STATISTICAL OPTIMIZATION OF FEL PERFORMANCE
I. Agapov *, G. Geloni, European XFEL GmbH, Hamburg, Germany
I. Zagorodnov, DESY, Hamburg, Germany

Abstract
Modern FEL facilities such as the European XFEL will serve a large number of users, thus understanding and optimizing their performance parameters such as the output power is important. In this work we describe the statistical approach to such optimization under assumption that the possibility of modelling is limited by uncertainties. We present experience of such statistical optimization of SASE radiation power for FLASH and discuss how the results of empirical tuning can be fed back into the model used in simulations.

INTRODUCTION
Experience shows that extensive tuning of an FEL may be required to reach design parameters. The main objective of the present study is to understand methods and design software tools for automatic tuning of FEL parameters. Since many uncertainties are present, we propose to perform such optimization based on empirical methods using very little model information. This roughly mimics what a human operator is doing, only taking advantage of more powerful and faster computations. The possibility of using the model enters into the design of the empirical method. We call such approach statistical. It is described in the first two sections of the paper, including its demonstration at FLASH. The second objective is to try to deduce the model parameters from the measurements so that more realistic calculations can be done. Such problem is typically ill-posed since there is usually much less diagnostics than the potential causes of deviation from design performance. We discuss a possible approach to such model inference in the last section, although its practical feasibility remains to be demonstrated. The statistical tuning software is part of the OCELOT framework ([1,2]).

EMPIRICAL OPTIMIZATION AT FLASH
Optimization is implemented as an arbitrary sequence of optimization steps, each step maximizing the SASE pulse energy with a certain group of devices. A group of devices can be arbitrary, in practice such groups as all launch steerers, FODO quadrupoles, matching quadrupoles, steers between undulators etc. are used. Optimization using a group of devices is usually performed with the simplex (Nelder-Mead) method, although other methods can be used too. The objective function used in maximization is proportional to the SASE pulse energy averaged over several bunch trains. Beam losses approaching the alarm threshold are penalized so that in practice the optimization algorithm always avoids beam losses. To better understand the performance of the optimizer response functions of SASE energy to the control parameters can be studied. Examples of such response functions for launch steerers and FODO quadrupoles are shown in Figs. 1 and 2. The scans are done such that starting from some average value the magnet current is first driven up, then down, and then up again. One can see a certain “hysteresis” effect, which is mostly due to the drift in the radiation power. Figure 3 shows such fluctuations when the machine is not interfered with apart from some feedbacks running. When present, this drift sets a limit to the optimizer performance.
Figure 2 also shows the presence of quadrupole misalignment through the coupling of the quadrupole strength to the orbit, mostly in the vertical direction.

Figure 1: SASE response functions to launch steerers. Green is the set and blue is the read back values.

Figure 2: SASE and orbit response functions to FODO quadrupole strength.
The optimization has been successfully demonstrated at FLASH at several wavelengths (see Fig. 4, 5).

Due to high cost of machine time, it is desirable to study optimization methods in advance in simulation. This particularly applies to European XFEL, where the number of potential control parameters is much larger than at FLASH. At FLASH the optimization speed is mostly limited by the magnet response time, which is about 1 sec in the case of orbit correctors or FODO quadrupoles and can be longer for stronger magnets. The expected performance can be first tested in OCELOT flight simulator (see screenshot on Fig. 6). An example of simulated SASE optimization with quadrupole alignment is presented in Fig 7. The usual time-dependent FEL calculations are computationally demanding, and when done on a high-performance cluster their cost approaches the machine time cost when high precision is required. For optimization method studies, even steady state 3D FEL calculations are not suitable for speed reasons. In the flight simulator, simple approximate formulae for radiation power dependence on optics errors are used. These are used to estimate the complexity of tuning methods and are not suitable for predicting radiation parameters. More precise fitting formulae are being introduced to the flight simulator. This indicates that the simplex method should be also applicable to optimization using quadrupole alignment, where the response time is proportional to the distance over which the magnet is moved.

