Machine learning-based surrogate model construction for optics matching at European XFEL injector

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DESY MXL

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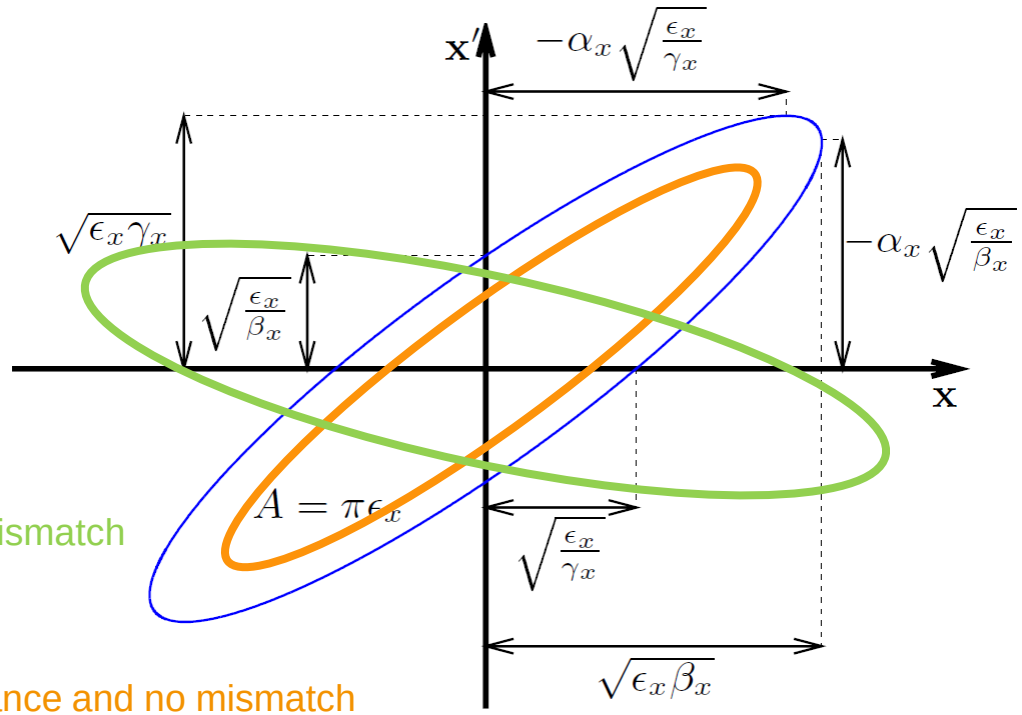
Emittance and twiss parameters

- Emittance is the area in phase space coverd by particle distribution
  - Ellipse is introduced to describe the distribution
  - Emittance is a conserved quantity if beam only subjected to conservative forces (Liouville's Theorem)
- The beam orientation can be described using the Twiss parameters α, β, γ
- Mismatch: beam distribution does not have the same orientation as the design optics

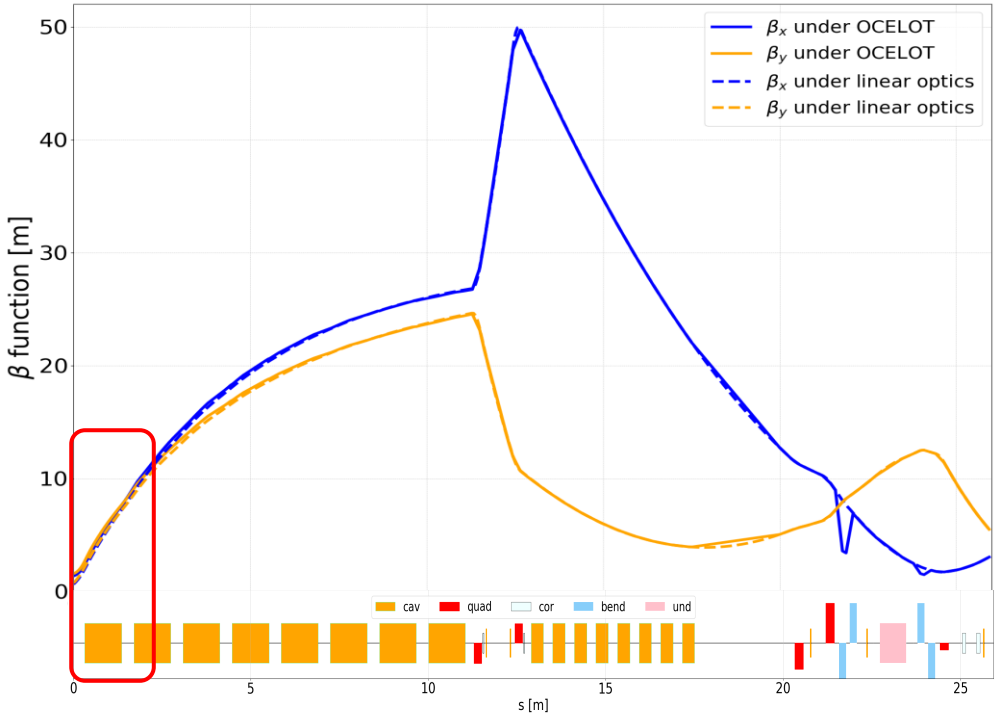


same emittance with mismatch

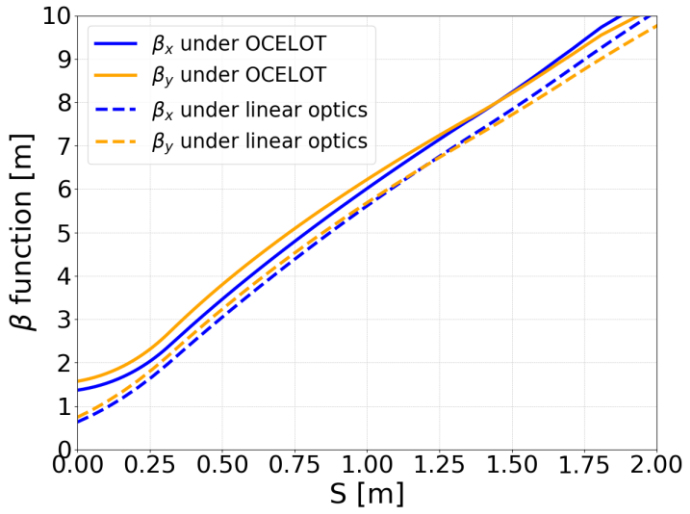
smaller emittance and no mismatch

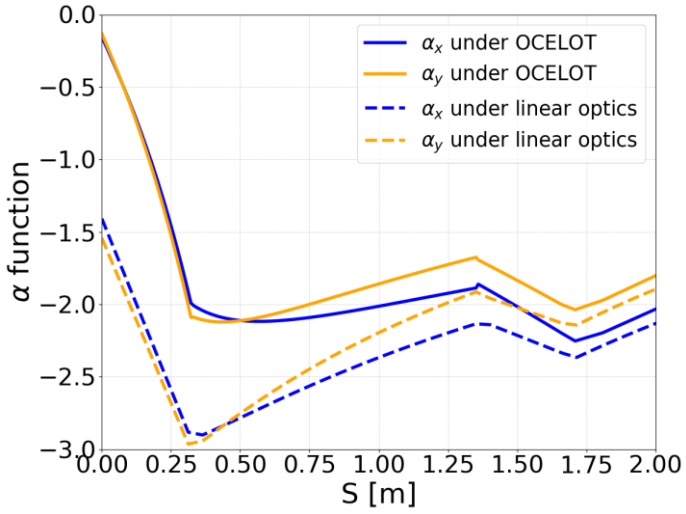
Motivations

- Optics matching in the injector section is essential to the downstream beam transport and final FEL lasing performance.
  - Linear optics model
  - No access to get beam optics properties at gun cavity exit



