# Large deviations and population dynamics: finite-population effects

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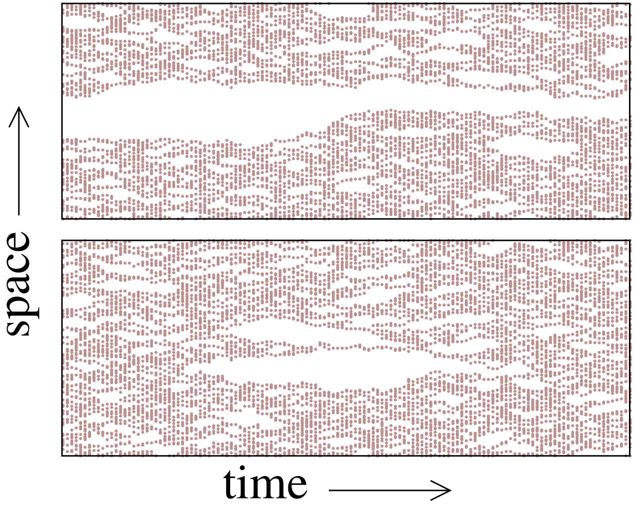
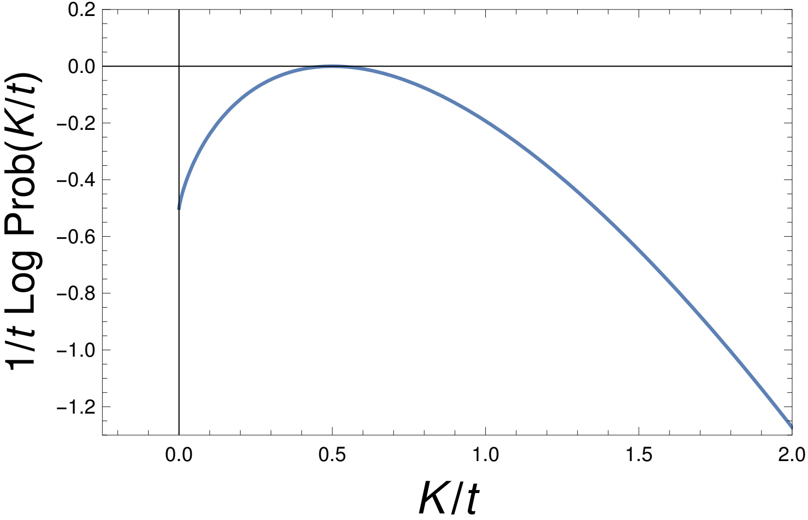
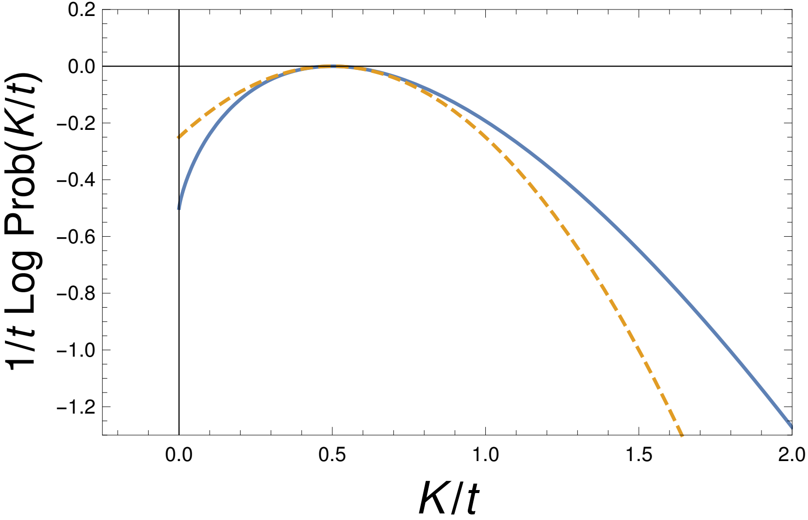



[Merrolle, Garrahan and Chandler, 2005]

Order parameter: additive observable $K$ (= number of events)




