Population dynamics and rare events

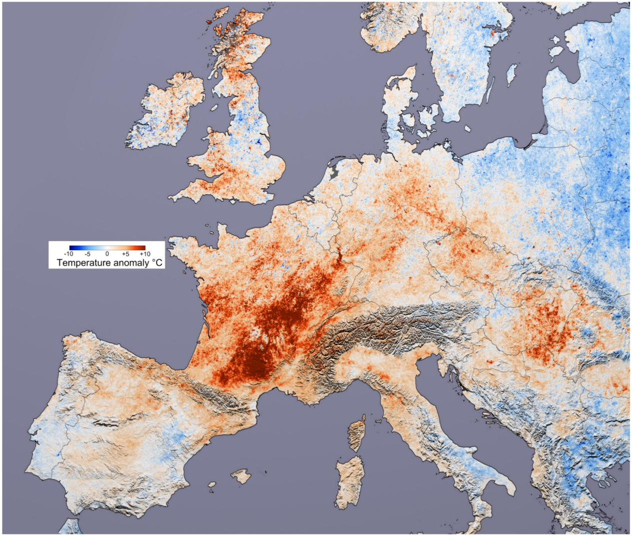
Esteban Guevara[(1)], Takahiro Nemoto[(2)],

Freddy Bouchet[(3)], Rob L Jack[(4)], Vivien Lecomte[(5)]

[(1)] IJM, Paris [(2)] ENS, Paris [(3)] ENS, Lyon
[(4)] Bath University & Cambridge University [(5)] LIPhy, Grenoble

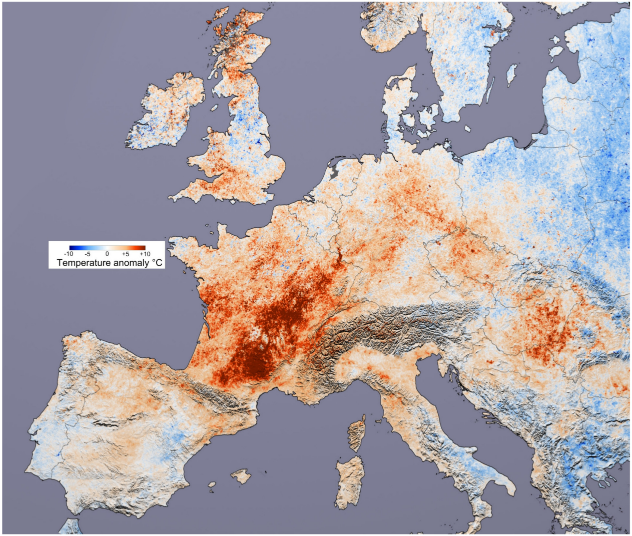
University of Oldenburg — January 24, 2019

Why studying rare events?



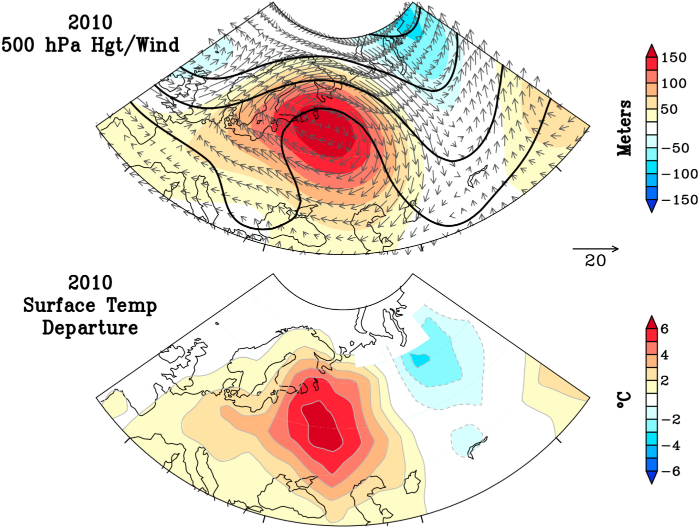
2003 heat wave, Europe [Terra MODIS]

Why studying rare events?



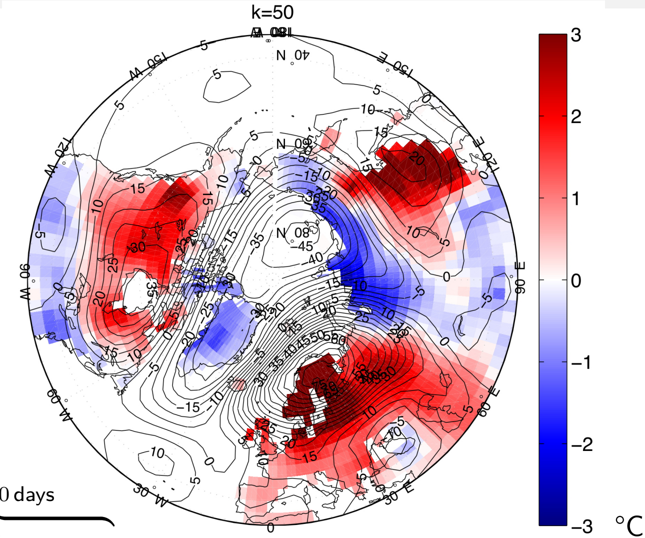
[Anomaly for **1-month** average] 2003 heat wave, Europe [Terra MODIS]

Why studying rare events?



2010 heat wave in Western Russia [Dole *et al.*, 2011]

Why studying rare events?



$$\overbrace{\frac{1}{t_{\max}}\int_0^{t_{\max}}}^{t_{\max}=40\text{ days}} dt\,\Delta T(t) > 2^\circ C \Rightarrow$$ « Teleconnection patterns » [Bouchet *et al.*]

How to study rare events?

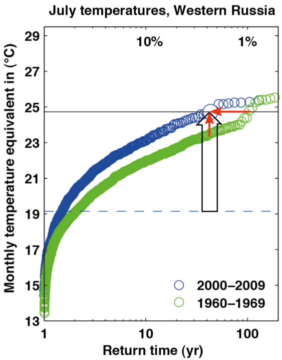
Questions for physicists and mathematicians:

- Probability and **dynamics** of rare events?
- How to **sample** these in numerical modelisation?
- Numerical **tools** and methods to understand their **formation**?

How to study rare events?

Questions for physicists and mathematicians:

- Probability and **dynamics** of rare events?
- How to **sample** these in numerical modelisation?
- Numerical **tools** and methods to understand their **formation**?



Evolution of the return time
of the monthly averaged temperature

$$\frac{1}{t_{\max}} \int_0^{t_{\max}} dt \; T(t)$$

$\longleftrightarrow$ anthropogenic impact on climate?

[Otto *et al.*, 2012]

Outline

- **Introduction**
- **Tools and algorithm**:
  Large deviation functions
  Ingredient 1/2: population dynamics
  Ingredient 2/2: change of ensemble
- **Use, extensions and limitations of population dynamics**:
  Different averages
  Feedback method
  Finite-time and finite-population scalings
- **Open questions**

Outline

- **Introduction**
- **Tools and algorithm**:
  - Large deviation functions
  - Ingredient 1/2: population dynamics
  - Ingredient 2/2: change of ensemble
- **Use, extensions and limitations of population dynamics**:
  - Different averages
  - Feedback method
  - Finite-time and finite-population scalings
- **Open questions**

Time-extensive observable on a time window $[0, t_f]$

- Climate dynamics:

$$\int_0^{t_f} dt \ \text{temperature}(t)$$

- Fluctuating thermodynamics:

$$\text{work} = \int_0^{t_f} dt \ \textbf{force}(t) \cdot \textbf{velocity}(t)$$

- Road traffic:

$$\#\{\text{cars passing through a gate}\}$$

- Molecular transport:

$$\#\{\text{steps of a motor on a filament}\}$$

- Lattice gases in 1d:

$$\text{“current”} = \#\{\text{jumps to the right}\} - \{\text{jumps to the left}\}$$
$$\text{“activity”} = \#\{\text{jumps to the right}\} + \{\text{jumps to the left}\}$$

Time-extensive observable on a time window $[0, t_\mathrm{f}]$

- Climate dynamics:

$$\int_0^{t_\mathrm{f}} dt\ \text{temperature}(t)$$

- Fluctuating thermodynamics:

$$\text{work} = \int_0^{t_\mathrm{f}} dt\ \textbf{force}(t) \cdot \textbf{velocity}(t)$$

- Road traffic:

$$\#\{\text{cars passing through a gate}\}$$

- Molecular transport:

$$\#\{\text{steps of a motor on a filament}\}$$

- Lattice gases in 1d:

$$\text{“current”} = \#\{\text{jumps to the right}\} - \{\text{jumps to the left}\}$$
$$\text{“activity”} = \#\{\text{jumps to the right}\} + \{\text{jumps to the left}\}$$

Time-extensive observable on a time window $[0, t_f]$

- Climate dynamics:

$$\int_0^{t_f} dt\ \text{temperature}(t)$$

- Fluctuating thermodynamics:

$$\text{work} = \int_0^{t_f} dt\ \textbf{force}(t) \cdot \textbf{velocity}(t)$$

- Road traffic:

$$\#\{\text{cars passing through a gate}\}$$

- Molecular transport:

$$\#\{\text{steps of a motor on a filament}\}$$

- Lattice gases in 1d:

$$\text{“current”} = \#\{\text{jumps to the right}\} - \{\text{jumps to the left}\}$$
$$\text{“activity”} = \#\{\text{jumps to the right}\} + \{\text{jumps to the left}\}$$

Time-extensive observable on a time window $[0, t_{\mathrm{f}}]$

- Climate dynamics:

$$\int_0^{t_{\mathrm{f}}} dt \ \text{temperature}(t)$$

- Fluctuating thermodynamics:

$$\text{work} \ = \ \int_0^{t_{\mathrm{f}}} dt \ \textbf{force}(t) \cdot \textbf{velocity}(t)$$

- Road traffic:

$$\#\{\text{cars passing through a gate}\}$$

- Molecular transport:

$$\#\{\text{steps of a motor on a filament}\}$$

- Lattice gases in 1d:

$$\text{“current”} \ = \ \#\{\text{jumps to the right}\} - \{\text{jumps to the left}\}$$
$$\text{“activity”} \ = \ \#\{\text{jumps to the right}\} + \{\text{jumps to the left}\}$$

Time-extensive observable on a time window $[0, t_\mathrm{f}]$

- Climate dynamics:

$$\int_0^{t_\mathrm{f}} dt \;\; \text{temperature}(t)$$

- Fluctuating thermodynamics:

$$\text{work} \;=\; \int_0^{t_\mathrm{f}} dt \;\; \textbf{force}(t) \cdot \textbf{velocity}(t)$$

- Road traffic:

$$\#\{\text{cars passing through a gate}\}$$

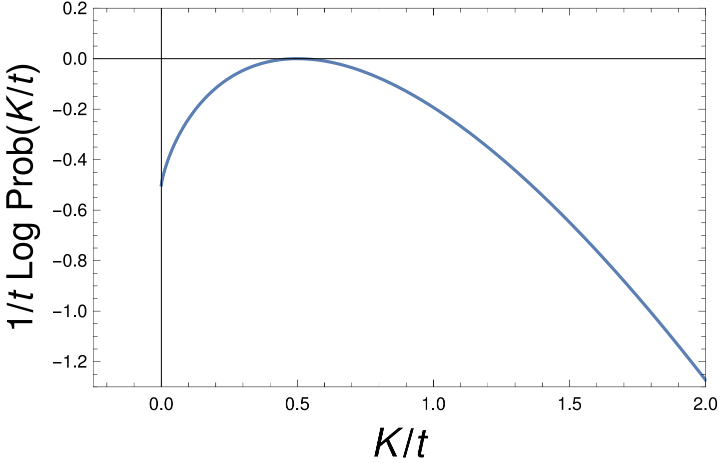
- Molecular transport:

$$\#\{\text{steps of a motor on a filament}\}$$

- Lattice gases in 1d:

