Direct evaluation of large-deviation functions

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We introduce a numerical procedure to evaluate directly the probabilities of large deviations of physical quantities, such as current or density, that are local in time. The large-deviation functions are given in terms of the typical properties of a modified dynamics, and since they no longer involve rare events, can be evaluated efficiently and over a wider ranges of values. We illustrate the method with the current fluctuations of the Totally Asymmetric Exclusion Process and with the work distribution of a driven Lorentz gas.

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In the last few years there has been a renewed interest in the theory of large deviations of nonequilibrium systems, with the development of general results concerning the fluctuations of soft modes [1], of nontrivial and rich analytic solutions of explicit models [2, 3, 4, 5, 6, 7, 8, 9, 10], and with the discovery of strikingly simple and general nonequilibrium relations [11, 12, 13, 14, 15, 16, 17, 18, 19] (the Fluctuation Theorem, Jarzynski's relation) obeyed by work fluctuations. Perhaps for the first time, we are gathering a few glimpses of truly general features of macroscopic systems well out of equilibrium.

The large-deviation function plays an essential role in the investigation of nonequilibrium systems—a role akin to the free energy in equilibrium ones. When available techniques do not allow for an exact evaluation of this function, one turns to simulations: but direct numerical simulation of large deviations is hard, since, by definition, they are rare. In equilibrium, this difficulty is often overcome by introducing biased (non-Boltzmann) sampling [20]. Here we show that a similar strategy can be introduced in systems out of equilibrium, in order to evaluate the large deviations function for quantities that are local in time, although not necessarily in space. We find that, in nonequilibrium, it is necessary not only to bias suitably the dynamics of the system, but also to introduce a process by which images (clones) of the system reproduce or die, a technique inspired by the Diffusion Monte Carlo method [21] of quantum mechanics. In the present work, after deriving the general formalism, we show its effectiveness by applying it to two nonequilibrium processes: a stochastic one, the Totally Asymmetric Exclusion Process (TASEP), and a deterministic one, a driven Lorentz gas. Our algorithm allows to compute the probability of obtaining a temporary large deviation (compared to the typical) value of the current in the first example and of the dissipated work in the second one.

We consider the general setup of a system evolving according to Markovian dynamics. Let $\mathcal{C}, \mathcal{C}'$ denote two configurations in the and let $U_{\mathcal{C}'\mathcal{C}}$ be the transition matrix of the discrete (eventually continuous) time dynamics. Denoting by $P_{\mathcal{C}}(t)$ the probability of being in the configuration $\mathcal{C}$ at time t, one has

$$P_{\mathcal{C}'}(t+1) = \sum_{\mathcal{C}} U_{\mathcal{C}'\mathcal{C}} P_{\mathcal{C}}(t)\,. \tag{1}$$

In a time interval of length T, a path $\mathcal{C}_0, \mathcal{C}_1, \ldots, \mathcal{C}_T$ in the configuration space, starting from a fixed $\mathcal{C}_0$, will have the probability

$$\mathrm{Prob}[\mathcal{C}_0, \mathcal{C}_1, \ldots, \mathcal{C}_T] = U_{\mathcal{C}_T\mathcal{C}_{T-1}} \cdots U_{\mathcal{C}_2\mathcal{C}_1} \cdot U_{\mathcal{C}_1\mathcal{C}_0}\,. \tag{2}$$

We shall consider physical quantities Q_T that are additive in time, i.e., which can be written as $Q_T = \sum_{t=0}^{T-1} J(\mathcal{C}_{t+1}, \mathcal{C}_t)$. For example, for a transition $\mathcal{C} \to \mathcal{C}'$ in a lattice system:

$$J_{\mathcal{C}'\mathcal{C}} = \begin{cases} 1, & \text{a particle jumps to the right;} \\ 0, & \text{nothing happens;} \\ -1, & \text{a particle jumps to the left.} \end{cases} \tag{3}$$