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

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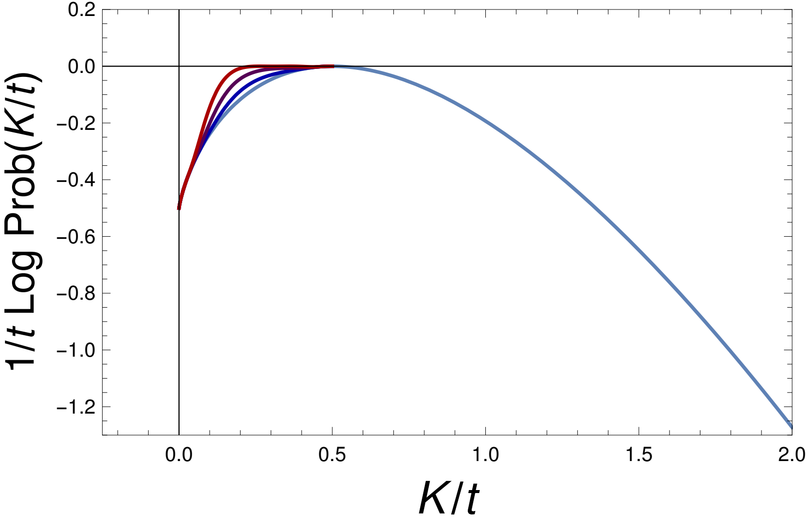


$\text{Prob}[K] \sim e^{t\,\varphi(K/t)}$ Finite-time & -size scalings matter.

# $s$-modified dynamics

- Markov processes:

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

# $s$-modified dynamics    $K$ =activity

- Markov processes:

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

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

- Canonical description: $s$ 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]

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

# Numerical method [with J. Tailleur]

## Evaluation of large deviation functions [*à la* Monte-Carlo diffusion]

$$Z(s,t) = \sum_{\mathcal{C}} \hat{P}(\mathcal{C}, s, t) = \langle e^{-s K} \rangle \sim e^{-t\,\psi(s)}$$

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

## Cloning dynamics

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

- $W_s(\mathcal{C}' \to \mathcal{C}) = e^{-s} W(\mathcal{C}' \to \mathcal{C})$
- $r_s(\mathcal{C}) = \sum_{\mathcal{C}'} W_s(\mathcal{C} \to \mathcal{C}')$
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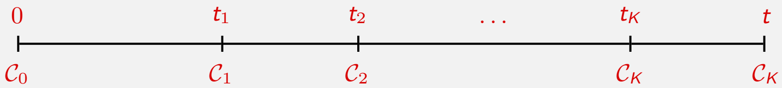
# Explicit construction (1/3)




## Probability-preserving contribution

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

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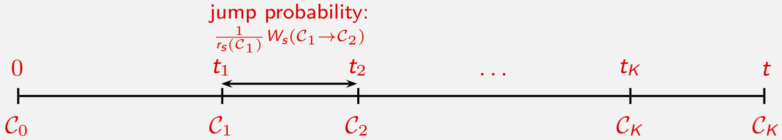



## Which configurations will be visited?

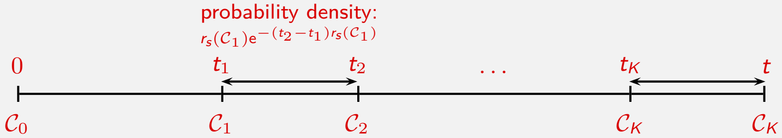
Configurational part of the trajectory: $\mathcal{C}_0 \to \dots \to \mathcal{C}_K$

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

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 $t_n - t_{n-1}$

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

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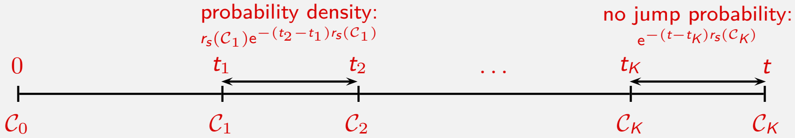


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- probability density for the time interval $t_n - t_{n-1}$

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

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

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

# 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?

- make evolve a large number of copies of the system
- implement a selection rule: on a time interval $\Delta t$ 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 un-biased pruning/cloning

