ISBN: 978-3-95450-247-9 ISSN: 2673-5490 doi: 10.18429/JACoW-IPAC2024-MOPS14

COMPARISON OF BAYESIAN OPTIMIZATION AND THE REDUCTION OF RESONANCE DRIVING TERMS IN THE OPTIMIZATION OF THE DYNAMIC APERTURE OF THE BESSY III MBA LATTICE

B. Kuske*, M. Arlandoo, M. Ries, A. Schälicke, Helmholtz-Zentrum Berlin, Berlin, Germany
A. Santamaria Garcia, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Abstract

Helmholtz-Zentrum Berlin (HZB) is currently designing the lattice for BESSY III, the successor of the 1.7 GeV electron storage ring that has been running in Berlin since 1998. HZB follows a deterministic lattice design strategy, where the natural substructures of a multi-bend achromat (MBA) lattice with distributed sextupoles are optimized separately. The substructures consist of only a few parameters, that can be derived from the strategic goals of the project. In the next step, the focusing and defocusing sextupole families are split to optimize the longitudinal and the transverse apertures. The paper compares two approaches to select the optimal sextupole strengths. One is Bayesian optimization, where the dynamic aperture area from tracking simulations is used as an objective to be maximized. The other does not involve tracking and minimizes the geometric resonance driving terms. The comparison of the two results includes their quality in terms of the size of the achievable 2D dynamic aperture and the computational effort involved.

INTRODUCTION

Modern light sources, like BESSY III [1, 2], are designed to reach pico-meter emittance. This is achieved by incorporating many dipoles and strong focusing into the lattices. As a result, the small dispersion function and the large natural chromaticity cause large sextupole strength, limiting the momentum acceptance (MA) and the dynamic aperture (DA), sometimes to an extent where expensive technical solutions become unavoidable, such as swap-in-swap-out injection schemes or bunch lengthening techniques. Therefore, much effort is spent optimizing the settings of the sextupole-, octupole-, and sometimes even decapole fields in the lattice.

A common, but resource-intensive approach is to perform tracking studies, combined with machine learning approaches, such as multi-objective genetic algorithms (MOGAs) [3, 4]. Often, these approaches are improved by requiring the lower-order resonance driving terms (RDTs) to be small. The characterization of non-linear single-particle dynamics by RDTs started in the late 1980s [5] and was further developed by different authors, including experiments [6, 7]. Small 1st-order RDTs were shown to be a necessary, but not sufficient, condition for a large DA [8, 9]. This is confirmed by considering the simple example of a 7-BA lattice with five identical unit cells with a phase advance of 0.4 and 0.1 and no additional sextupoles outside of the unit cells, creating a perfect higher-order achromat (HOA). All geometric driving terms are exactly zero, except for the amplitude-dependent tune-shift terms and h_{20020} [10], which will limit the dynamic aperture. [9, 11] introduce the concept of 'RDT fluctuations', or 'local RDTs', i.e. the development of the RDTs over a super period, in contrast to the 'global RDTs', i.e. the value after one turn.

The determination of the *absolute* DAs of a machine is non-trivial. Usually, it is a statistical evaluation of many error seeds. It depends on the number of turns tracked, the type of errors included, the step size, etc. A criterion allowing for *relative* comparisons of the DAs of different non-linear realizations of the same linear lattice is to limit the tune shift associated with amplitudes and momentum offsets. A stricter tune confinement stands for a larger DAs. The limit of stable motion, (momentum and amplitude) in this paper is $\sqrt{\Delta Q_x^2 + \Delta Q_y^2} \leq 0.1$. The measure for comparing different DAs is their enclosed area. Fig. 1 shows an example of an DA defined by particle loss and by the tune shift criterion. This paper compares apertures maximized using two different tracking approaches and by minimizing different driving terms. The goal is to investigate how much aperture can be gained by investing more computing power.

