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Machine learning of coarse-grained molecular dynamics force fields

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Atomistic or ab initio molecular dynamics simulations are widely used to predict thermodynamics and kinetics and relate them to molecular structure. A common approach to go beyond the time- and length-scales accessible with such computationally expensive simulations is the definition of coarse-grained molecular models. Existing coarse-graining approaches define an effective interaction potential to match defined properties of high-resolution models or experimental data. In this paper, we reformulate coarse-graining as a supervised machine learning problem. We use statistical learning theory to decompose the coarse-graining error and cross-validation to select and compare the performance of different models. We introduce CGnets, a deep learning approach, that learns coarse-grained free energy functions and can be trained by a force-matching scheme. CGnets maintain all physically relevant invariances and allow one to incorporate prior physics knowledge to avoid sampling of unphysical structures. We show that CGnets can capture all-atom explicit-solvent free energy surfaces with models using only a few coarse-grained beads and no solvent, while classical coarse-graining methods fail to capture crucial features of the free energy surface. Thus, CGnets are able to capture multibody terms that emerge from the dimensionality reduction.