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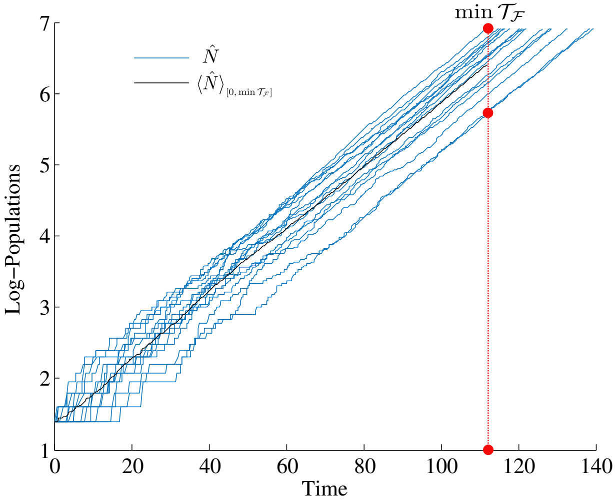
# Non-constant population [with E Guevara]



# Questions

Source of errors when evaluating the CGF $\psi(s)$:

1. Diversity issue
2. Finite-time and finite-population issues

CGF = (scaled) Cumulant Generating Function

# How to perform averages? (1/2) [with R Jack, F Bouchet, T Nemoto]

⋆ **Final-time distribution**: *proportion* of copies in $\mathcal{C}$ at $t$

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

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

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

[$N_{\text{nc}}$ = number in non-constant population dynamics]

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

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

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

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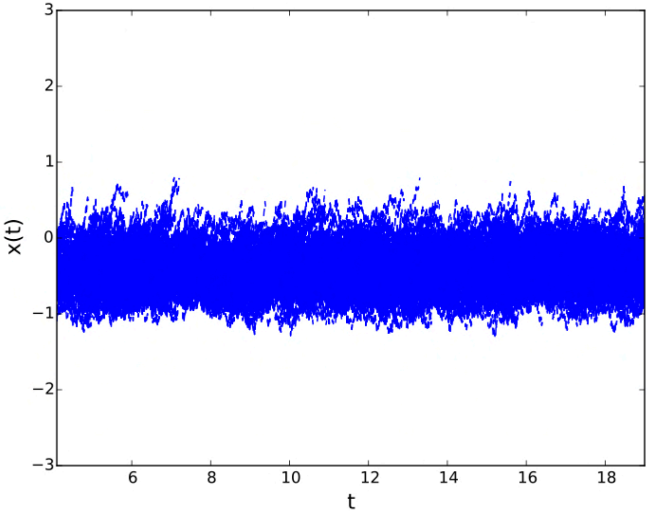
$$p_{\rm end}(\mathcal{C},t) = \frac{\langle N_{\rm nc}(\mathcal{C},t)\rangle_s}{\langle N_{\rm nc}(t)\rangle_s} \underset{t\to\infty}{\sim} \langle \mathcal{C}|R\rangle \equiv p_{\rm end}(\mathcal{C})$$

[$N_{\rm nc}$ = number in non-constant population dynamics]

Final-time distribution governed by **right** eigenvector of $\mathbb{W}_s$.


3
2
1
0
−1
−2
−3
x(t)
6
8
10
12
14
16
18
t

# How to perform averages? (2/2)

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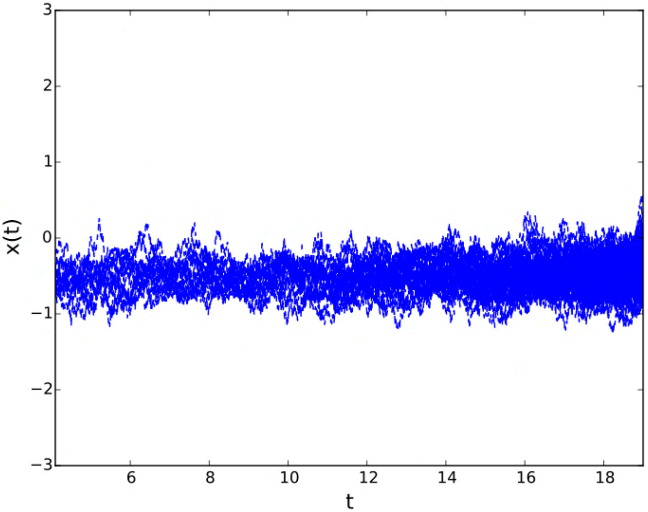
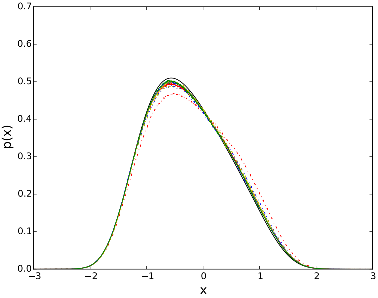
Mid-time distribution governed by **left** and **right** eigenvectors of $\mathbb{W}_s$.

