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Unsupervised machine learning on atomistic configurations: examples on amorphous defects and energy landscapes EKIN CUBUK, Harvard University, SAMUEL SCHOENHOLZ, ANDREA LIU, University of Pennsylvania, EFTHIMIOS KAXIRAS, Harvard University — Due to the recent availability of very large datasets, machine learning (ML) methods are gaining popularity as approximation and optimization tools in solid state physics. We have recently shown that supervised ML can also be used to identify and analyze soft particles, particles susceptible to rearrangement, in amorphous solids [1]. Our method can be used to understand what makes certain configurations of particles more prone to rearrangement, and design stronger materials. We use unsupervised ML and nonlinear dimensionality reduction methods, where we do not need a "training set" to train the algorithm, to explore better representations of atomic configurations. These representations are shown to provide important physical insights into the structure of soft spots and stable regions in several computational and experimental glassy systems, as well as the energy landscapes of quantum mechanical systems based on Density Functional Theory calculations. By discovering an improved representation and visualization of relevant energy landscapes, discovery and optimization efforts can be simplified.

[1] arXiv: 1409.6820

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