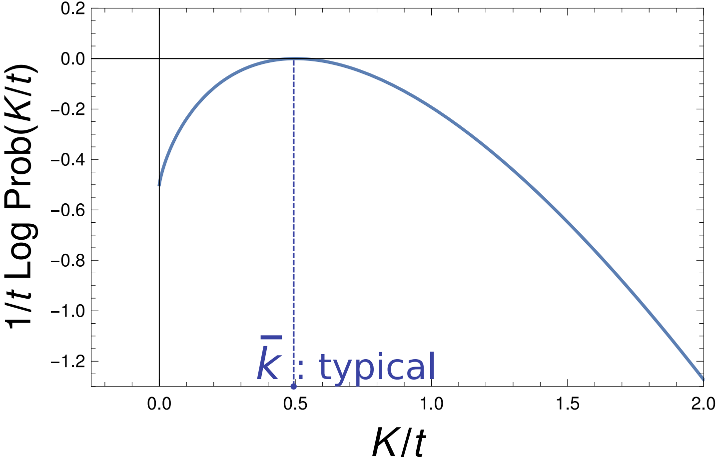
$$\begin{aligned} \text{“current”} \;&=\; \#\{\text{jumps to the right}\} - \{\text{jumps to the left}\} \\ \text{“activity”} \;&=\; \#\{\text{jumps to the right}\} + \{\text{jumps to the left}\} \end{aligned}$$

Distribution of a time-extensive observable K on $[0, t]$



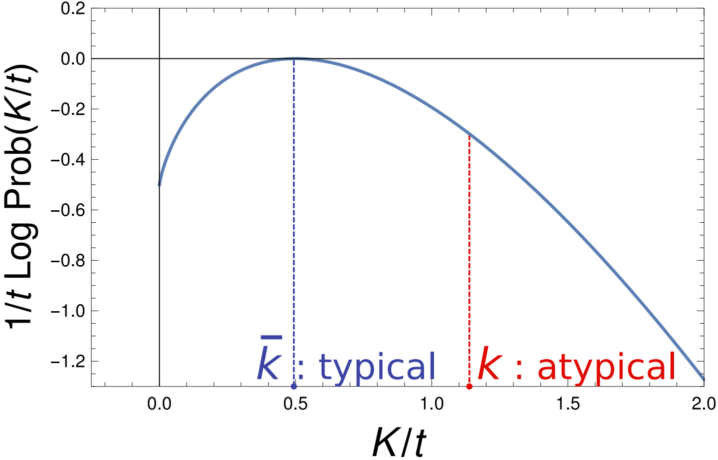
$\text{Prob}[K, t] \sim e^{t\,\varphi(K/t)}$ as $t \to \infty$ $\qquad$ $\varphi(k)$ = large deviation function

Distribution of a time-extensive observable K on $[0, t]$



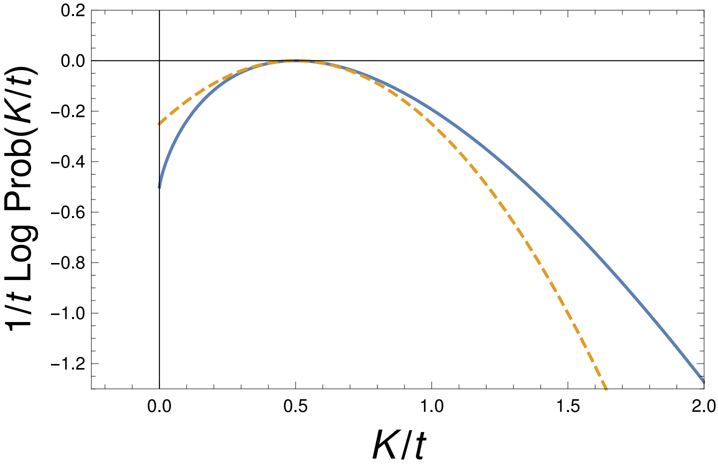
$\mathrm{Prob}[K, t] \sim e^{t\varphi(K/t)}$ as $t \to \infty$ $\qquad$ $\varphi(k) =$ large deviation function

Distribution of a time-extensive observable K on $[0, t]$



$\text{Prob}[K, t] \sim e^{t\,\varphi(K/t)}$ as $t \to \infty$ $\varphi(k) =$ large deviation function

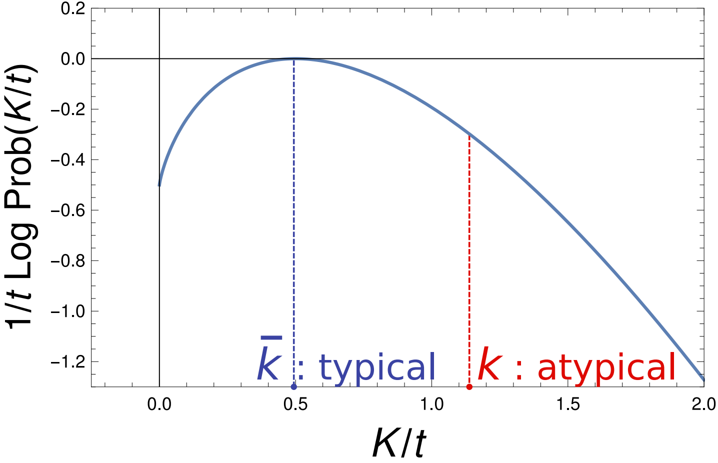
Distribution of a time-extensive observable K on $[0, t]$



$\text{Prob}[K, t] \sim e^{t\,\varphi(K/t)}$ as $t \to \infty$ $\varphi(k) =$ large deviation function

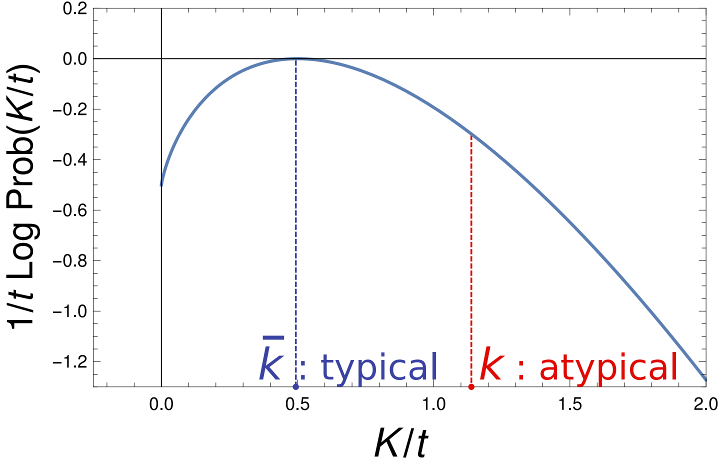
quadratic approx. $\varphi(k) = \frac{(k-\bar{k})^2}{2\sigma^2} + \dots$ $\leftrightarrow$ Gaussian fluctuations

Aim: modify dynamics to make atypical values k typical



Original dynamics: $\bar{k}$ is typical and k atypical

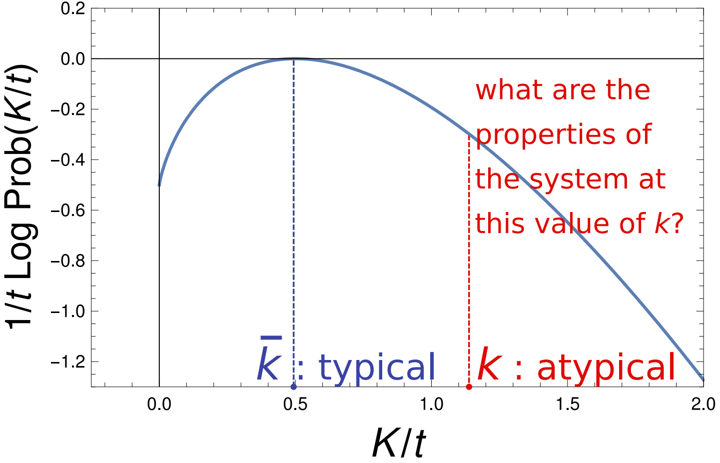
Aim: modify dynamics to make atypical values k typical



Original dynamics: $\bar{k}$ is typical and k atypical

$\exists$ modified dynamics where k is now **typical**?

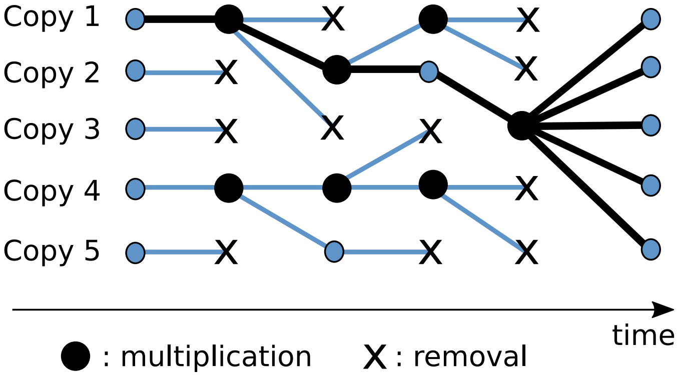
Aim: modify dynamics to make atypical values k typical



Original dynamics: $\bar{k}$ is typical and k atypical

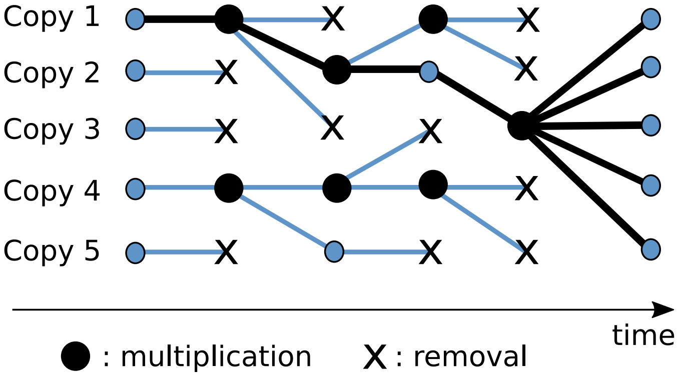
∃ modified dynamics where k is now **typical**?

Ingredient 1/2: population dynamics



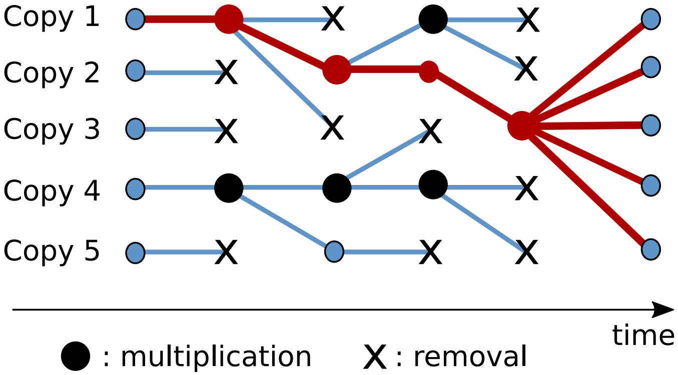
Many copies of the system of interest evolve in parallel.