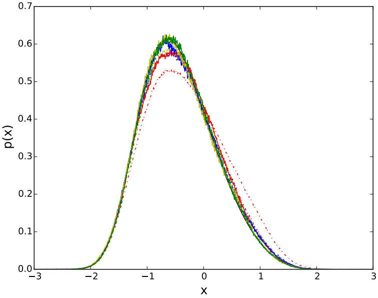



Huge sampling issue

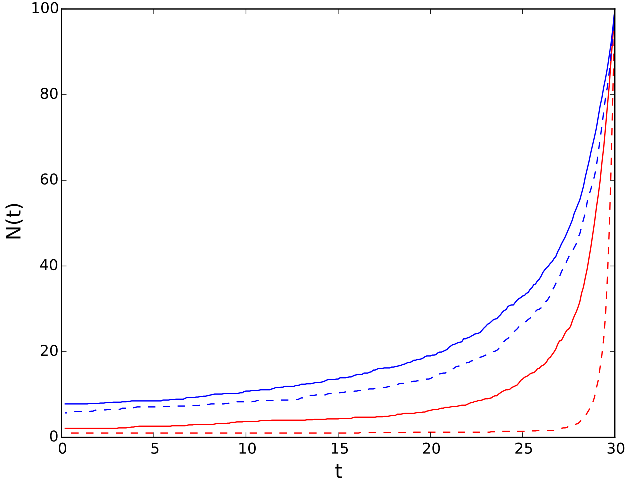
# Example distributions for a simple Langevin dynamics




$p_{\text{end}}(x)$




$p_{\text{ave}}(x)$




$N(t)$ = number of surviving trajectories on $[t, t_{\text{final}}]$

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

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

- Probability preserving
- No mismatch between $p_{\text{ave}}$ and $p_{\text{end}}$
- Constructed as: [$\hat{L}$ = diagonal matrix of elements $L$]

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- Issue: determining $L$ is difficult
- Solution: evaluate $L$ as $L_{\text{test}}$ on the fly and simulate

$$\mathbb{W}_s^{\text{test}} = L_{\text{test}}\,\mathbb{W}_s\,L_{\text{test}}^{-1}$$

- Whichever $L_{\text{test}}$, the simulation is still correct.

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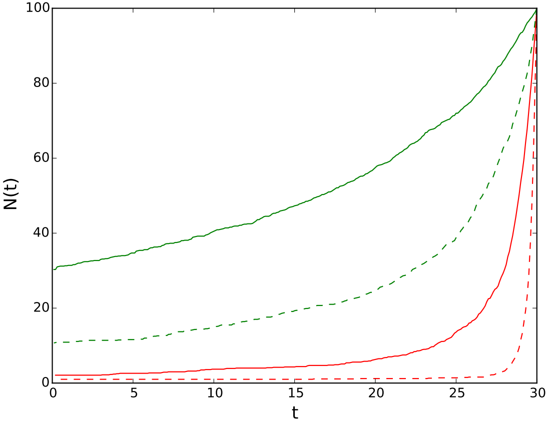
Similar in spirit to **multi-canonical** (e.g. Wang-Landau) approach in static thermodynamics

Improvement of the depletion-of-ancestors problem:

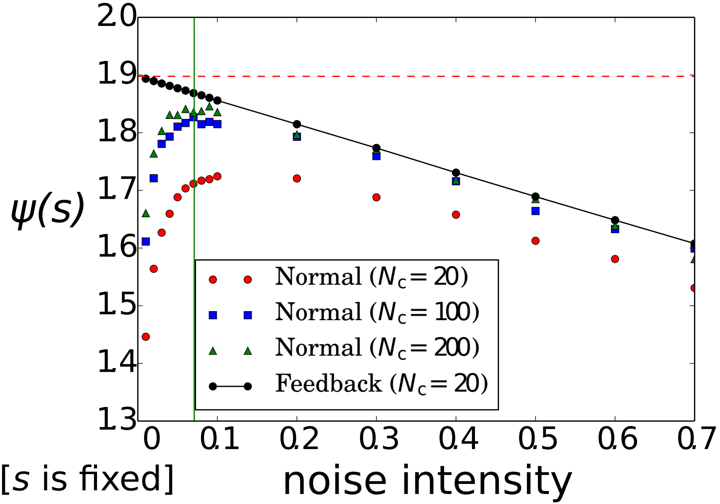



Red: without multicanonical sampling.