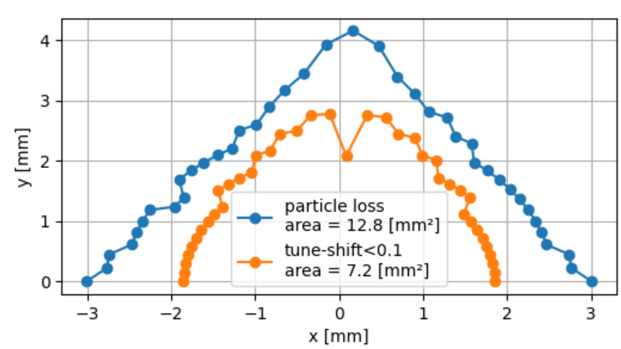

Figure 1: DA of BIII with two families of sextupoles, without errors, defined by particle loss, blue, and by the limited tune shift of the tracked particles, orange.

THE BESSY III LATTICE

The linear lattice for BESSY III, a 2.5 GeV, low emittance, MBA, was developed deterministically, i.e. without computer-assisted optimization [12]. The lattice is a 6-Bend-Achromat following the design criteria of HOAs, with distributed sextupoles. The phase advance of the unit cells is 0.4 and 0.1 for control of the lower-order RDTs. The phase advance of each of the two dispersion suppression cells (con-

* bettina.kuske@helmholtz-berlin.de

ISBN: 978-3-95450-247-9 ISSN: 2673-5490 doi: 10.18429/JACoW-IPAC2024-MOPS14

stituting the 5th unit cell) is 0.386 and 0.061 , a compromise with other design criteria. The deviating phase advance disturbs the perfect cancellation of the RDTs. The 1st - 3rd order RDTs (in perturbation theory), $h^{(1)}$ to $h^{(3)}$, for a scheme of two families of chromatic sextupoles only (located at 8 symmetric positions), are listed in Table 1. All RDTs are small, except those driving the tune-shift with amplitude (tswa).

Table 1: RDTs for 2 Chromatic Sextupole Families

$h^{(1)}$	< 6.0
$h^{(2)}$	< 80.000
$h^{(3)}$	< 1800

OPTIMIZING THE RDTS

To enlarge the on-momentum DA, it should therefore be sufficient to minimize the tswa terms, a_{xx}, a_{xy}, and a_{yy}, while keeping the other terms small. The tswa terms (2nd-order in perturbation theory) are related to the 1st-order geometric terms, h_{21000}, h_{30000}, h_{10110}, h_{10020}, and h_{10200}, in a non-trivial way.

Using two families of sextupoles with equal integrated strength is the minimalistic approach to compensate for chromaticity, and it is used as the initial configuration for the RDT minimization. The 'Powell's method' was found to be the most successful. Six sextupole pairs per super period were optimized, while the two innermost were used for chromaticity compensation. Table 2 lists the results for different boundaries on the sextupole strength, from ± 30 to 60% and no boundaries. The objective function is the rms value of the 3 tswa terms, and its reduction is listed in the first column. The other columns list the stable area of the DA, determined by particle loss and by the tune shift criterion, and the momentum acceptance as the other critical parameter for the non-linear robustness of the lattice. Optimal convergence is achieved for ≥ 60% variation range. These cases also enlarge the momentum acceptance of the lattice. This is a feature of the linear lattice [13]. The corresponding sextupole strengths show a significant increase in SF3, SD4 and SD5. These magnets are the outer sextupoles, in or near the dispersion suppression cell, i.e. the location of the disturbed phase advance. This follows 'hands-on' optimization experience using OPA [10].

Table 2: Minimization of the tswa Terms

SX limit	reduction to %	area by loss mm²	area by ΔQ mm²	mom. acc. %
start	100	12.8	7.2	3.0
30%	6	33.5	29.2	2.0
40%	23	43.6	39.3	2.0
50%	23	43.8	39.4	2.0
60%	5e-6	29.9	27.4	3.5
no limit	0	29.7	27.2	3.5

Starting from these optimized values, different objective functions were compared, Fig. 2. Minimizing the tswa terms, from two different start values (labels 'start', 'opt') seek identical results, as well as including the local 1st-order geometric terms in the objective function (label hjklm-loc-ajk). Minimizing only the global 1st-order geometric RDTs is the least successful. Using only the local 1st-order geometric RDTs seeks the largest dynamic aperture for reduced MA.

