A numerical approach to large deviations in continuous-time

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Abstract

Over the last decade, there has been a growing interest within the physics community in the use of large deviation functions to describe the fluctuations of physical observables. This tools proved especially well-suited to probe transient or non-equilibrium phenomena, for which one lacks a general approach such as the Boltzmann-Gibbs thermodynamics of equilibrium.

We present an algorithm to evaluate the large deviation functions associated to history-dependent observables. Instead of relying on a time discretisation procedure to approximate the dynamics, we provide a direct continuous-time algorithm, valuable for systems with multiple time scales, thus extending the work of Giardinà, Kurchan and Peliti [1]. The procedure yields a direct access to typical configurations giving birth to deviations, which we illustrate on a driven lattice gas.

We also show how the method can be used to probe large deviation functions in systems with a dynamical phase transition – revealed in our context through the appearance of a non-analyticity in the large deviation functions and a discontinuity of the (dynamical) order parameter.

Large Deviations: Motivations

- *Boltzmann-Gibbs* thermodynamics

$$\Omega(E,L) = \left| \begin{array}{l}\text{number of configurations}\\ \text{with energy } E\end{array}\right. \qquad \text{(large volume } L)$$

$$Z(\beta,L) = \sum_E \Omega(E,L)\,\mathrm{e}^{-\beta E} \qquad \text{(partition function)}$$

- Statistics over histories (in the spirit of Ruelle, Gaspard)

$$\Omega_{\rm dyn}(A,t) = \left| \begin{array}{l}\text{number of histories with a given value of the}\\ \text{time-extensive observable } A \text{ between 0 et } t\end{array}\right. \qquad \text{(large time } t)$$

$$Z_A(s,t) = \sum_A \Omega_{\rm dyn}(A,t)\,\mathrm{e}^{-sA} \qquad \text{(dynamical partition function)}$$

Examples: A= integrated current, number of events.

Markov Stochastic Dynamics

- Dynamics
  - ⋆ Probability of being in configuration $\mathcal{C}$ at time t

$$\partial_t P(\mathcal{C},t) = \sum_{\mathcal{C}'} W(\mathcal{C}'\to\mathcal{C})P(\mathcal{C}',t) \;-r(\mathcal{C})P(\mathcal{C},t) \qquad \text{(master equation)}$$

$$r(\mathcal{C}) = \sum_{\mathcal{C}'} W(\mathcal{C}\to\mathcal{C}'). \qquad \text{(escape rate from } \mathcal{C})$$

  - ⋆ Histories (**Fig. 1**)

Probability of a jump $\mathcal{C}_k \to \mathcal{C}_{k+1}$:

$$\text{Prob}[\mathcal{C}_k\to\mathcal{C}_{k+1}] = \frac{W(\mathcal{C}_k\to\mathcal{C}_{k+1})}{r(\mathcal{C}_k)}$$

Waiting time probability density: $\text{prob}[t_{k+1}-t_k] = r(\mathcal{C}_k)e^{-(t_{k+1}-t_k)r(\mathcal{C}_k)}$

