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VIRTUAL PHOTON PULSE CHARACTERISATION USING MACHINE LEARNING METHODS

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Abstract

The use of fast computational tools is important in the operation of X-ray free electron lasers, in order to predict the output of diagnostics when they are either destructive or unavailable. Physics-based simulations can be computationally intensive to provide estimates on a real-time basis. This proposed work explores the use of machine learning to provide operators with estimates of key photon pulse characteristics related to beam pointing. A data pipeline is set up and the method is applied to the SASE1 undulator line at the European XFEL. This case study evaluates the performance of the model for different amounts of training data.

INTRODUCTION

Free electron lasers (FELs) are powerful light sources that can produce high-intensity, high-energy laser beams over a wide range of wavelengths. FELs are used in a wide range of scientific research applications, including material science, chemistry, biology, and physics. To measure the beam properties during acceleration, transport, and delivery to users, diagnostic tools require increased accuracy. However, extreme beam conditions and the increased complexity of experiments pose challenges to the current state-of-the-art diagnostics. At the European XFEL in Hamburg [1], machine learning (ML) techniques have been applied to conduct beam optics matching [2], predict occurrences of breakdowns of the superconducting radio-frequency cavities [3] and to calibrate diagnostic devices [4]. Virtual diagnostic tools offer non-invasive measurements of the beam when the diagnostic has limited resolution or availability, using readily available input data. Such tools have the potential to aid in experiment design, setup, and optimization, saving valuable operation time, and interpreting experimental results, especially when current diagnostics cannot provide necessary information.

This work explores the use of an artificial neural network (ANN) to estimate photon pulse pointing properties at the user site based on beam position monitor (BPM) and x-ray gas monitor detector (XGMD) measurements at the photon generation side. The photon properties are extracted from images captured by the FEL radiation imager, which is used to align the FEL beam by controlling and optimising its shape and position. This preliminary work explores the effect of different training dataset sizes in relation to the accuracy of the model, as carried out for the SASE1 undulator. Determining the minimal data that needs to be acquired on each run is important to make the process more efficient.

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METHODS

The acquisition, processing, modelling and evaluation of data is hosted on the Maxwell High-Performance Computing (HPC) cluster, allowing flexibility for data access and control. The complete data pipeline from data ingestion to model predictions is shown in Fig. 1. Data from the two acquisition systems is filtered and merged, followed by model tuning, training and finally evaluation of the trained model. In this section, the main components of this data pipeline are described in detail.

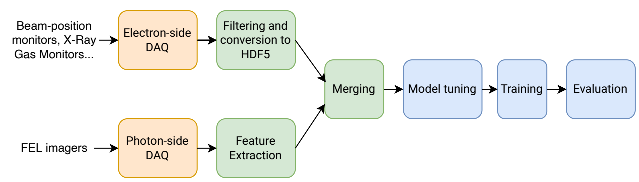

Figure 1: Data pipeline hosted on the Maxwell HPC cluster.

Data Acquisition

In order to train the model for a range of different photon pulse conditions, orbit correctors placed upstream of the initial undulator cell are controlled to generate angular and spatial offsets. Each offset configuration is measured for a period of five seconds. All data is acquired at 10 Hz from two main sources: the DOOCS DAQ, which captures the BPMs and XGMDs, whilst the Karabo DAQ captures the FEL radiation imager images. BPMs along all the undulator cells are recorded as well as XGMs at the end of the undulator. The FEL imager uses a YAG:Ce screen and a Basler acA2500-14gm camera [5].

Feature Extraction

The predicted photon pulse properties are extracted from the FEL radiation imager frames. Each frame is a pixel matrix with size 2592 x 1944 (columns x lines) with a 12-bit resolution. Since the region-of-interest (ROI) in this case is much smaller than the whole frame, the image is initially cropped by calculating a rough estimate of the centre-of-mass. This is done by averaging the pixel intensities along the rows and columns and fitting a Gaussian curve. The pixel at the peak of the curve is considered as the center and the region is expanded to six times the curve's standard deviation from the calculated centre. An example of a raw image is shown in Fig. 2a) and an example of a cropped image in Fig. 2b).

Follow the cropping, a Gaussian curve is refitted on the reduced image as shown in Fig 3. The extracted features

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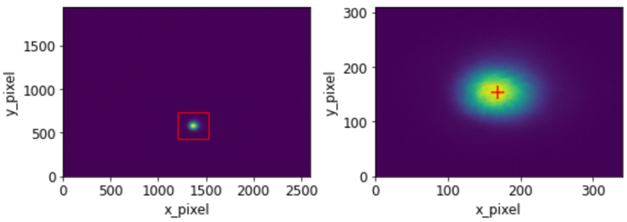

Figure 2: (a) Raw image and (b) image after ROI cropping.

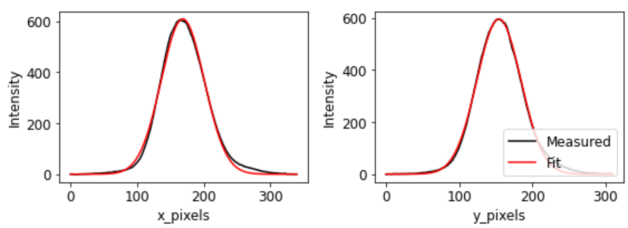

Figure 3: Average pixel intensity along (a) x-direction and (b) y-direction in black and the fitted curve in red.

from the fit include the centre-of-mass, beam size, skewness and kurtosis in both x (horizontal) and y (vertical) positions.