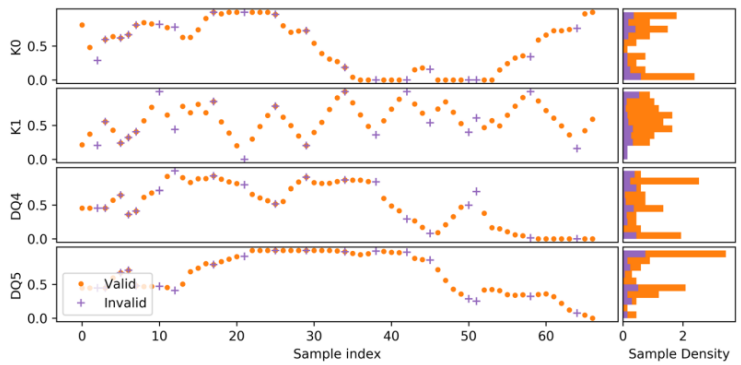
- Samples from OCELOT simulation
  - Start from 6 MeV
  - Collective effects (space charge, wakefields)
  - Second-order optics





Motivations

- Machine learning techniques are mature enough to be applied to accelerators
  - Anomaly detection and machine protection
  - **System modeling**
  - Virtual diagnostics
  - Online tuning and control
  - Advanced data analysis
- Introducing the ML-based technique to construct a surrogate model
  - an alterative to the existing linear optics toolkit
  - A virtual diagnostic tool for beam transverse properties at gun exit



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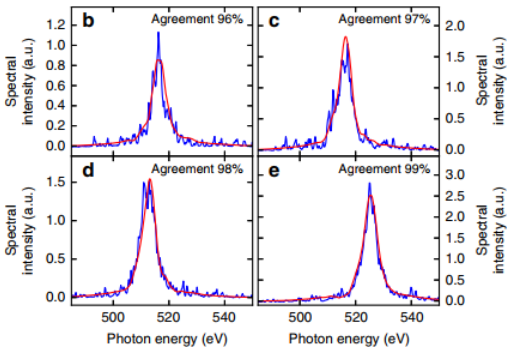

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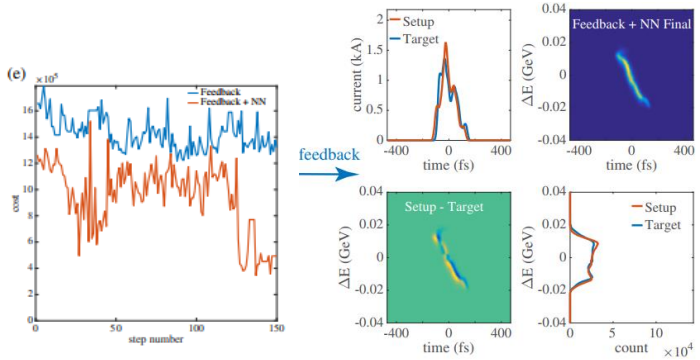

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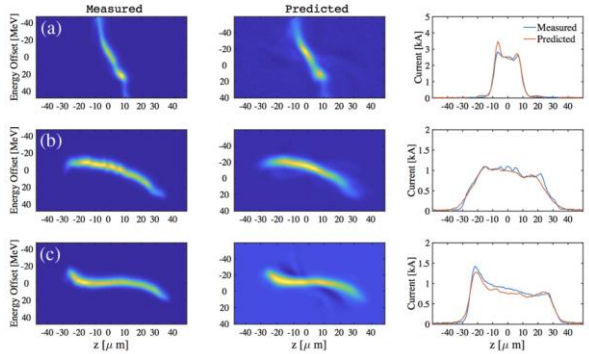

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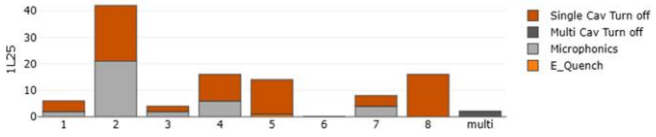

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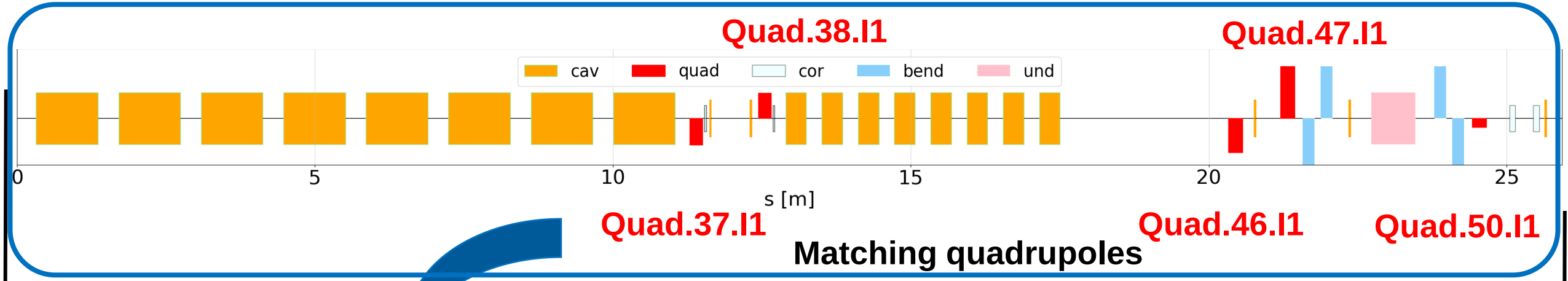
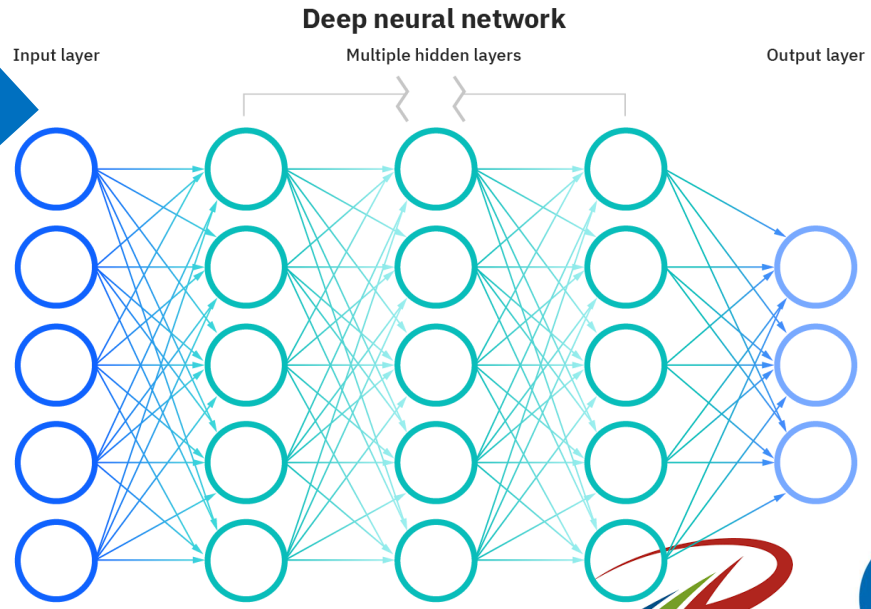


Matching quadrupoles

Initial point
Twiss parameter:
α_{xi}, α_{yi}, β_{xi}, β_{yi}

Reference point
Twiss parameter:
α_{xr}, α_{yr}, β_{xr}, β_{yr}



- Input parameters:
  - Initial twiss parameters: α_{xi}, α_{yi}, β_{xi}, β_{yi}
  - Matching quads settings: **Q37.k1, Q38.k1, Q46.k1, Q47.k1, Q50.k1**

