Interpretable Machine Learning at the European XFEL

Danilo Ferreira de Lima and *many many others* from the European XFEL

Data Analysis group, European XFEL

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How do we see Machine Learning at the EuXFEL?

- Goal: maximize scientific outcome.
- But ... not all approaches are equal.
- Users have the last word on how to do their experiments.
- Let's manufacture consensus.

Characteristics:

- *interpretability* → what do the results mean?
- *context-aware* → connects to the science?
- *quality control* → conditions for operation?

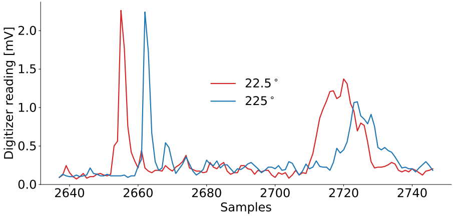
How to achieve it:

- Clarify inner workings.
- Shape it based on science.
- Estimate region of validity.

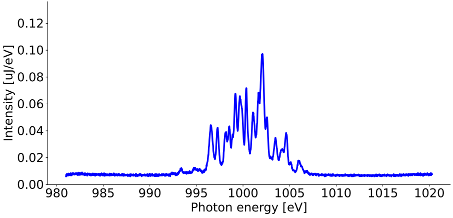
Virtual Spectrometer

Enhancing non-invasive X-ray diagnostics

Photo-Electron Spectrometer (PES)



Grating Spectrometer (GS)

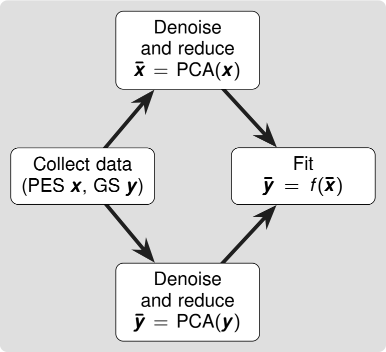


- Non-invasive.
- Pulse-resolved.
- Complex calibration.
- Low resolution.

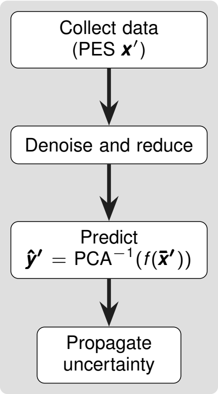
- Invasive.
- Train-resolved.
- Simple calibration.
- High resolution.

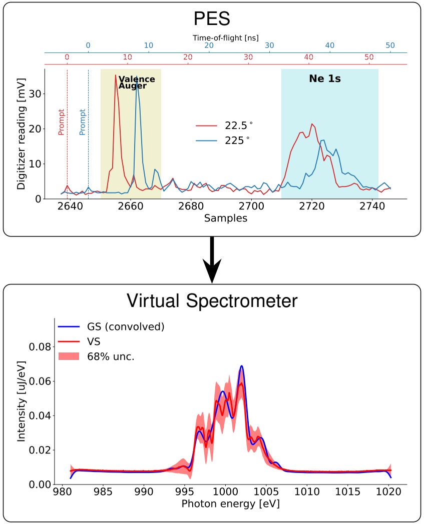
Enhancing non-invasive X-ray diagnostics: method