Green: with multicanonical sampling ($L_{\text{test}}$ evaluated on the fly)

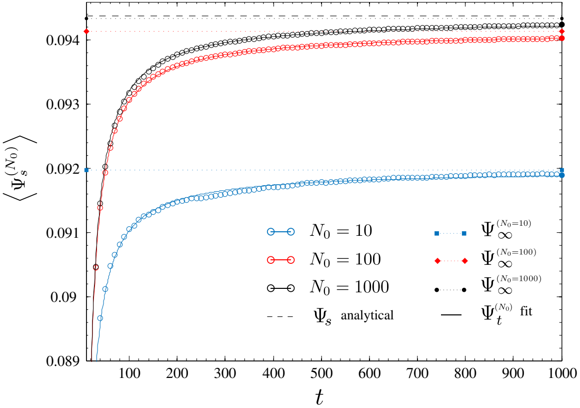
Dashed: lower temperature

Improvement of the small-noise crisis:



# Numerical observations (1/3) [with T. Nemoto & E. Guevara]

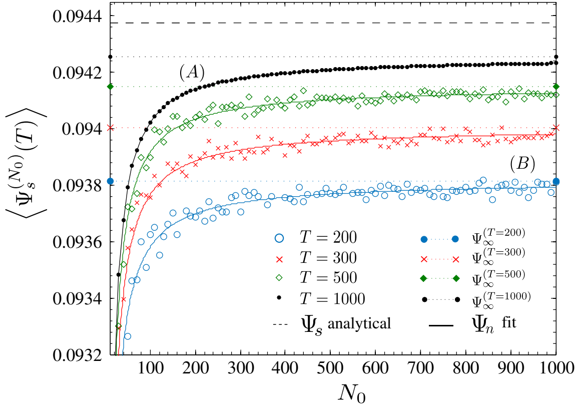
**Large-$t$ asymptotics** at fixed population size $N_0$.




$$\underbrace{\left\langle \Psi_s^{(N_0)}(t) \right\rangle}_{\text{numerical estimator}} = \Psi_s^{(N_0)} + \frac{1}{t} \Delta\Psi_s^{(N_0)}$$

# Numerical observations (2/3) [with T. Nemoto & E. Guevara]

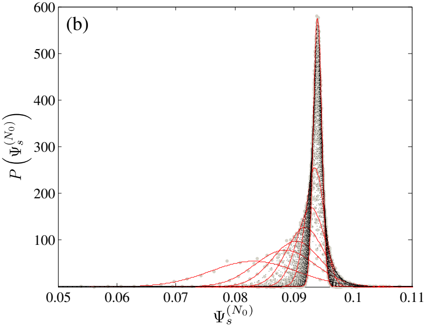
**Large-$N_0$ asymptotics** at fixed final time $T$.

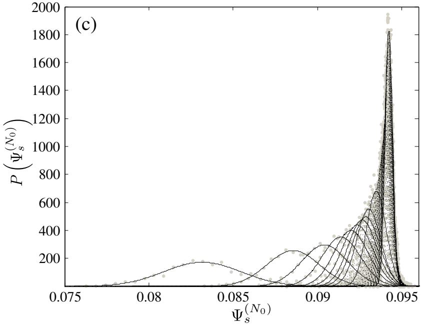



$$\underbrace{\left\langle \Psi_s^{(N_0)}(T) \right\rangle}_{\text{numerical estimator}} = \Psi_s^{(\infty)} + \frac{1}{N_0} \Delta\Psi_s^{(\infty)}$$

