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Discerning multiple order parameters with interpretable machines: towards the automation of phase classification

Machine learning techniques can boost the exploration of complicated phase diagrams in many-body systems. To date, most studies are tied to situations involving only one phase transition and one order parameter. Systems accommodating multiple phases of coexisting and competing orders remain largely unexplored. Using Support Vector Machines (SVMs) we focus on multipolar orders and their tensorial order parameters, whose identification is difficult with traditional methods. The key property that allows one to make progress is the *interpretability* of the decision function, from which the physical order parameter can be deduced. Furthermore, we discuss a second intrinsic parameter of the SVM, the *bias*, which allows one to make an unsupervised graph analysis of the topology of the phase diagram. We illustrate our tool for the frustrated classical XXZ model on the pyrochlore lattice. Unexpectedly, the machine could also learn local constraints hinting at various types of spin liquids resulting in a complete classification of all types of behavior for this model.

References:
Greitemann, J. *et al. Identification of emergent constraints and hidden order in frustrated magnets using tensorial kernel methods of machine learning. Phys. Rev. B* **100,** 467 (2019), https://journals.aps.org/prb/abstract/10.1103/PhysRevB.100.174408.