Spectrometer Alignment via Machine Learning

Peter Feuer-Forson, Philippe Wernet, Gregor Hartmann, Rolf Mitzner

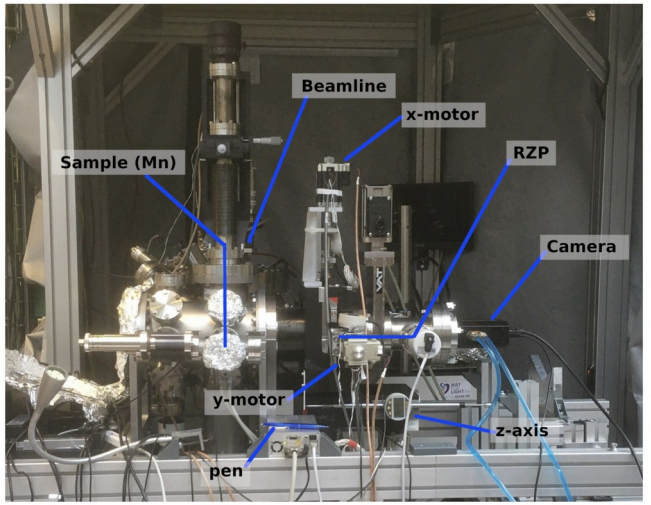
The SXP instrument at the European XFEL: status and perspectives 24.01.2022

MLP as Surrogate model

Aim

- Manual Spectrometer Alignment is slow – automate process.
- 3 motors (x, y, z) – find perfect position.
- Use NN trained only with simulation data (Ray-UI).
- Find offset between Simulation and Experiment.

SPECTROMETER



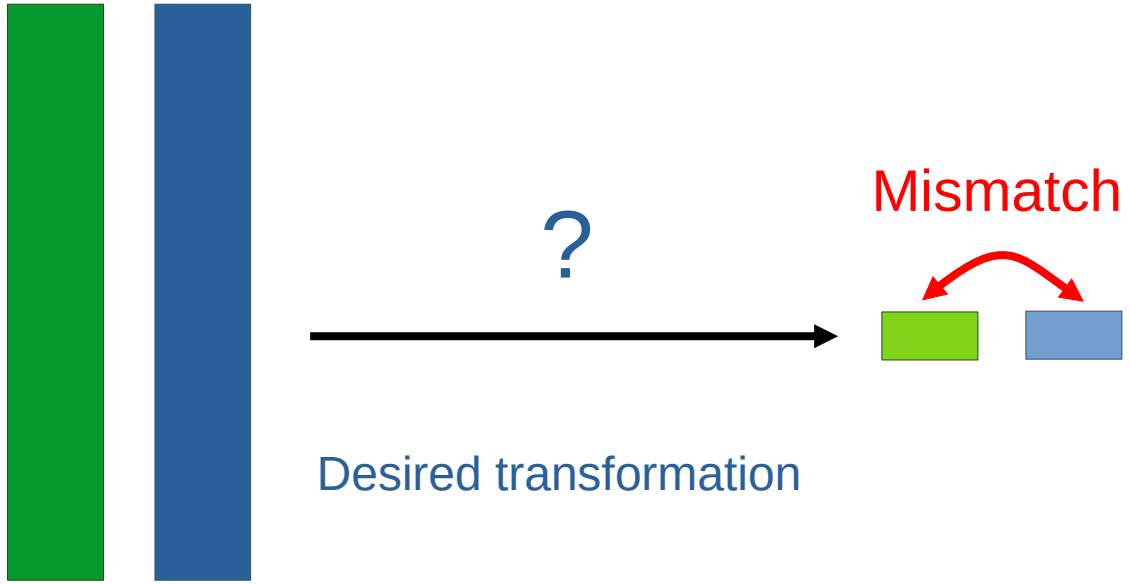
Challenge

- Experiment data is ‘dirty’ - noise, backlash, camera pos.
- Parameter Space not fully explorable.
- Mismatch between simulation and reality.

EXPERIMENT VS SIMULATION

High dimensional experiment data.

Simulation data.