# Numerical observations (3/3) [with T. Nemoto & E. Guevara]

**Distribution** of large-deviation estimators.



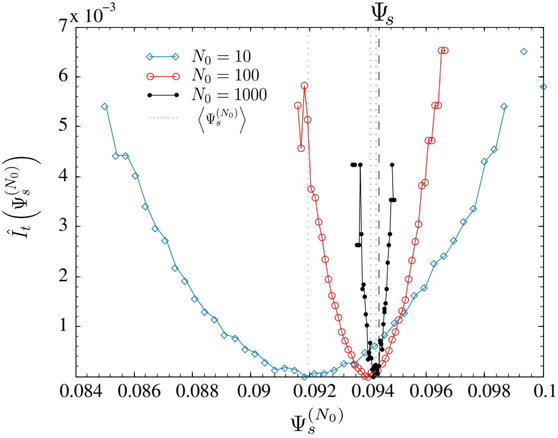




$N_0 = 100$ $N_0 = 1000$

Stochastic errors **and** systematic errors at finite $N_0$.

# Numerical observations (3/3) [with T. Nemoto & E. Guevara]

**Large deviations** of large-deviations.




$$\mathbb{P}\left(\Psi_s^{(N_0)}\right) \sim e^{-t\,\hat{I}(\Psi_s^{(N_0)})}$$

# Analytical approach (1/3) [with T. Nemoto & E. Guevara]

(Fixed $N_0$) **death-birth** process to represent the population dynamics:

- Preserves probability.
- LDF estimator is $(\frac{1}{t}\times)$ an additive observable of the trajectory.

$$\Psi_s^{(N_0)} = \frac{1}{t} \log \prod_{\text{events}} \frac{N_0 + \overbrace{\text{number of } \textit{offsprings}}^{\in\{-1,0,1,\ldots\}}}{N_0}$$

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- Large-deviation principle applies to the distribution of $\Psi_s^{(N_0)}$:

$$\mathbb{P}\big(\Psi_s^{(N_0)}\big) \sim e^{-t\,\hat{I}(\Psi_s^{(N_0)})}$$

- Aim:

$$\underbrace{\langle \Psi_s^{(N_0)} \rangle}_{\substack{\text{death-birth}\\ \text{process}}} \to \underbrace{\psi(s)}_{\substack{\text{original}\\ \text{CGF}}}$$

# Analytical approach (2/3) [with T. Nemoto & E. Guevara]

Route to follow:

- Determine the rates of the death-birth process (at fixed $N_0$).
- Write the steady-state equation for the death-birth process.
- Project on the occupation number.
- Show that, in the steady-state the fractions

$$p_{\mathcal{C}} \equiv \left\langle \frac{\text{number of copies in configuration } \mathcal{C}}{N_0} \right\rangle$$

  **obey the original $s$-modified master equation**.
- Hypothesis: at large $N_0$, independence

$$\left\langle \frac{\text{number of copies in configuration } \mathcal{C}}{N_0} \frac{\text{number of copies in configuration } \mathcal{C}'}{N_0} \right\rangle \propto \delta_{\mathcal{C}\mathcal{C}'}$$

# Analytical approach (3/3) [with T. Nemoto & E. Guevara]

Infinite-$N_0$ limit and large-$N_0$ asymptotics:

$$\text{fluctuating} \quad x_{\mathcal{C}} \equiv \frac{\substack{\text{number of copies} \\ \text{in configuration } \mathcal{C}}}{N_0} \qquad \left( \Rightarrow p_{\mathcal{C}} = \langle x_{\mathcal{C}} \rangle \right)$$

- Large $N_0$ expansion (*à la* van Kampen)
- At infinite $N_0$: the $x_{\mathcal{C}}$ **obey deterministic equations**.

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- Large $N_0$ expansion (*à la* van Kampen)
- At infinite $N_0$: the $x_{\mathcal{C}}$ **obey deterministic equations**.
- At large $N_0$: noise of amplitude $\sqrt{N_0}$.
- Large-deviation principle

$$\boxed{\mathbb{P}\big(\Psi_s^{(N_0)}\big) \sim e^{-tN_0\, J(\Psi_s^{(N_0)})}}$$

*i.e.*

$$\lim_{N_0\to\infty} \lim_{t\to\infty} \frac{1}{N_0 t} \log \mathbb{P}\big(\Psi_s^{(N_0)}\big) = J\big(\Psi_s^{(N_0)}\big)$$

# Averaging

Exercise/riddle for you:

$$\Big\langle \underbrace{\log \prod_{\text{events}} \frac{N_0 + \substack{\text{number of}\\ \textit{offsprings}}}{N_0}}_{\text{this is } \Psi_s^{(N_0)}} \Big\rangle \quad \textit{vs.} \quad \log \Big\langle \prod_{\text{events}} \frac{N_0 + \substack{\text{number of}\\ \textit{offsprings}}}{N_0} \Big\rangle$$

Which is the “best” estimator of the CGF $\psi(s)$?

