

Tutorial "Active Learning with Bayesian Optimization"

Monday, 13 September 2021 17:00 (1 hour)

Gaussian process regression (GPR) is a kernel-based regression tool with intrinsic uncertainty estimation, which makes it well-suited to natural science datasets. In Bayesian optimization, GPR is coupled with acquisition functions for an active learning approach, where models are iteratively refined by addition of new data points with high information content. This tutorial will use the BOSS code to demonstrate the basic principles of Bayesian optimization and how it can be applied in N-dimensional atomistic structures search.

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Session Classification: Machine Learning - Theory