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Elementary, my dear Zernike: model order reduction for accelerating optical dimensional microscopy

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Abstract. Dimensional microscopy is an essential tool for non-destructive and fast inspection of manufacturing processes. Standard approaches process only the measured images. By modelling the imaged structure and solving an inverse problem, the uncertainty on dimensional estimates can be reduced by orders of magnitude. At the same time, the inverse problem needs to be solved in a timely manner. Here we present a method of accelerating the inverse problem by reducing images to their elementary features, thereby extracting the relevant information and distinguishing it from noise. The resulting reduction in complexity allows the inverse problem to be solved more efficiently by utilize cutting edge machine learning based optimization techniques. By employing the techniques presented here, we are able to perform for highly accurate and fast dimensional microscopy.

1 Introduction

Dimensional microscopy is an essential tool for non-destructive and fast inspection of manufacturing processes. One important application is the bidirectional measurement of line structures [1]. The current state of the art involves analysing the image data using threshold techniques. In many measurements, information about the sample and microscope is also available but remains unused. A more accurate estimate of the structure dimensions can be obtained by modelling the light interaction with the structure and comparing the simulated structure images to their experimental counterparts. By varying the model's structure dimension parameters (i.e. line width, particle diameter), the parameters which minimise the difference between model and experiment can be determined. This process is called solving the inverse problem.

In order for the inverse problem to be solvable, the model needs to be able to describe the measurements to a high degree of accuracy. To this end, we have developed a forward model using the finite element solver *JCMwave* [2], which takes into account an efficient sampling of the microscope's illumination pupil, nanooptical scattering at the structure and phase aberrations effects due to the imaging system [3]. Due to the sophistication of the model, we require a method of solving the potentially multi-dimensional inverse problem with relatively few model evaluations. Recently, the Bayesian target vector optimization (BTVO) method has been shown to both efficiently solve the inverse problem and provide information on the uncertainties of the predicted dimensional parameters such as line widths and particle diameters [4].

2 Method

Typical methods of solving the inverse problem attempt to globally minimise χ^2 (chi-squared) calculated from the simulated data and measured data and variances (denoted as σ^2). In the case of images the simulated and measured data consists of the intensity on each pixel (I_{sim} and I_{meas}, respectively) in multiple focal and afocal measurement planes. For high resolution images, the number of pixel data points can run in to the tens of thousands. Using these data points, χ^2 can be calculated by summing up the contribution of each i^{th} pixel to the overall χ^2,

$$\chi^2(\vec{x}) = \sum_{i=1}^{N} \frac{(I_{\mathrm{sim}}^{(i)}(\vec{x}) - I_{\mathrm{meas}}^{(i)})^2}{\sigma_i^2}. \quad (1)$$

The inverse problem is then solved by finding the free model input parameters (represented by the vector $\vec{x}$), such as the line width or diameter, which minimize the total χ^2 for all N pixel data points. The method of Bayesian optimization (BO) performs this minimization by building a surrogate model (called Gaussian process regression) for χ^2, which can then be used to find the global minimum efficiently. However, in building our surrogate model for the sum of the χ^2 contributions, we lose information on the individual pieces of measurement data, and we approximate a multivariate Gaussian distribution for χ^2.

Alternatively, the BTVO method creates a surrogate model (i.e. Gaussian process regression) for each piece of

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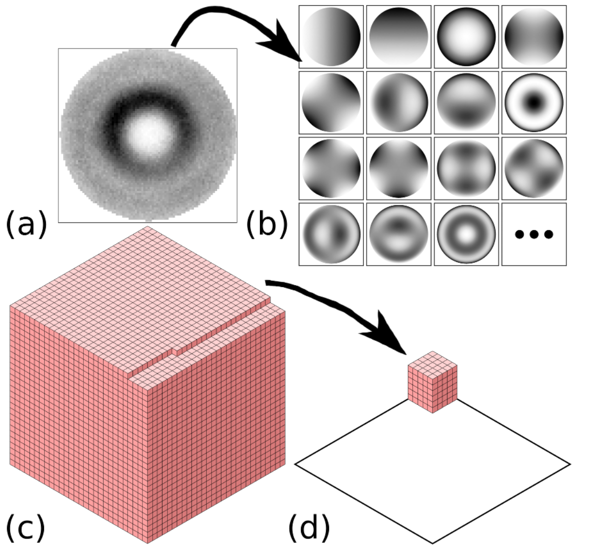

Figure 1. (a) Image of a Cr particle in a plane 2 μm from the focal plane, (b) first few Zernike basis functions used to expand the image in (a). (c-d) Schematic image displaying the number of Gaussian processes needed for different model approaches (one cube represents one Gaussian process). (c) If every pixel in the image stack is modelled with a Gaussian process, (d) if the coefficients of the image expansion are modelled with a Gaussian process.

measured data, which are then used to evaluate χ^2. This has the advantage of providing the correct distribution for χ^2 which results in accurate uncertainties on the reconstructed parameters.

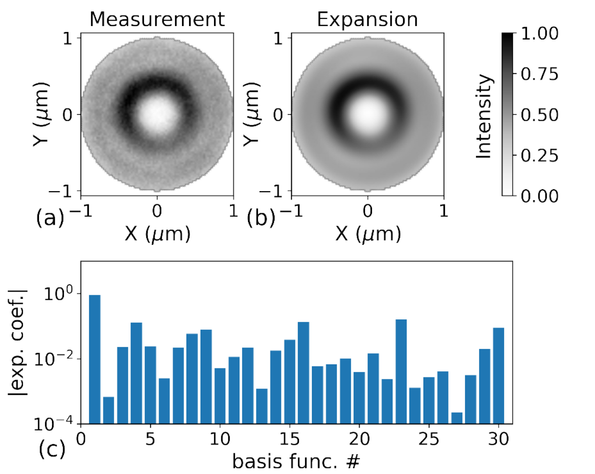

Figure 2. (a) Image of a Cr particle in a plane 2 μm from the focal plane. (b) The expansion of the image using Zernike polynomials. (c) The absolute value of the expansion coefficients used to in the expansion for (b).

The BTVO approach has a larger computational overhead, needing to train N Gaussian processes rather than a single one in the case of BO. In the example of our pixel data, training tens of thousands of Gaussian processes (one for each pixel) would be much too computationally demanding, as shown schematically in figure 1. Instead we seek to extract the essential information contained in the images, while removing the noise, by expanding the images in each plane in a set of orthogonal basis functions. For the particle Zernike polynomials are chosen due to the radial symmetry of the images. The coefficients of the basis function expansion then become the new measurement data. Expanding our simulated images in the same basis, we can solve the inverse problem by minimizing χ^2 for the basis coefficients instead of the pixel intensities.

3 Results

Figure 2 presents an example image expansion in a series of Zernike polynomials. Also shown are the absolute values of the basis coefficients determining the expansion. These values represent our dimensionally reduced measurement data which we use for solving the inverse problem in place of the pixels intensities of the image depicted in (a).

In this contribution, we will demonstrate the effectiveness of employing the Bayesian target vector optimization method for dimensional microscopy. We present results for model based estimates of line widths based on bidirectional optical measurements and compare with estimates based on other experimental techniques.

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