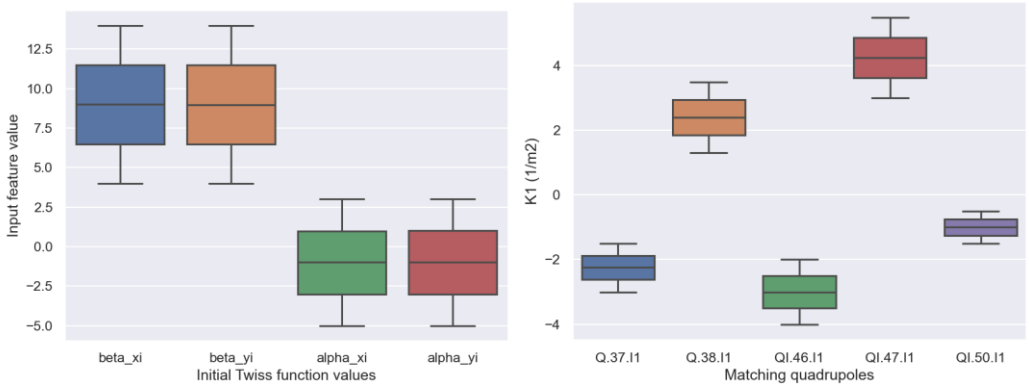
- Output parameters:
  - Final twiss parameters: α_{xr}, α_{yr}, β_{xr}, β_{yr}

Sample generation for training

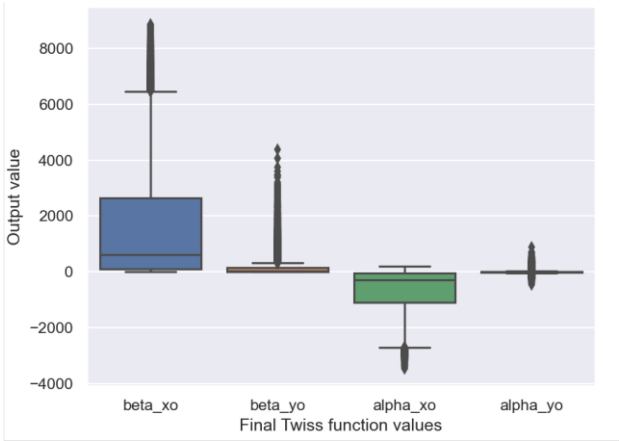
- Difficulty in the sample generation

Most time spent on generating those useless samples ☹

  - Input features



  - Output parameters

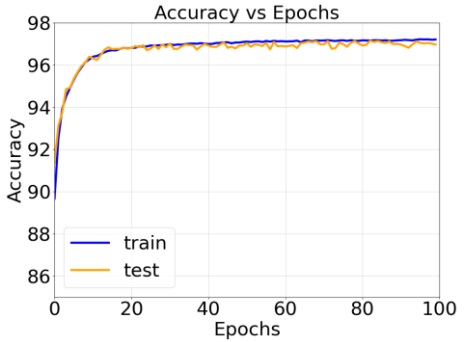


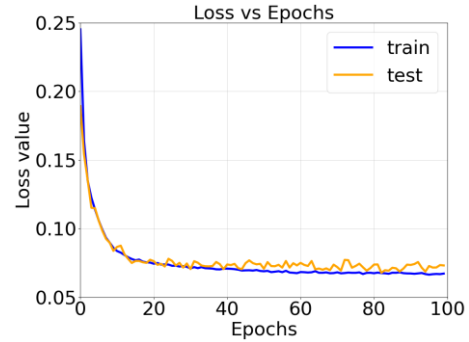
α_{xr}: [-10,10]
α_{yr} : [-10,10]
β_{xr}: [0,20]
β_{yr}: [0,20]

- Binary classification NN

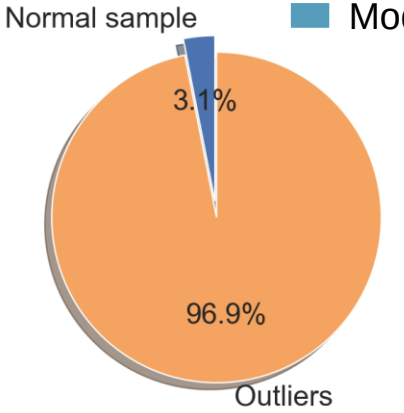
This model acts as a filter for efficient samples generation

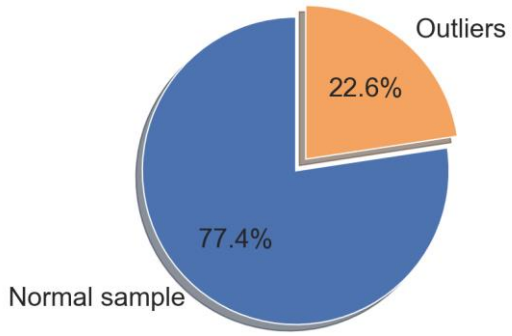
  - Label assignment for the whole sample set
  - Model training and validation





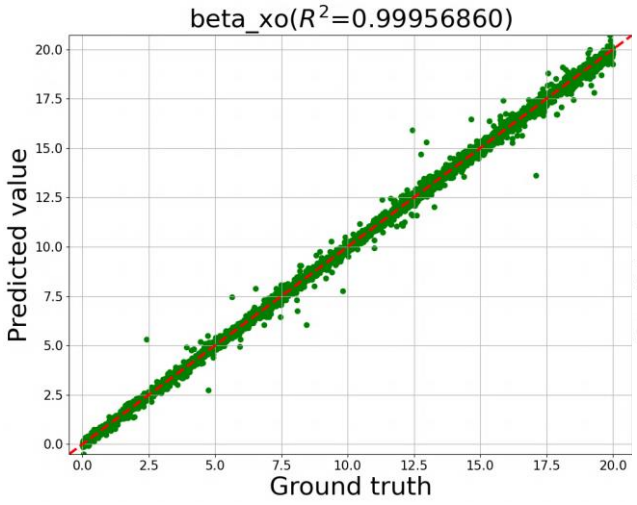
  - Model application for sample generation

