Unsupervised Machine Learning for Phase Classification in Strongly Correlated Electron System

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We investigate the finite-temperature phase diagram of the spinless two-dimensional Falicov-Kimball model using unsupervised machine learning methods. In strongly correlated systems, traditional methods often struggle to capture the full phase diagram without prior knowledge of the order parameters. Here, we demonstrate that simple unsupervised methods can accurately identify phase boundaries using only raw particle occupation snapshots from Monte Carlo simulations [1].

We test several approaches, including Principal Component Analysis (PCA), neural network predictors, and autoencoders. First, all methods successfully identify the phase boundary between the ordered phase and the disordered phases, independent of the transition order. Second, and more remarkably, we distinguish between the weakly localized regime and the Anderson-localized insulator within the disordered phase. This crossover is challenging to detect using standard methods.

Surprisingly, the linear PCA method outperforms more complex neural network architectures in resolving these boundaries. Our results highlight the potential of straightforward, interpretable unsupervised learning techniques for exploring phase diagrams in strongly correlated electron systems.

References:

[1] L. Frk, P. Baláž, E. Archemashvili, M. Žonda, Phys. Rev. B 111 (2025) 205116