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MACHINE LEARNING BASED SURROGATE MODEL CONSTRUCTION FOR OPTICS MATCHING AT THE EUROPEAN XFEL

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Abstract

Beam optics matching is a daily routine in the operation of an X-ray free-electron laser facility. Usually, linear optics is employed to conduct the beam matching in the control room. However, the collective effects like space charge dominate the electron bunch in the low-energy region which decreases the accuracy of the existing tool. Therefore, we proposed a scheme to construct a surrogate model with nonlinear optics and collective effects to speed up the optics matching in the European XFEL injector section. Furthermore, this model also facilitates further research on beam dynamics for the space-charge dominated beam.

INTRODUCTION

The X-ray free-electron laser facilities around the world aim at generating high-brightness and coherent X-ray pulses [1], which facilitate the ultra-fast scientific research with atomic spatial resolution [2–4]. The European X-ray Free-Electron Laser (EuXFEL), which is in the operational stage since 2017, is designed to generate X-rays from 0.25 to 25 keV[5]. It is driven by a superconductive accelerator that is able to produce up to 27,000 electron bunches per second with maximum electron beam energy up to 17.5 GeV. As the source of electron bunches, the photoinjector section aims at generating the bunches with low emittance and matched optics with design values which is essential to the downstream beam delivery to the undulators. Therefore, it is required to measure and optimize these transverse phase space parameters by tuning the several injector settings, which is one of the routine procedures of accelerator operation.

Usually, the multi-quadrupole scan method is applied to optics measurement. These optical functions are calculated based on the beam size measurement on the intercepting screen whilst varying the upstream machine lattice. The deduction is based on the linear optics model to track the beam from the first matching quadrupole to the final reference point. However, collective effects such as space charge and wakefields are not taken into account in this approach, which might lead to inaccuracy. Moreover, the beam tracking with these collective effects would take more computational resources for one single simulation, making it not applicable to be introduced in the online optimization of beam optics matching. Therefore, the machine learning-based approach is proposed to construct the surrogate model to deal with this problem. The model involves the second-order optics and the beam collective effects, aiming to act as an alternative to the existing tool to execute the optics matching in the control room.

The machine learning technique has been applied to power many scientific domains in these two decades due to the improvements in computational resources and the theory of algorithms. As one of the classical approaches in machine learning, supervised learning builds a function that maps the input features to the output parameters using the sample set. In the accelerator community, this method has been introduced to tackle system modeling in several projects. Its most useful strength is the fast execution of high-fidelity beam simulations with sufficient accuracy. Based on it, it facilitates the fast offline beam dynamics optimization and design (i.e. dynamics aperture maximization for storage ring, the emittance, and energy spread in wakefield accelerator linacs) [6, 7], as well as providing on-the-fly prediction of the realistic machine, for instance, switching between different operation modes [8]. Hence, the machine learning-based surrogate model is introduced to assist the online optics matching at the injector section to replace the time-consuming beam tracking with collective effects, as presented in Fig. 1. The proof-of-principle experiment in the control room demonstrates the accuracy of the surrogate model and it paves the path for further exploration of machine learning applications on accelerators.

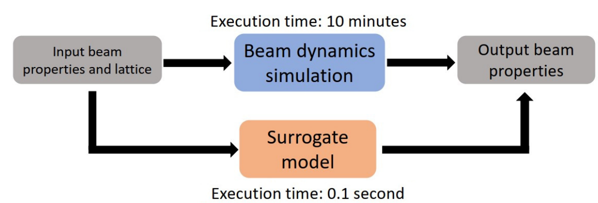

Figure 1: The built surrogate model can substitute the slow physical simulation and largely improve the evaluation efficiency, which facilitates the beam dynamics optimization both in offline design and online control.

SURROGATE MODEL CONSTRUCTION

The injector section of the EuXFEL consists of a photocathode electron gun, a booster accelerator, a third harmonic cavity, and a laser heater chicane. In the following beam diagnostic section, the transverse deflecting cavity is deployed to resolve the beam longitudinal properties. The surrogate model is constructed under a deep neural network with the

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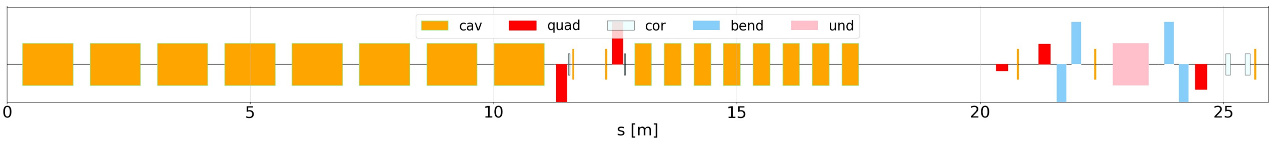

