \mapsto K+1$

$$\underbrace{\partial_t \sum_{n,K} K P(n,K,t)}_{\text{by definit}^\circ:\ \langle K \rangle} = \sum_K \left\{ cKP(0,K-1,t) + K(1-c)P(1,K-1,t) - cKP(0,K,t) - (1-c)KP(1,K,t) \right\}$$

$\underbrace{\langle K \rangle}_{\text{averages over histories on } [0,t]}$

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

$$\partial_t \langle K \rangle = c\,P(0,t) + (1-c)\,P(1,t) \qquad \begin{cases} \sum_K P(0,K,t) = P(0,t) \\ \sum_K P(1,K,t) = P(1,t) \end{cases}$$

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

this relation is generic Check it!

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

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

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: $\psi_K(s) = \frac{1}{t}\log\langle e^{-sK}\rangle = \text{Max } S_p\, \mathbb{W}_K(s)$

$$\left(\mathbb{W}_K(s)\right)_{\mathcal{C}\mathcal{C}'} = e^{-s} W(\mathcal{C}' \to \mathcal{C}) - r(\mathcal{C})\,\delta_{\mathcal{C}\mathcal{C}'}, \text{ hence } \boxed{\mathbb{W}_K(s) = \begin{pmatrix} -c & e^{-s}(1-c) \\ e^{-s}c & -(1-c) \end{pmatrix}}$$

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

No surprise here: everything is analytic

from which one gets for instance

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

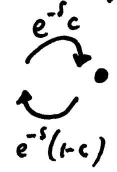
$$(t\to\infty) \quad \frac{1}{t}\langle K^2 \rangle_c = 4c(1-c)\left(1-2c(1-c)\right)$$

$$\vdots$$

Population algorithm to measure $\psi_K(s)$: for $s \leftrightarrow K$

$$\partial_t \hat{P}(n,s,t) = \underbrace{e^{-s}\left[cn + (1-c)(1-n)\right]\hat{P}(1-n,s,t) - e^{-s}\big(c(1-n)+n(1-c)\big)\hat{P}(n,s,t)}_{\text{death \& birth process with rates}}$$

$$+ \underbrace{\left(e^{-s}-1\right)\underbrace{\big(c(1-n)+n(1-c)\big)}_{r(n)}\hat{P}(n,s,t)}_{\text{cloning at rate } (e^{-s}-1)\,r(n)}$$



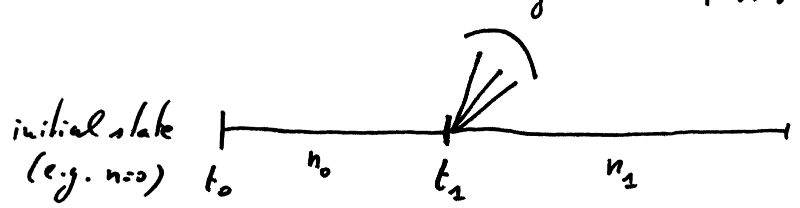
For this simple example, we keep total population $\mathcal{N}(t)$ non-constant.

Start with $\mathcal{N}_0$ copies of the system ($\mathcal{N}_0 \gg 1$, typically 10^2-10^3)

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

Each copy of the system evolves as follow:

gives rise to p offsprings: $p+1 = \underbrace{\lfloor (e^{-s}-1)\, r(n_0) \rfloor}_{\text{this is}}$ ← lower integer part



and so on

$P(t_1) = r_s(n_0)\, e^{-t_1/r_s(n_0)}$

↑ there is only one choice for n_1: $1-n_0$

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

Each of the offsprings evolves independently afterwards.

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