A framework for the direct evaluation of large deviations in non-Markovian processes

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Introduction

- In non-equilibrium physics we target trajectories in space-time rather than static configurations.
- The details of the time evolution take on a major role and temporal correlations can have dramatic effects on fluctuations of time-extensive observables, such as the current J [1].
- Numerical tools to explore systematically large deviations in non-Markovian processes are needed.
- We extend the "cloning" procedure of Ref. [2] to such processes.

Themodynamics of trajectories

- Trajectory:

$$w(t) := (t_0, x_0,\ t_1, x_1,\ t_2, x_2\ \dots\ t_n, x_n,\ t).$$

- Probability density:

$$\varrho[w(t)] = \phi_{x_n}[t - t_n|w(t_n)]\psi_{x_n,x_{n-1}}[t_n - t_{n-1}|w(t_{n-1})]\dots \times \psi_{x_1,x_0}[t_1 - t_0|w(t_0)]P_{x_0}(t_0).$$

- "Canonical" partition function:

$$Z(s,t) = \int e^{-sJ[w(t)]}\varrho[w(t)]dw(t).$$

- Large deviation principle:

$$\mathrm{Prob}\{J/t = j\} \asymp e^{-t\hat{e}(j)}.$$

- Dynamical free energy:

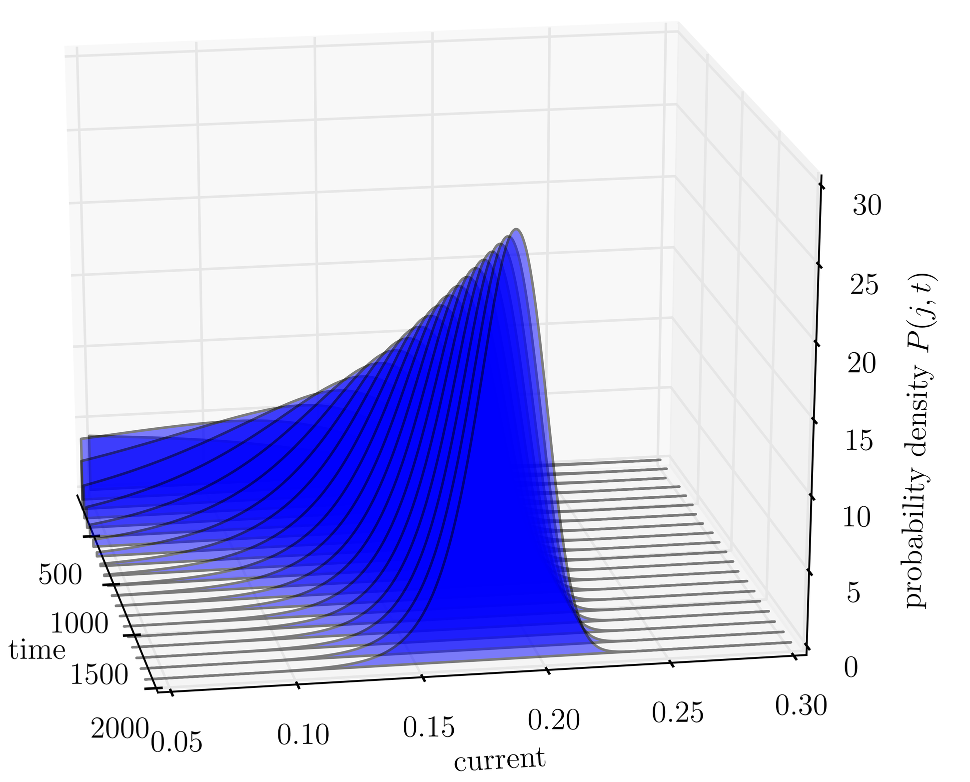
$$e(s) = -\lim_{t\to\infty}\frac{1}{t}\ln Z(s,t).$$

- Rate function (Gärtner-Ellis theorem):

$$\hat{e}(j) = \sup_s\{e(s) - sj\}.$$

Cloning approach

- We wish to find $Z(s,t)$.
- Problem: exponentially fast loss of information on rare trajectories (see figure).
- Solution: cloning/pruning of relevant trajectories [2, 3].



- In non-Markovian processes:
$e^{-sJ[w(t)]}\varrho[w(t)] = \phi_{x_n}[t - t_n|w(t_n)]e^{-s\theta_{x_n,x_{n-1}}}p_{x_n,x_{n-1}}[t_n - t_{n-1}|w(t_{n-1})]\psi_{x_n,x_{n-1}}[t_n - t_{n-1}|w(t_{n-1})]\dots\times e^{-s\theta_{x_1,x_0}}p_{x_1,x_0}[t_1 - t_0|w(t_0)]\psi_{x_1,x_0}[t_1 - t_0|w(t_0)]P_{x_0}(t_0)$.