Ingredient 1/2: population dynamics



Many copies of the system of interest evolve in parallel.
Selection rules favor the normally atypical value of k

Ingredient 1/2: population dynamics



Many copies of the system of interest evolve in parallel.
Selection rules favor the normally atypical value of k
$\rightarrow$ **typical** population trajectories sample the original system at atypical k

Ingredient 2/2: dynamical change of ensemble @$t \to \infty$

Consider an observable $\mathcal{O}[\text{trajectory}]$.

$$\underbrace{\frac{\left\langle \mathcal{O}[\text{traj.}]\, \delta\!\left(\frac{1}{t} K[\text{traj.}] - k\right)\right\rangle}{\left\langle \delta\!\left(\frac{1}{t} K[\text{traj.}] - k\right)\right\rangle}}_{\substack{\text{average of } \mathcal{O} \text{ for trajectories} \\ \text{with atypical } k = K/t}}$$

Ingredient 2/2: dynamical change of ensemble $@t \to \infty$

Consider an observable $\mathcal{O}[\text{trajectory}]$. One can show:

$$\underbrace{\frac{\left\langle \mathcal{O}[\text{traj.}]\, \delta\left(\frac{1}{t}K[\text{traj.}] - k\right)\right\rangle}{\left\langle \delta\left(\frac{1}{t}K[\text{traj.}] - k\right)\right\rangle}}_{\substack{\text{average of } \mathcal{O} \text{ for trajectories} \\ \text{with atypical } k = K/t}} = \underbrace{\frac{\left\langle \mathcal{O}[\text{traj.}]\, \mathrm{e}^{-s\,K[\text{traj.}]}\right\rangle}{\left\langle \mathrm{e}^{-s\,K[\text{traj.}]}\right\rangle}}_{\substack{\text{average of } \mathcal{O} \text{ for trajectories} \\ \text{with a bias } \mathrm{e}^{-s\,K}}}$$

For s and k suitably “conjugated”.

Ingredient 2/2: dynamical change of ensemble @$t \to \infty$

Consider an observable $\mathcal{O}[\text{trajectory}]$. One can show:

$$\underbrace{\frac{\Big\langle \mathcal{O}[\text{traj.}]\, \delta\Big(\frac{1}{t}K[\text{traj.}] - k\Big)\Big\rangle}{\Big\langle \delta\Big(\frac{1}{t}K[\text{traj.}] - k\Big)\Big\rangle}}_{\substack{\text{average of } \mathcal{O} \text{ for trajectories} \\ \text{with atypical } k = K/t \\ \textbf{conditionned ensemble}}} = \underbrace{\frac{\Big\langle \mathcal{O}[\text{traj.}]\, \mathrm{e}^{-s\,K[\text{traj.}]}\Big\rangle}{\Big\langle \mathrm{e}^{-s\,K[\text{traj.}]}\Big\rangle}}_{\substack{\text{average of } \mathcal{O} \text{ for trajectories} \\ \text{with a bias } \mathrm{e}^{-s\,K} \\ \textbf{biased ensemble}}}$$

For s and k suitably “conjugated”.

Ingredient 2/2: dynamical change of ensemble @$t \to \infty$

Consider an observable $\mathcal{O}[\text{trajectory}]$. One can show:

$$\underbrace{\frac{\left\langle \mathcal{O}[\text{traj.}]\, \delta\!\left(\frac{1}{t}K[\text{traj.}] - k\right)\right\rangle}{\left\langle \delta\!\left(\frac{1}{t}K[\text{traj.}] - k\right)\right\rangle}}_{\substack{\text{average of } \mathcal{O} \text{ for trajectories} \\ \text{with atypical } k = K/t \\ \textbf{conditionned ensemble}}} = \underbrace{\frac{\left\langle \mathcal{O}[\text{traj.}]\, e^{-s\,K[\text{traj.}]}\right\rangle}{\left\langle e^{-s\,K[\text{traj.}]}\right\rangle}}_{\substack{\text{average of } \mathcal{O} \text{ for trajectories} \\ \text{with a bias } e^{-s\,K} \\ \textbf{biased ensemble}}}$$

Next goal: show that $\quad \ldots = \underbrace{\big\langle \mathcal{O}[\text{traj.}] \big\rangle_{\text{population dynamics}}}_{\substack{\text{average of } \mathcal{O} \text{ for trajectories} \\ \text{in fixed-size population} \\ \text{dynamics}}}$

For s and k suitably “conjugated”.

Ingredient 2/2: dynamical change of ensemble @$t \to \infty$

Consider an observable $\mathcal{O}[\text{trajectory}]$. One can show:

$$\underbrace{\frac{\left\langle \mathcal{O}[\text{traj.}]\,\delta\left(\frac{1}{t}K[\text{traj.}]-k\right)\right\rangle}{\left\langle \delta\left(\frac{1}{t}K[\text{traj.}]-k\right)\right\rangle}}_{\substack{\text{average of } \mathcal{O} \text{ for trajectories} \\ \text{with atypical } k=K/t \\ \textbf{conditionned ensemble} \\ \textbf{microcanonical ensemble}}} = \underbrace{\frac{\left\langle \mathcal{O}[\text{traj.}]\,\mathrm{e}^{-s\,K[\text{traj.}]}\right\rangle}{\left\langle \mathrm{e}^{-s\,K[\text{traj.}]}\right\rangle}}_{\substack{\text{average of } \mathcal{O} \text{ for trajectories} \\ \text{with a bias } \mathrm{e}^{-s\,K} \\ \textbf{biased ensemble} \\ \textbf{canonical ensemble}}}$$

Next goal: show that $\quad \ldots = \underbrace{\left\langle \mathcal{O}[\text{traj.}]\right\rangle_{\text{population dynamics}}}_{\substack{\text{average of } \mathcal{O} \text{ for trajectories} \\ \text{in fixed-size population} \\ \text{dynamics}}}$

For s and k suitably “conjugated”.

Analogy: $k \equiv$ energy/volume; $s \equiv$ inverse temperature β

Ingredient 2/2: dynamical change of ensemble @$t \to \infty$

Main message:

Fixed $k = K/t \quad \Longleftrightarrow \quad$ bias by e^{-sK}

Ingredient 2/2: dynamical change of ensemble @$t \to \infty$

Main message:

Fixed $k = K/t$ $\iff$ bias by e^{-sK} $\iff$ Selection rules in population dynamics

Ingredient 2/2: dynamical change of ensemble @$t \to \infty$

Main message:

Fixed $k = K/t$ $\iff$ bias by e^{-sK} $\iff$ Selection rules in population dynamics

Relation between s and k; Cumulant Generating Function (CGF):

$$\mathrm{Prob}\left[K/t = k\right] \sim \mathrm{e}^{t\varphi(k)} \qquad \iff \qquad \left\langle \mathrm{e}^{-sK} \right\rangle \sim \mathrm{e}^{t\overbrace{\psi(s)}^{\textbf{CGF}}}$$

Ingredient 2/2: dynamical change of ensemble @$t \to \infty$

Main message:

Fixed $k = K/t$ $\iff$ bias by e^{-sK} $\iff$ Selection rules in population dynamics

Relation between s and k; Cumulant Generating Function (CGF):

$$\mathrm{Prob}\left[K/t = k\right] \sim \mathrm{e}^{t\varphi(k)} \qquad \iff \qquad \left\langle \mathrm{e}^{-sK} \right\rangle \sim \mathrm{e}^{t\overbrace{\psi(s)}^{\text{CGF}}}$$

Saddle-point at large t:

$$\max_{k} \left\{ \varphi(k) - s\,k \right\} \;=\; \psi(s)$$

Maximum reached for k conjugated to s

Ingredient 2/2: dynamical change of ensemble @$t \to \infty$

Main message:

Fixed $k = K/t$ $\iff$ bias by e^{-sK} $\iff$ Selection rules in population dynamics

Relation between s and k; Cumulant Generating Function (CGF):

$$\text{Prob}\left[K/t = k\right] \sim e^{t\varphi(k)} \qquad \iff \qquad \left\langle e^{-sK}\right\rangle \sim e^{t\overbrace{\psi(s)}^{\textbf{CGF}}}$$

Saddle-point at large t:

$$\max_k \left\{\varphi(k) - s\,k\right\} \;=\; \psi(s)$$

Maximum reached for k conjugated to s

Remaining question: how to represent e^{-sK} by pop. dynamics?

s-modified dynamics (for discrete stochastic processes)

- Markov processes: Configs. $\mathcal{C}$, jump rates $W(\mathcal{C} \to \mathcal{C}')$

$$\partial_t P(\mathcal{C}, t) = \sum_{\mathcal{C}'} \Big\{ \underbrace{W(\mathcal{C}' \to \mathcal{C}) P(\mathcal{C}', t)}_{\text{gain term}} - \underbrace{W(\mathcal{C} \to \mathcal{C}') P(\mathcal{C}, t)}_{\text{loss term}} \Big\}$$

s-modified dynamics $\qquad K = \text{activity} = \#\text{events}$

- Markov processes: Configs. $\mathcal{C}$, jump rates $W(\mathcal{C} \to \mathcal{C}')$

$$\partial_t P(\mathcal{C}, t) = \sum_{\mathcal{C}'} \Big\{ \underbrace{W(\mathcal{C}' \to \mathcal{C}) P(\mathcal{C}', t)}_{\text{gain term}} - \underbrace{W(\mathcal{C} \to \mathcal{C}') P(\mathcal{C}, t)}_{\text{loss term}} \Big\}$$

- More detailed dynamics for $P(\mathcal{C}, K, t)$:

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

s-modified dynamics $\quad K = \text{activity} = \#\text{events}$

- Markov processes: Configs. $\mathcal{C}$, jump rates $W(\mathcal{C} \to \mathcal{C}')$

$$\partial_t P(\mathcal{C}, t) = \sum_{\mathcal{C}'} \Big\{ \underbrace{W(\mathcal{C}' \to \mathcal{C}) P(\mathcal{C}', t)}_{\text{gain term}} - \underbrace{W(\mathcal{C} \to \mathcal{C}') P(\mathcal{C}, t)}_{\text{loss term}} \Big\}$$

- More detailed dynamics for $P(\mathcal{C}, K, t)$:

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

- Biased ensemble: s conjugated to K (canonical description)

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

s-modified dynamics $\qquad K = \text{activity} = \#\text{events}$

- Markov processes: Configs. $\mathcal{C}$, jump rates $W(\mathcal{C} \to \mathcal{C}')$

$$\partial_t P(\mathcal{C}, t) = \sum_{\mathcal{C}'} \Big\{ \underbrace{W(\mathcal{C}' \to \mathcal{C}) P(\mathcal{C}', t)}_{\text{gain term}} - \underbrace{W(\mathcal{C} \to \mathcal{C}') P(\mathcal{C}, t)}_{\text{loss term}} \Big\}$$

- More detailed dynamics for $P(\mathcal{C}, K, t)$:

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

- Biased ensemble: s conjugated to K (canonical description)

$$\hat{P}(\mathcal{C}, s, t) = \sum_{K} \mathrm{e}^{-sK} P(\mathcal{C}, K, t)$$

- s-modified dynamics [probability non-conserving] $\partial_t |\hat{P}\rangle = \mathbb{W}_s |\hat{P}\rangle$

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

s-modified dynamics $\quad K = k_{\mathcal{C}_0\mathcal{C}_1} + k_{\mathcal{C}_1\mathcal{C}_2} + \ldots$

- Markov processes: Configs. $\mathcal{C}$, jump rates $W(\mathcal{C} \to \mathcal{C}')$

$$\partial_t P(\mathcal{C},t) = \sum_{\mathcal{C}'} \Big\{ \underbrace{W(\mathcal{C}' \to \mathcal{C}) P(\mathcal{C}',t)}_{\text{gain term}} - \underbrace{W(\mathcal{C} \to \mathcal{C}') P(\mathcal{C},t)}_{\text{loss term}} \Big\}$$

- More detailed dynamics for $P(\mathcal{C},K,t)$:

$$\partial_t P(\mathcal{C},K,t) = \sum_{\mathcal{C}'} \Big\{ W(\mathcal{C}' \to \mathcal{C}) P(\mathcal{C}',K - k_{\mathcal{C}'\mathcal{C}},t) - W(\mathcal{C} \to \mathcal{C}') P(\mathcal{C},K,t) \Big\}$$

- Biased ensemble: s conjugated to K

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

- s-modified dynamics [probability non-conserving] $\quad \partial_t |\hat{P}\rangle = \mathbb{W}_s |\hat{P}\rangle$

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

Numerical method [JB Anderson; D Aldous; P Grassberger; P Del Moral; ...]

