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# Thermodynamic Integration along interpolant ML-potentials

*Wednesday, 23 October 2024 10:00 (40 minutes)*

We propose to machine learn an interpolating family of potential functions between two Hamiltonians and to perform thermodynamic integration along it. The approach requires the functional forms of the Hamiltonians and samples from the corresponding Boltzmann distributions. We then define an interpolation between the distributions at the level of samples and optimize a neural network potential to match the corresponding equilibrium potential, i.e. the negative log-likelihood, at every intermediate time-step. Once the alignment between the interpolating samples and potentials is sufficiently accurate, the free energy difference between the two Hamiltonians can be estimated using (neural) thermodynamic integration. We experimentally validate the proposal on the estimation of solvation free energies.

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