Bayesian Optimization Applied to Calibration of Electron Microscope

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Jilles van Hulst[1,*], Roy van Zuijlen[1], Duarte Antunes[1], and Maurice Heemels[1]

[1]Control Systems Technology Section, Dept. of Mechanical Engineering, Eindhoven University of Technology, The Netherlands

[*]Email: j.s.v.hulst@tue.nl

1 Introduction

Electron Microscopes (EMs) can create images at atomic level which continue to enable breakthroughs in a multitude of scientific fields. The quality of the images is a direct result of the quality of the electron beam focus. This focus quality is often imperfect due to fundamental physical limitations. These imperfections can be quantified and are referred to as aberrations. Hardware components can be introduced to compensate the aberrations, but this results in an increased number of calibration parameters, which in turn introduces the need for frequent and lengthy re-calibration by an expert operator. This motivates the need for automatic calibration.

2 Problem Formulation

The aim of this research is to automate the EM calibration process based on its output, which are images. This goal is challenging since these images are high-dimensional and the output is a non-injective mapping of the aberrations. This means that one image can correspond to different aberration configurations.

3 Approach

The proposed method consists of two steps: interpretation of the images, and decision-making based on the interpretation. The first step is performed by feature extraction based on physical insights, which reduces the high-dimensionality of the images first to a low-dimensional vector of features, and then to a scalar cost, similar to [1]. The second step uses Bayesian optimization (BO) [2] with a Gaussian process (GP) estimate to simultaneously estimate and optimize the unknown cost function. The GP uses data gathered from the EM to estimate the cost as a smooth function, while BO selects where to sample next based on the expected improvement which can be computed from the GP estimate.

4 Results

When applying the proposed method to a dataset of synthetic images produced by a high-fidelity model, we verify that the cost function produced by the first step is smooth, symmetrical, and has a unique global minimum. Fig. 1 shows that the cost function is well-estimated in very few samples and that the sample selection converges to the minimizer after initially exploring. In fact, the proposed method is able to calibrate two aberrations in 100% out of 50 attempts, and in 10 or fewer samples 92% of the time.

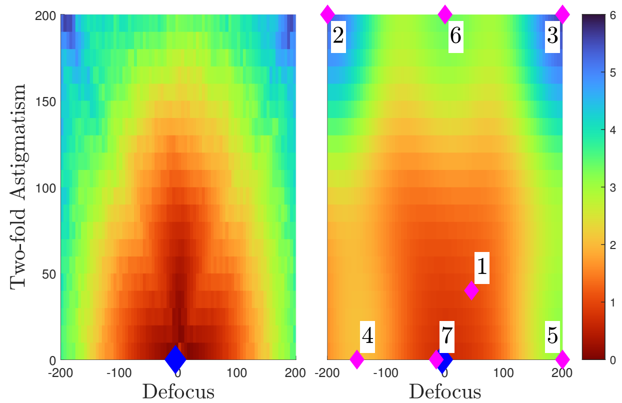

Figure 1: On the left: cost function resulting from feature extraction with minimizer (♦). On the right: GP approximation of the cost function. The indexed sample locations (♦) are selected using BO.

5 Conclusion and Outlook

This research introduces a method for the automatic calibration of EMs that interprets the microscope images and makes decisions that balance improving estimates and exploiting promising current beliefs. Future research avenues include automating the feature extraction process, incorporating more prior knowledge into the optimization scheme, and analyzing the stochastic optimization problem.

References

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