Algorithm

1. Set up an ensemble of N clones and initialise each with a given time t_0, a random configuration x_0, and a counter $n = 0$. Set a variable C to zero. For each clone, draw a time t of the next jump from the density $\psi_{x_0}[t - t_0|w(t_0)]$, and then choose the clone with the smallest value of t.
2. For the chosen clone, update n to $n + 1$, and x_{n-1} to x_n according to the probability mass $p_{x_n,x_{n-1}}[t - t_{n-1}|w(t_{n-1})]$.
3. Generate a new waiting time τ for the updated clone according to $\psi_{x_{n-1}}[\tau|w(t_{n-1})]$ and increment t to $t + \tau$.
4. **Cloning step.** Compute $y = \lfloor e^{-s\theta_{x_n,x_{n-1}}} + u\rfloor$, where u is drawn from a uniform distribution in $[0, 1)$.

4.1 If $y = 0$, prune the current clone. Then replace it with another one, uniformly chosen among the remaining $N - 1$.

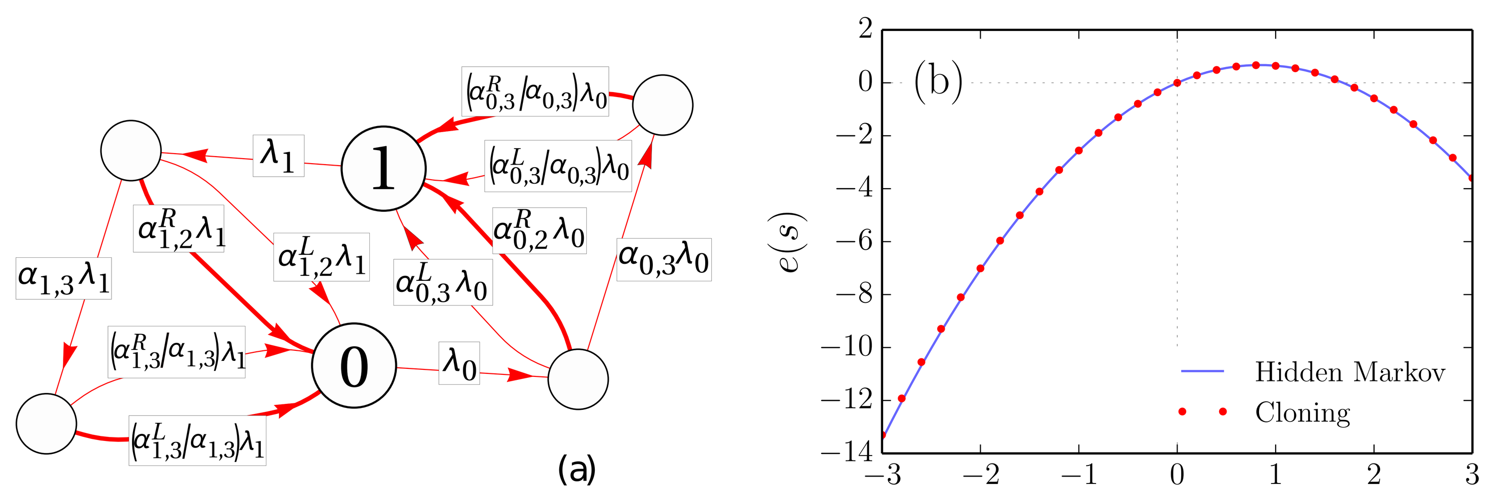
4.2 If $y > 0$, produce y copies of the current clones. Then, prune a number y of elements, uniformly chosen among the existing $N + y$.

5. Increment C to $C + \ln[(N + e^{-s\theta_{x_n,x_{n-1}}} - 1)/N]$. Choose the clone with the smallest t, and repeat from 2) until the chosen t reaches the desired simulation time T.

$Z(s,t)$ is finally recovered as $-C/T$ for large T.