Evaluation of large deviation functions [*à la* "Diffusion Monte-Carlo"]

$$\sum_{\mathcal{C}} \hat{P}(\mathcal{C}, s, t) = \langle e^{-s K} \rangle \sim e^{t\psi(s)} \qquad (\psi(s)\text{=CGF=max eigenv. } \mathbb{W}_s)$$

- discrete time: Giardinà, Kurchan, Peliti [PRL **96**, 120603 (2006)]
- continuous time: VL, Tailleur [JSTAT P03004 (2007)]

Cloning dynamics

$$\partial_t \hat{P}(\mathcal{C}, s) = \underbrace{\sum_{\mathcal{C}'} W_s(\mathcal{C}' \to \mathcal{C}) \hat{P}(\mathcal{C}', s) - r_s(\mathcal{C}) \hat{P}(\mathcal{C}, s)}_{\text{modified dynamics}} + \underbrace{\delta r_s(\mathcal{C}) \hat{P}(\mathcal{C}, s)}_{\text{cloning term}}$$

- $W_s(\mathcal{C}' \to \mathcal{C}) = e^{-s} W(\mathcal{C}' \to \mathcal{C})$
- $r_s(\mathcal{C}) = \sum_{\mathcal{C}'} W_s(\mathcal{C} \to \mathcal{C}')$ $\qquad r(\mathcal{C}) = \sum_{\mathcal{C}'} W(\mathcal{C} \to \mathcal{C}')$
- $\delta r_s(\mathcal{C}) = r_s(\mathcal{C}) - r(\mathcal{C})$

Numerical method [JB Anderson; D Aldous; P Grassberger; P Del Moral; ...]

Evaluation of large deviation functions [*à la* "Diffusion Monte-Carlo"]

$$\sum_{\mathcal{C}} \hat{P}(\mathcal{C}, s, t) = \left\langle \mathrm{e}^{-s\,K} \right\rangle \sim \mathrm{e}^{t\,\psi(s)} \qquad (\psi(s) = \text{CGF} = \text{max eigenv. } \mathbb{W}_s)$$

- discrete time: Giardinà, Kurchan, Peliti [PRL **96**, 120603 (2006)]
- continuous time: VL, Tailleur [JSTAT P03004 (2007)]

Cloning dynamics

$$\partial_t \hat{P}(\mathcal{C}, s) = \underbrace{\sum_{\mathcal{C}'} W_s(\mathcal{C}' \to \mathcal{C}) \hat{P}(\mathcal{C}', s) - r_s(\mathcal{C}) \hat{P}(\mathcal{C}, s)}_{\text{modified dynamics}} + \underbrace{\delta r_s(\mathcal{C}) \hat{P}(\mathcal{C}, s)}_{\text{cloning term}}$$

- $W_s(\mathcal{C}' \to \mathcal{C}) = \mathrm{e}^{-s} W(\mathcal{C}' \to \mathcal{C})$
- $r_s(\mathcal{C}) = \sum_{\mathcal{C}'} W_s(\mathcal{C} \to \mathcal{C}')$ $\qquad r(\mathcal{C}) = \sum_{\mathcal{C}'} W(\mathcal{C} \to \mathcal{C}')$
- $\delta r_s(\mathcal{C}) = r_s(\mathcal{C}) - r(\mathcal{C})$

Explicit construction

$$\partial_t \hat{P}(\mathcal{C},s) = \underbrace{\sum_{\mathcal{C}'} W_s(\mathcal{C}' \to \mathcal{C})\hat{P}(\mathcal{C}',s) - r_s(\mathcal{C})\hat{P}(\mathcal{C},s)}_{\text{modified dynamics}} + \underbrace{\delta r_s(\mathcal{C})\hat{P}(\mathcal{C},s)}_{\text{cloning term}}$$

How to take into account loss/gain of probability?

- handle a large number N_c of copies of the system
- implement a selection rule: on a time interval Δt
  a copy in config $\mathcal{C}$ is replaced by $Y = e^{\Delta t\, \delta r_s(\mathcal{C})}$ copies
- $\psi(s)$ = the rate of exponential growth/decay of the total population
- optionally: keep population constant by non-biased pruning/cloning

Explicit construction

$$\partial_t \hat{P}(\mathcal{C},s) = \underbrace{\sum_{\mathcal{C}'} W_s(\mathcal{C}' \to \mathcal{C})\hat{P}(\mathcal{C}',s) - r_s(\mathcal{C})\hat{P}(\mathcal{C},s)}_{\text{modified dynamics}} + \underbrace{\delta r_s(\mathcal{C})\hat{P}(\mathcal{C},s)}_{\text{cloning term}}$$

How to take into account loss/gain of probability?

- handle a large number N_c of copies of the system
- implement a selection rule: on a time interval Δt
  a copy in config $\mathcal{C}$ is replaced by $Y = \lfloor e^{\Delta t\, \delta r_s(\mathcal{C})} + \varepsilon \rfloor$ copies, $\varepsilon \sim [0,1]$
- $\psi(s)$ = the rate of exponential growth/decay of the total population
- optionally: keep population constant by non-biased pruning/cloning

Explicit construction

$$\partial_t \hat{P}(\mathcal{C},s) = \underbrace{\sum_{\mathcal{C}'} W_s(\mathcal{C}' \to \mathcal{C})\hat{P}(\mathcal{C}',s) - r_s(\mathcal{C})\hat{P}(\mathcal{C},s)}_{\text{modified dynamics}} + \underbrace{\delta r_s(\mathcal{C})\hat{P}(\mathcal{C},s)}_{\text{cloning term}}$$

How to take into account loss/gain of probability?

- handle a large number N_c of copies of the system
- implement a selection rule: on a time interval Δt
  a copy in config $\mathcal{C}$ is replaced by $Y = \lfloor e^{\Delta t\, \delta r_s(\mathcal{C})} + \varepsilon \rfloor$ copies, $\varepsilon \sim [0,1]$
- $\psi(s)$ = the rate of exponential growth/decay of the total population
- optionally: keep population constant by non-biased pruning/cloning

Explicit construction

$$\partial_t \hat{P}(\mathcal{C},s) = \underbrace{\sum_{\mathcal{C}'} W_s(\mathcal{C}'\to\mathcal{C})\hat{P}(\mathcal{C}',s) - r_s(\mathcal{C})\hat{P}(\mathcal{C},s)}_{\text{modified dynamics}} + \underbrace{\delta r_s(\mathcal{C})\hat{P}(\mathcal{C},s)}_{\text{cloning term}}$$

How to take into account loss/gain of probability?

- handle a large number N_c of copies of the system
- implement a selection rule: on a time interval Δt
  a copy in config $\mathcal{C}$ is replaced by $Y = \lfloor e^{\Delta t\, \delta r_s(\mathcal{C})} + \varepsilon \rfloor$ copies, $\varepsilon \sim [0,1]$
- $\psi(s)$ = the rate of exponential growth/decay of the total population
- optionally: keep population constant by non-biased pruning/cloning

CGF estimator: $\psi(s) = \langle \Psi(s) \rangle$ with $\Psi(s) = \log \underbrace{\prod_t \frac{N_c + Y_t - 1}{N_c}}_{\text{reconstituted population size}}$

Explicit construction

$$\partial_t \hat{P}(\mathcal{C},s) = \underbrace{\sum_{\mathcal{C}'} W_s(\mathcal{C}' \to \mathcal{C})\hat{P}(\mathcal{C}',s) - r_s(\mathcal{C})\hat{P}(\mathcal{C},s)}_{\text{modified dynamics}} + \underbrace{\delta r_s(\mathcal{C})\hat{P}(\mathcal{C},s)}_{\text{cloning term}}$$

Biological interpretation

- copy in configuration $\mathcal{C}$ $\equiv$ organism of **genome** $\mathcal{C}$
- dynamics of rates W_s $\equiv$ **mutations**
- cloning at rates δr_s $\equiv$ **selection** rendering typical the rare histories

Explicit construction

$$\partial_t \hat{P}(\mathcal{C},s) = \underbrace{\sum_{\mathcal{C}'} W_s(\mathcal{C}' \to \mathcal{C})\hat{P}(\mathcal{C}',s) - r_s(\mathcal{C})\hat{P}(\mathcal{C},s)}_{\text{modified dynamics}} + \underbrace{\delta r_s(\mathcal{C})\hat{P}(\mathcal{C},s)}_{\text{cloning term}}$$

Biological interpretation

- copy in configuration $\mathcal{C} \equiv$ organism of **genome** $\mathcal{C}$
- dynamics of rates $W_s \equiv$ **mutations**
- cloning at rates $\delta r_s \equiv$ **selection** rendering typical the rare histories
- the CGF $\psi(s)$ is a measure of the **fitness** of the population

Explicit construction

$$\partial_t \hat{P}(\mathcal{C},s) = \underbrace{\sum_{\mathcal{C}'} W_s(\mathcal{C}' \to \mathcal{C})\hat{P}(\mathcal{C}',s) - r_s(\mathcal{C})\hat{P}(\mathcal{C},s)}_{\text{modified dynamics}} + \underbrace{\delta r_s(\mathcal{C})\hat{P}(\mathcal{C},s)}_{\text{cloning term}}$$

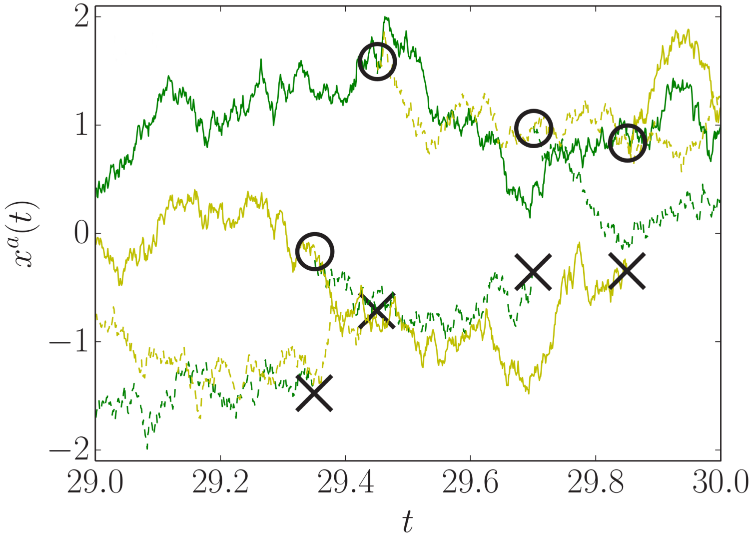
Biological interpretation

- copy in configuration $\mathcal{C} \equiv$ organism of **genome** $\mathcal{C}$
- dynamics of rates $W_s \equiv$ **mutations**
- cloning at rates $\delta r_s \equiv$ **selection** rendering typical the rare histories
- the CGF $\psi(s)$ is a measure of the **fitness** of the population