Figure 2: Schematic layout of partial EuXFEL injector from the gun cavity exit to the optics matching position.

sample set generated by beam dynamics simulations using the tracking code OCELOT with all the collective effects taken into account[9]. In Fig.2 the beam tracking region, which starts from the gun cavity exit and ends in the optics matching reference position, is presented. The beam dynamics from the cathode to the end of the gun cavity are simulated with ASTRA[10]. The sample generation is an essential part of supervised learning. Here, the same standard beam distribution simulated by ASTRA is used as the input beam distribution for the OCELOT simulation. The initial optical functions are varied randomly within a reasonable range, and the strengths of the five matching quadrupoles downstream of the accelerating cavity are also generated randomly based on the information from the machine database during operation. Each input parameter and its range can be found in Table 1. These beam optical functions at the initial position and quadrupole strengths are fed to the neural network as the input features. The beam final optical properties at the matching position are treated as the output parameters.

Table 1: The Nine Input Features and These Value Ranges for Simulation

Parameters	Range	Unit
Optics function α_{xi}	[-10, 3]	
Optics function α_{yi}	[-10, 3]	
Optics function β_{xi}	[1, 16]	m
Optics function β_{yi}	[1, 16]	m
Quadrupole strength Q37.k1	[-3, 1.5]	m^{-2}
Quadrupole strength Q38.k1	[1.3, 3.5]	m^{-2}
Quadrupole strength Q46.k1	[-4, 1.2]	m^{-2}
Quadrupole strength Q47.k1	[-1, 5.5]	m^{-2}
Quadrupole strength Q50.k1	[-2, 2]	m^{-2}

The simulations are executed in the DESY Maxwell HPC. The sample set contains 190,000 simulation results and 80% of them are used for training and the other 20% are used for testing. The surrogate model is constructed under the deep neural network architecture which is implemented based on the Pytorch framework[11]. It contains four hidden layers, each with 128 nodes and the tanh activation function. The batch size is 4,000 and the Adam is selected as the optimizer. The model is trained by minimizing the loss function, chosen to be the mean squared error. The performance of the model on the testing set can be found in Fig.3.

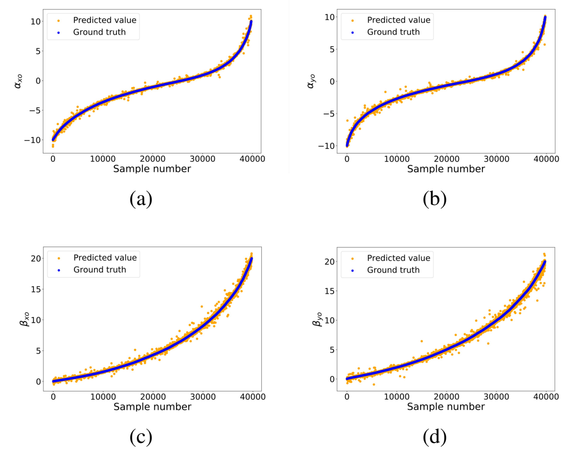

Figure 3: The performance of the neural network on the testing set. The orange dots are the model prediction and the blue dots are the ground truth values.

PROOF-OF-PRINCIPLE EXPERIMENT

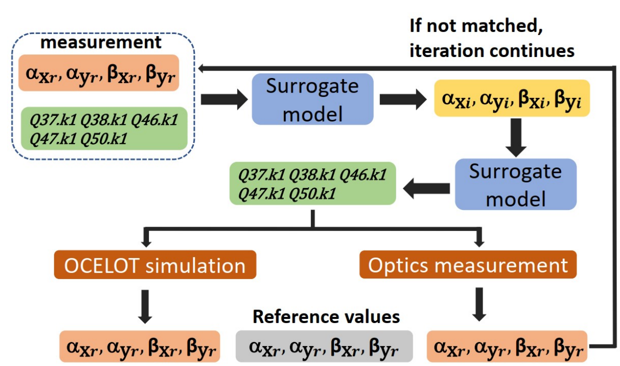

Figure 4: The workflow of model application in the control room. There are two different ways of validation: OCELOT simulation and optics measurement.

