Linear tensor fits and marginalized graph kernels as means for novel machine learning molecular dynamics

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As part of a molecular dynamics machine learning pipeline, distributions of force constant matrices that describe atomic interactions in bcc materials were abstracted from linear fits performed to the atomic configurations of each timestep of a quantum simulation. Once symmetry operations are enforced on the system to reduce our distributions according to the primitive unit cell, these fits yield means that were then utilized to calculate the harmonic approximation. As a further development of the pipeline, gaussian process regression was performed on a molecular graph kernel (Tang, 2019) to construct a relation between the energy of the system and the atomic configurations. The distribution of displacements and force constant fits are approximately gaussian in accordance with the central limit theorem. Training of the graph kernel in 400 randomly selected timesteps yields a mean error of 5meV, with a standard deviation of 8meV. Obtaining effective forces from this potential though the central difference theorem, Python's Atomic Simulation Environment (ase) is leveraged to perform molecular dynamics through our novel method.