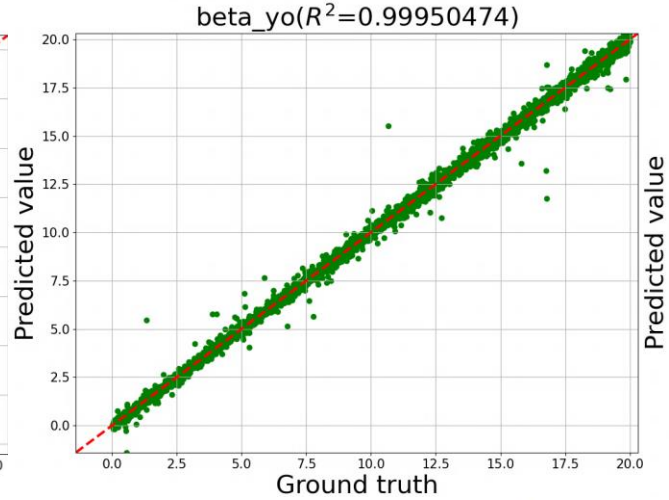


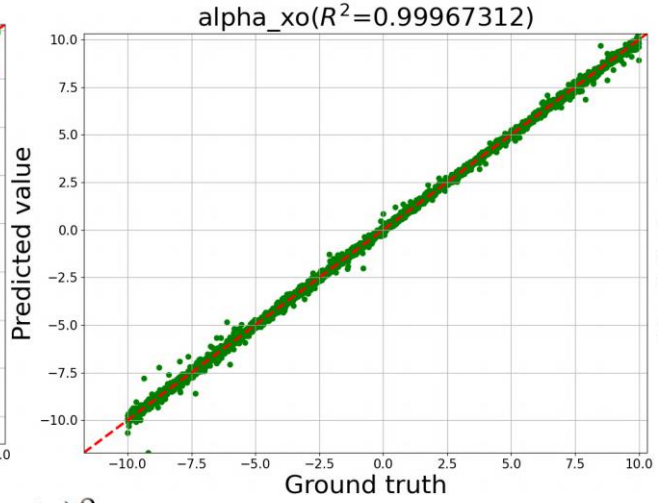


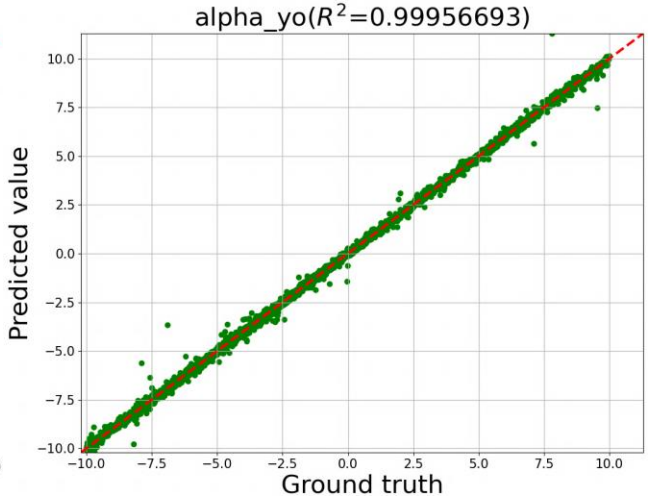
Surrogate model construction

- Samples under OCELOT simulation in Maxwell
  - simulation in parallel in 20 nodes (40 CPUs in each)
  - Spent ~ 13 h to get sample sets of 40k
- Neural network architecture and hyperparameters
  - 200k samples in total (20% for testing)
  - 3 hidden layers with 128 neurons in each
  - Loss function: Mean square error
  - Activation function: Tanh
  - Optimizer: Adam



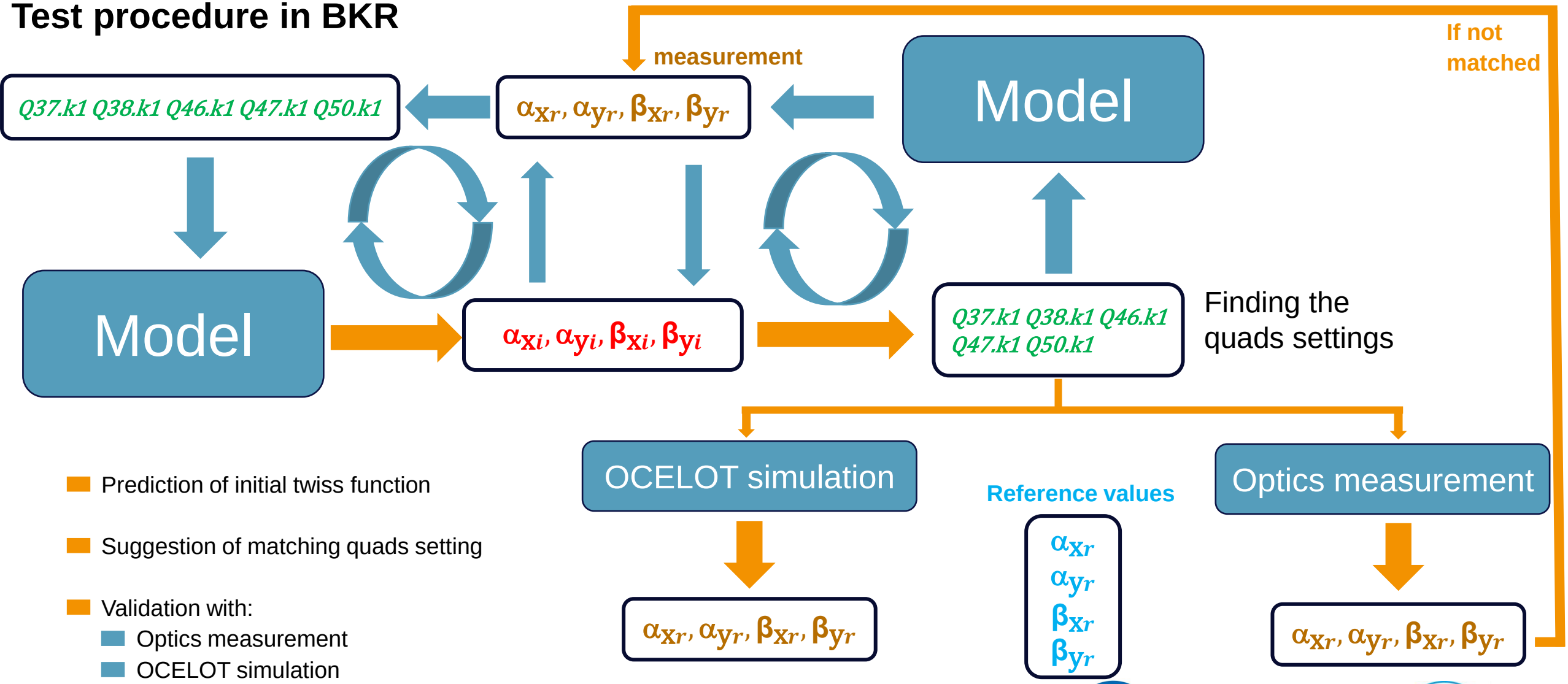






$$R^2 = 1 - \frac{SS_{RES}}{SS_{TOT}} = 1 - \frac{\sum_i (y_i - \hat{y}_i)^2}{\sum_i (y_i - \overline{y})^2}$$

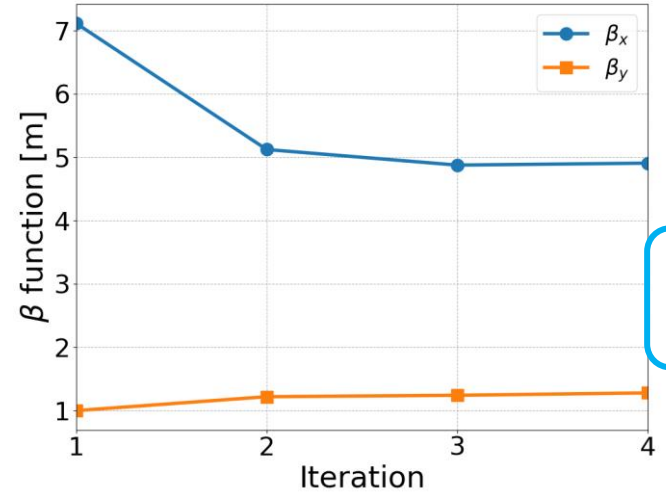
Test procedure in BKR

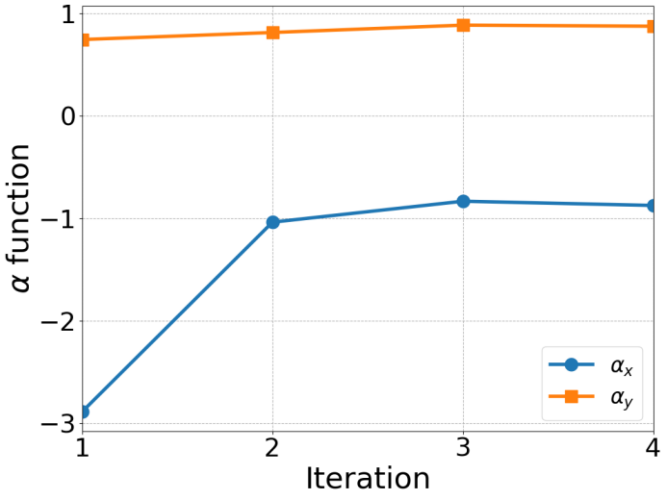


- Prediction of initial twiss function
- Suggestion of matching quads setting
- Validation with:
  - Optics measurement
  - OCELOT simulation

CASE 1: Solenoid current of 344A (nominated strength)