We are interested in calculating the probability of having a current Q_T in the time interval T, i.e., a current $q = Q_T/T$ per unit time. Denoting with angular brackets the average over trajectories, we have

$$\begin{aligned} P\left(\frac{Q_T}{T} = q\right) &= \langle \delta(J_{\mathcal{C}_1\mathcal{C}_0} + \cdots + J_{\mathcal{C}_T\mathcal{C}_{T-1}} - qT) \rangle \\ &= \frac{1}{2\pi i} \int_{-i\infty}^{+i\infty} d\lambda\, e^{T\,[\,\mu(\lambda) - \lambda q\,]}, \end{aligned} \tag{4}$$

where we used the integral representation of delta function and we have defined

$$\begin{aligned} e^{T\mu(\lambda)} &= \left\langle e^{\lambda(J_{\mathcal{C}_1\mathcal{C}_0} + \cdots + J_{\mathcal{C}_T\mathcal{C}_{T-1}})} \right\rangle \\ &= \sum_{\mathcal{C}_1, \ldots, \mathcal{C}_T} U_{\mathcal{C}_T\mathcal{C}_{T-1}} \cdots U_{\mathcal{C}_1\mathcal{C}_0} e^{\lambda(J_{\mathcal{C}_1\mathcal{C}_0} + \cdots + J_{\mathcal{C}_T\mathcal{C}_{T-1}})}. \end{aligned} \tag{5}$$

In the limit $T \to \infty$, by applying the steepest descent method to Eq. (4) (and assuming that the imaginary contour line can be deformed to the real line),

one obtains that the large deviation function $f(q) = \lim_{T\to\infty} \ln P(Q_T)/T$ and $\mu(\lambda)$ are Legendre transforms of each other:

$$f(q) = \max_{\lambda}[\mu(\lambda) - \lambda q], \tag{6}$$

so that $q = \mu'(\lambda^*)$ where λ^* is the saddle. We introduce the bias (7) of the original measure by defining the new matrix

$$\tilde{U}_{\mathcal{C}'\mathcal{C}} \equiv e^{\lambda J_{\mathcal{C}'\mathcal{C}}} U_{\mathcal{C}'\mathcal{C}}, \tag{7}$$

so that

$$e^{T\mu(\lambda)} = \sum_{\mathcal{C}_1,\ldots,\mathcal{C}_T} \tilde{U}_{\mathcal{C}_T\mathcal{C}_{T-1}} \cdots \tilde{U}_{\mathcal{C}_1\mathcal{C}_0} = \sum_{\mathcal{C}_T} \left[\tilde{U}^T\right]_{\mathcal{C}_T\mathcal{C}_0}. \tag{8}$$

Introducing the spectral decomposition $\tilde{U} = \sum_j e^{\Lambda_j} |\Lambda_j^R\rangle\langle\Lambda_j^L|$ where we assumed a complete biorthogonal set of the matrix $\tilde{U}$ exists, i.e. $\tilde{U}|\Lambda_j^R\rangle = e^{\Lambda_j}|\Lambda_j^R\rangle$ $\langle\Lambda_j^L|\tilde{U} = e^{\Lambda_j}\langle\Lambda_j^L|$ and denoting by e^{Λ} the eigenvalue of $\tilde{U}$ with the largest real part, and by $|\Lambda^R\rangle$, $|\Lambda^L\rangle$ the corresponding right and left eigenvectors, we have, for large times T,

$$e^{T\mu(\lambda)} = \sum_{\mathcal{C}_T} \langle\mathcal{C}_T|\Lambda^R\rangle\langle\Lambda^L|\mathcal{C}_0\rangle\, e^{T\Lambda}, \tag{9}$$

so that $\Lambda = \mu(\lambda)$. In order to compute $\mu(\lambda)$, one possibility is to perform path-sampling over the trajectories with weight (7). Such a procedure has been proposed in the context of the work distributions [22] on nonequilibrium trajectories. In this paper we propose a different strategy: the idea is to define a new effective dynamics whose expectation values directly give the large deviations. As we shall see, the new dynamics involves the parallel evolution of clones which reproduce and die, a procedure inspired by the "Diffusion Monte Carlo" method of simulation of the Schrödinger equation [21]. In order to write eq. (8) as expectation on the new dynamics, let us put $K_{\mathcal{C}} \equiv \sum_{\mathcal{C}'} \tilde{U}_{\mathcal{C}'\mathcal{C}}$, and define the stochastic matrix

$$U'_{\mathcal{C}'\mathcal{C}} \equiv \tilde{U}_{\mathcal{C}'\mathcal{C}} K_{\mathcal{C}}^{-1}. \tag{10}$$

