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Bayesian Approach to Uncertainty Quantification of Interatomic Models in OpenKIM Database KINAMO WILLIAMS, YONATAN KURNIAWAN, CODY PETRIE, MARK TRANSTRUM, Brigham Young University — Interatomic models (IMs) are used in molecular modeling to predict material 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 take a Bayesian approach to uncertainty quantification. Using Monte Carlo methods, I sample from the posterior distribution of the parameters when trained on data. I demonstrate this method on Lennard-Jones and Morse potentials fit to triclinic crystal configurations from the OpenKIM database. These examples illustrate several subtleties related to the selection of Bayesian prior and choice of model parameterization. In particular, IMs are often sloppy, i.e., have likelihood surfaces with long, narrow canyons and broad, flat plateaus. Because of these features, the posterior can depend strongly on the prior and model parameterization. I discuss implications of sloppiness for uncertainty quantification in molecular modeling.

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