- Optics function values evolution during the optimization





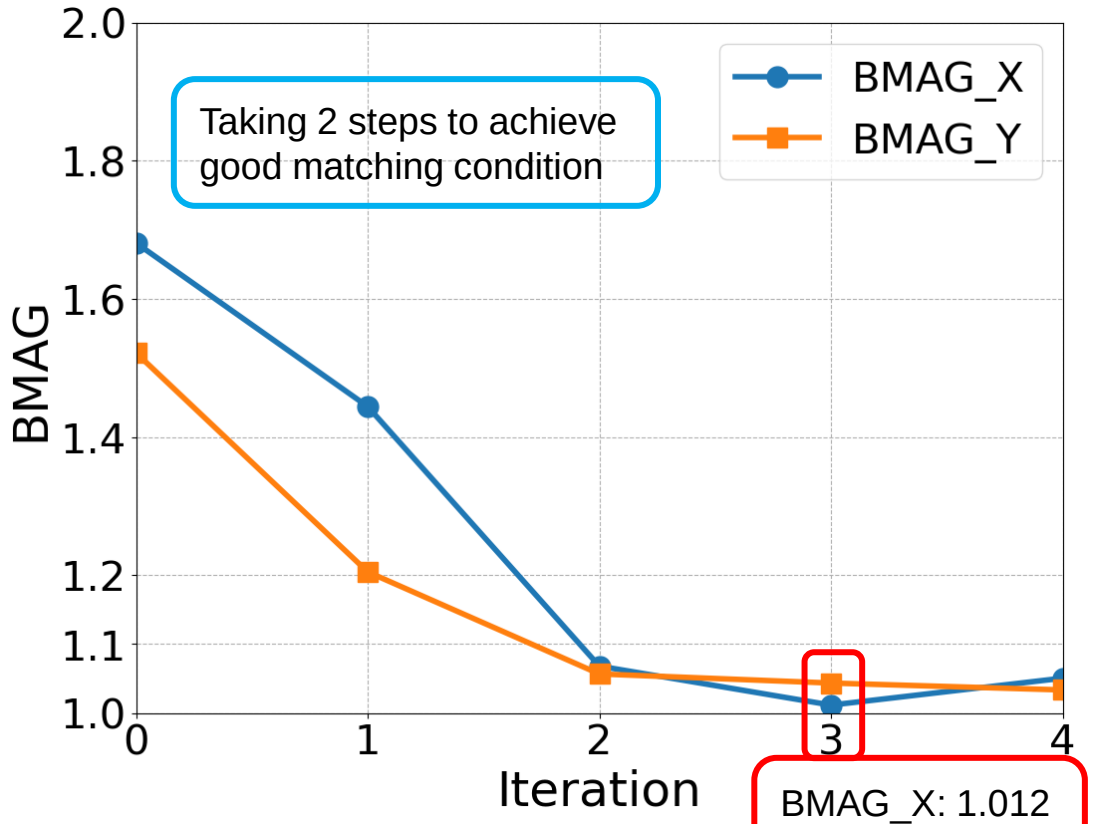
Asymmetry between the transverse planes

$$\xi = \frac{1}{2}\left(\gamma\beta_0 - 2\alpha\alpha_0 + \beta\gamma_0\right)$$

$$\mathrm{BMAG} = \xi + \sqrt{\xi^2 - 1}$$

$$\frac{\beta_0}{\mathrm{BMAG}} < \beta < \mathrm{BMAG} \cdot \beta_0$$

- Mismatch parameters evolution during the optimization



Taking 2 steps to achieve good matching condition

BMAG_X: 1.012
BMAG_Y: 1.044

CASE 1: Solenoid current of 344A (nominated strength)

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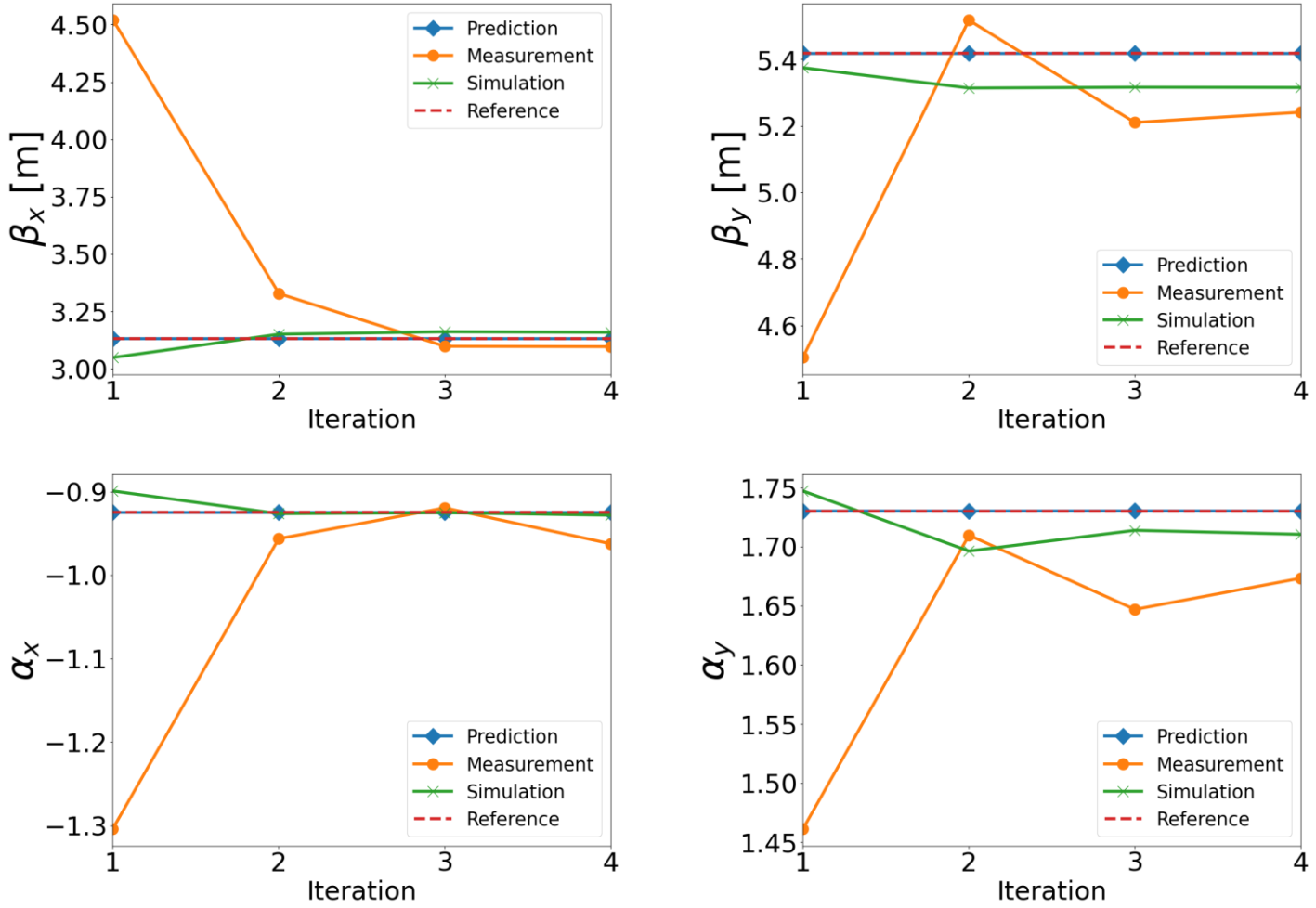
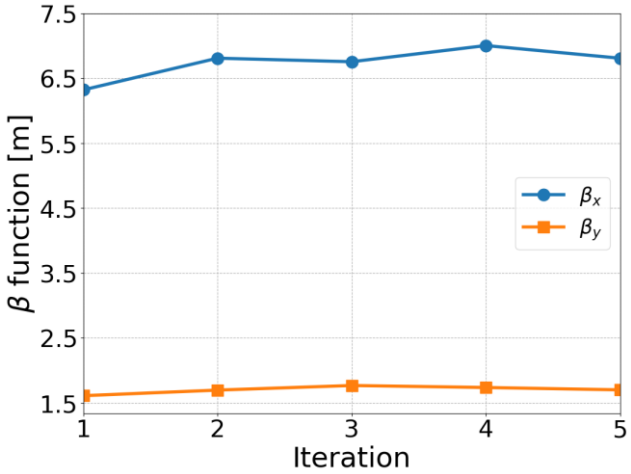
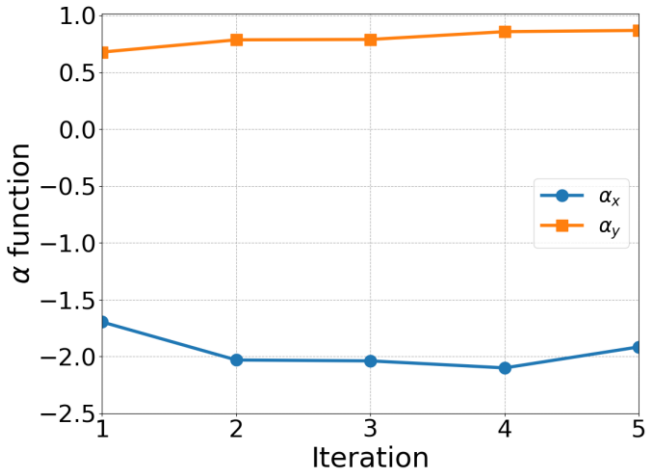


