

From Thermodynamic Ensembles to Conditioned Dynamics via Reweighting Principle

Salvatore Romano^{1,2}, Christoph Dellago¹

¹University Of Vienna, Vienna, Austria, ²Vienna Doctoral School in Physics, Vienna, Austria

Reweighting of probability measures provides a unifying perspective on several fundamental constructions in statistical mechanics [1,2]. Starting from a reference ensemble, both conditioning (hard constraints) and exponential tilting (soft constraints) can be formulated as instances of Bayesian reweighting, where prior probabilities are updated through the introduction of information encoded in a weight functional. This viewpoint places ensemble transformations, maximum entropy principles, and inference on the same conceptual footing [3].

To make this connection explicit, we introduce an enlarged space in which observables are promoted to independent variables. In this setting, the joint distribution is defined through a structural prior enforcing the relation between microstates and observables. After exponential reweighting in the observable sector, microcanonical and canonical ensembles are recovered naturally as conditional and marginal distributions, respectively. This construction highlights that thermodynamic ensembles arise from different projections of a single underlying probabilistic object.

Within this framework, the thermodynamic limit acquires a transparent interpretation: the observable marginal of the tilted ensemble concentrates through a saddle-point mechanism, revealing how hard constraints emerge from the competition between entropy and bias. This provides a direct interpretation of ensemble equivalence as a concentration phenomenon, connecting directly to the large-deviation approach [4].

The same reweighting principle extends naturally to path space. Reweighting trajectory measures by boundary functionals or time-integrated observables generates conditioned dynamical ensembles [5,6]. In particular, in the context of rare events, conditioning leads to Committor functions [7,8], while exponential tilting connects to Feynman–Kac representations [9,10]. This establishes a bridge between equilibrium thermodynamics and the conditioned stochastic processes.

Overall, this work suggests a unified view of statistical mechanics as inference under constraints via reweighting, connecting static ensembles, dynamical trajectories, and rare-event phenomena within a single probabilistic framework.

References:

- [1] Bennett, C. H., Efficient estimation of free energy differences from Monte Carlo data (1976)
- [2] Frenkel, D. and Smit, B., Understanding Molecular Simulation: From Algorithms to Applications (2023)
- [3] Jaynes, E. T., Information Theory and Statistical Mechanics (1957)
- [4] Touchette, H., The large deviation approach to statistical mechanics (2009)
- [5] Doob, J. L., Classical Potential Theory and Its Probabilistic Counterpart (1984)
- [6] Girsanov, I. V., On transforming a certain class of stochastic processes by absolutely continuous substitution of measures (1960)
- [7] E, W. and Vanden-Eijnden, E., Transition-Path Theory and Path-Finding Algorithms for the Study of Rare Events (2010)
- [8] Triplett, L. and Lu, J., Diffusion Methods for Generating Transition Paths (2023)
- [9] Kac, M., On distributions of certain Wiener functionals (1949)
- [10] Singh, A. N., Das, A. and Limmer, D. T., Variational Path Sampling of Rare Dynamical Events (2025)