Part II.

Evaluation of Large Deviation Functions
Population Dynamics Algorithm

II.1 Complexity Summer School Warwick 2013

Outline:

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

"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 btw 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 $\mathcal{C} \curvearrowright \mathcal{C}'$ 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 before the "jump" $P(\mathcal{C}, K, t)$:

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

However not 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

Linear evolution:
$$\partial_t \overbrace{|\hat{P}(s,t)\rangle}^{\text{vector of components } \hat{P}(\mathcal{C},s,t)} = \overbrace{\mathbb{W}(s)}^{\text{matrix}}\, |\hat{P}(s,t)\rangle$$
$$(\mathbb{W}(s))_{\mathcal{C}\mathcal{C}'} = e^{-s}\, W(\mathcal{C}' \to \mathcal{C}) - r(\mathcal{C})\, \delta_{\mathcal{C}\mathcal{C}'}$$

× <u>Eigenvector & eigenvalue problem</u>:

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

In the large-time limit: $\left[\partial_t |\hat{P}\rangle = \mathbb{W}|\hat{P}\rangle \text{ is solved by } |\hat{P}\rangle = e^{t\mathbb{W}}|\hat{P}\rangle_{t=0}\right]$

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

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

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

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

× <u>Remark</u>: 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

$$e^{-s\alpha(\mathcal{C}\to\mathcal{C}')} W(\mathcal{C}\to\mathcal{C}')$$

2. EVALUATING $\Psi(s)$ THROUGH A "CLONING" ALGORITHM.

II.4 Complexity Summer School

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:

$$\partial_t \hat{P}(\mathcal{C},s,t) = \underbrace{\sum_{\mathcal{C}'} W_s(\mathcal{C}'\to\mathcal{C}) \hat{P}(\mathcal{C}',s,t) - r_s(\mathcal{C}) \hat{P}(\mathcal{C},s,t)}_{\text{(Probability-preserving) evolution with s-modified rates } W_s(\mathcal{C}'\to\mathcal{C})} + \underbrace{[r_s(\mathcal{C}) - r(\mathcal{C})] \hat{P}(\mathcal{C},s,t)}_{\text{reproduction at a rate } r_s(\mathcal{C})-r(\mathcal{C})}$$

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

"mutations" "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.b. 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 $\langle \mathcal{O} \rangle_s$.

Remark: in practice, one uses tricks to keep total population constant!
[↔ linked with Wright-Fischer process - see Tobias Galla's lecture.]

2-c Implementation in discrete time :

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

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