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Classifying Pattern Formation in Materials via Machine Learning

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ABSTRACT

Scanning probe experiments such as scanning tunneling microscopy (STM) and atomic force microscopy (AFM) on strongly correlated materials often reveal complex pattern formation that occurs on multiple length scales. We have shown in two disparate correlated materials that the pattern formation is driven by proximity to a disorder-driven critical point. We developed new analysis concepts and techniques that relate the observed pattern formation to critical exponents by analyzing the geometry and statistics of clusters observed in these experiments and converting that information into critical exponents. Machine learning algorithms can be helpful correlating data from scanning probe experiments to theoretical models of pattern formation. We analyze the use of machine learning algorithms for the identification of critical behavior and universality underlying scanning probe data sets taken from correlated materials. This method has complementary strengths to the cluster analysis methods. The cluster techniques have a clear physical interpretation while machine learning algorithms require less expertise from the user and are faster to implement. The complementary nature of the two techniques further facilitates our understanding of correlated materials. The training of machine learning algorithms has been done through artificial neural networks. The neural net was trained using data from theoretical simulations of percolation and Ising models. The trained net had a 3.00% average classification error during testing. This proves that machine learning algorithms can successfully distinguish whether the complex pattern formation of a specific novel material is governed by uncorrelated percolation or by an interaction model fixed point.

KEYWORDS

strongly correlated electronic systems, correlated materials, pattern formation, scanning probe, machine learning