- Model can find the solution based on its knowledge
- Prediction from the surrogate model agrees well with the simulation

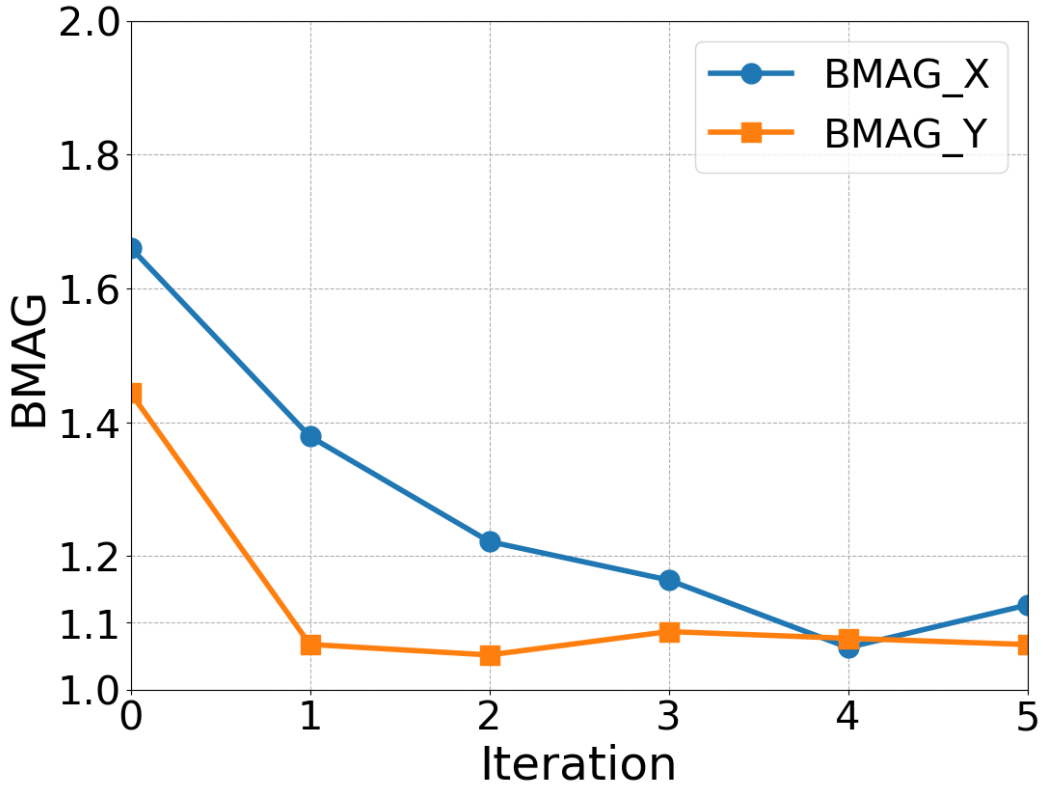
CASE 3: Solenoid current of 343.5 A

- Optics function values evolution during the optimization
  - Beam initial condition changed after solenoid tuning
  - Keep the Q.50 strength fixed, adjust the other 4 quads
  - Matching achieved, but see some limitations





- Mismatch parameters evolution during the optimization



CASE 3: Solenoid current of 343.5 A

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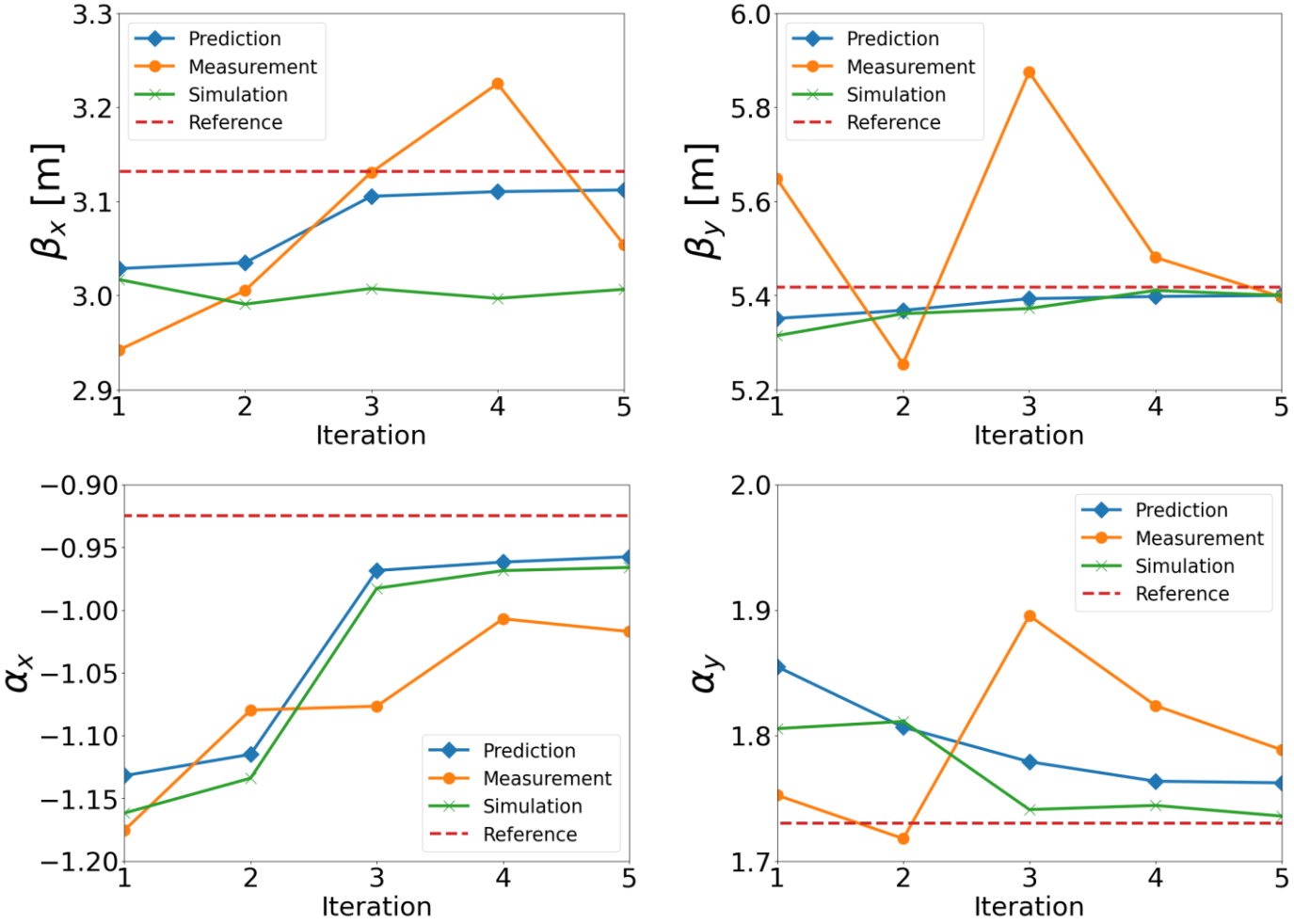
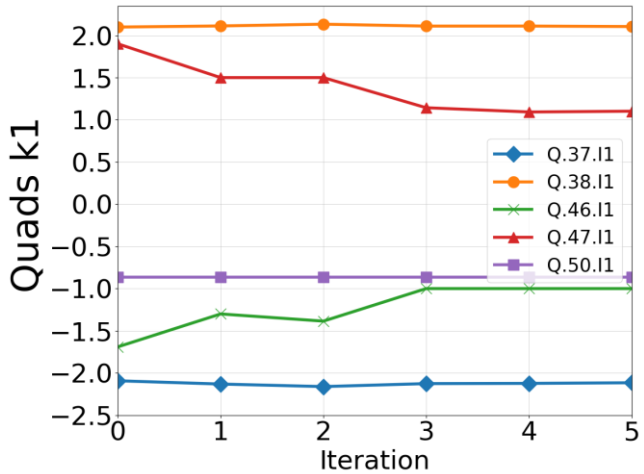


