A machine learning method for efficient optimization and parameter reconstruction of nano-structures

P.-I. Schneider,[a] M. Hammerschmidt,[a] X. Garcia Santiago,[ab] V. Soltwisch,[c] C. Rockstuhl,[b] S. Burger[ad]

[a] JCMwave GmbH, Bolivarallee 22, 14 050 Berlin, Germany

[b] Karlsruhe Institute of Technology (KIT), Kaiserstraße 7, 76 131 Karlsruhe, Germany

[c] Physikalisch-Technische Bundesanstalt (PTB), Abbestraße 2-12, 10 587 Berlin, Germany

[d] Zuse Institute Berlin (ZIB), Takustraße 7, 14 195 Berlin, Germany

Numerical optimization is a fundamental task for many scientific and industrial applications. In nano-optics it is employed, e. g., for the optimization of lithographic masks[1] or for scatterometric shape reconstruction[2] (see Fig. 1). The computation of the objective function often requires to rigorously solve Maxwell's equations for multiple frequencies or incoming light-field directions while the parameter space can consist of ten or more degrees of freedom and contains in general a large number of local extrema. This makes numerical optimization in nano-optics very demanding and time consuming.

We demonstrate that the application of Bayesian optimization (BO), a method that has gained popularity in the field of machine learning,[3] can significantly speed up optimization. BO uses previous evaluations of the objective in order to train a stochastic model. The model, a Gaussian process,[4] is subsequently used to derive promising parameter values by means of Bayesian inference. This search strategy uses data on *all* previous function evaluations, which is in contrast to other local or stochastic optimization methods. In order to demonstrate the advantages of the method, we benchmark BO against other commonly used optimization methods such as the downhill simplex algorithm, particle swarm optimization and differential evolution.[5]

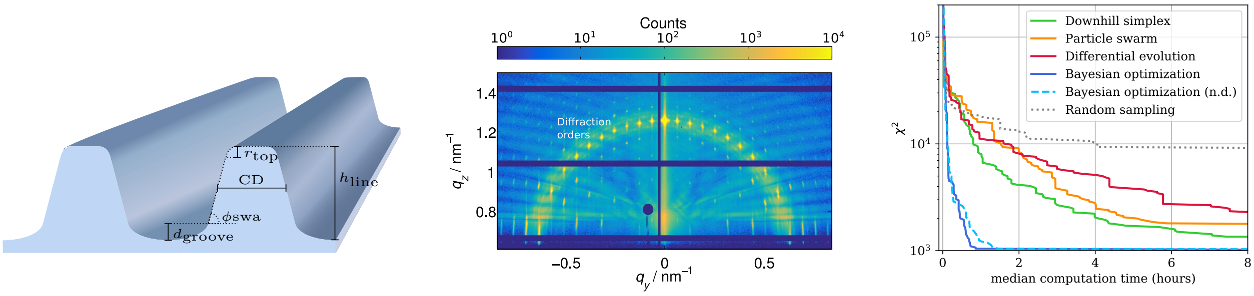

Figure 1. A scatterometric parameter reconstruction problem that consists of identifying the shape parameters of a lamellar grating (left) that correspond to a measured x-ray scattering response (center). The scattering process is simulated on the basis of Maxwell's equations for different parameter values in order to minimize the deviation χ^2 between the measured and simulated response. Bayesian optimization requires significantly less time to identify the optimal parameter values (right).

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