Generic idea

- **Different dynamics can share equivalent statistical properties.**
- Constrained trajectories (fixed atypical $k = K/t$) $\equiv$ pop. dynamics

An example: 4 copies, 1 degree of freedom $\mathcal{C} = x \in \mathbb{R}$



How to perform averages? (i) [spectral analysis]

⋆ Final-time distribution $p_{\text{end}}(\mathcal{C})$: *proportion* of copies in $\mathcal{C}$ at t

$$\langle N_{\text{nc}}(t)\rangle_s$$

$$\langle N_{\text{nc}}(\mathcal{C},t)\rangle_s$$

$$p_{\text{end}}(\mathcal{C},t) = \frac{\langle N_{\text{nc}}(\mathcal{C},t)\rangle_s}{\langle N_{\text{nc}}(t)\rangle_s}$$

[N_{nc} = number of copies in non-constant population dynamics]

How to perform averages? (i) [spectral analysis]

$$\partial_t|\hat{P}\rangle \;=\; \mathbb{W}_s|\hat{P}\rangle$$

⋆ Final-time distribution $p_{\text{end}}(\mathcal{C})$: *proportion* of copies in $\mathcal{C}$ at t

$$\langle N_{\text{nc}}(t)\rangle_s$$

$$\langle N_{\text{nc}}(\mathcal{C},t)\rangle_s$$

$$p_{\text{end}}(\mathcal{C},t) = \frac{\langle N_{\text{nc}}(\mathcal{C},t)\rangle_s}{\langle N_{\text{nc}}(t)\rangle_s}$$

[N_{nc} = number of copies in non-constant population dynamics]

How to perform averages? (i) [spectral analysis]

$$\partial_t|\hat{P}\rangle \;=\; \mathbb{W}_s|\hat{P}\rangle$$

$$\mathbb{W}_s|R\rangle = \psi(s)|R\rangle$$

$$\langle L|\mathbb{W}_s = \psi(s)\langle L|$$

$$[\quad \langle L| = \langle -| \;\; @\, s=0 \quad]$$

⋆ Final-time distribution $p_{\text{end}}(\mathcal{C})$: *proportion* of copies in $\mathcal{C}$ at t

$$\langle N_{\text{nc}}(t)\rangle_s$$

$$\langle N_{\text{nc}}(\mathcal{C},t)\rangle_s$$

$$p_{\text{end}}(\mathcal{C},t) = \frac{\langle N_{\text{nc}}(\mathcal{C},t)\rangle_s}{\langle N_{\text{nc}}(t)\rangle_s}$$

[N_{nc} = number of copies in non-constant population dynamics]

How to perform averages? (i) [spectral analysis]

$$\partial_t|\hat{P}\rangle = \mathbb{W}_s|\hat{P}\rangle \qquad \mathbb{W}_s|R\rangle = \psi(s)|R\rangle$$

$$e^{t\mathbb{W}_s} \underset{t\to\infty}{\sim} e^{t\psi(s)}|R\rangle\langle L| \qquad \langle L|\mathbb{W}_s = \psi(s)\langle L|$$

$$[\quad \langle L| = \langle -| \;\; @\, s=0 \quad]$$

⋆ Final-time distribution $p_{\text{end}}(\mathcal{C})$: *proportion* of copies in $\mathcal{C}$ at t

$$\langle N_{\text{nc}}(t)\rangle_s$$

$$\langle N_{\text{nc}}(\mathcal{C},t)\rangle_s$$

$$p_{\text{end}}(\mathcal{C},t) = \frac{\langle N_{\text{nc}}(\mathcal{C},t)\rangle_s}{\langle N_{\text{nc}}(t)\rangle_s}$$

[N_{nc} = number of copies in non-constant population dynamics]

How to perform averages? (i) [spectral analysis]

$$\partial_t |\hat{P}\rangle = \mathbb{W}_s |\hat{P}\rangle \qquad \mathbb{W}_s |R\rangle = \psi(s)|R\rangle$$

$$e^{t\mathbb{W}_s} \underset{t\to\infty}{\sim} e^{t\psi(s)}|R\rangle\langle L| \qquad \langle L|\mathbb{W}_s = \psi(s)\langle L|$$

$$[\quad \langle L| = \langle -| \;\; @\, s=0 \quad]$$

⋆ Final-time distribution $p_{\text{end}}(\mathcal{C})$: *proportion* of copies in $\mathcal{C}$ at t

$$\langle N_{\text{nc}}(t)\rangle_s = \langle -|e^{t\mathbb{W}_s}|P_{\text{i}}\rangle N_0 \underset{t\to\infty}{\sim} e^{t\psi(s)}\langle L|P_{\text{i}}\rangle N_0$$

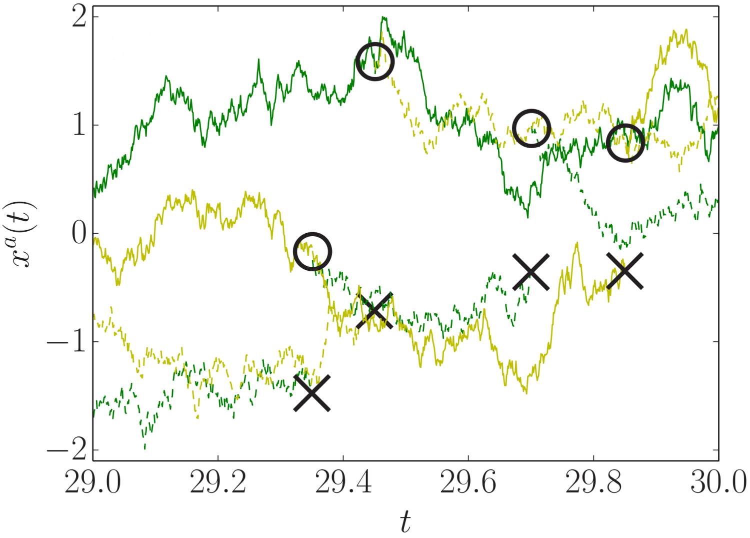
$$\langle N_{\text{nc}}(\mathcal{C},t)\rangle_s = \langle \mathcal{C}|e^{t\mathbb{W}_s}|P_{\text{i}}\rangle N_0 \underset{t\to\infty}{\sim} e^{t\psi(s)}\langle \mathcal{C}|R\rangle\langle L|P_{\text{i}}\rangle N_0$$

$$p_{\text{end}}(\mathcal{C},t) = \frac{\langle N_{\text{nc}}(\mathcal{C},t)\rangle_s}{\langle N_{\text{nc}}(t)\rangle_s} \underset{t\to\infty}{\sim} \langle \mathcal{C}|R\rangle \equiv p_{\text{end}}(\mathcal{C})$$

[N_{nc} = number of copies in non-constant population dynamics]

Final-time distribution $p_{\text{end}}(\mathcal{C})$ governed by **right** eigenvector.

An example: 4 copies, 1 degree of freedom $\mathcal{C} = x \in \mathbb{R}$



How to perform averages? (ii) Intermediate times

$$\partial_t|\hat{P}\rangle = \mathbb{W}_s|\hat{P}\rangle$$

$$e^{t\mathbb{W}_s} \underset{t\to\infty}{\sim} e^{t\psi(s)}|R\rangle\langle L|$$

$$\mathbb{W}_s|R\rangle = \psi(s)|R\rangle$$

$$\langle L|\mathbb{W}_s = \psi(s)\langle L|$$

$$[\quad \langle L| = \langle -| \ \ @\, s=0 \quad]$$

- ⋆ Mid-time distribution $p_{\text{ave}}(\mathcal{C})$: *proportion* of copies in $\mathcal{C}$ at $t_1 \ll t$

$$\langle N_{\text{nc}}(t)\rangle_s$$

$$\langle N_{\text{nc}}(t|\mathcal{C},t_1)\rangle_s$$

$$p(t|\mathcal{C},t_1) = \frac{\langle N_{\text{nc}}(t|\mathcal{C},t_1)\rangle_s}{\langle N_{\text{nc}}(t)\rangle_s}$$

How to perform averages? (ii) Intermediate times

$$\partial_t|\hat{P}\rangle = \mathbb{W}_s|\hat{P}\rangle \qquad \mathbb{W}_s|R\rangle = \psi(s)|R\rangle$$

$$e^{t\mathbb{W}_s} \underset{t\to\infty}{\sim} e^{t\psi(s)}|R\rangle\langle L| \qquad \langle L|\mathbb{W}_s = \psi(s)\langle L|$$

$$[\quad \langle L| = \langle -| \ \ @\, s=0 \quad]$$

⋆ Mid-time distribution $p_{\text{ave}}(\mathcal{C})$: *proportion* of copies in $\mathcal{C}$ at $t_1 \ll t$

$$\langle N_{\text{nc}}(t)\rangle_s = \langle -|e^{t\mathbb{W}_s}|P_{\text{i}}\rangle N_0 \underset{t\to\infty}{\sim} e^{t\psi(s)}\langle L|P_{\text{i}}\rangle N_0$$

$$\langle N_{\text{nc}}(t|\mathcal{C},t_1)\rangle_s = \langle -|e^{(t-t_1)\mathbb{W}_s}|\mathcal{C}\rangle\langle\mathcal{C}|e^{t_1\mathbb{W}_s}|P_{\text{i}}\rangle N_0 \sim e^{t\psi(s)}\langle L|\mathcal{C}\rangle\langle\mathcal{C}|R\rangle\langle L|P_{\text{i}}\rangle N_0$$

$$p(t|\mathcal{C},t_1) = \frac{\langle N_{\text{nc}}(t|\mathcal{C},t_1)\rangle_s}{\langle N_{\text{nc}}(t)\rangle_s} \underset{t\to\infty}{\sim} \langle L|\mathcal{C}\rangle\langle\mathcal{C}|R\rangle \equiv p_{\text{ave}}(\mathcal{C})$$

How to perform averages? (ii) Intermediate times

$$\partial_t|\hat{P}\rangle = \mathbb{W}_s|\hat{P}\rangle \qquad \mathbb{W}_s|R\rangle = \psi(s)|R\rangle$$

$$e^{t\mathbb{W}_s} \underset{t\to\infty}{\sim} e^{t\psi(s)}|R\rangle\langle L| \qquad \langle L|\mathbb{W}_s = \psi(s)\langle L|$$

$$[\quad \langle L| = \langle -| \ @\, s=0 \quad]$$

⋆ Mid-time distribution $p_{\text{ave}}(\mathcal{C})$: *proportion* of copies in $\mathcal{C}$ at $t_1 \ll t$

