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On-the-Fly Optimization of Synchrotron Beamlines Using Machine Learning

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ABSTRACT

Synchrotron beamline alignment is often a cumbersome and time-intensive task due to the many degrees of freedom and the high sensitivity to misalignment of each optical element. We develop an online learning model for autonomous optimization of optical parameters using data collected from the Tender Energy X-ray Absorption Spectroscopy (TES) beamline at the National Synchrotron Light Source-II (NSLS-II). We test several optimization methods, and discuss the effectiveness of each approach, as well as their application to different optimization problems and benchmarks for beamline performance. We also discuss the practical concerns of implementing autonomous alignment systems at NSLS-II, and their potential use at other facilities.

Keywords: synchrotron radiation, x-ray optics, beamline alignment, beamline control, machine learning

1. INTRODUCTION

One of the largest factors limiting research done at synchrotron beamlines is the limited time available to users. This issue is only compounded by the time needed technical operation of beamlines, much of which is spent aligning and re-aligning beamlines for different experiments. Beamline alignment can be time-consuming, due to the large number of degrees of freedom and high degree of sensitivity of the optical systems of each beamline and that the optical characteristics of the beam can change with different energies, as well as gradually over time. This alignment is typically carried out manually by a member of the beamline staff.

There are thus several benefits of an autonomously-aligned beamline over traditional means. The most obvious is that machine learning-guided alignment is able to both operate the beamline and navigate the high-dimensional parameter space more quickly and knowlegeably than any human, which amounts to time savings that can be reallocated to actual research. Another benefit is that an autonomous beamline is potentially able to find an alignment with more optimal beam characteristics (e.g. a smaller spot size). Lastly, an autonomous beamline avails itself to researcher without an intimate knowledge of the specific beamline being used.

This paper demonstrates with a proof-of-concept that autonomous beamline alignment is feasible, and that it can consistently optimize portions of the Tender-Edge X-Ray Absorption Spectroscopy (TES) beamline at NSLS-II with up to four dimensions.

2. THE TES BEAMLINE

The TES beamline[1] is an X-ray beamline that can perform spectroscopy at energies between 2 and 5.5 keV at micron scales. The full TES beamline has thirteen degrees of freedom for beamline alignment; however, we focus our efforts on applying optimization methods to the toroidal mirror preceding the secondary-source aperture (SSA) and the two Kirkpatrick-Baez (KB) mirrors directly preceding the endstation (see Figure 1), each with four degrees of freedom.

The toroidal mirror is intended to manipulate the beam before it passes through the secondary source aperture (SSA), which then removes all unwanted artifacts (e.g. diffraction) from the periphery of the beam. The toroid's

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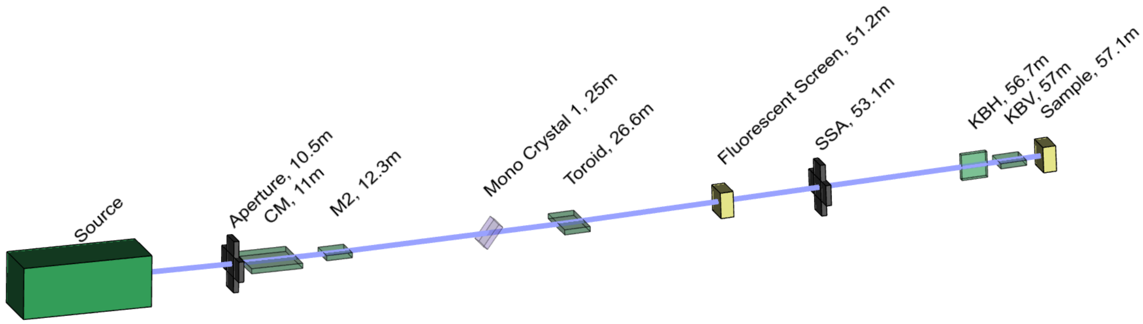

Figure 1: A diagram of the optical configuration of the Tender-Edge X-Ray Absorption Spectroscopy (TES) beamline at NSLS-II.