These results can be explained using the derivations in [11]. The tswa terms can be determined using the 1st-order RDTs. They can be decomposed into two parts, a_{ij}=A+B, following the notation of [11]. While A is an integral over the development of the driving terms over one super-period of the lattice, i.e. uses the local RDTs, B only depends on the global RDTs, i.e. the values after one turn. For a HOA lattice, A is the dominant term. Therefore, minimizing the global RDTs, only acts on term B which is already small, whereas minimizing the local RDTs acts on the dominant part A. Minimizing the tswa terms does not further reduce the local RDTs and is less favorable.

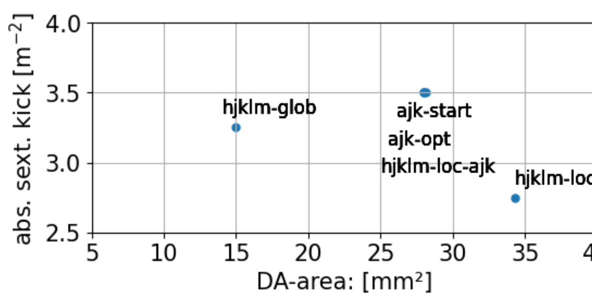

Figure 2: MA over the area of the DA, determined by limited ΔQ. Different objective functions are compared.

BAYESIAN OPTIMIZATION APPROACH

Bayesian optimization (BO) is a black-box, iterative optimization algorithm that has become popular in the accelerator community in recent years due to its effectiveness in solving common tuning tasks [14]. It is a model-based method where a statistical surrogate model of the objective, usually Gaussian processes (GP), is iteratively built with data samples. This optimization method is commonly used to find the global optimum of expensive-to-evaluate functions due to its sample-efficiency. Nevertheless, finding such a global optimum can become increasingly challenging depending on the dimensionality of the problem and the complexity of the objective function. On the one hand, the parameter hypervolume to optimize grows exponentially with the number of dimensions n^d, where n are the data samples and d the dimensionality of the problem. This means that the number of samples required to make reliable inferences grows exponentially. On the other hand, if the optimization objective landscape is highly nonconvex, the presence of many local minima can trap the optimization process in suboptimal regions. In conjunction with the sample sparsity present in high dimensions, the objective might be difficult to model with GP.

ISBN: 978-3-95450-247-9 ISSN: 2673-5490 doi: 10.18429/JACoW-IPAC2024-MOPS14

In this study, we want to maximize the DA using six chromatic sextupole pairs, while matching the chromaticity to zero with two additional sextupoles, as in the RDT approach. We use newly developed Python libraries in the accelerator community: Xopt [15] as BO framework and Xsuite [16] for chromaticity matching and DA estimations. This problem is nonlinear with $d = 6$, where the size of the parameter hypervolume will depend on the allowed sextupole strength range. The matching of the chromaticity presents an additional challenge in this optimization since it requires the change of the strength of two sextupoles, which will, in turn, affect the DA. This introduces contextual parameters (i.e., cannot be varied by the algorithm but affect the objective) that change non-monotonically in every iteration.

The chromaticity was matched to zero with a tolerance of 10^{-1}, the DA calculations used 512-turn tracking, and the acquisition function used was expected improvement (EI). Two optimization runs were performed, one initialized with 200 random samples and full sextupole strength range, and the other initialized with 500 samples and a reduced sextupole strength range, centered around pre-optimized sextupole values, Fig. 3. We observed that the run with more initial samples and reduced actuator range obtained on average a higher DA area, due to the simplification of the problem by localizing the search in the parameter hypervolume. Nevertheless, we see no meaningful improvement trend over time, which reflects the inability of the algorithm to learn properly due to the complexity of the problem. The best DA area achieved was 24 mm^2. To apply BO to DA optimization the problem needs to be simplified to develop a competitive data-driven approach. This can be done by incorporating domain knowledge through informed priors and constraints to guide the optimization more efficiently and/or advanced kernel functions, as well as by reducing the complexity of the objective function and parameter hypervolume.

