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Machine Learning Discovery of Computational Model Efficacy Boundaries MICHAEL MURILLO, Michigan State University, LIAM STANTON, San Jose' State University, MATHIEU MARCIANTE, CEA — Computational models are formulated in hierarchies of variable fidelity, often with no quantitative rule for defining the fidelity boundaries. We have constructed a dataset from a wide range of atomistic computational models to reveal the accuracy boundary between higher-fidelity models and a simple, lower-fidelity model. The symbolic decision boundary is discovered by optimizing a support vector machine on the data through iterative feature engineering. This data-driven approach reveals two important results: (1) a symbolic rule emerges that is independent of the algorithm, and (2) the symbolic rule provides a deeper understanding of the fidelity boundary. Specifically, our dataset is composed of radial distribution functions from seven high-fidelity methods that cover wide ranges in the features (element, density and temperature); high-fidelity results are compared with a simple pair-potential model to discover the nonlinear combination of the features, and the machine learning approach directly reveals the central role of atomic physics in determining accuracy. From the learned symbolic rule, transferability of the result is used to understand accuracy boundaries for diffusion and viscosity calculations in non-ideal plasmas.

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