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Optimizing Beamline Performance: The Bayesian Approach

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The BAMline, a beamline for material science research at BESSY II, has been operated by the Bundesanstalt für Materialforschung und -prüfung for over two decades. In the last few years, Bayesian optimization (BO) with Gaussian processes (GP) has been introduced as a transformative method in this setting. This contribution highlights the integration and impact of BO and GP in refining BAMline operations.

We will explore the impact of integrating Bayesian methods, especially when combined with Gaussian processes, on the operational efficiency of the BAMline. Our discussion commences with an overview of the fundamental concepts of active learning and optimization. This is followed by an in-depth analysis of specific case studies, drawing on our direct experience with these innovative methods.

For this our focus is on three key applications:

- Alignment of Optical Elements (DCM and DMM): The implementation of Bayesian optimization using Gaussian processes has revolutionized the alignment process for the Double Crystal Monochromator (DCM) and the Double Multilayer Monochromator (DMM). This approach greatly reduced manual effort and enhanced the efficiency and effectiveness of the alignment procedure.
- Optimal Spot Selection for Spatial Mapping in XRF Studies: In X-ray fluorescence (XRF) experiments, determining the most informative sampling spots is crucial. The introduction of BO, informed by GP, has significantly improved the selection process, especially in large or heterogeneous samples. This methodology ensures maximum information gain, optimizing the balance between comprehensive mapping and resource management.
- Selection of Optimal Energies for XANES Measurements in GEXANES Geometry: In the specific context of X-ray Absorption Near Edge Structure (XANES) studies using Grazing Exit (GEXANES) geometry, the Bayesian approach with Gaussian processes is now utilized to identify the most effective energy settings. This results in detailed spectral data acquired in a much shorter time.

We also address challenges and limitations encountered during implementation. Additionally, the versatility of this approach in addressing a range of different research questions will be demonstrated.

Primary author: RADTKE, Martin

Co-authors: GUILHERME BUZANICH, Ana (BAM Bundesanstalt für Materialforschung und -prüfung); Mr CAKIR, Cafer Tufan (BAM Bundesanstalt für Materialforschung und -prüfung)

Presenter: RADTKE, Martin

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