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Pareto fronts for multiobjective optimization design on materials data ABHIJITH GOPAKUMAR, PRASANNA BALACHANDRAN, JAMES E. GUBERNATIS, TURAB LOOKMAN, Los Alamos Natl Lab — Optimizing multiple properties simultaneously is vital in materials design. Here we apply infor- mation driven, statistical optimization strategies blended with machine learning methods, to address multi-objective optimization tasks on materials data. These strategies aim to find the Pareto front consisting of non-dominated data points from a set of candidate compounds with known character- istics. The objective is to find the pareto front in as few additional measurements or calculations as possible. We show how exploration of the data space to find the front is achieved by using uncer- tainties in predictions from regression models. We test our proposed design strategies on multiple, independent data sets including those from computations as well as experiments. These include data sets for Max phases, piezoelectrics and multicomponent alloys.

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