Mini-projet II -

Cloning algorithm for the determination of a large-deviation function - example.

I - Settings - [See part IIb of the lecture]

(1) × System of configurations $\{\mathcal{C}\}$; transition rates $\{\mathcal{C}\}$

× Evolution equation for the proba. to be in $\mathcal{C}$ at time t, having observed a value K of the activity: $P(\mathcal{C},K,t)$

$$\boxed{\partial_t P(\mathcal{C},K,t) = \sum_{\mathcal{C}'} W(\mathcal{C}'\to\mathcal{C})\, P(\mathcal{C}',K-1,t) \quad - \quad r(\mathcal{C})\, P(\mathcal{C},K,t)} \quad (*)$$

× Laplace transform: $\hat{P}(\mathcal{C},s,t) = \sum_K e^{-sK} P(\mathcal{C},K,t)$

allowing to recover $\underbrace{\langle e^{-sK}\rangle}_{\text{Average on histories of duration } t} = \sum_{\mathcal{C}} \hat{P}(\mathcal{C},s,t)$

a × $\hat{P}(\mathcal{C},s{=}0,t) = ?$

× Aim: Determine the cumulant generating function $\psi(s)$ defined from:

$$\boxed{\psi(s) = \lim_{t\to\infty} \frac{1}{t} \log \langle e^{-sK}\rangle}$$

× Method: use a cloning algorithm

× Starting point: the equation of evolution for $\hat{P}(\mathcal{C},s,t)$:

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

derived from (*) above.

b × Question: if detailed balance is verified $W(\mathcal{C}\to\mathcal{C}')P_{eq}(\mathcal{C}) = W(\mathcal{C}'\to\mathcal{C})P_{eq}(\mathcal{C}')$

find (as in the case $s=0$) a $\hat{P}^{sym}(\mathcal{C},s,t)$ whose evolution

writes $\partial_t \underbrace{|\hat{P}^{sym}(s,t)\rangle}_{\text{Vector of components } \hat{P}^{sym}(\mathcal{C},s,t)} = \mathbb{W}_s^{sym}\, |\hat{P}^{sym}(s,t)\rangle$ where $\mathbb{W}_s^{sym}$ is a symmetric matrix.

② Rewriting of the evolution equation

$$\partial_t \hat{P}(\mathcal{C},s,t) = \begin{cases} \sum_{\mathcal{C}'} W_s(\mathcal{C}'\to\mathcal{C})\,\hat{P}(\mathcal{C}',s,t) \quad - \; r_s(\mathcal{C})\,\hat{P}(\mathcal{C},s,t) \\ + \;(r_s(\mathcal{C}) - r(\mathcal{C}))\,\hat{P}(\mathcal{C},s,t) \end{cases} \qquad (***)$$

where $W_s(\mathcal{C}\to\mathcal{C}') = e^{-s}\,W(\mathcal{C}\to\mathcal{C}')$ and $r_s(\mathcal{C}) = \sum_{\mathcal{C}'} W_s(\mathcal{C}\to\mathcal{C}')$

× Why does the first line preserve probability?

[a] × Defining $\mathcal{N}(s,t) = \sum_{\mathcal{C}} \hat{P}(\mathcal{C},s,t)$:

- Show that $\mathcal{N}(s,0) = 1$ explicitly. Show that $\mathcal{N}(s,t) = \langle e^{-sK}\rangle$.
- From (***) above, show that

$$\partial_t \mathcal{N}(s,t) = \sum_{\mathcal{C}} (r_s(\mathcal{C}) - r(\mathcal{C}))\,\hat{P}(\mathcal{C},s,t) \qquad \left(\begin{smallmatrix}**\\**\end{smallmatrix}\right)$$

[b] × Average in the s-ensemble: $\langle \mathcal{O}(\mathcal{C})\rangle_s := \dfrac{\sum_{\mathcal{C}} \mathcal{O}(\mathcal{C})\hat{P}(\mathcal{C},s,t)}{\sum_{\mathcal{C}} \hat{P}(\mathcal{C},s,t)} = \dfrac{\sum_{\mathcal{C}} \mathcal{O}(\mathcal{C})\hat{P}(\mathcal{C},s,t)}{\mathcal{N}(s,t)}$

depends implicitly on t

- Show that $\langle \mathcal{O}(\mathcal{C})\rangle_s = \dfrac{\langle \mathcal{O}(\mathcal{C})e^{-sK}\rangle}{\langle e^{-sK}\rangle}$, explicitly.

- From $\left(\begin{smallmatrix}**\\**\end{smallmatrix}\right)$, show that $\partial_t \log \mathcal{N}(s,t) = \langle r_s(\mathcal{C}) - r(\mathcal{C})\rangle_s$.
- We admit that $\langle \mathcal{O}(\mathcal{C})\rangle_s$ converges to a limit as $t\to\infty$ [Bonus: show this property, using $\mathbb{W}_s$.]