- There is always gap between the predicted values and reference value
- Good matching condition achieved in 4th step

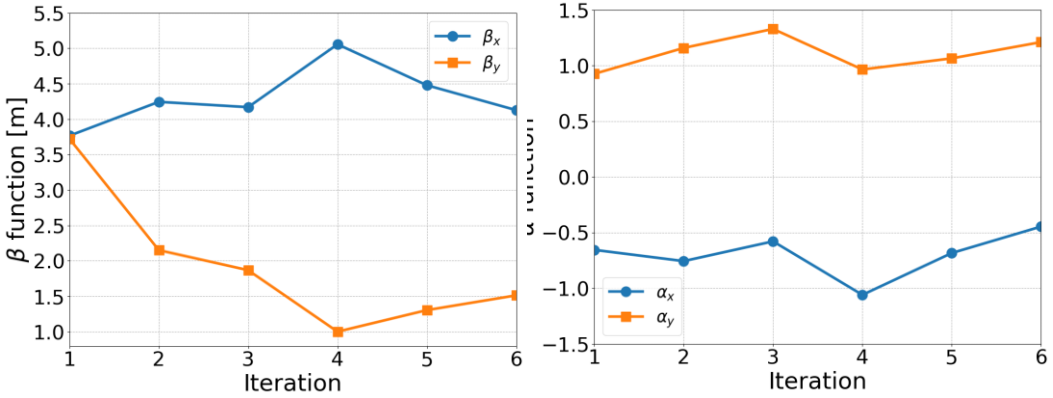


Q47: Adjust the lower bound from 1.5 to 1.0

Q46: hit the upper bound (-1.0)

CASE 2: Solenoid current of 344.5 A

- Optics function values evolution during the optimization



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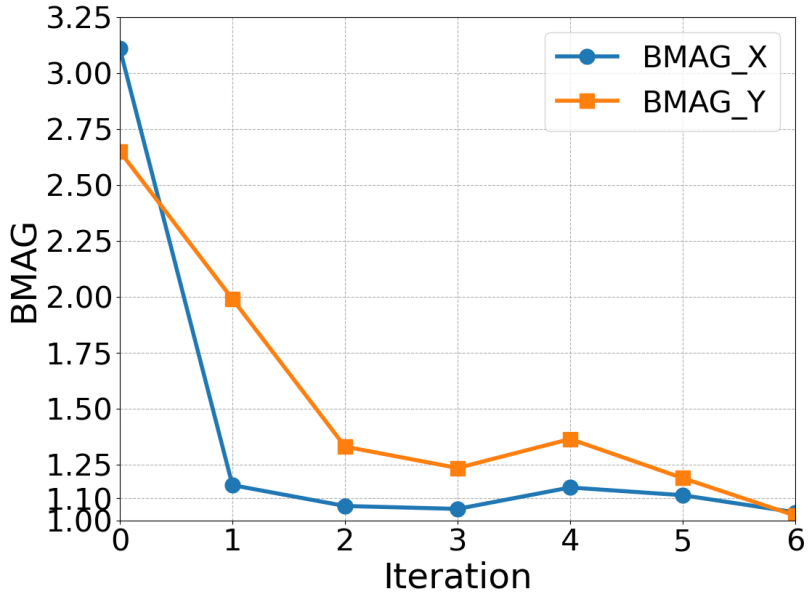

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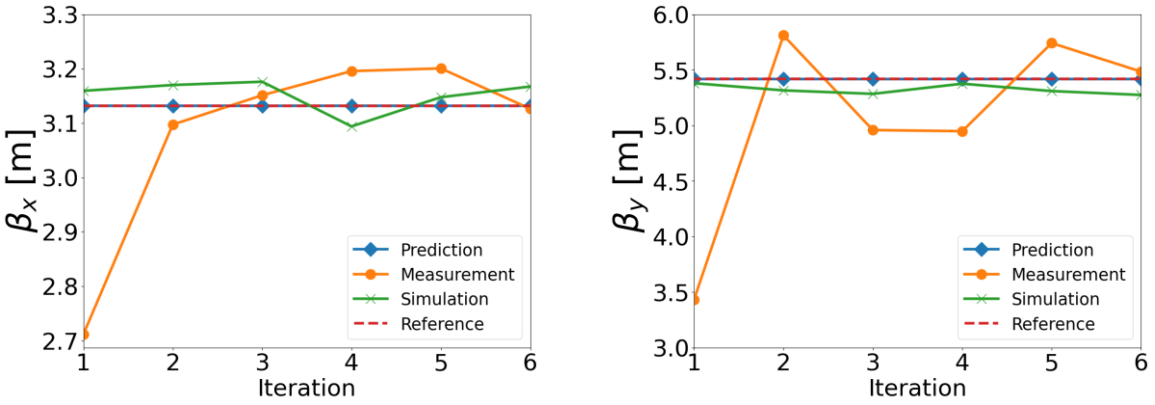
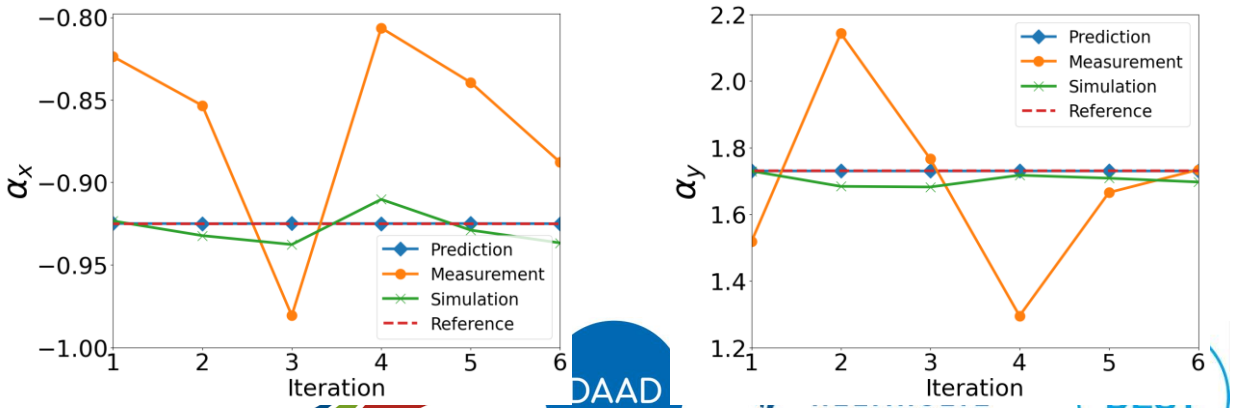
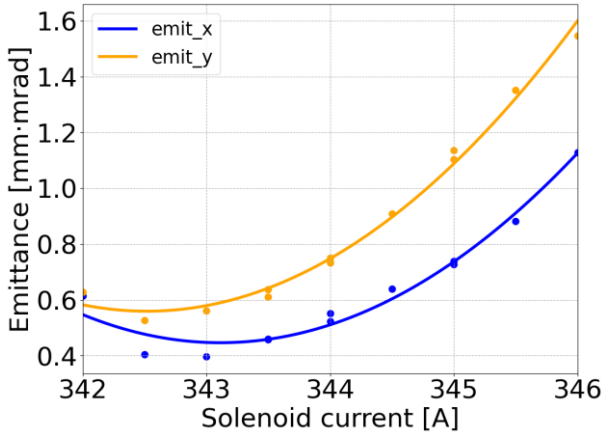
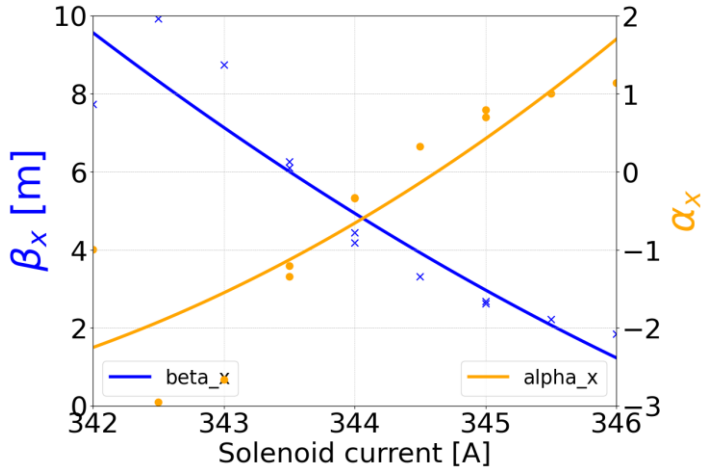