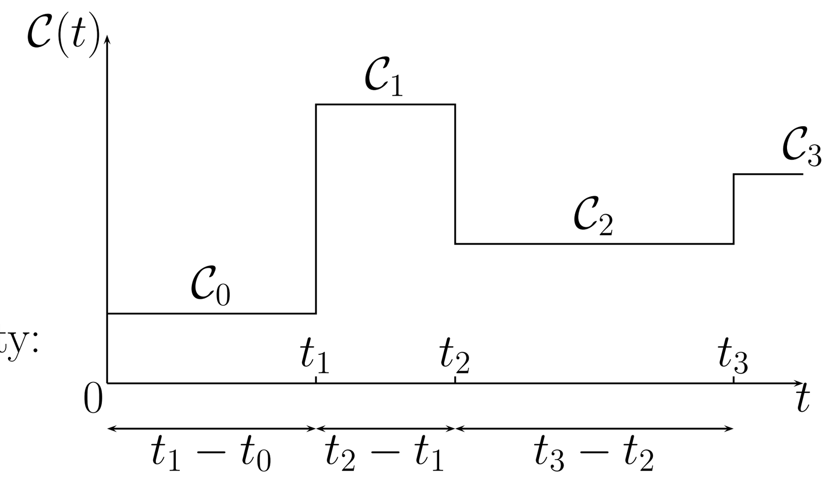


Figure 1: an history in continuous time

- Time-extensive observable A[hist] and large-deviation functions

$$A[\text{hist}] = \sum_{k=0}^{K-1} \alpha(\mathcal{C}_k,\mathcal{C}_{k+1})$$

$$P(A/t=a,t) \sim e^{t\,\pi(a)} \qquad (\pi(a)\text{: dynamical entropy})$$

$$Z_A(s,t) = \langle e^{-sA}\rangle \sim e^{t\,\psi_A(s)} \qquad (-\psi_A(s)\text{: dynamical free-energy})$$

- Observable $\mathcal{O}$ in the s-ensemble: $\langle\mathcal{O}\rangle_s = \langle\mathcal{O}\,e^{-sA}\rangle / \langle e^{-sA}\rangle$

Algorithm

- Microcanonical and canonical point of view ($\hat{P}_A(\mathcal{C},s,t) = \sum_A e^{-sA}P(\mathcal{C},A,t)$)

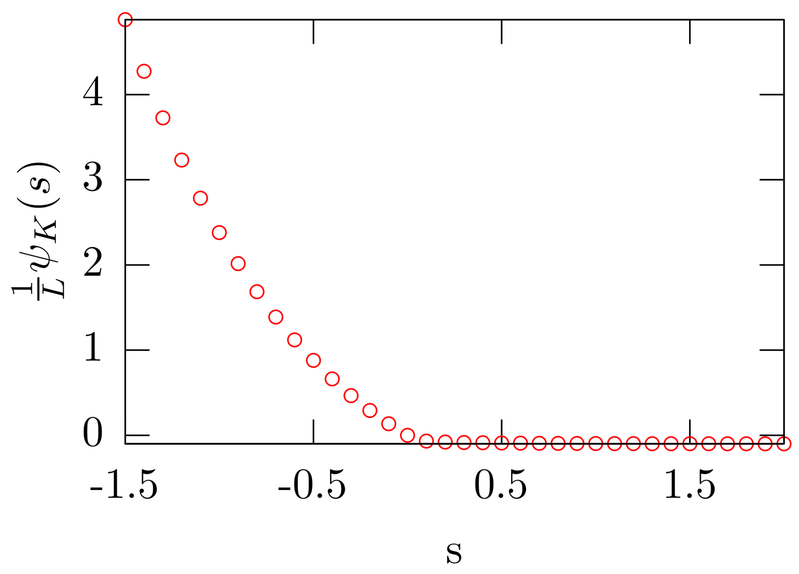
$$\partial_t P(\mathcal{C},A,t) = \sum_{\mathcal{C}'} W(\mathcal{C}'\to\mathcal{C})P\big(\mathcal{C}',A-\alpha(\mathcal{C}',\mathcal{C}),t\big) \;-r(\mathcal{C})P(\mathcal{C},A,t)$$

$$\partial_t \hat{P}_A(\mathcal{C},s,t) = \underbrace{\sum_{\mathcal{C}'} W_s(\mathcal{C}'\to\mathcal{C})\hat{P}_A(\mathcal{C}',s,t) - r_s(\mathcal{C})\hat{P}_A(\mathcal{C},s)}_{s\text{-modified dynamics}} \;+ \underbrace{\delta r_s(\mathcal{C})\hat{P}_A(\mathcal{C},s,t)}_{\text{cloning term}}$$

