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Why is uncertainty quantification of sloppy models challenging?[1] YONATAN KURNIAWAN, CODY PETRIE, KINAMO WILLIAMS, MARK TRANSTRUM, Brigham Young University — Interatomic models (IMs) are used in materials modeling to predict material's properties of interest. The development of a single IM can take anywhere from several months to years and relies on expert intuition, and yet these potentials are usually only valid for a particular application of interest. Extending existing IMs to new applications is an active area of research. Quantifying the uncertainty of an IM can tell us how much we can trust the predictions it makes. I compare Bayesian (Markov Chain Monte Carlo) and Frequentist (profile likelihood) methods to quantify uncertainty of IM's parameters. I demonstrate these methods on Lennard-Jones and Morse potentials in predicting the energy and forces of the bases atoms of a triclinic body-centered crystal structure from the OpenKIM database. Results indicate that these models are "sloppy" in some of their parameters, i.e., likelihood surfaces have long, narrow canyons and broad, flat plateaus. I discuss difficulties and challenges from applying these uncertainty quantification methods to sloppy models.

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