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Neural-network-biased genetic algorithms for materials design[1]

TARAK PATRA, VENKATESH MEENAKSHISUNDARAM, DAVID SIMMONS, The University of Akron — Machine learning tools have been progressively adopted by the materials science community to accelerate design of materials with targeted properties. However, in the search for new materials exhibiting properties and performance beyond that previously achieved, machine learning approaches are frequently limited by two major shortcomings. First, they are intrinsically interpolative. They are therefore better suited to the optimization of properties within the known range of accessible behavior than to the discovery of new materials with extremal behavior. Second, they require the availability of large datasets, which in some fields are not available and would be prohibitively expensive to produce. Here we describe a new strategy for combining genetic algorithms, neural networks and other machine learning tools, and molecular simulation to discover materials with extremal properties in the absence of pre-existing data. Predictions from progressively constructed machine learning tools are employed to bias the evolution of a genetic algorithm, with fitness evaluations performed via direct molecular dynamics simulation. We survey several initial materials design problems we have addressed with this framework and compare its performance to that of standard genetic algorithm approaches.

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