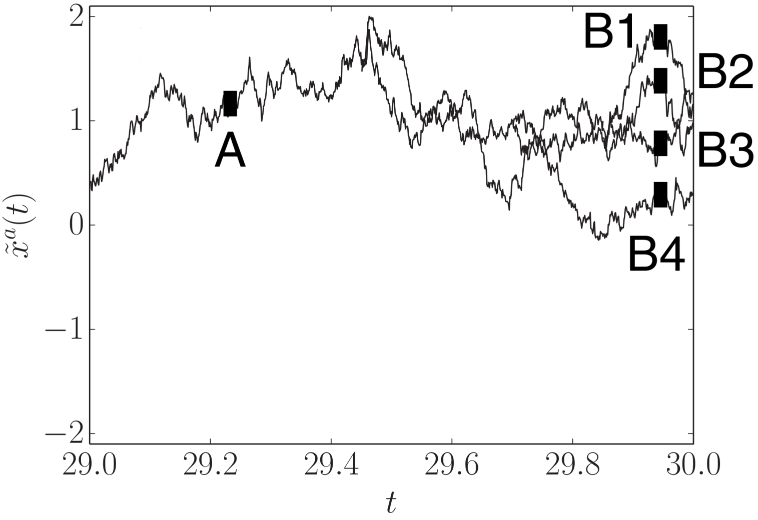
$$\langle N_{\text{nc}}(t)\rangle_s = \langle -|e^{t\mathbb{W}_s}|P_{\text{i}}\rangle N_0 \underset{t\to\infty}{\sim} e^{t\psi(s)}\langle L|P_{\text{i}}\rangle N_0$$

$$\langle N_{\text{nc}}(t|\mathcal{C},t_1)\rangle_s = \langle -|e^{(t-t_1)\mathbb{W}_s}|\mathcal{C}\rangle\langle\mathcal{C}|e^{t_1\mathbb{W}_s}|P_{\text{i}}\rangle N_0 \sim e^{t\psi(s)}\langle L|\mathcal{C}\rangle\langle\mathcal{C}|R\rangle\langle L|P_{\text{i}}\rangle N_0$$

$$p(t|\mathcal{C},t_1) = \frac{\langle N_{\text{nc}}(t|\mathcal{C},t_1)\rangle_s}{\langle N_{\text{nc}}(t)\rangle_s} \underset{t\to\infty}{\sim} \langle L|\mathcal{C}\rangle\langle\mathcal{C}|R\rangle \equiv p_{\text{ave}}(\mathcal{C})$$

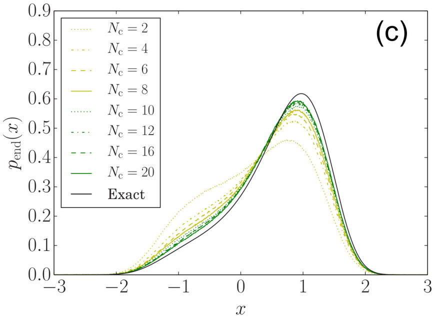
Mid-time distribution $p_{\text{ave}}(\mathcal{C})$ governed by **left** and **right** eigenvecs.

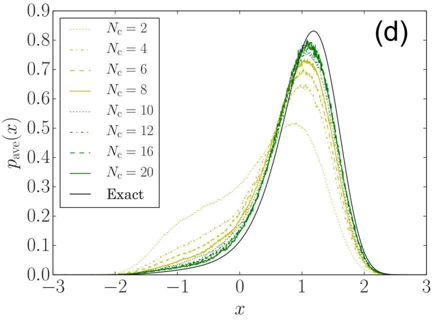
An example: 4 copies, 1 degree of freedom $\mathcal{C} = x \in \mathbb{R}$



Huge sampling issue

Example distributions for a simple Langevin dynamics



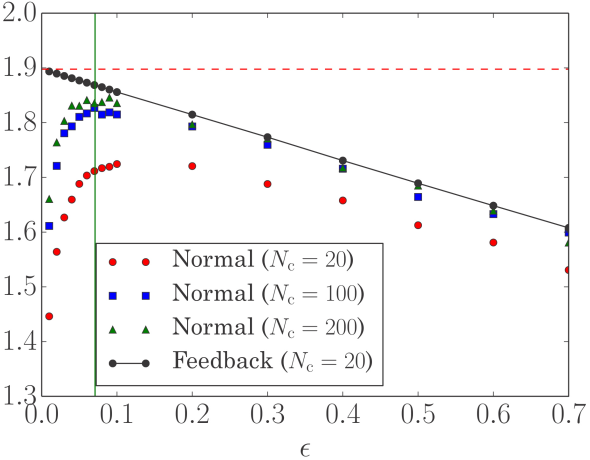


final-time: $p_{\text{end}}(x)$
$(= R(x))$

intermediate-time: $p_{\text{ave}}(x)$
$(= R(x)L(x))$

The small-noise crisis: systematic errors grow as $\epsilon \to 0$

CGF as a function of the noise amplitude ϵ:



Cause: as $\epsilon \to 0$, $p_{\text{ave}}(x)$ & $p_{\text{end}}(x)$ $\to$ sharply peaked at *different points*

i.e. the clones do not sample correctly the phase space

The feedback method

How to make mid- and final-time distribution closer?

Driven/auxiliary dynamics: [Maes, Jack&Sollich, Touchette&Chetrite]

- Probability preserving
- No mismatch between p_{ave} and p_{end}
- Constructed as **[Different dynamics can share ≡ statistical properties.]**

$$\mathbb{W}_s^{\text{aux}} = L\mathbb{W}_s L^{-1} - \psi(s)\mathbf{1}$$

How to make mid- and final-time distribution closer?

Driven/auxiliary dynamics: [Maes, Jack&Sollich, Touchette&Chetrite]

- Probability preserving
- No mismatch between p_{ave} and p_{end}
- Constructed as **[Different dynamics can share ≡ statistical properties.]**

$$\mathbb{W}_s^{\text{aux}} = L\mathbb{W}_s L^{-1} - \psi(s)\mathbf{1}$$

How to make mid- and final-time distribution closer?

Driven/auxiliary dynamics: [Maes, Jack&Sollich, Touchette&Chetrite]

- Probability preserving
- No mismatch between p_{ave} and p_{end}
- Constructed as **[Different dynamics can share ≡ statistical properties.]**

$$\mathbb{W}_s^{\text{aux}} = L\mathbb{W}_s L^{-1} - \psi(s)\mathbf{1}$$

- Issue: determining L is difficult
- Solution: evaluate L as L_{test} on the fly **[feedback]** and simulate

$$\mathbb{W}_s^{\text{test}} = L_{\text{test}}\mathbb{W}_s L_{\text{test}}^{-1} \qquad \text{(induces \textit{effective forces})}$$

- **Iterate.** [For any L_{test}, the simulation is in principle correct.]

How to make mid- and final-time distribution closer?

Driven/auxiliary dynamics: [Maes, Jack&Sollich, Touchette&Chetrite]

- Probability preserving
- No mismatch between p_{ave} and p_{end}
- Constructed as **[Different dynamics can share ≡ statistical properties.]**

$$\mathbb{W}_s^{\text{aux}} = L\mathbb{W}_s L^{-1} - \psi(s)\mathbf{1}$$

- Issue: determining L is difficult
- Solution: evaluate L as L_{test} on the fly **[feedback]** and simulate

$$\mathbb{W}_s^{\text{test}} = L_{\text{test}}\mathbb{W}_s L_{\text{test}}^{-1} \qquad \text{(induces \textbf{\textit{effective forces}})}$$

- **Iterate.** [For any L_{test}, the simulation is in principle correct.]

How to make mid- and final-time distribution closer?

Driven/auxiliary dynamics: [Maes, Jack&Sollich, Touchette&Chetrite]

- Probability preserving
- No mismatch between p_{ave} and p_{end}
- Constructed as **[Different dynamics can share ≡ statistical properties.]**

$$\mathbb{W}_s^{\text{aux}} = L \mathbb{W}_s L^{-1} - \psi(s)\mathbf{1}$$

- Issue: determining L is difficult
- Solution: evaluate L as L_{test} on the fly **[feedback]** and simulate

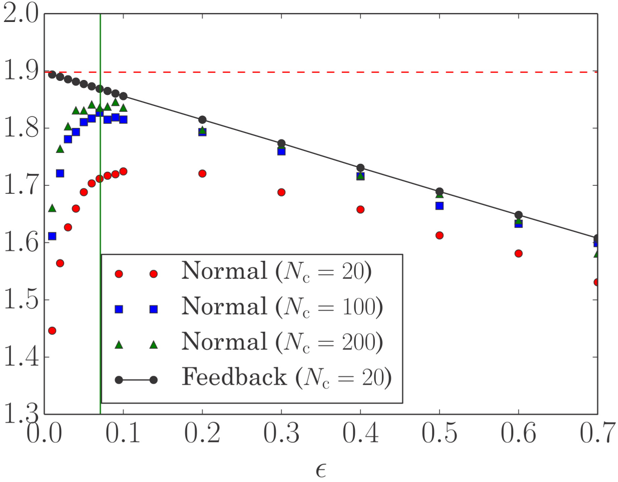
$$\mathbb{W}_s^{\text{test}} = L_{\text{test}} \mathbb{W}_s L_{\text{test}}^{-1} \qquad \text{(induces \textbf{\textit{effective forces}})}$$

- **Iterate.** [For any L_{test}, the simulation is in principle correct.]

Similar in spirit to **multi-canonical** (*e.g.* Wang–Landau) approaches in static thermodynamics. [Here, one flattens the left-eigenvector of $\mathbb{W}_s^{\text{test}}$.]

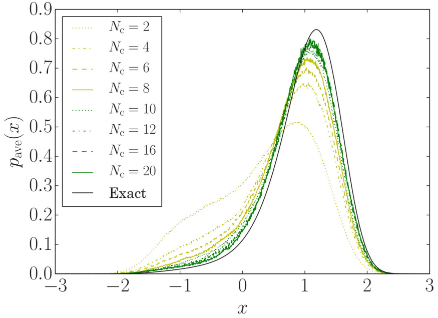
Improvement of the small-noise crisis (i.i)

CGF as a function of the noise amplitude ϵ:

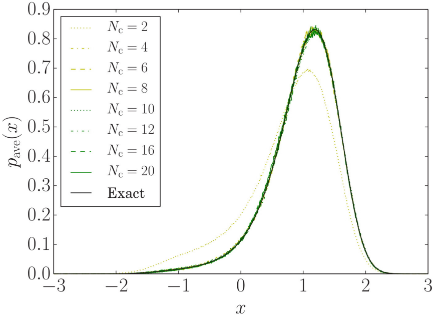


Physical insight: probability loss transformed into *effective forces*.

Improvement of the small-noise crisis (i.ii)



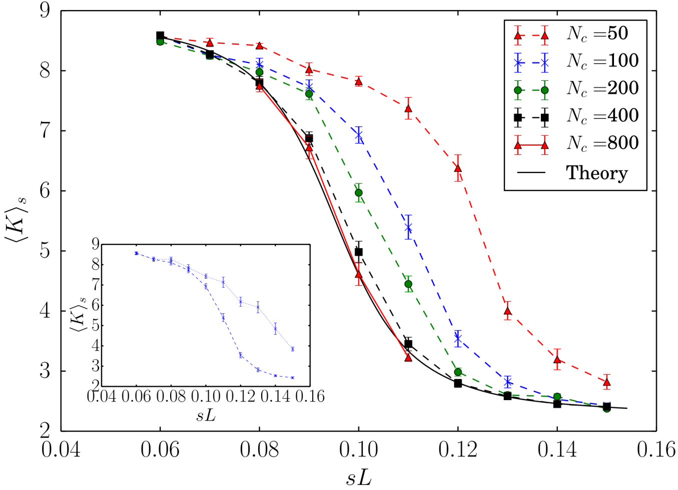
Without feedback



With feedback

Much more efficient evaluation of the biased distribution.
Even for a very crude (polynomial) approximation of the effective force.