# Summary and questions

(1) Multicanonical approach [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 chaos/large number of degrees of freedom?

# Summary and questions

### (1) Multicanonical approach [with F Bouchet, R Jack, T Nemoto]

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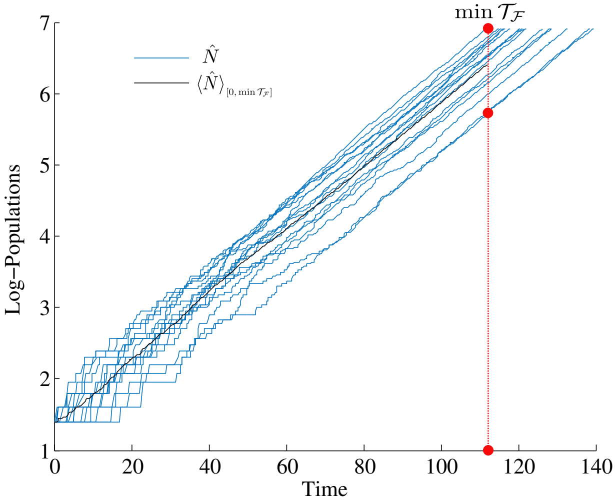
### (2) Finite-time $t$ and finite-population $N_0$ [with E Guevara, T Nemoto]

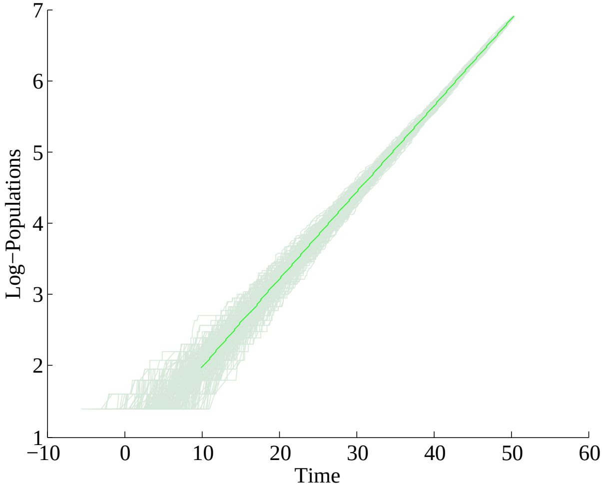
- LDF estimator converges at (i) $t \to \infty$ (ii) $N_0 \to \infty$
- Order of the correction understood
- Gives an interpolation procedure for the numerics
- Phase transitions? Absence of steady-state?
- Combine (1) and (2)?

# Initial transient regime [with E. Guevara]

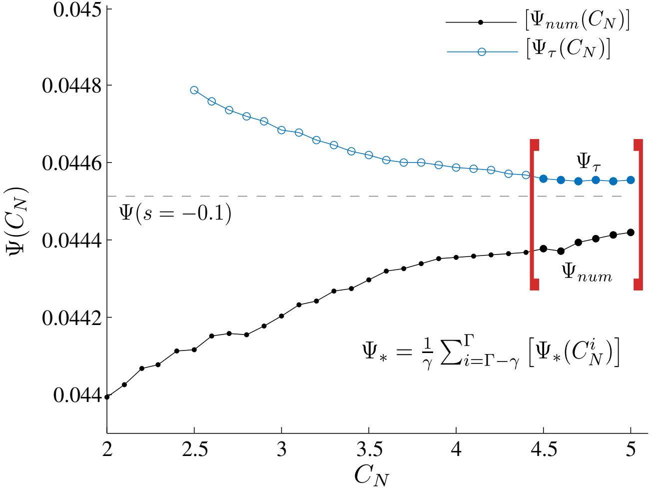
Non-constant population dynamics



# Time-delay



# Improvement of the numerical evaluation of $\psi(s)$



# Distribution of time delays