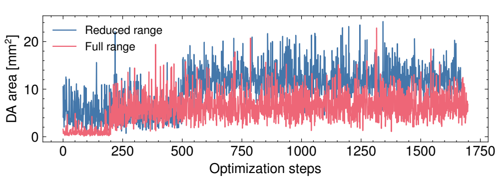

Figure 3: Two BO runs: 200 samples and full sextupole range (pink) and 500 samples and a reduced range (blue).

RESULTS

Additionally, an optimization strategy based on *skopt.learning.ExtraTreesRegressor* was used to maximize the DA [17, 18]. The objective function was changed from using the area of the DA to applying a frequency-map analysis, i.e. minimizing the diffusion rate over the sampled particle map [19]. Unlike BO, this approach does not suffer from increasing computation time with proceeding optimization, therefore enabling significantly more evaluations of different sextupole settings. 13.000 sextupole settings were evaluated, taking ≈ four hours using four nodes of the HPC of the HZB accelerator division.

Figure 4 shows the results of the two approaches. The DA using the 'ExtraTree' optimization and particle loss is much larger than the one defined by RDT minimization, but it is associated with large tune shifts and will be largely reduced when errors are applied. The additional area compared to the RDT-method, when applying the tune confinement criterion, lies mostly in the vertical plane, which will be limited by undulator gaps. The DA defined by RDT minimization is larger in the horizontal plane needed for injection and it is more robust against errors.

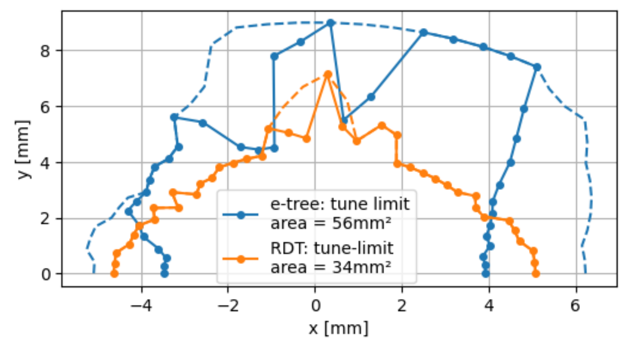

Figure 4: comparison of the DA resulting from the 'Extra-Tree' optimization (blue) and by RDT minimization, orange. Dashed lines indicate the DA determined by particle loss, solid lines the ones by the tune confinement.

CONCLUSION

This paper compared different approaches to optimizing the dynamic aperture for the BIII lattice. The optimization of RDTs corresponds to finding the minimum of a smooth 6D surface, where the projection onto each axis (RDTs) is a polynomial of the sextupole strength. The minimization is straightforward and fast, seconds to a few minutes, but it is an indirect approach, confining the tune space covered by the different amplitudes. The straightforward use of BO with the DA-area as the objective, was not successful. More work has to be invested in confining the complexity of the problem, as the objective surface is highly non-linear, and the method runs into CPU issues due to the high dimension of the problem. The third approach optimizes the diffusion rate, calculating 13.000 DAs. Although a large DA is found, the result lacks robustness. We conclude that for a linear lattice optimized as HOA the minimization of the RDTs is a robust approximation of the DA, well-suited to compare different lattices during the design stage. Tracking optimizations can therefore be postponed to fine-tuning and when the focus is shifted to the effect of errors.

The next step is to include the momentum acceptance and off-momentum DA in the optimization. For the RDT minimization, chromatic RDTs and the 2$^{\text{nd}}$-order chromaticity have to be included in the objective function. For the tracking approaches, the off-momentum dynamic apertures over the desired momentum acceptance need to be calculated in every step as well.