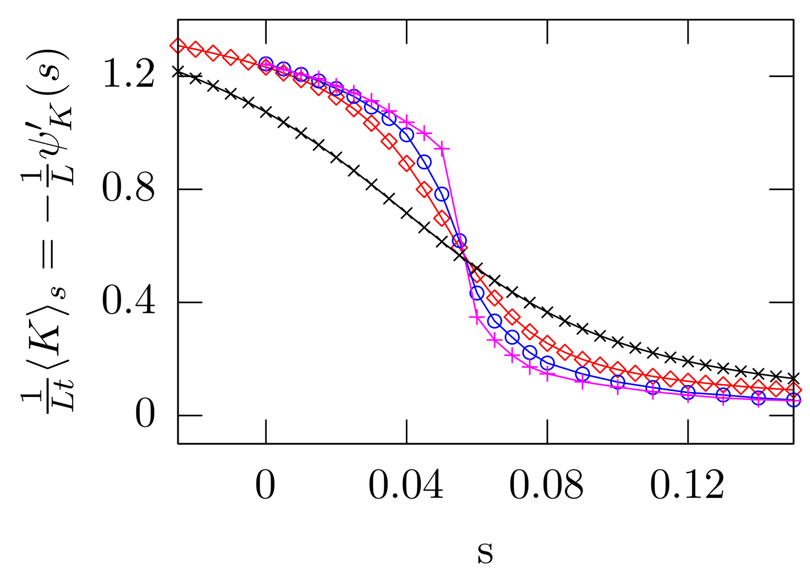
- s-modified dynamics $\left\{\begin{array}{l} W_s(\mathcal{C}'\to\mathcal{C}) = e^{-s\alpha(\mathcal{C}',\mathcal{C})}W(\mathcal{C}'\to\mathcal{C})\\ r_s(\mathcal{C}) = \sum_{\mathcal{C}'} W_s(\mathcal{C}\to\mathcal{C}')\end{array}\right.$ and $\delta r_s = r_s - r$
- Dynamical partition function obtained by: $Z_A(s,t) = \sum_{\mathcal{C}} \hat{P}_A(\mathcal{C},s,t)$
- Numerical procedure: $\mathcal{N} \gg 1$ copies of the system evolving *in parallel*
  - ⋆ each copy evolves *continuously in time* (*cf.* **Fig. 1**) with s-modified rates
  - ⋆ over each time interval $[t_k,t_{k+1}]$, each copy is killed/cloned with rate δr_s
  - ⋆ total number of copies is kept constant by (un)zooming in the space of copies
- $Z_A(s,t)$ equal to the product of these (un)zooming factors.

Contact Process with a Field

- Model:
  - ⋆ 1D lattice of L sites with periodic boundary conditions
  - ⋆ Each site i is empty ($n_i=0$) or occupied ($n_i=1$)
  - ⋆ Dynamics: $\left\{\begin{array}{l} W(n_i=1\to n_i=0)=1\\ W(n_i=0\to n_i=1)=\lambda(n_{i-1}+n_{i+1})+h\end{array}\right.$
- Phenomenology at zero field ($h=0$):
  - ⋆ the system spends a long ($\sim L$) time in an *active* (density>0) state
  - ⋆ before reaching an absorbing *inactive* (density$=0$) state
- Phenomenology for $h>0$: the absorbing state disappears.
- Statistics over histories with a weak $h>0$ field ($h=0.1$, $\lambda=3.5$), with s conjugated to K: **phase transition** at $s_c\simeq 0.057$, in the large size limit ($L\to\infty$).



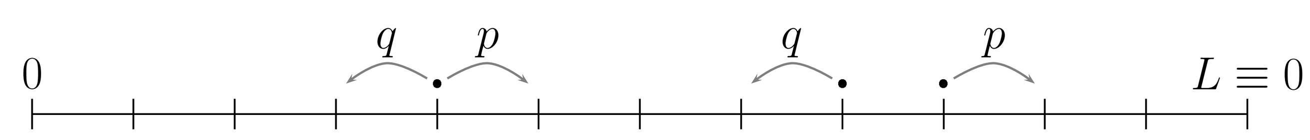
Dynamical free energy $\frac{1}{L}\psi_K(s)$
– active branch ($s<s_c$)
– inactive branch ($s>s_c$)



