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TT-Metadynamics: Tensor Train Enhanced Sampling for High-Dimensional Molecular Systems

Tensor networks offer powerful tools for compressing and manipulating high-dimensional functions, but their application outside quantum many-body theory remains relatively unexplored. In this work, we introduce TT-metadynamics, a novel adaptive biasing algorithm for classical molecular dynamics that leverages tensor train (TT) decompositions to overcome the curse of dimensionality in enhanced sampling. Standard metadynamics accumulates a bias potential by summing Gaussians in a low-dimensional collective variable space. However, the cost of evaluating and storing this bias grows rapidly with dimension, rendering such methods impractical beyond 4–5 variables. TT-metadynamics circumvents this bottleneck by periodically compressing the accumulated bias into a TT format, enabling linear scaling with the number of collective variables, independent of the number of accumulated Gaussians. We demonstrate the scalability and effectiveness of this approach on a range of benchmark systems, from alanine dipeptide (2D) to ditryptophan (8D) and Aib9 (10D–14D), showing that TT-metadynamics matches or exceeds the accuracy of standard metadynamics over long simulations. Our results establish TT-metadynamics as a promising interdisciplinary application of tensor networks, with potential implications for nonequilibrium statistical mechanics, complex energy landscapes, and scalable high-dimensional modeling in chemistry and biophysics.

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