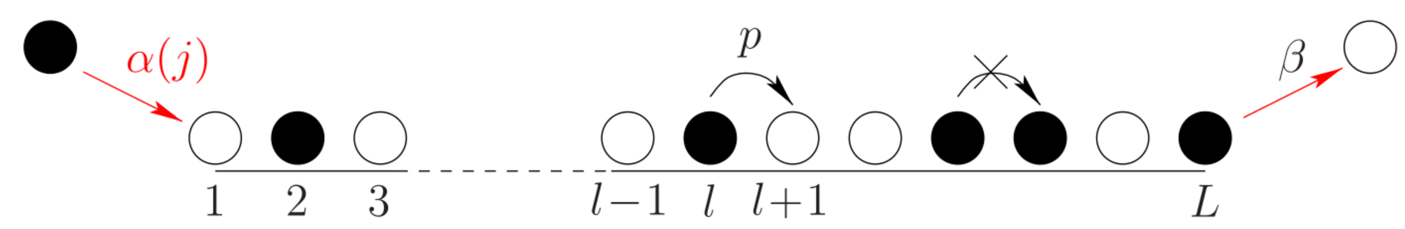
Example: two-state toy model

- The system can be in either state 0 or 1. Transitions triggered by two mechanisms with Gamma distributed inter-event times [4].
- After each transition, memory is reset (semi-Markov process).

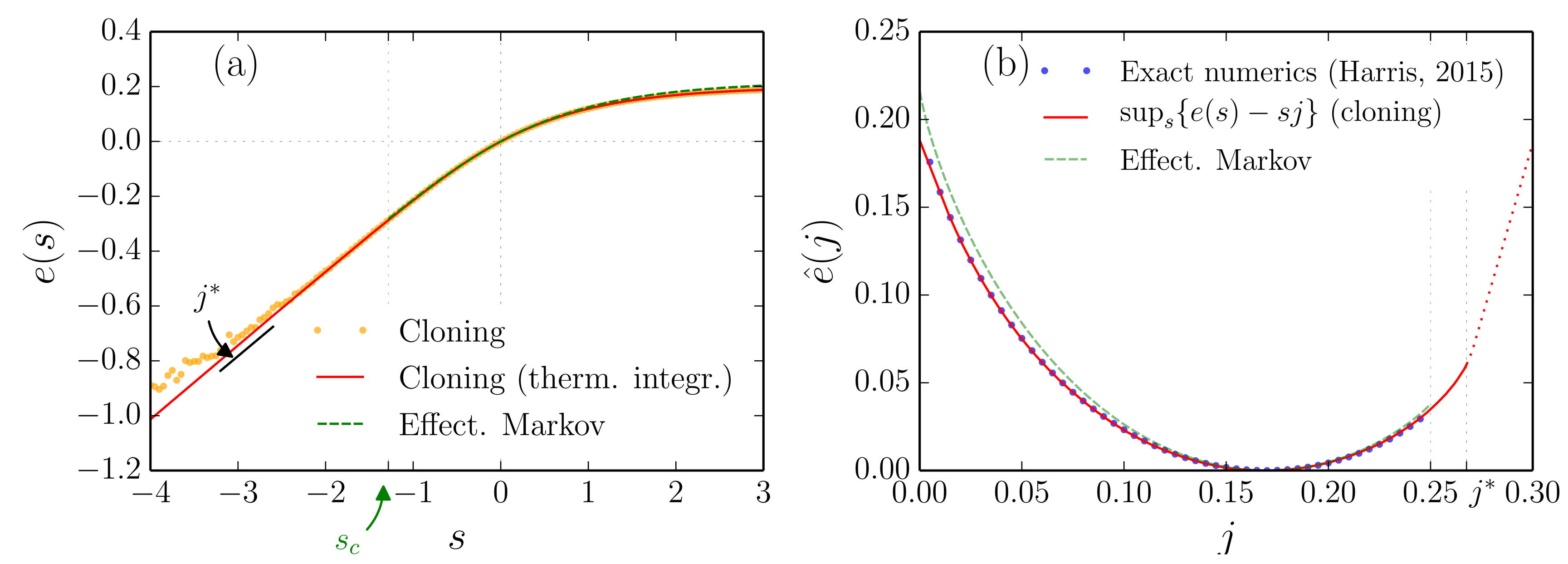


(a) Formulation in terms of Markov process with hidden variables serves as test.
(b) Excellent agreement between the cloning procedure and the exact numerics.

Example: trajectory-dependent TASEP



- Totally Asymmetric Simple Exclusion Process with open boundaries.
- A mechanism injects particles with time-dependent rate $\alpha[j(t)]$.
- Numerical results for the low density phase with positive feedback.



(a) Threshold value j^* detected. Dynamical transition to a "maximal-current" phase [4].
(b) Cloning results in excellent agreement with temporal additivity principle [5].

Discussion

- "Cloning" is a continuous-time sequential Monte Carlo method [6] to explore large-deviation events.
- It can be applied consistently to both Markovian and non-Markovian dynamics.
- Its efficacy has been extensively tested on models whose large deviations can be obtained by other means.
- Further details in Ref. [4].
- Applications to teletraffic engineering in Ref. [7].

References

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