Improvement of the small-noise crisis (ii)

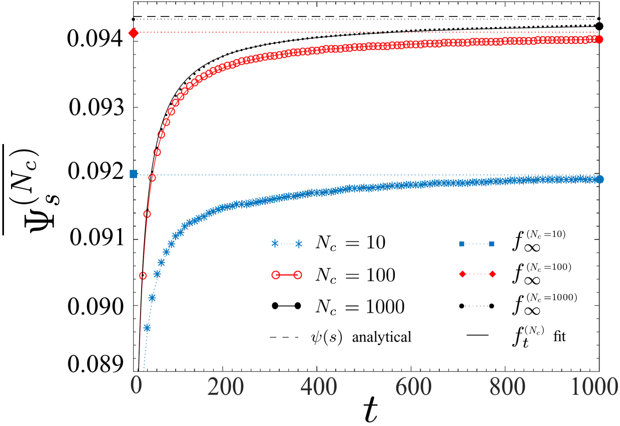


Interacting system in 1D.

Effective force: 1-, 2-, 3- body interactions only [also crude approx.].

Finite-time and -population effects

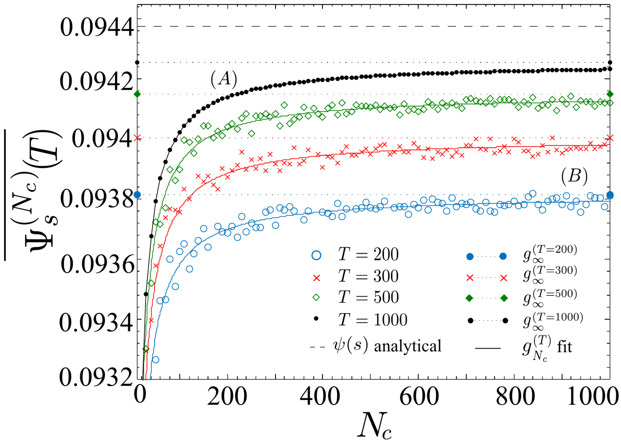
Finite-time scaling [fixed population N_c]



Estimator converges in $1/t$ to its infinite-time limit

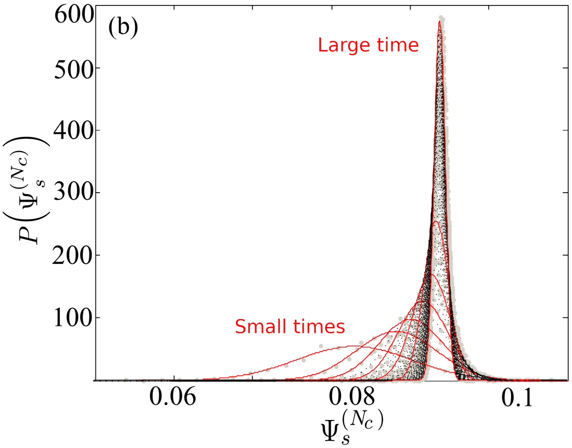
Understanding: the estimator is an additive observable of the pop. dyn.

Finite-N_c scaling [fixed time]



Estimator converges in $1/N_c$ to its infinite-population limit
Understanding: large N_c expansion, small-noise description

Distribution of the CGF estimator **[fixed population N_c]**



In the numerics: $\approx$ Gaussian when finite-N_c scaling is $O(1/N_c)$
A way to check why one is / is not in that regime

Summary and open questions (1)

Feedback method [with F Bouchet, R Jack, T Nemoto]

- Sampling problem (depletion of ancestors)
- On-the-fly evaluated auxiliary dynamics
- Solution to the small-noise crisis
- Systems with large number of degrees of freedom

Summary and open questions (1)

Feedback method [with F Bouchet, R Jack, T Nemoto]

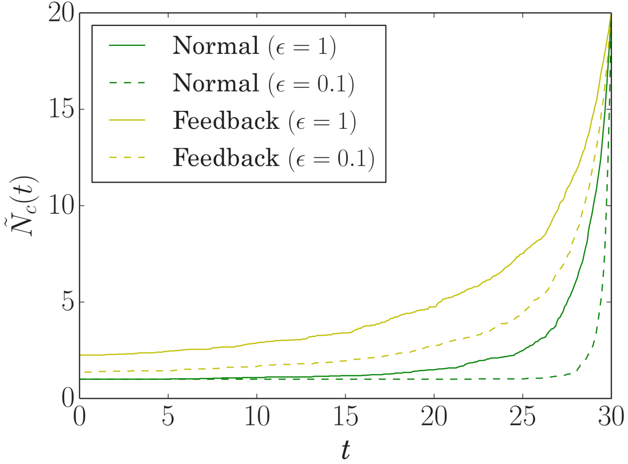
- Sampling problem (depletion of ancestors)
- On-the-fly evaluated auxiliary dynamics
- Solution to the small-noise crisis
- Systems with large number of degrees of freedom

Finite-population effects [with E Guevara, T Nemoto]

- Quantitative finite-N_{clones} scaling $\to$ interpolation method
- Initial transient regime due to small population
- Analogy with biology: many small islands *vs.* few large islands?
- Question: effective forces $\leftarrow$ selection?

Open questions (2): why is the feedback working?

Improvement of the depletion-of-ancestors problem:



Dashed line: lower noise   Continuous line: higher noise

Open questions (3)

Finite-population and -time scalings

- Anomalous fluctuations (invalid $1/N_c$ asymptotics)
- Correct description of the meta-dynamics?
- Finite-N_c and -t scaling **with feedback**
- Phase transition in the distribution of the CGF estimator?

Thank you for your attention!

References:

- ⋆ *Population dynamics method with a multi-canonical feedback control*
  Takahiro Nemoto, Freddy Bouchet, Robert L. Jack and Vivien Lecomte
  PRE **93** 062123 (2016)
- ⋆ *Finite-time and finite-size scalings in the evaluation of large deviation functions: Analytical study using a birth-death process*
  Takahiro Nemoto, Esteban Guevara Hidalgo and Vivien Lecomte
  PRE **95** 012102 (2017)
- ⋆ *Finite-size scaling of a first-order dynamical phase transition: adaptive population dynamics and effective model*
  Takahiro Nemoto, Robert L. Jack and Vivien Lecomte
  PRL **118** 115702 (2017)
- ⋆ *Finite-time and finite-size scalings in the evaluation of large deviation functions: Numerical approach in continuous time*
  Esteban Guevara Hidalgo, Takahiro Nemoto and Vivien Lecomte
  PRE **95** 062134 (2017)

Supplementary material

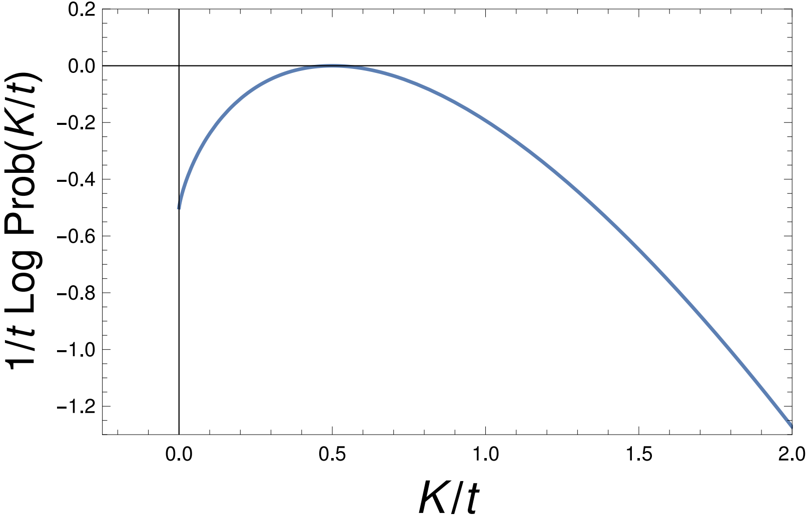
How to perform averages?

⋆ Mid-time ancestor distribution:

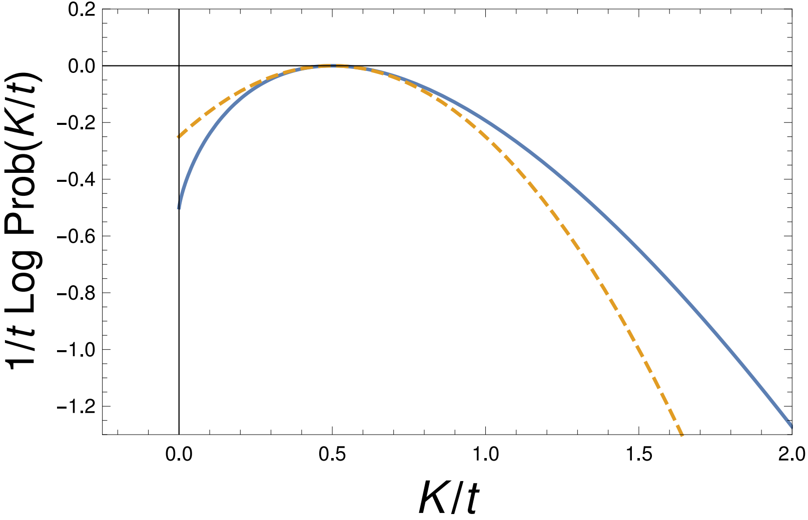
fraction of copies (at time t_1) which were in configuration $\mathcal{C}$, knowing that there are in configuration $\mathcal{C}_\mathsf{f}$ at final time t_f:

$$p_{\mathsf{anc}}(\mathcal{C}, t_1; \mathcal{C}_\mathsf{f}, t_\mathsf{f}) = \frac{\langle N_{\mathsf{nc}}(\mathcal{C}_\mathsf{f}, t_\mathsf{f} | \mathcal{C}, t_1) \rangle_s}{\sum_{\mathcal{C}'} \langle N_{\mathsf{nc}}(\mathcal{C}_\mathsf{f}, t_\mathsf{f} | \mathcal{C}', t_1) \rangle_s} \underset{t_{\mathsf{f},1} \to \infty}{\sim} \langle L | \mathcal{C} \rangle \langle \mathcal{C} | R \rangle = p_{\mathsf{ave}}(\mathcal{C})$$

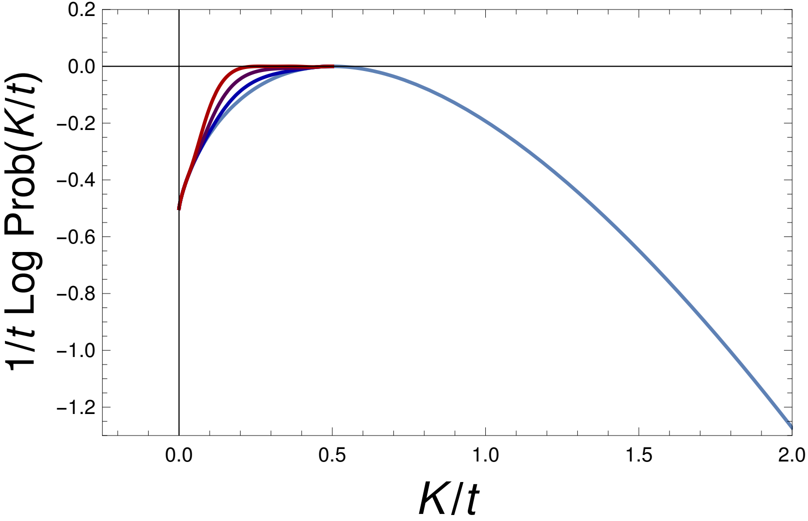
The “ancestor statistics” of a configuration $\mathcal{C}_\mathsf{f}$ is thus independent (far enough in the past) of the configuration $\mathcal{C}_\mathsf{f}$.