From the last equality you have shown, explain why

$$\boxed{\psi(s) = \langle r_s(\mathcal{C}) - r(\mathcal{C})\rangle_s^{st.st.}}$$

steady-state, i.e. @ $t\to\infty$

[c] × From the definition $\psi(s) = \lim_{t\to\infty} \frac{1}{t}\log\langle e^{-sK}\rangle$ show that

$$\boxed{\psi'(s) = \lim_{t\to\infty} -\frac{1}{t}\langle K\rangle_s}$$

Mini proj II

II - An example: Fermionic birth & death process

$$0 \underset{1-c}{\overset{c}{\rightleftarrows}} 1 \qquad \{\mathcal{C}\} = \{0,1\}$$

[a] - Write the equation for $|\hat{P}(s,t)\rangle = \begin{pmatrix} \hat{P}(0,s,t) \\ \hat{P}(1,s,t) \end{pmatrix}$ in the form

$$\partial_t |\hat{P}(s,t)\rangle = \mathbb{W}_s |\hat{P}(s,t)\rangle$$ where $\mathbb{W}_s$ is a 2×2 matrix that you have to explicit.

[b] - Show that $\psi(s)$ is the maximal eigenvalue of $\mathbb{W}_s$ (in general).

[c] - Using this result, compute $\psi(s)$ explicitly in our example.
Check that $\psi(0)=0$

$\psi'(0) = -\langle r(\mathcal{C})\rangle$ ← average in the equilibrium state [that you have determined in a previous hw.]

[d] Bonus: determine $\hat{P}(0,s,t)$ & $\hat{P}(1,s,t)$ analytically at all times

those are the state of the system.

with initial condition $P(\mathcal{C},t=0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$.

[e] - Plot $-\psi'(s)$ as a function of s.
Comment, using the property $\frac{1}{t}\langle K\rangle_s = -\psi'(s)$.

[f] - Bonus: determine the "dynamical entropy" $\pi(k)$ of

$$P(K,t) \sim e^{t\,\pi(K/t)}$$

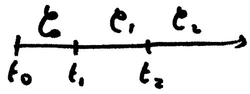
from $\psi(s)$, using Legendre transform.

III - Cloning Algorithm at non-constant population -

① **Algorithm:** One starts from a large number $\mathcal{N}_0$ of copies of the system.

× each copy of the system evolves with the modified rates $W_s(\mathcal{C}\to\mathcal{C}')$

→ . visit sequences of configurations $\mathcal{C}_0, \mathcal{C}_1, \dots, \mathcal{C}_k, \dots, \mathcal{C}_K$
with jumps $\mathcal{C}_k \to \mathcal{C}_{k+1}$ at time t_{k+1}



. waiting time $t_{k+1}-t_k$ in $\mathcal{C}_k$ distributed with exponential law of rate $r_s(\mathcal{C}_k)$.

(You've simulated this evolution in the previous homework for $0 \underset{1-c}{\overset{c}{\rightleftarrows}} 1$.)

× each copy is "cloned" at a rate $r_s(\mathcal{C}) - r(\mathcal{C})$, namely, between $\underbrace{t_k \text{ and } t_{k+1}}$, the copy is replaced by $Y = e^{\Delta t_k\, r(\mathcal{C}_k)}$ at the end of the interval.

We define $\boxed{\Delta t_k = t_{k+1}-t_k}$

[a] × A small computation: if $n(t)$ verifies $\partial_t n(t) = R\, n(t)$ (R being constant)
show that $n(t'') = e^{R(t''-t')}\, n(t')$.

[b] × Noting that, for an individual copy, $\mathcal{C}$ is constant ($=\mathcal{C}_k$) between t_k and t_{k+1}, show that the number of copies of the system in configuration $\mathcal{C}$ $\mathcal{N}(\mathcal{C},s,t)$ evolves according to:

$$\partial_t \mathcal{N}(\mathcal{C},s,t) = \begin{cases} \sum_{\mathcal{C}'} W_s(\mathcal{C}'\to\mathcal{C})\,\mathcal{N}(\mathcal{C}',s,t) & - r(\mathcal{C})\,\mathcal{N}(\mathcal{C},s,t) \\ & + \left(r_s(\mathcal{C}) - r(\mathcal{C})\right)\mathcal{N}(\mathcal{C},s,t) \end{cases}$$

for the cloning dynamics proposed above. (Use [a].)

× This equation is the same as the one followed by $\hat{P}(\mathcal{C},s,t)$.

[c] × Justify thus that the total population $\mathcal{N}(s,t) = \sum_{\mathcal{C}} \mathcal{N}(\mathcal{C},s,t)$ behaves at large time as $\mathcal{N}(s,t) \sim \exp(t\,\psi(s))$.

