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Free energy calculation from umbrella sampling using Bayesian inference NOAM BERNSTEIN, Naval Research Laboratory, THOMAS STECHER, GÁBOR CSÁNYI, Department of Engineering, University of Cambridge — Using simulations to obtain information about the free energy of a system far from its free energy minima requires biased sampling, for example using a series of harmonic umbrella confining potentials to scan over a range of collective variable values. One fundamental distinction between existing methods that use this approach is in what quantities are measured and how they are used: histograms of the system's probability distribution in WHAM, or gradients of the potential of mean force for umbrella integration (UI) and the single-sweep radial basis function (RBF) approach. Here we present a method that reconstructs the free energy from umbrella sampling data using Bayesian inference that effectively uses all available information from multiple umbrella windows. We show that for a single collective variable, our method can use histograms, gradients, or both, to match or outperform WHAM and UI in the accuracy of free energy for a given amount of total simulation time. In higher dimensions, our method can effectively use gradient information to reconstruct the multidimensional free energy surface. We test our method for the alanine polypeptide model system, and show that it is more accurate than a RBF reconstruction for sparse data, and more stable for abundant data.

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