Complexity Summer School

Warwick 2013

Part II. EVALUATION OF LARGE DEVIATION FUNCTIONS — POPULATION DYNAMICS ALGORITHM

Outline:

1. "Operator Formalism" and $\psi(s)$ as a maximal eigenvalue
2. Evaluating $\psi(s)$ using a "cloning algorithm"

1. "OPERATOR FORMALISM" & $\psi(s)$ AS A MAXIMAL EIGENVALUE

1. a. Generic Observables.

System with discrete configurations $\{\mathcal{C}\}$ (↳ even, a finite number)

× Dynamics of the system: given by transition rates $W(\mathcal{C}\to\mathcal{C}')$

ie b/w t & $t+dt$: (small dt)

$$\begin{cases} \mathcal{C} \curvearrowright \mathcal{C}' & \text{with probability} \quad dt\, W(\mathcal{C}\to\mathcal{C}') \\ \mathcal{C} \curvearrowright \mathcal{C} \ [\text{no event}] & \text{———} \quad 1 - \sum_{\mathcal{C}'} dt\, W(\mathcal{C}\to\mathcal{C}') \end{cases}$$

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

$dt \to 0$ ↳ $$\partial_t P(\mathcal{C}, t) = \sum_{\mathcal{C}'} W(\mathcal{C}'\to\mathcal{C})\, P(\mathcal{C}', t) - r(\mathcal{C})\, P(\mathcal{C}, t)$$

↳ $r(\mathcal{C}) = \sum_{\mathcal{C}'} W(\mathcal{C}\to\mathcal{C}')$ [$r(\mathcal{C})$ is called the "escape rate"]

× Description of the dynamics [see Tibor's lecture]

. the system stays in conf $\mathcal{C}$ for a duration Δt [↳ not small] with prob. $r(\mathcal{C})e^{-\Delta t\, r(\mathcal{C})}$

. the system then jumps from $\mathcal{C} \to \mathcal{C}'$ with prob. $\dfrac{W(\mathcal{C}\to\mathcal{C}')}{r(\mathcal{C})}$

× Generic observable: $$A = \sum_{k=0}^{K-1} \alpha(\mathcal{C}_k \to \mathcal{C}_{k+1})$$

for a history $\mathcal{C}_0 \dots \mathcal{C}_K$ of the system;

i.e. at each "jump" (or event) $A \mapsto A + \alpha(\mathcal{C}\to\mathcal{C}')$

1. b – The simplest case : $A = K$ (activity)

ie, upon each event $K \mapsto K+1$

× evolution of the probability density of being in $\mathcal{C}$ at time t, having observed a value K of the activity $P(\mathcal{C},K,t)$:

$$\partial_t P(\mathcal{C},K,t) = \underbrace{\sum_{\mathcal{C}'} P(\mathcal{C}', \overset{\text{before the "jump"}}{K-1}, t)\, W(\mathcal{C}'\to\mathcal{C})}_{\substack{\text{the problem is difficult to solve}\\ \text{because this term is non-diagonal}\\ \text{along direction } K}} - r(\mathcal{C})\, P(\mathcal{C},K,t) \quad (*)$$

However note that if one obtains $P(\mathcal{C},K,t)$, one has $P(K,t) = \sum_{\mathcal{C}} P(\mathcal{C},K,t)$

As Tobias said: this def. of the generating function is akin to Fourier transforms.

× Going to the s-ensemble : $\boxed{\hat{P}(\mathcal{C},s,t) = \sum_{K\geq 0} e^{-sK} P(\mathcal{C},K,t)}$

Remarks – this is a "Laplace transform" ($\Leftrightarrow$ generating functions)

– by definition $\langle e^{-sK}\rangle = \sum_{K\geq 0}\sum_{\mathcal{C}} e^{-sK} P(\mathcal{C},K,t) = \sum_{\mathcal{C}} \underbrace{\hat{P}(\mathcal{C},s,t)}_{\text{not normalized!}}$

