Finite-time and -size scalings in the evaluation of large deviation functions. Numerical analysis in continuous time

E. Guevara[1], T. Nemoto[2], V. Lecomte[3]

[1]Universite Paris Diderot, France

[2]École Normale Supérieure & PSL Research University, France

[3]Université Grenoble Alpes & CNRS, France

Rare events and rare trajectories can be analyzed through a variety of numerical approaches, ranging from importance sampling, adaptive multilevel splitting to transition path sampling. Population dynamics provide a numerical tool allowing their study, by means of simulating a large number of copies of the system, which are subjected to a selection rule that favors the rare trajectories of interest. By exponentially biasing their probability it makes possible to render typical the rare trajectories of the original dynamics in the simulated dynamics.

The idea is to perform the numerical simulation of a large number of copies N_c of the original dynamics, supplemented with selection rules which favour the rare trajectories of interest. The version of the population dynamics algorithm introduced by Giardin, Kurchan and Peliti provides a method to evaluate the large deviation function (LDF) associated to the distribution of a trajectory-dependent observable. The LDF is obtained as the exponential growth rate that the population would present if it was not kept constant. Under this approach, the corresponding LDF estimator is in fact valid only in the limits of infinite simulation time t and infinite population size N_c. The usual strategy that is followed in order to obtain those limits is to increase the simulation time and the population size until the average of the estimator over several realizations does not depend on those two parameters, up to numerical uncertainties.

In a previous analytical study of a discrete-time version of the population dynamics algorithms, we derived its convergence-speed in the large-N_c, and -t limits to be $1/N_c$ and $1/t$, respectively. In principle, knowing the scaling a priori means that the asymptotic limit of the estimator in the $t \to \infty$ and $N_c \to \infty$ limits may be interpolated from the data at finite t and N_c. However, whether this idea is actually useful or not is a non-trivial question, as there is always a possibility that onset values of N_c and t-scalings are too large to use these scalings. Here, we consider a continuous-time version of the population dynamics algorithms. We show numerically that one can indeed make use of these scaling properties in order to improve the estimation of LDF, in an application to a many-body system (contact process).

[l] E. Guevara, V. Lecomte, J. Phys. A **49**, 205002 (2016).

[2] T. Nemorto, E. Guevara, V. Lecomte, Phys. Rev. E **95**, 012102 (2017).

[3] E. Guevara, T. Nemorto, V. Lecomte, under revision, arXiv:1607.08804 (2017).