Desired transformation

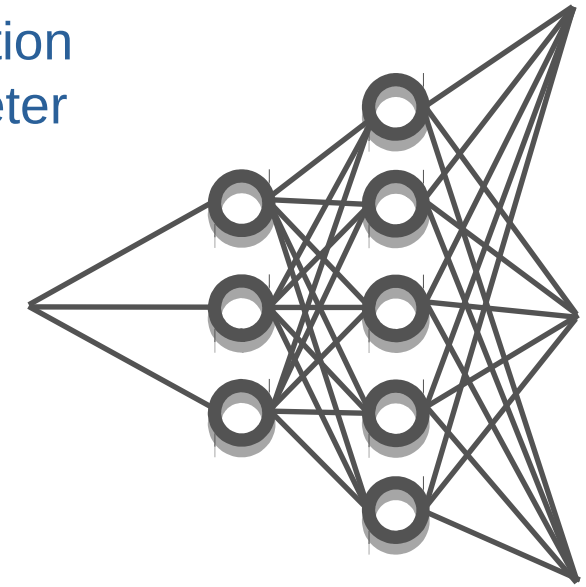
Low dimensional desired information.

Simulation parameter.

SURROGATE MODEL: RAY-TRACING

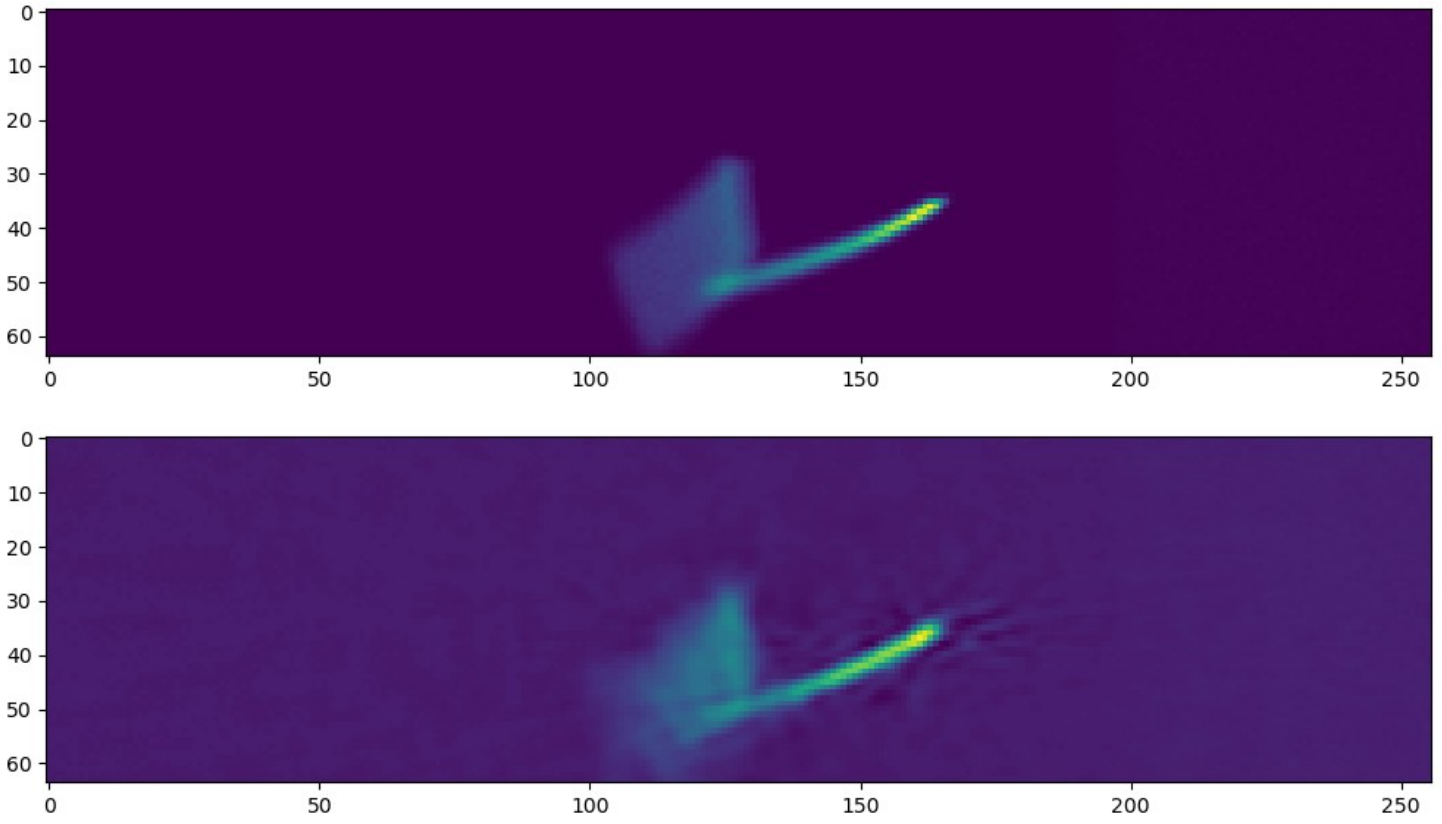
Simulation
Data (image)

