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Gausian processes for system-agnostic construction of high-dimensional PES with sparse ab initio data JUN DAI, University of British Columbia, HIROKI SUGISAWA, TOMONORI IDA, Kanazawa University, ROMAN KREMS, University of British Columbia — Gaussian process (GP) regression has recently been proposed as a system-agnostic tool for building global potential energy surfaces (PES) of polyatomic systems. As with other machine-learning tools, the accuracy of GP regression can be improved by increasing the number of training points. However, this presents significant challenges for applications of GPs in physics. Here, we show that the accuracy of GP models of PES can be improved by increasing the complexity of GP kernels instead of the number of ab initio points. This allows us to build accurate global PES for molecular systems with 4 and 19 atoms, using 500 and 5000 quantum chemistry calculations, respectively. We show that GP models of the PES thus constructed have generalization power, allowing us to extrapolate global PES from low energies to high energies. We illustrate an algorithm to enhance the accuracy of PES by simultaneously optimizing the distributions of ab initio points and the complexity of GP kernels. References: arXiv:1907.08717; arXiv:2001.07271

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