As discussed above, the FEL performance characteristics can be optimized empirically even if the electron transport
errors are not fully understood. However it is more desirable to understand and correct the source of errors. Alignment errors are one such case and in the following we will consider an example of quadrupole alignment in a FODO channel. If the BPMs are perfectly aligned and are placed after each quadrupole one can reconstruct the misalignments easily. However if the BPMs can be misaligned so that the number of free parameters is larger than the number of measurements the problem may become ill-posed in the sense that solution is not unique. The problem is symptomatic for any sort of optics parameter reconstruction as soon as we allow uncertainties in the transport parameters. Imposing constraints such as regularization penalty one can get a unique solution which however does not need to have anything to do with reality. It thus seems logical to develop methods which produce not specific output values but sets of parameters which are consistent with measurements. As more measurements become available the parameter set can be refined. In the following these methods will be called Bayesian. The classical Bayesian methods estimate probability densities of parameters which reflect the degree of belief. The Bayes theorem is used to compute the aposteriori estimate \( f(\theta | Y) \) of probability of parameter \( \theta \) after measurement \( Y \) using the apriori estimate \( f(\theta) \) and the probability \( f(Y|\theta) \) of observation \( Y \) given model parameters \( \theta \)

\[
f(\theta | Y) = \frac{f(Y|\theta) f(\theta)}{\int f(Y|\theta) f(\theta) d\theta}
\]

Evaluation of \( f(Y|\theta) \) is easy since we typically have the appropriate model. Dealing with multi-dimensional densities (dimension equals number of free parameters) is problematic. If certain features such as the model linearity can be exploited the difficulty can be overcome. For a FODO channel with initial beam coordinates \( x, x' \), BPM offsets \( \delta_1 \) and quadrupole offsets \( \Delta_1, \Delta_2, \ldots, \Delta_n \), the parameter vector is then \( \theta = \{ x, x', \delta_1, \Delta_1, \ldots, \delta_n, \Delta_n \} \). The BPM reading vector is \( Y_1 \). For a fixed quadrupole strength one easily computes the response matrix \( A_1 \) of \( Y \) with respect to \( \theta \) and the parameters are a solution to a linear system of equations \( Y = A_1 \theta \). Now if we assume that any BPM can be offset, any position measurement introduces an additional free parameter, and there are always infinite number of solutions (unless different measurements are performed e.g. at different energy or with different optics setup). A unique solution can be obtained by a regularized least square fit (solution with minimum norm).

\[
\theta_0 = (A_1^T A_1 + \lambda I)^{-1} A_1^T Y_1
\]

where \( \lambda \) is a small regularization parameter. The uniqueness of the solution is, as discussed above, artificial. However, all solutions of the system can be represented as a direct sum of a particular solution and the null space of \( A_1 \)

\[
\theta = U_1 \theta_1 + \theta_0 \quad \theta_1 \in \mathbb{R}^{dim(null(A_1))}
\]

where \( U_1 \) is a matrix whose columns are an orthogonal basis of the null space of \( A_1 \) and \( \theta_1 \) is arbitrary. The null space can be calculated via SVD decomposition in practice. Now if we are given a second measurement we look for the least squares solution in the subspace given by Eq. 3. If the matrix \( A_2 \) in the second measurement is the same as \( A_1 \), then the measurement is only consistent if \( Y_1 = Y_2 \), in which case no new information is gained. Otherwise we proceed to determine a particular solution of \( A_2 \theta = Y_2 \)

\[
\theta_1 = (U_1^T A_2^T A_2 U_1 + \lambda I)^{-1} U_1^T A_2^T (Y_2 - A_2 \theta_0)
\]

and this process is continued for each new set of measurements. The basis of the linear manifold to which the possible misalignments belong is thus iteratively evaluated and should yield a solution if the measurements are properly designed. It can be shown that this procedure can be used for determining quadrupole and BPM misalignments simultaneously. However it is then completely equivalent to piling up all the measurements and performing a single least squares fit. The advantage would appear if the procedure yields a low dimensional manifold and one can use other measurements such as the SASE power to produce an interpretable probability density of parameters. If the approach is feasible in practice remains to be seen.

CONCLUSION AND OUTLOOK

We developed automatic FEL tuning software based on empirical principles and demonstrated it at FLASH for optimizing SASE pulse energy. Operator friendly tools are under development. More advanced optimization methods including FEL spectrum control, undulator gap tuning, pointing control will be studied in simulation and experimentally both for FLASH and for the European XFEL.

ACKNOWLEDGEMENTS

The authors wish to thank S. Molodtsov for support of this work, A. Bozhevolnov and V. Rybnikov for help with the controls interface and the whole FLASH team for support during measurements.

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