– More generally, $\langle \Theta(\mathcal{C}) e^{-sK}\rangle = \sum_{\mathcal{C}} \Theta(\mathcal{C})\, \hat{P}(\mathcal{C},s,t)$

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

this is the only difference with the $s=0$ dynamics

vector of components $\hat{P}(\mathcal{C},s,t)$ — matrix

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

× Eigenvector & eigenvalue problem :

let's call $\psi(s)$ the largest eigenvalue of $\mathbb{W}(s)$, of eigenvector $|\hat{P}_0(s)\rangle$

$\left[\partial_t|\hat{P}\rangle = \mathbb{W}|\hat{P}\rangle \text{ is solved by } |\hat{P}\rangle = e^{t\mathbb{W}}|\hat{P}\rangle_{t=0}\right]$

In the large-time limit :

[See remark 2 bellow for a demonstration]

$$\underbrace{|\hat{P}(s,t)\rangle}\ = e^{t\mathbb{W}(s)}|\hat{P}(s,0)\rangle \underset{t\to\infty}{\sim} e^{t\psi(s)}|\hat{P}_0(s)\rangle \quad (*)$$

Hence: all components $\hat{P}(\mathcal{C},s,t)$ evolve exponentially in time $\sim e^{t\psi(s)}$

$$\hookrightarrow \boxed{\langle e^{-sK}\rangle \sim e^{t\psi(s)}, \quad \psi(s) = \underbrace{\max Sp}_{\text{Maximal eigenvalue}}\ \mathbb{W}(s)}$$

$= \sum_{\mathcal{C}} \hat{P}(\mathcal{C},s,t)$, see p II.2

> The problem of determining the fluctuations of K thus amounts to finding the extremal eigenvalue of a matrix.

One can thus borrow methods from quantum mechanics & mathematics where this sort of problems occurs rather regularly.

× **Remark 1**: everything we wrote also works for the l.d.f $\psi(s)$ of quantities $A = \sum_{k=0}^{K-1} \alpha(\mathcal{C}_k \to \mathcal{C}_{k+1})$:

One simply has to replace $e^{-s}W(\mathcal{C}\to\mathcal{C}')$ by $e^{-s\alpha(\mathcal{C}\to\mathcal{C}')}W(\mathcal{C}\to\mathcal{C}')$

× **Remark 2**: To show (*) above, decompose $|\hat{P}(s,0)\rangle$ on a basis where $\mathbb{W}$ is diagonal : $|\hat{P}(s,0)\rangle = \alpha_0|P_0(s)\rangle + \alpha_1|P_1(s)\rangle + \dots + \alpha_k$

where $(\psi(s) = \lambda_0 > \lambda_1 \geq \dots \lambda_k \dots \geq \dots)$ are eigv. of eigv. $(|P_0(s)\rangle, \dots, |P_k(s)\rangle \dots)$

then $$e^{t\mathbb{W}(s)}|\hat{P}(s,0)\rangle = \underbrace{\alpha_0 e^{t\psi(s)}|P_0(s)\rangle + \alpha_1 e^{t\lambda_1(s)}|P_1(s)\rangle + \dots + \alpha_k e^{t\lambda_k(s)}|P_k\rangle \dots}_{\text{this finite sum is dominated by } e^{t\psi(s)} \text{ as } t\to\infty}$$

2. Evaluating $\psi(s)$ through a "Cloning" Algorithm

Consider the equation of evolution of $\hat{P}(\mathcal{C},s,t)$ $\left\{ r(\mathcal{C}) = \sum_{\mathcal{C}'} W(\mathcal{C}\to\mathcal{C}') \right.$

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

It does not correspond to a Markov evolution of a probability $\hat{P}(\mathcal{C},s,t)$

because: $r(\mathcal{C}) = \sum_{\mathcal{C}'} W(\mathcal{C}\to\mathcal{C}')$ and not $\sum_{\mathcal{C}'} W_s(\mathcal{C}\to\mathcal{C}')$

