Karlsruher Institut für Technologie

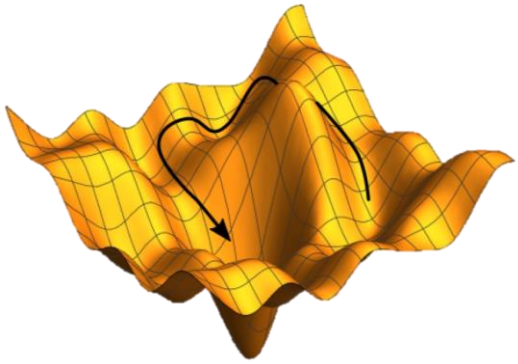
IAM
Institut für Angewandte Materialien

Bachelor Thesis

Optimization strategies enhancing an active learning framework for data-driven material design

Background:

In materials design, traditional trial-and-error methods are often computationally and resources-expensive. Data-driven approaches offer a cost-effective alternative, however their success relies on the ability to guide data collection effectively. Active learning allows to guide the exploration of the search space, prioritizing data points that maximize information gain, thus optimizing the design process while conserving resources.



Your task:

Extension of an active learning Bayesian framework implemented within KadiAI. Study and application of different optimization methods, tuning and investigation for best performances. Customization and validation tests with real material science problems.

Keywords:

Active Learning, Bayesian Optimization, Kadi4Mat, Materials Science

Prerequisites:

Basic knowledge of Linux system and Python is desirable. Interest in machine learning as well as in familiarization with new methods and topics should be present.

What we offer:

- Intensive supervision
- Modern work stations and high performance computers as work environment
- Productive and dynamic atmosphere in a team
- Cooperations with international research groups
- Career options as junior scientist

Curious?

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