We now have, instead of eq. (9),

$$e^{T\mu(\lambda)} = \sum_{\mathcal{C}_2,\ldots,\mathcal{C}_T} U'_{\mathcal{C}_T\mathcal{C}_{T-1}} K_{\mathcal{C}_{T-1}} \cdots U'_{\mathcal{C}_1\mathcal{C}_0} K_{\mathcal{C}_0}. \tag{11}$$

This can be realized by considering an *ensemble* of L copies ("clones") of the system, and by successively going, for all of them, through a process defined by the following three steps:

- A cloning step:

$$P_{\mathcal{C}}(t+1/2) = K_{\mathcal{C}} P_{\mathcal{C}}(t), \tag{12}$$

where the configuration $\mathcal{C}$ of the selected copy gives rise to G identical clones, $G = [K_{\mathcal{C}}] + 1$ with probability $K_{\mathcal{C}} - [K_{\mathcal{C}}]$, and $G = [K_{\mathcal{C}}]$ otherwise ($[x]$ denotes the integer part of x). If $[K_{\mathcal{C}}] = 0$, the copy may be killed and leave no offspring.

- A shift step without cloning of all the offspring of $\mathcal{C}'$ with the modified dynamics U'

$$P_{\mathcal{C}'}(t+1) = \sum_{\mathcal{C}} U'_{\mathcal{C}'\mathcal{C}} P_{\mathcal{C}}(t+1/2). \tag{13}$$

- An overall cloning step with an adjustable rate $M_t = L/(L+G)$ (at each time the same for all configurations), so as to keep the total number of clones constant. This amounts to multiplying $\tilde{U}$ by M_t times an identity, at each time.

It is easy to see that, in the long-time limit, the compensatory factor gives us $\mu(\lambda)$ through

$$-\ln[M_T \cdots M_2 \cdot M_1] = T\mu(\lambda). \tag{14}$$

Remark 1: We note that, if the quantity Q_T, whose deviations we wish to compute, depends on a single configuration rather than on a pair of configurations, such as for the density $Q_T = \sum_{t=1}^{T} \rho(\mathcal{C}_t)$, the same derivation goes through with the substitution $J_{\mathcal{C}'\mathcal{C}} \to \rho(\mathcal{C})$.

Remark 2: The configurations obtained in the course of the simulation are representative of the typical ones *at the end* ($t = T$), *rather than within* ($0 \ll t \ll T$) the interval of time T during which the large deviations are observed. (Their probabilities are proportional to$\langle\mathcal{C}|\Lambda^R\rangle$ and $\langle\Lambda^L|\mathcal{C}\rangle\langle\mathcal{C}|\Lambda^R\rangle$, respectively).

We now turn to two examples: the Totally Asymmetric Exclusion Process, and the Lorenz gas.

A stochastic system: The Totally Asymmetric Exclusion Process (TASEP). The TASEP [10] consists of particles on a ring with discrete sites with occupancy zero or one. A given particle chosen at random does not attempt to move with probability $(1-\alpha)$, and with probability α attempts to move to the right and succeeds if the corresponding site is empty. The parameter α can be made small to approach the continuous time limit. Here we shall set it to unity. Let us denote by $X_{\mathcal{C}}$ the number of different configurations that can be reached by making a one-particle move (1PM) from $\mathcal{C}$. Then the non-zero entries of $U_{\mathcal{C}'\mathcal{C}}$ are given by

$$U_{\mathcal{C}'\mathcal{C}} = \begin{cases} \alpha/N, & \text{if } \mathcal{C} \to \mathcal{C}' \text{ is a 1PM;} \\ 1 - (X_{\mathcal{C}}\alpha/N), & \text{if } \mathcal{C}' = \mathcal{C}. \end{cases} \tag{15}$$

This implies for $\tilde{U}$

$$\tilde{U}_{\mathcal{C}'\mathcal{C}} = \begin{cases} \alpha e^{\lambda}/N, & \text{if } \mathcal{C} \to \mathcal{C}' \text{ is a 1PM;} \\ 1 - (X_{\mathcal{C}}\alpha/N) & \text{if } \mathcal{C}' = \mathcal{C}. \end{cases} \tag{16}$$