Model Tuning

Once the data from both acquisition systems is merged based on the train ID, the dataset is divided into a training, validation and testing set (60%, 20%, 20% respectively). Different combinations of hyperparameters are then tested on a sample of the training dataset. Hyperparameters are the model variables that the user can modify to tune the model, such as the number of hidden layers and the number of nodes in the hidden layer. In this work a grid search is carried out before the model is trained, which uses a different combination of all the specified hyperparameters and their values and calculates the performance for each combination and selects the best value for training the model. For the dataset presented in this work, a neural network with three hidden layers and 84 nodes in each layer is found to be optimal.

Model Training

The neural network is constructed using the PyTorch framework [6]. The model input features include 13 BPMs (x and y positions) and one XGM. The target features are the eight extracted photon properties. An early stopping approach is applied, where the training is stopped when the validation error starts increasing. This ensures the model is neither underfit nor overfit. The patience parameter controls how many epochs the training process will continue without any improvement in the validation loss. If the validation loss doesn't improve after 'patience' number of epochs, the training process is stopped.

Evaluation

Once the trained model is saved, it can be used to predict the eight photon pulse properties for different BPM/XGMD

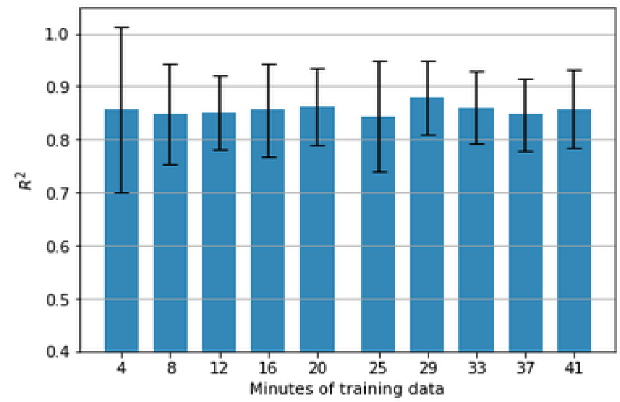

Figure 4: Average R^2 for the eight predicted outputs with varying amounts of training data

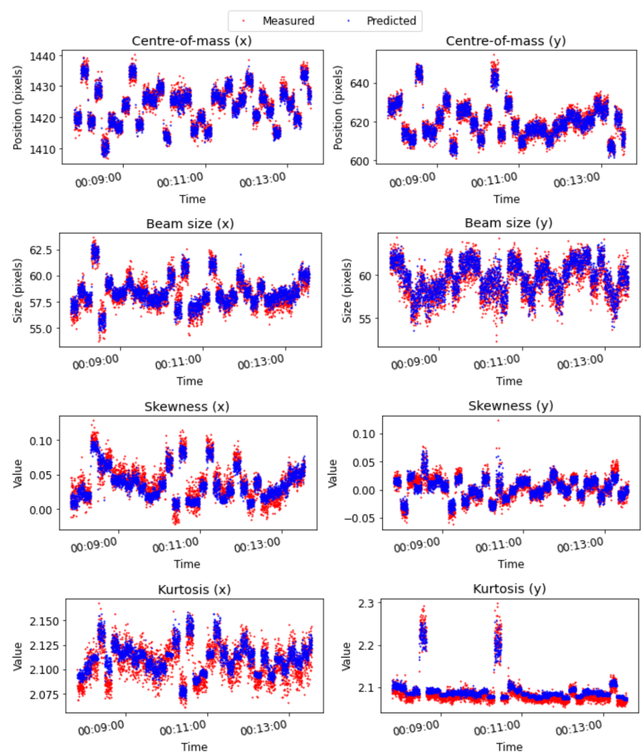

Figure 5: Measured (red) and predicted (blue) properties for the model trained with 20 minutes of machine data.

values. The performance of the model is evaluated by calculating the average coefficient of determination (R^2) and root mean square error (RMSE) for the eight properties. As a case study in this work, the performance of the model is tested when it is trained using different amounts of data, ranging from 4 minutes (10 %) to 41 minutes (100 %). Figure 4 shows the resulting average R^2 and standard deviation calculated for the eight predicted outputs.

The average and deviation in performance is noted to converge after 12 minutes. In Fig. 5 the individual measured and predicted photon pulse properties are shown for the

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recorded testing dataset, when trained with 16 minutes of data.

CONCLUSION

The use of machine learning techniques, such as ANNs, can aid in beam optics matching, predict breakdown occurrences, and calibrate diagnostic devices. The presented work explored the use of an ANN to estimate photon pulse pointing properties at the user site based on BPM and XGMD measurements at the photon generation side. The study investigated the effect of different training dataset sizes in relation to the accuracy of the model for the SASE1 undulator. This work demonstrated the potential for virtual diagnostic tools to aid in experiment design, setup, and optimization, saving valuable operation time and interpreting experimental results, especially when current diagnostics cannot provide necessary information. Future work is still required to determine the extent of how such models can be used and under which conditions models can be trained and used during machine operation or setup.

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