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An Information Geometry Approach to Uncertainty Quantification of Sloppy Interatomic Models[1] CODY PETRIE, YONATAN KURNIAWAN, KINAMO WILLIAMS, MARK TRANSTRUM, Brigham Young University — Atomistic simulations often use fitted Interatomic Models (IMs) due to their ability to quickly compute the energy and forces on collections of atoms. Estimating the uncertainty in the fitted parameters is important for assessing the reliability of a model's predictions. Multiparameter models, including many IMs, are often sloppy, i.e., exhibit an extreme insensitivity to coordinated changes in some of their parameter values. Consequently, fitted parameters often have large uncertainties and quantifying this uncertainty can be challenging when models are sloppy. We use an information geometry approach to systematically explore the parameter space of families of IMs, identifying regions of sloppiness. In this approach, a multiparameter model is interpreted as a manifold of potential predictions with parameters as coordinates. We numerically calculate geodesics on the model manifold and identify boundaries of the manifold that are associated with coordinated, extreme values of the parameters. We show how these boundaries are related to sloppiness and uncertainty in fitted parameter values and discuss implications for model selection and uncertainty quantification in atomistic simulations.

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