Simulation
parameter
(x, y, z)



Small MLP for fast
inference.

Simulation



Prediction

EXPERIMENT PROCEDURE

Function to minimise

$$\text{diff} = \sum_{i=1}^{N} (Image_i^{exp} - NN(T_i^{exp} + T^{off}, C^{off}, RZP^{off}, Ratio))^2$$

Parameters:

- T_exp = x,y,z coords experiment
- T_off = offset to determine
- C_off = camera offset
- Ratio = ratio of Oxygen to Manganese

Process

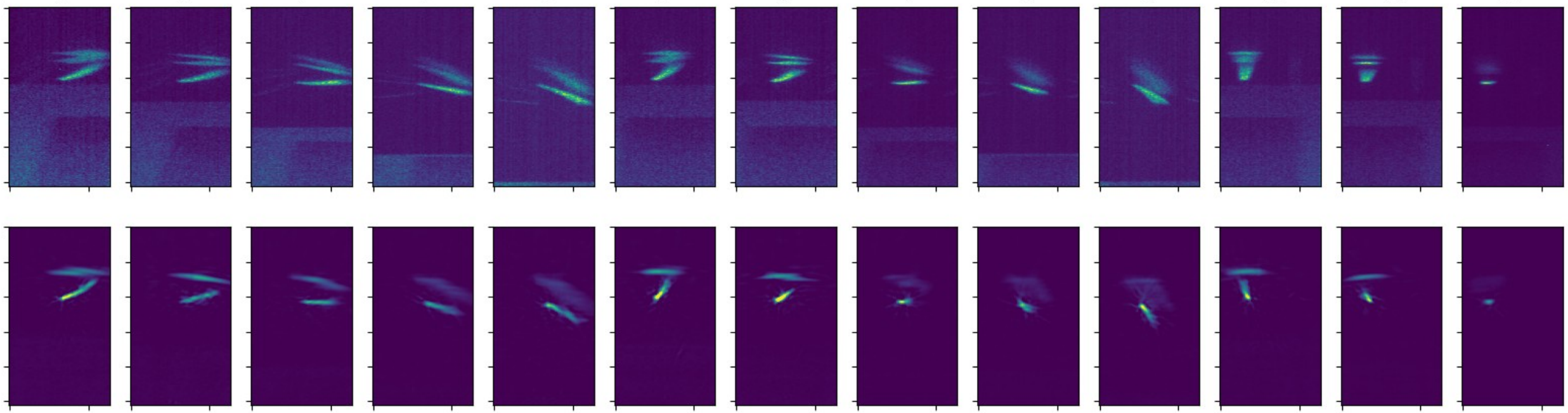
- Record N images and their corresponding T_exp (10).
- Use Optimiser to minimise diff by searching for T_off.
- Result of T_off => Absolute position of perfect alignment.

10 images and coords → Basin Hopping Optimiser → x,y,z perfect alignment

APPLICATION OF SURROGATE MODEL

Experiment

Precision: ~0.01mm
Runtime: ~10 min



Optimiser

OUTLOOK

- Improve runtime.
- Test robustness with different setups (Iron, multi-RZP, -1 Order).
- Publish
- Use ML to optimise design of new Spectrometer
  - Find optimal setups for large design space by optimising design parameters to maximise specific design goals – intensity, separation, number of photons.
  - Reduce cost.