After the construction, the surrogate model is introduced in the control room for optics matching in the operational machine. The workflow of the experiment is present in Fig.4. In the beginning, the optics measurement at the reference position is conducted, and the measured optics function values together with the strength of the matching quadrupoles are fed to the model. Based on the simplex numerical optimization [12], the beam optics values at the initial position can be predicted. Then the surrogate model can provide the

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suggestion of matching quadrupoles settings which are supposed to match the beam to the design optics values at the reference point. The optimization iterations will continue according to the updated optics measurement results and the machine lattice.

The optical mismatch parameters BMAG is calculated as [13]

$$\xi = \frac{1}{2}(\gamma\beta_0 - 2\alpha\alpha_0 + \beta\gamma_0)$$
$$\mathrm{BMAG} = \xi + \sqrt{\xi^2 - 1}, \tag{1}$$

where α_0, β_0, γ_0 are the design optics function values at the matching position, the α, β, γ are the measured optics functions. The optimization objective involves getting the BMAG parameters below 1.1 in both horizontal and vertical planes. The experimental result is presented in Fig.5. In the initial condition, the good SASE lasing performance is achieved with these working points whose beam mismatch parameters in the transverse directions are 1.56 and 1.69 in x and y planes, respectively. After four iterations with the constructed surrogate model, the two BMAG parameters are optimized to be 1.05 and 1.03, indicating that the perfect beam matching scenario is achieved using the surrogate model. Fig.6 presents the evolution of the four optical functions, in which good agreement between the model prediction and beam dynamics simulation can be found.

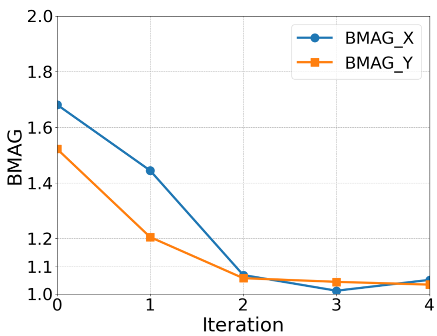

Figure 5: The mismatch parameters BMAG values evolution during the optimization. Iteration 0 denotes the initial condition. The BMAG parameters below 1.1 in both the transverse planes are considered to be good matching conditions.

DISCUSSION AND CONCLUSION

In this paper, the machine learning-based surrogate model for optics matching at European XFEL is constructed. The experimental result demonstrates that the deep neural network can be applied to fulfill the beam optics matching in the injector efficiently. The surrogate model, which involves the beam collective effects during the construction, also has the potential to provide a fast beam diagnostic of transverse properties at the gun cavity exit where the beam is dominated by the space charge effect. Furthermore, the robustness of the model can also be improved through introducing more

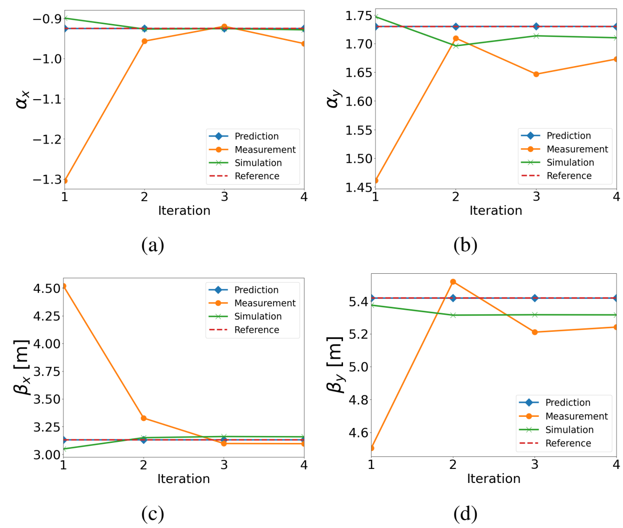

Figure 6: The evolution of the optical functions at the reference point during the optimization iterations. The surrogate model prediction is shown in blue, the red dashed line is the optics design values, the orange line is the optics values acquired from optics measurement server, and OCELOT simulation results are shown in green as the second validation.

machine settings (such as RF parameters within the gun cavity and solenoid strength) that are able to adjust the beam transverse phase space distributions to the features. Some relevant proposals are scheduled in the following research plan.

In conclusion, the machine learning technique has great potential to improve the operation efficiency of XFEL facilities. Here the proposed approach establishes the available toolkit to facilitate online optics matching in the injector section. It lays the foundation for further exploration of machine learning applications in the accelerator operation.

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