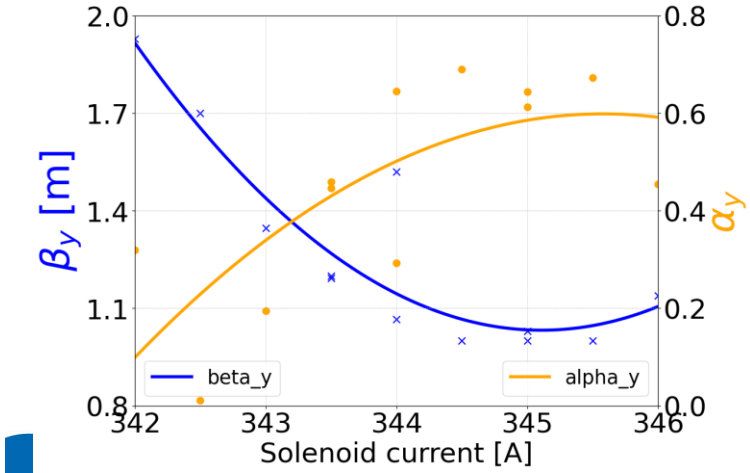


Solenoid strength scan

- Transverse emittance at the matching position dependent on solenoid strength
  - ± 2 A around the nominated strength (344 A)
  - Keep the machine lattice the same during the scan
- Prediction of initial twiss function values

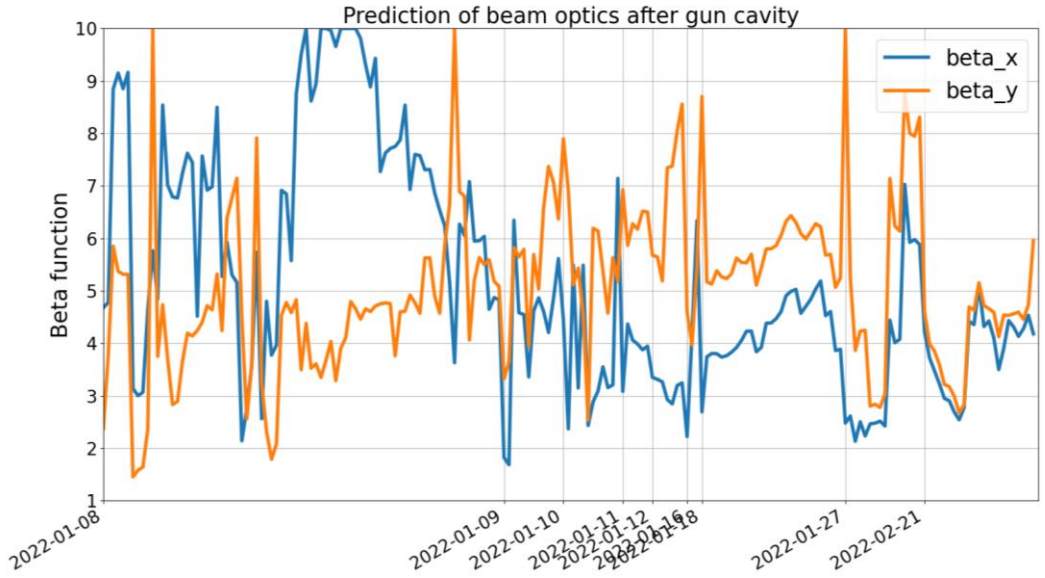




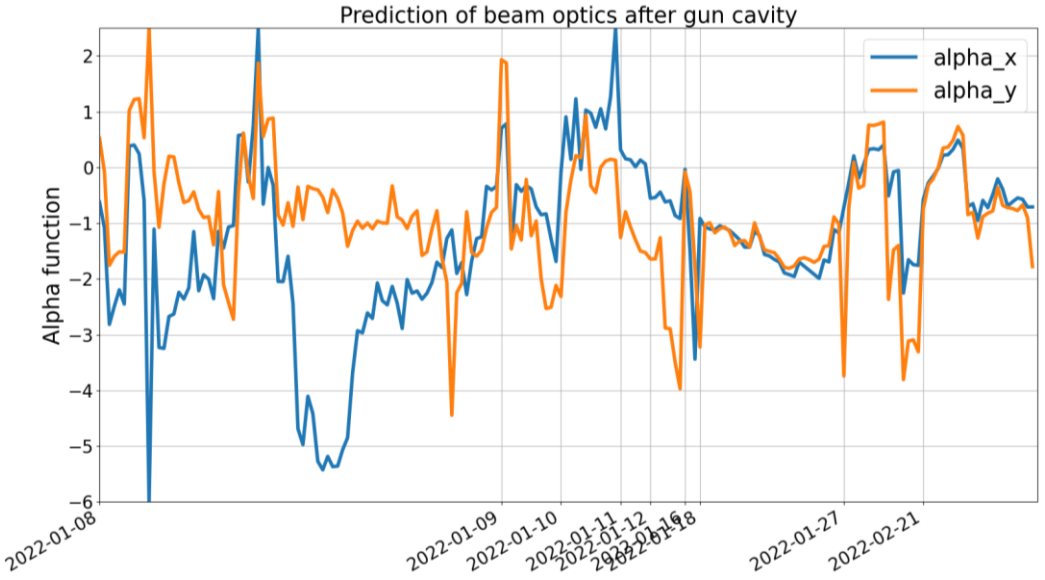


Applicaton to beam diagnostics at gun cavity

- Collection of all the optics measurement data in BKR from 08/01/2022 to 21/02/2022 (189 samples in total)
- Prediction of initial twiss function values from each samples
- Potential further application for research on:
  - Beam transverse properties optimization at gun cavity
  - Laser stability on the cathode
  - Emittance compensation with solenoid



Set-up the machine after shutdown | Beam delivery, SASE2 tuning | Gun study



Summary

- Achievements
  - The prediction of the constructed model agrees well with the result from OCELOT simulation
  - The surrogate model can achieve good matching scenario (BMAG < 1.1 in two planes) under multiple solenoid settings
  - The model can be applied as a diagnostics tool towards beam transverse properties at the gun cavity exit.

- Outlook
  - Improvenment of model capability (wider parameters search space)
  - Involving knobs in the gun cavity to the surrogate model
  - Exploration of more machine learning based online optimization and virtual diagnostic application.