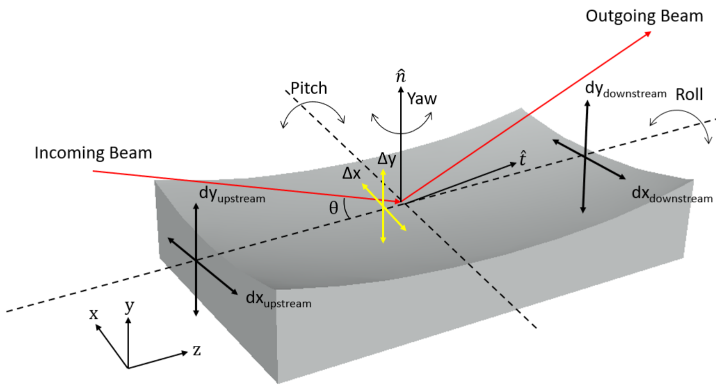

Figure 2: A diagram of the degrees of freedom of the TES beamline's toroidal mirror. This figure is taken from Nash et al.[2]

four degrees of degrees of freedom (two tranverse translation with respect to the beam, as well as pitch and yaw) are shown in Figure 2. The KB mirrors consist of two orthogonal mirrors, and are intended to focus the beam horizontally and vertically after the secondary source aperture (SSA). Each KB mirror can be translated and rotated with respect to the beam (summing to four total degrees of freedom), analogously to the pitch and Δy degrees of freedom for the toroid. The positions of all of the mirrors are manipulated using motors, which can be modulated by set increments. Because these variations are typically small, the vector of optical coordinates describing the beamline (using the convention outlined in this section) are effectively a linear transformation of the vector of the motor positions.

As a proof of concept, we devote our efforts to optimizing these two subsections of the beamline separately; these two subsets of the optical system are classically optimized separately and determine much of the beam quality.

We do not consider variation in energies in this work; all the data herein was taken at 3 keV. We note the importance of an integrated approach to beamline optimization, where we are capable of automatically every part of the beamline. This work is in the context of the larger goal of being able to sequentially optimize optical parameters along the propagation of the beam.

3. DATA COLLECTION AND PREPROCESSING

Data were taken in two sessions. The variation in beam characteristics by the toroidal mirror were measured by inserting a fluorescent screen immediately preceding the SSA, and observing the shape and intensity of the spot as the mirror was misaligned in each degree of freedom. This dataset consisted of 90,000 images which were processed to account for the the skew of the detector's field of view with respect to the optical axis. The images themselves were minimally processed.

The effects of the KB mirrors were similarly measured by observing the beam at the endstation with various misalignments, after the toroidal mirror had been classically optimized. This dataset consisted of 50,000 images which were processed analogously to the first data set.

4. METHODS FOR OFFLINE MODELS

Ideally, the beamline optimization methods would be tested on the beam itself. However, time using the beamline is limited due to to high demand from other researchers. We note two alternative approaches, namely, fiducial simulations and neural network-aided interpolation of real data. Software for simulating synchrotron radiation and beamline outputs include SRW[3] and SHADOW,[4] but often have an expensive trade-off between accuracy and speed (though improvements in efficiency are a very active area of research). We might alternatively "simulate" the intensity output of a beamline for a specific set of optical parameters by interpolating one a sufficiently densely sampled dataset of real images corresponding to real parameters by training a neural network on real images to produce the output image for a respective set of motor positions. Successful methods typically use deconvolutional neural networks, which are well-suited for image generation from a vector input. Further works will explore simulation-aided optimization, as well as machine-learning aided simulation methods.

In this work, however, we distill each beam into a set of statistics (the vertical and horizontal centroids and spreads, the peak intensity, the total flux, etc.) and use them as proxies for a full beam profile. In the interest of analytical simplicity and fast training times, we model the effects of the toroidal and KB mirrors on the TES beam by interpolating the beam statistics in the parameter space of optical misalignments using a Gaussian Process regressor.

5. DIFFERENT OPTIMIZATION METHODS

The motor positions were then optimized using a simple of objective function that preferred the beam to be located in the center of the field of view, as well as minimizing the sum of its vertical width, horizontal width, and difference between those widths (creating a small, round spot). The value of the objective function for unviable beams (e.g. those not entirely contained in the field of view) were additionally penalized. In principle, this approach works for any general objective function that can be mapped to from a profile of the beam intensity. We tested both a gradient descent method, as well as a genetic method (in the differential evolution method). We find that both methods are capable of optimizing both the toroidal and KB mirrors. A visualization of this optimization is found in Figure ??: images consist of collected beam intensity closest in parameter space to the optimal result, while the red squares denote the optimal center of the beam. The number of elapsed iterations for each panel is shown above the plot, where each misaligment was optimized within 64 iterations (implying a real-world optimization time of a few minutes).

6. RESULTS, CONCLUSIONS, AND FURTHER DEVELOPMENT

While we have demonstrated that a straightforward objective function and optimization strategy can quickly find the optimum, and that autonomous beamline alignment is consistently efficient and effective (with a similar optimum being found for differing initial misalignments) and is able to quickly align the predicted beam statistics of the TES beamline. We note that a significant confounding factor in the optimization of proxy datasets is in the assumption that the real data are densely enough sampled (or, in the case of simulation, that the simulated data is accurate).