ISBN: 978-3-95450-247-9 ISSN: 2673-5490 doi: 10.18429/JACoW-IPAC2024-MOPS14

REFERENCES

[1] A. Vollmer, P. Goslawski, A. Jankowiak, F. Krawatzek, M. Sauerborn, and O. Schwarzkopf, "Materials Discovery at BESSY," *Synchrotron Radiat. News*, vol. 37, pp. 12–17, 2024. doi:10.1080/08940886.2024.2312051

[2] *BESSY III - The Materials Discovery Facility*, 2022. https://www.helmholtz-berlin.de/media/media/angebote/bibliothek/reports/r0004-bessy-iii-the-materials-discovery-facility.pdf

[3] M. Borland, L. Emery, V. Sajaev, and A. Xiao, "Direct Methods of Optimization of Storage Ring Dynamic and Momentum Aperture," in *Proc. PAC'09*, Vancouver, Canada, May 2009, pp. 3850–3852. https://jacow.org/PAC2009/papers/TH6PFP062.pdf

[4] M. P. Ehrlichman, "Genetic algorithm for chromaticity correction in diffraction limited storage rings," *Phys. Rev. Accel. Beams*, vol. 19, no. 4, p. 044 001, 2016. doi:10.1103/PhysRevAccelBeams.19.044001

[5] J. Bengtsson, "Non-linear transverse dynamics for storage rings with applications to the low-energy antiproton ring (LEAR) at CERN," Ph.D. dissertation, Lund U., 1998. doi:10.5170/CERN-1988-005

[6] R. Bartolini and F. Schmidt, "Normal form via tracking or beam data," *Part. Accel.*, vol. 59, pp. 93–106, 1998.

[7] R. Bartolini, "Resonance Driving Term Experiments: An Overview," in *Proc. ICAP'06*, Chamonix, Switzerland, Oct. 2006, pp. 22–27. https://jacow.org/icap06/papers/MOM1MP03.pdf

[8] L. Yang, Y. Li, W. Guo, and S. Krinsky, "Multiobjective optimization of dynamic aperture," *Phys. Rev. Spec. Top. Accel. Beams*, vol. 14, p. 054 001, 2011. doi:10.1103/PhysRevSTAB.14.054001

[9] B. Wei, Z. Bai, L. Tan J.and Wang, and G. Feng, "Minimizing the fluctuation of Resonance Driving Terms in Dynamic Aperture Optimization," *Phys. Rev. Spec. Top. Accel. Beams*, vol. 26, p. 084 001, 2023. doi:10.1103/PhysRevAccelBeams.26.084001

[10] A. Streun, *OPA Lattice Design Code*. https://ados.web.psi.ch/opa/.

[11] M. Arlandoo, "Transverse Resonance Island Buckets in Advanced Light Sources," Ph.D. dissertation, Humboldt-Universität zu Berlin, to be published.

[12] B. Kuske and P. Goslawski, "Deterministic Approach to MBA Lattice Design," in *iFAST – 9th Low Emittance Workshop, CERN, Switzerland*, 2024. https://indico.cern.ch/event/1326603/contributions/5773933

[13] "BESSY III Progress," in *Contribution list of the 3rd Workshop on on Low Emittance Lattices, LEL2022, Barcelona, Spain*, 2022. https://indico.cells.es/event/1072/contributions

[14] R. Roussel *et al.*, "Bayesian Optimization Algorithms for Accelerator Physics," 2023. doi:10.48550/arXiv.2312.05667

[15] R. Roussel, A. Edelen, A. Bartnik, and C. Mayes, "Xopt: A simplified framework for optimization of accelerator problems using advanced algorithms," in *Proc. IPAC'23*, Venezia, 2023, pp. 4796–4799. doi:10.18429/jacow-ipac2023-thpl164

[16] G. Iadarola *et al.*, "Xsuite: An Integrated Beam Physics Simulation Framework," in *Proc. HB2023*, 2024, TUA2I1. doi:10.18429/JACoW-HB2023-TUA2I1

[17] G. Louppe, *Understanding random forests: From theory to practice*, 2015.

[18] *skopt.learning.ExtraTreesRegressor*, https://scikit-optimize.github.io/0.8/modules/generated/skopt.learning.ExtraTreesRegressor.html, Accessed: 2024-05-14.

[19] *pyAT frequency map analysis*, https://atcollab.github.io/at/p/apiat.physics.frequency_maps.html\#module-at.physics.frequency_maps, Accessed: 2024-05-14.