Thus, for a configuration $\mathcal{C}$ with $X_{\mathcal{C}}$ mobile particles, we have

$$K_{\mathcal{C}} = 1 + \frac{X_{\mathcal{C}}\alpha}{N}(e^{\lambda} - 1), \tag{17}$$

and finally

$$U'_{\mathcal{C}'\mathcal{C}} = \begin{cases} (\alpha e^{\lambda}/N)/K_{\mathcal{C}}, & \text{if } \mathcal{C} \to \mathcal{C}' \text{ is a 1PM,} \\ (1 - X_{\mathcal{C}'}\alpha/N)/K_{\mathcal{C}}, & \text{if } \mathcal{C}' = \mathcal{C}. \end{cases} \tag{18}$$

Thus, with probability $(1 - X_{\mathcal{C}}\alpha/N)/K_{\mathcal{C}}$ no move is made; otherwise we move a particle randomly chosen with uniform probability among the $X_{\mathcal{C}}$ mobile particles.

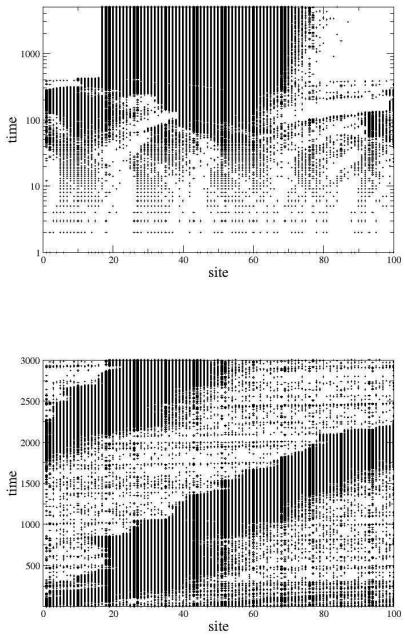

FIG. 1: Space-time diagram for a ring of $N = 100$ sites. Top: $\lambda = -50$ and density 0.5; the shock is dense and does not advance. Bottom: $\lambda = -30$ and density 0.3; the shock drifts to the right.

In Figure 1 (top) we show a space-time diagram of the system with $N = 100$ particles, density 0.5 and $\lambda = -50$. The simulation was done with $L = 1000$ clones, each of them initialized with random (uniform) occupancy numbers, such that the configuration has density 0.5. We notice that the configurations rapidly become inhomogeneous, exhibiting an alternation of a regions with high density with regions of slow density, as in traffic jams or in shock waves. The high-density regions eventually coalesce into a single one. The figure does not quite represent the evolution of a shock (because of Remark 2 above), but rather the configuration at the end of the time-interval for time intervals ending at progressively longer times. As predicted by the theory for this value of the density, the shock does not drift, although different initial conditions lead to different shock positions. Bottom of Figure 1 shows the case $\lambda = -30$, and density 0.3: we see that the shock has a net drift to the right, again as predicted by the theory [3]. Finally, in figure 2 we show the numerical results obtained for $\mu(\lambda)$, and compare them to the analytic ones of Ref. [3]. The agreement is excellent, and the numerical effort corresponds to tens of minutes of a pe

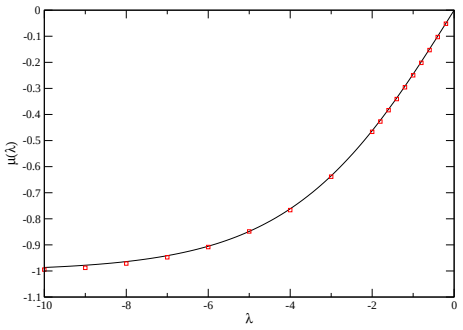

FIG. 2: Plot of $\mu(\lambda)$ vs. λ for the TASEP at density one-half. Numerical results and analytic results of ref. [3], with points and full line, respectively.