Moreover, this optimization method can be directly implemented into the current NSLS-II data acquisition framework, which uses the Bluesky to perform scans. In particular, using the Adaptive Bluesky package, we can seamlessly integrate an optimization scheme into a data collection plan, which will then iteratively optimize itself. Further development will consist of autonomous optimization of real beamlines using the Bluesky framework, instead of the statistical proxies used in this work. In addition, the development of this tool can be easily extended to all other NSLS-II beamlines for testing and adaptation.

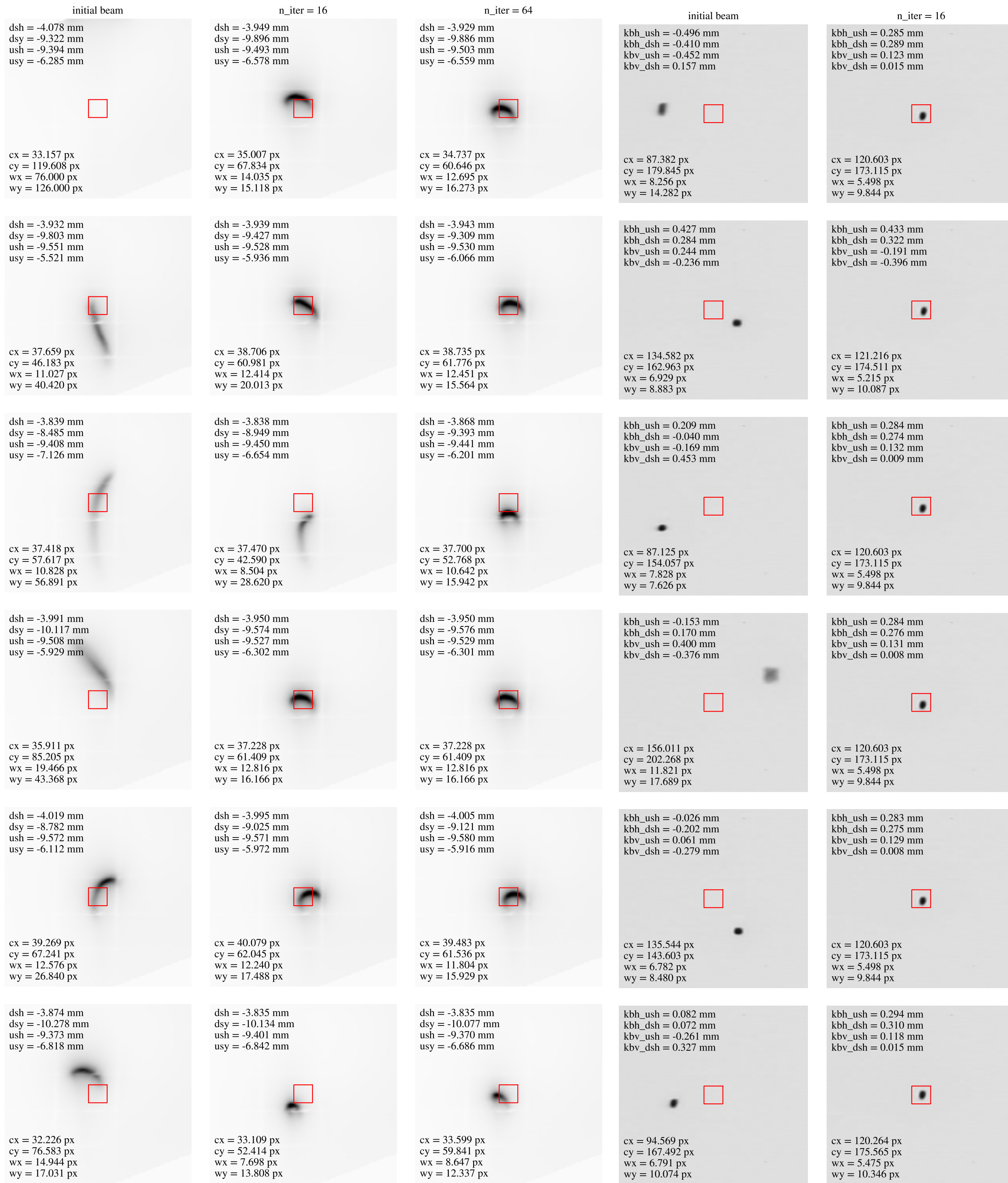

Figure 3: *Left:* Auto-alignment of the toroidal mirror. *Right:* Auto-alignment of the KB mirrors. The evolution of the beam shape and position can be seen clearly for the toroidal optimization. Motor positions are indicated at the top left of each panel, and the beam statistics (the vertical and horizontal centroids and widths) are indicated at the bottom left.

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