→ $\boxed{\text{This allows to evaluate } \psi(s) \text{ from the growth rate of the pop.}}$

(2) Practical implementation :

[a] × Cloning procedure : for an individual copy

- At the end of $[t_k, t_{k+1}]$, just before the configuration change, the copy has to be replaced by $Y = \exp\left((t_{k+1} - t_k)\, r(\mathcal{C}_k)\right)$
- The problem is that Y is not an integer in general
- Justify that taking $y = \lfloor Y + \varepsilon \rfloor$ — lower integer part; ε: real number (random) uniformly distributed on $[0,1]$ — is a reasonable choice.

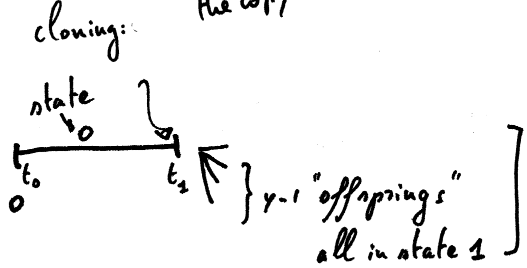
[b] × Expressions for the death & birth process :

Show that
- $W_s(0 \to 1) = e^{-s} c = r_s(0)$
- $W_s(1 \to 0) = e^{-s}(1-c) = r_s(1)$
- $r_s(\mathcal{C}) - r(\mathcal{C}) = (e^{-s} - 1)\, r(\mathcal{C})$ (cloning rate)

× We focus on the case $s < 0$ so that the cloning rate is always > 0

[c] × Implement the procedure, starting from $N_0 = 1$ copy of the system, in state 0 .

The copy is replaced by $y = \lfloor Y + \varepsilon \rfloor$ where $Y = e^{(t_1 - t_0)\, r_s(0)}$



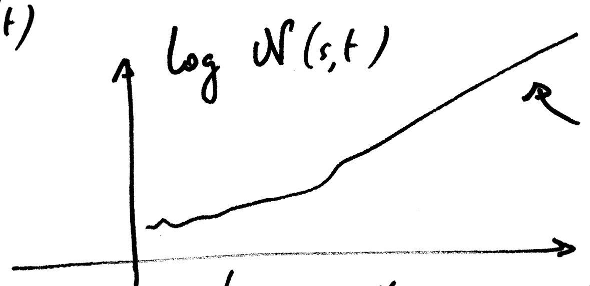
at time t_1, all copies (there are y of them) go into state 1. their next change of configuration will occur at a time t_2 which depends on the copy [each of the $t_2 - t_1$ is taken from an exponential distribution of rate $r_s(1)$].

and so on, for all copies.

× Remark: restrict on the range $s \in [-0{,}1\,, 0]$, otherwise the population grows too quickly.

(3) Determination of $\Psi(s)$:

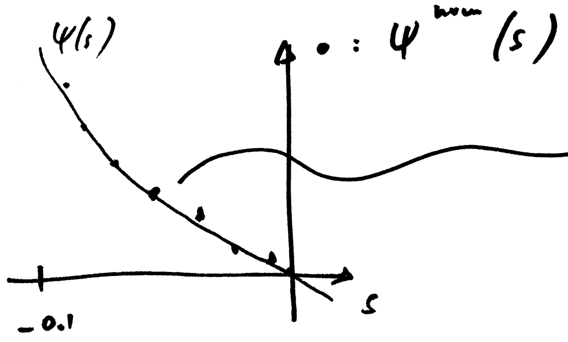
[a] × Wait long enough so that the total population size, $\mathcal{N}(s,t)$, is increasing exponentially in time



determine $\Psi^{num}(s)$ from the slope.

Show a few instances of this curve for varied values of s.

[b] × Compare the numerical evaluation $\Psi^{num}(s)$ to the theoretical one for various $s \in [-0.1, 0]$



(Each point is determined by the average of $\Psi^{num}(s)$ evaluated as above on several runs [don't forget to update the random seed ⚠].

numerically : average $r_s(\mathcal{C}) - r(\mathcal{C}) = (e^{s}-1)\, r(\mathcal{C})$ over the copies of the system, at final time.

[c] × Use the equality $\Psi(s) = \langle r_s(\mathcal{C}) - r(\mathcal{C}) \rangle_s$ to get another numerical evaluation of $\Psi(s)$

Plot the same graph as previously, in b.

[d] × **Bonus**: study finite time. Compare to analytical prediction of II-d-.

[e] × **Bonus**: How would you evaluate $\langle K \rangle_s$?

(Hint: attach a value of K to each copy]

Compare $\underbrace{\frac{1}{t} \langle K \rangle_s}_{\text{evaluated numerically}}$ to $\underbrace{-\Psi'(s)}_{\text{evaluated analytically for our system}}$.

they should be the same [see question I-②-c]