(And indeed: $\sum_{\mathcal{C}} \hat{P}(\mathcal{C},s,t) \underset{t\to\infty}{\sim} e^{t\psi(s)}$: "probability is not conserved")

2-a. Rewriting in terms of a population dynamics:

$$\partial_t \hat{P}(\mathcal{C},s,t) = \underbrace{\sum_{\mathcal{C}'} W_s(\mathcal{C}'\to\mathcal{C}) \hat{P}(\mathcal{C}',s,t) - r_s(\mathcal{C}) \hat{P}(\mathcal{C},s,t)}_{} + \underbrace{[r_s(\mathcal{C}) - r(\mathcal{C})] \hat{P}(\mathcal{C},s,t)}_{}$$

with $r_s(\mathcal{C}) = \sum_{\mathcal{C}'} W_s(\mathcal{C}\to\mathcal{C}')$

(Probability-preserving) evolution with s-modified rates $W_s(\mathcal{C}'\to\mathcal{C})$

$\boxed{\text{"mutations"}}$

reproduction at a rate $r_s(\mathcal{C}) - r(\mathcal{C})$

$\boxed{\text{"selection"}}$

Physical interpretation: [don't forget we study a large deviation characterized by s]

- s-dependent transition rates slightly biasing the trajectories ("mutations" allowing to probe the available space of configurations)
- selection rules actually favor the configurations, which render the large deviation (determined by s) typical.

↳ In case of phase coexistence, this allows to select a phase and to study its properties

2.6. Implementation in continuous time:

. Start from a large number N_0 of copies of the system

- evolve each copy of the system with rates $W_s(\mathcal{C} \to \mathcal{C}')$

↳ . time Δt before one exits from a configuration $\mathcal{C}$ distributed exponentially with rate $r_s(\mathcal{C})$

. after this, change $\mathcal{C} \to \mathcal{C}'$ with probability $\frac{W_s(\mathcal{C} \to \mathcal{C}')}{r_s(\mathcal{C})}$

- "clone" with rate $r_s(\mathcal{C}) - r(\mathcal{C})$:
on each interval Δt during which $\mathcal{C}$ does not change, replicate the copy by a factor $e^{\Delta t . (r_s(\mathcal{C}) - r(\mathcal{C}))}$.

↳ with those rules, the number $\mathcal{N}(\mathcal{C}, t)$ of copies of the system in configuration $\mathcal{C}$ evolves with the same eq. as $\hat{P}(\mathcal{C}, s, t)$

Hence $\mathcal{N}(\mathcal{C}, t) \sim \underbrace{e^{t\psi(s)}}_{\text{measure the exponential evolution its rate yields } \psi(s)}$

Besides, average among the set of copies yields $\langle O \rangle_s$.

<u>Remark</u>: in practice, one uses tricks to keep total population <u>constant</u>!

[$\leftrightarrow$ linked with Wright-Fischer process - see Tobias Galla's lecture.]

2-c Implementation in discrete time:

$$\hat{P}(\mathcal{C}, s, t+dt) = \sum_{\mathcal{C}'} \underbrace{dt\, W_s(\mathcal{C}' \to \mathcal{C})}_{\substack{\text{change } \mathcal{C}' \to \mathcal{C} \text{ with} \\ \text{probability } dt W_s(\mathcal{C}' \to \mathcal{C})}} \hat{P}(\mathcal{C}', s, t) + \underbrace{\left[1 - dt\, r_s(\mathcal{C})\right]}_{\substack{\text{make no change} \\ \text{with probability} \\ 1 - dt\, r_s(\mathcal{C})}} \hat{P}(\mathcal{C}, s, t) + \underbrace{dt\left[r_s(\mathcal{C}) - r(\mathcal{C})\right]}_{\substack{\text{in any case,} \\ \text{duplicate the} \\ \text{copy with} \\ \text{rate } dt(r_s(\mathcal{C}) - r(\mathcal{C}))}} \hat{P}$$

⚠ **CAVEAT**: depending on s, the choice of dt might require a very small dt !
→ better to use continuous-time –