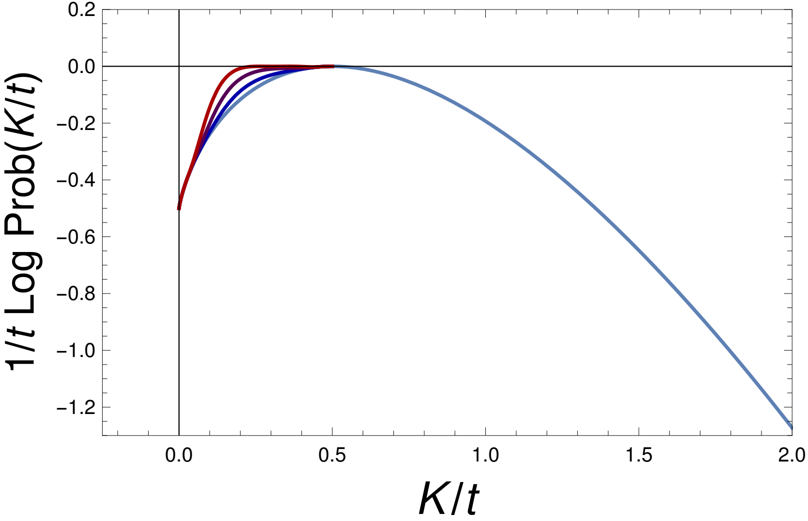
$$\mathrm{Prob}[K] \sim e^{t\,\varphi(K/t)}$$



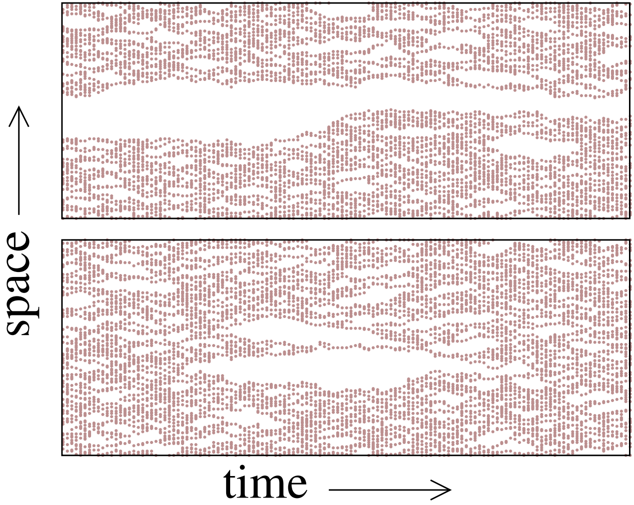
$\text{Prob}[K] \sim e^{t\,\varphi(K/t)}$



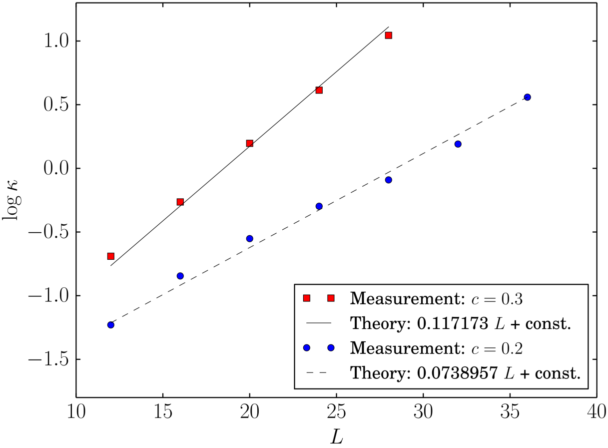
$\text{Prob}[K] \sim e^{t\,\varphi(K/t)}$



$\mathrm{Prob}[K] \sim e^{t\,\varphi(K/t)}$ Finite-time & -size scalings matter.

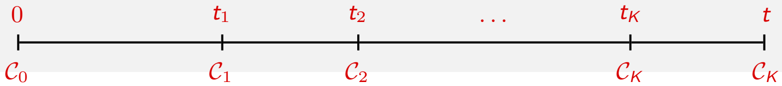


[Merolle, Garrahan and Chandler, 2005]



Exponential divergence of the susceptibility

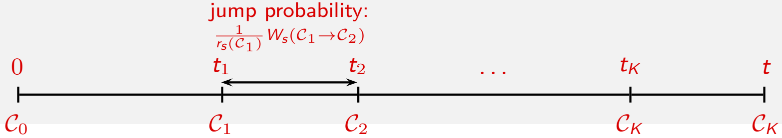
Explicit construction (1/3)



Probability-preserving contribution

$$\partial_t \hat{P}(\mathcal{C},t) = \sum_{\mathcal{C}'} \Big\{ \underbrace{W_s(\mathcal{C}' \to \mathcal{C})\hat{P}(\mathcal{C}',t)}_{\text{gain term}} - \underbrace{W_s(\mathcal{C} \to \mathcal{C}')\hat{P}(\mathcal{C},t)}_{\text{loss term}} \Big\}$$

Explicit construction (1/3)



Which configurations will be visited?

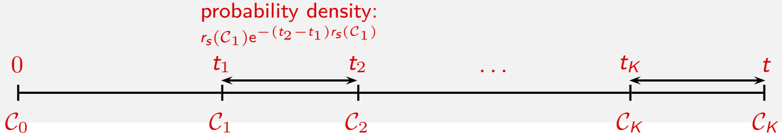
Configurational part of the trajectory: $\mathcal{C}_0 \to \dots \to \mathcal{C}_K$

$$\text{Prob}\{\text{hist}\} = \prod_{n=0}^{K-1} \frac{W_s(\mathcal{C}_n \to \mathcal{C}_{n+1})}{r_s(\mathcal{C}_n)}$$

where

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

Explicit construction (2/3)

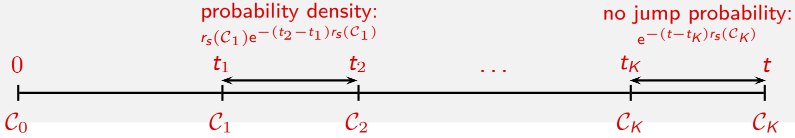


When shall the system jump from one configuration to the next one?

- probability density for the time interval $t_n - t_{n-1}$

$$r_s(\mathcal{C}_{n-1})\mathrm{e}^{-(t_n-t_{n-1})r_s(\mathcal{C}_{n-1})}$$

Explicit construction (2/3)



When shall the system jump from one configuration to the next one?

- probability density for the time interval $t_n - t_{n-1}$

$$r_s(\mathcal{C}_{n-1})\mathrm{e}^{-(t_n-t_{n-1})r_s(\mathcal{C}_{n-1})}$$

- probability not to leave $\mathcal{C}_K$ during the time interval $t - t_K$

$$\mathrm{e}^{-(t-t_K)r_s(\mathcal{C}_K)}$$

Explicit construction (3/3)

$$\partial_t \hat{P}(\mathcal{C},s) = \underbrace{\sum_{\mathcal{C}'} W_s(\mathcal{C}' \to \mathcal{C})\hat{P}(\mathcal{C}',s) - r_s(\mathcal{C})\hat{P}(\mathcal{C},s)}_{\text{modified dynamics}} \;+\; \underbrace{\delta r_s(\mathcal{C})\hat{P}(\mathcal{C},s)}_{\text{cloning term}}$$

How to take into account loss/gain of probability?

- handle a large number of copies of the system
- implement a selection rule: on a time interval Δt a copy in config $\mathcal{C}$ is replaced by $e^{\Delta t\,\delta r_s(\mathcal{C})}$ copies
- $\psi(s)$ = the rate of exponential growth/decay of the total population
- optionally: keep population constant by non-biased pruning/cloning

Explicit construction (3/3)

$$\partial_t \hat{P}(\mathcal{C},s) = \underbrace{\sum_{\mathcal{C}'} W_s(\mathcal{C}' \to \mathcal{C})\hat{P}(\mathcal{C}',s) - r_s(\mathcal{C})\hat{P}(\mathcal{C},s)}_{\text{modified dynamics}} \; + \; \underbrace{\delta r_s(\mathcal{C})\hat{P}(\mathcal{C},s)}_{\text{cloning term}}$$

How to take into account loss/gain of probability?

- handle a large number of copies of the system
- implement a selection rule: on a time interval Δt
  a copy in config $\mathcal{C}$ is replaced by $\lfloor e^{\Delta t\, \delta r_s(\mathcal{C})} + \varepsilon \rfloor$ copies, $\epsilon \sim [0,1]$
- $\psi(s)$ = the rate of exponential growth/decay of the total population
- optionally: keep population constant by non-biased pruning/cloning

Explicit construction (3/3)

$$\partial_t \hat{P}(\mathcal{C},s) = \underbrace{\sum_{\mathcal{C}'} W_s(\mathcal{C}' \to \mathcal{C})\hat{P}(\mathcal{C}',s) - r_s(\mathcal{C})\hat{P}(\mathcal{C},s)}_{\text{modified dynamics}} \; + \; \underbrace{\delta r_s(\mathcal{C})\hat{P}(\mathcal{C},s)}_{\text{cloning term}}$$

How to take into account loss/gain of probability?

- handle a large number of copies of the system
- implement a selection rule: on a time interval Δt
  a copy in config $\mathcal{C}$ is replaced by $\lfloor e^{\Delta t\,\delta r_s(\mathcal{C})} + \varepsilon \rfloor$ copies, $\epsilon \sim [0,1]$
- $\psi(s)$ = the rate of exponential growth/decay of the total population
- optionally: keep population constant by non-biased pruning/cloning

Explicit construction (3/3)

$$\partial_t \hat{P}(\mathcal{C},s) = \underbrace{\sum_{\mathcal{C}'} W_s(\mathcal{C}' \to \mathcal{C})\hat{P}(\mathcal{C}',s) - r_s(\mathcal{C})\hat{P}(\mathcal{C},s)}_{\text{modified dynamics}} \; + \; \underbrace{\delta r_s(\mathcal{C})\hat{P}(\mathcal{C},s)}_{\text{cloning term}}$$

How to take into account loss/gain of probability?

- handle a large number of copies of the system
- implement a selection rule: on a time interval Δt
  a copy in config $\mathcal{C}$ is replaced by $\lfloor e^{\Delta t\, \delta r_s(\mathcal{C})} + \varepsilon \rfloor$ copies, $\epsilon \sim [0,1]$
- $\psi(s)$ = the rate of exponential growth/decay of the total population
- optionally: keep population constant by non-biased pruning/cloning

Explicit construction (3/3)

$$\partial_t \hat{P}(\mathcal{C},s) = \underbrace{\sum_{\mathcal{C}'} W_s(\mathcal{C}' \to \mathcal{C})\hat{P}(\mathcal{C}',s) - r_s(\mathcal{C})\hat{P}(\mathcal{C},s)}_{\text{modified dynamics}} + \underbrace{\delta r_s(\mathcal{C})\hat{P}(\mathcal{C},s)}_{\text{cloning term}}$$

Biological interpretation

- copy in configuration $\mathcal{C} \equiv$ organism of **genome** $\mathcal{C}$
- dynamics of rates $W_s \equiv$ **mutations**
- cloning at rates $\delta r_s \equiv$ **selection** rendering atypical histories typical