A deterministic system: The Lorentz Gas and the Gallavotti-Cohen theorem. This system consists of a number of particles (in our case only one) moving inside a billiard as in figure 3, with periodic boundary conditions. The particle is under the action of a force field $\vec{E}$, and is subject to a deterministic thermostat that keeps the velocity modulus constant $|\vec{v}| = 1$. Between bounces, the equations of motion are:

$$\begin{aligned} \ddot{x}_i &= -E_i + \gamma(t)\dot{x}_i, \qquad i = 1, 2; \\ \gamma(t) &= \sum_i E_i \dot{x}_i. \end{aligned} \tag{19}$$

We wish to compute the generating function of the dissipated work $Q_T = \int_0^T \gamma(t)\, dt$, and check the Gallavotti-Cohen theorem, which states that $P(Q_T)/P(-Q_T) = \exp(Q_T)$, which is equivalent, thanks to Eq. (4), to the symmetry of $\mu(\lambda)$ around $\lambda = -\frac{1}{2}$.

The dynamics is deterministic, and hence cloned systems will evolve together and perform a poor sampling.

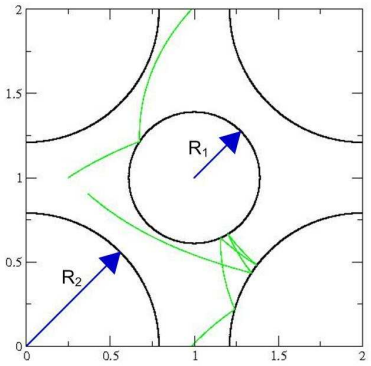

FIG. 3: The billiard. The radii are $R_1 = 0.39, R_2 = 0.79$. We also show an example of trajectory for the external field $\vec{E} = (1, 0)$.

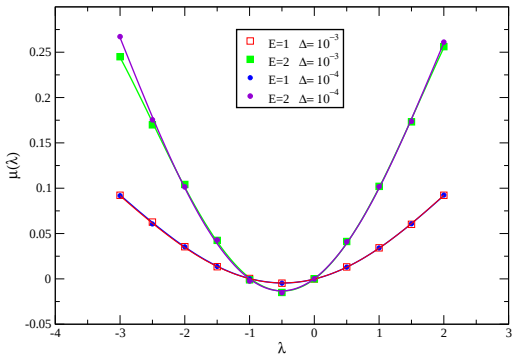

FIG. 4: Plot of $\mu(\lambda)$ vs. λ for the driven Lorentz gas. Data for $\vec{E} = (E, 0)$, $E = 1, 2$ and noise intensity $\Delta = 10^{-3}, 10^{-4}$. The Gallavotti-Cohen theorem implies the symmetry around $\lambda = -1/2$. The best fit (continuous lines) is quadratic for $E = 1$ (gaussian behavior), and a 4-th order polynomial for $E = 2$.

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To get around this problem, we introduce a small stochastic noise, and check the stability of results in the limit of small noise. We evolve the system for *macroscopic* intervals $\mathcal{T}$, and clone with a factor $K_t = e^{\lambda \Gamma_{\mathcal{T}}(t)}$, where $\Gamma_{\mathcal{T}}(t) = \int_t^{t+\mathcal{T}} \gamma(t)\, dt$ is the total dissipated work over the interval. Before each deterministic step of time $\mathcal{T}$, clones are given random kicks of variance Δ in position and/or velocity direction. *The time-interval $\mathcal{T}$ and the noise intensity Δ are chosen so that twin clones have a chance to separate during time $\mathcal{T}$*, and this depends on the chaotic properties of the system. In the present case, we checked that $0.1 \leq \mathcal{T} \leq 1$ allows for a few collisions, which guarantees clone diversity for $10^{-3} \leq \Delta \leq 10^{-4}$.

In Fig. 4 we show the results of $\mu(\lambda)$ for $-3 \leq \lambda \leq 2$, and for $\vec{E} = (E, 0)$ with $E = 1, 2$, corresponding to very large current deviations.

Diversity in a population of reproducing units is maintained by a balance between the natural loss due to sampling fluctuations and the increase introduced by mutations, represented in our case by noise [23]. Thus, if the noise level is too small in the billiard case, most of the clones correspond to too close configurations, and our results become noisy and unreliable. The same phenomenon explains why all clones exhibit shocks in essentially the same position for any given run in the TASEP (since they share a common ancestor): but we found that in this case the phenomenon poses no problem for the sampling, since the current does not depend on the position of the shock.

In conclusion, we have shown that sampling methods based on a modified dynamics with clones can be used to efficiently compute the large deviations function, in times and within ranges of values that cannot be reached in a direct simulation.

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