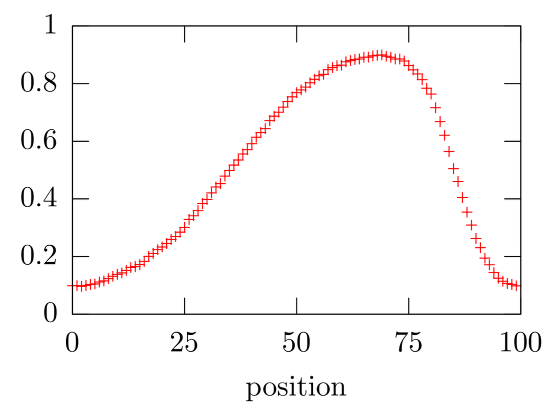
Order parameter of the first-order dynamical transition: mean activity $\frac{1}{Lt}\langle K\rangle_s$ around s_c. Discontinuity arises for $L\to\infty$.

- In the $h\to 0$ limit, the active ($s<0$) and inactive ($s>0$) branches correspond to the active and inactive periods of the histories at $h=0$.

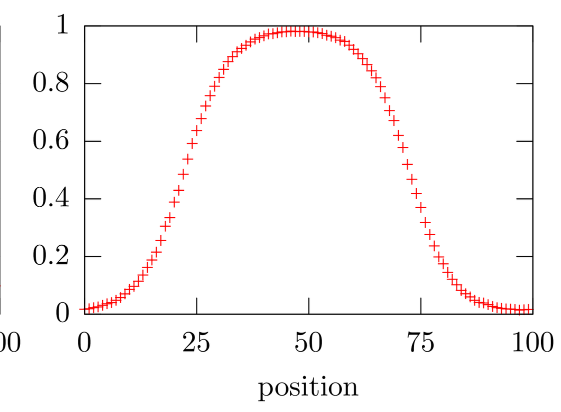
Asymmetric Exclusion Process



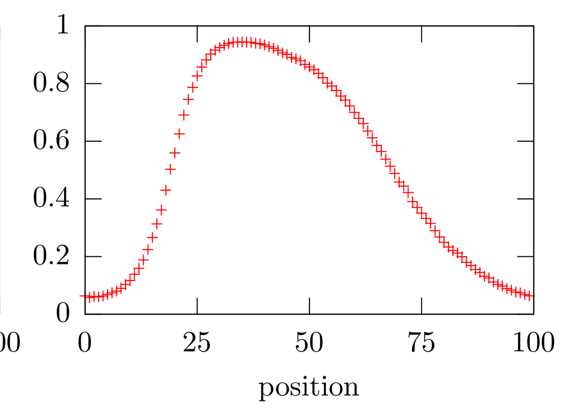
- Model:
  - ⋆ 1D lattice of L sites with periodic boundary conditions
  - ⋆ Each site i is empty ($n_i=0$) or occupied ($n_i=1$)
  - ⋆ Dynamics: particles jump to their right [left] neighbor (if unoccupied) with rate p [q].
- Phenomenology: the steady state has a flat profile, with a mean current $p-q$.
- Large deviations: s conjugated to total current Q. Typical profiles at low current:



At $s \lesssim \frac{1}{2}\log\frac{p}{q}$: typical profile given by asymmetric shock with current $\lesssim 0$



At $s=\frac{1}{2}\log\frac{p}{q}$ the large deviation presents no current on average.



At $s \gtrsim \frac{1}{2}\log\frac{p}{q}$: typical profile given by asymmetric shock with current $\gtrsim 0$

References

[1] Giardinà C, Kurchan J, and Peliti L, *Direct Evaluation of Large-Deviation Functions*, Phys. Rev. Lett. **96** 120603 (2006)

[2] Lecomte V, Tailleur J, *A numerical approach to large deviations in continuous-time*, J. Stat. Mech. (2007) P03004