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Analytical calculation of Jarzynski free-energy estimator bias MATTEO PALASSINI, Department of Fundamental Physics, University of Barcelona, NIKOS SKANTZOS, Instituut voor Theoretische Fysica, Katholieke Universiteit Leuven, FELIX RITORT, Department of Fundamental Physics, University of Barcelona — The Jarzynski equality connects the free-energy difference DF between two equilibrium states A and B of a system to the work done on the system in a non-equilibrium process that takes it from A to B, averaged exponentially over all possible realizations of the process. This provides an estimator for DF given N nonequilibrium experiments, which has been applied in a variety of contexts. Because of the exponential averaging, the Jarzynski estimator suffers a statistical bias for finite N, which can be substantial. Computing this bias is important for estimating correctly the free-energy, and is a notoriously difficult problem for which only results in the large-N limit are known. We propose an analytical method to estimate the bias and test it in the case of a Gaussian work distribution, for which it provides satisfactory estimates both in the large N and small N regimes. Finally, we discuss the applicability of these results to experimental studies on single biomolecules.

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