Title:

Active Machine Learning Approach to Adaptively Truncated Hilbert Space for an Impurity Solver

Abstract:

Dynamical mean field theory (DMFT) has effectively demonstrated many emergent phenomena in strongly correlated systems. However, its computational costs limit the number of orbitals in the impurity Hamiltonian, complicating the precise description of correlated materials. To address this issue, we introduce an active machine-learning approach to the configuration interaction-based impurity solver. We start with an initial training set for the classifier using restricted active space configuration interaction. Particle-hole substitution on key Slater determinants generates an unlabeled dataset. The classifier predicts the importance of this dataset, and based on the class probability of each instance, we select queries to construct the effective Hamiltonian. The effective Hamiltonian is then diagonalized using the Lanczos algorithm to determine the ground state energy. This process iterates until energy convergence, with updates to the training set incorporating new Slater determinants from the queries at each step. We benchmark this scheme on the one-dimensional Hubbard model. The new method, utilizing active learning, effectively reduces computational costs, outperforming the previous configuration interaction-based solver.