Training



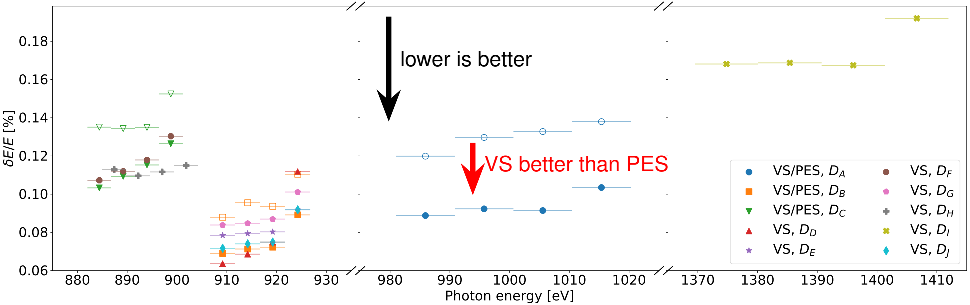
Inference





Virtual Spectrometer's resolution

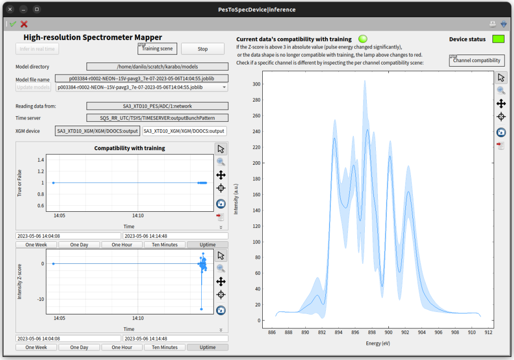
- Systematic resolution studies under several conditions done.
- Comparison with PES show better resolution.
- Resolution calculated after training to inform scientists.



PES: open symbols; VS: full symbols.

Deployment *online* and outlook

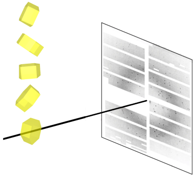
- Deployed in control system with simple interface to retrieve data and integrate ML projects.
- Combines advantages of low- and high-resolution devices:
  - Non-invasive.
  - Pulse-resolved.
  - Automated calibration.
  - Improved resolution.
- Adheres to self-defined guidelines:
  - Embedded **quality control**.
  - Resolution and uncertainty estimate $\Rightarrow$ **interpretability**.
  - SASE principle guides denoising $\Rightarrow$ **context-aware**.



- Outlook:
  - Expand project for hard photons.
  - Interpolate conditions to avoid pre-training stage.

Automated data analysis

Streamlining data analysis using ML



- Often data analysis pipelines have parameters.
- **Idea:** Simplify data analysis for non-experts.

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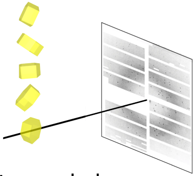
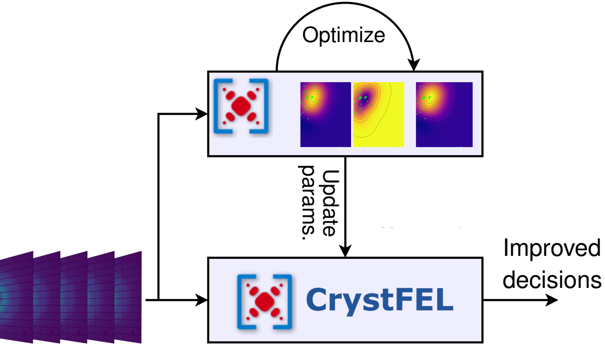
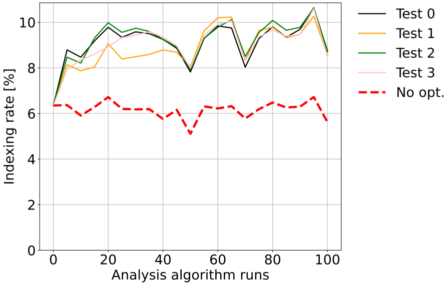
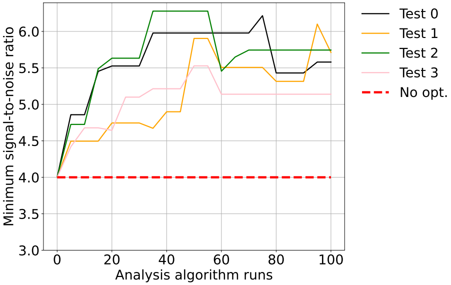




- **Goal:** Tune parameters to maximize a *metric*.
- This example: maximize the fraction of indexed frames f.
- *Online*: fast feedback, higher success chances.
- *Offline*: improved scientific findings.

Streamlining data analysis using ML: example



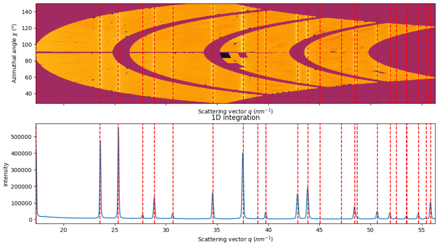


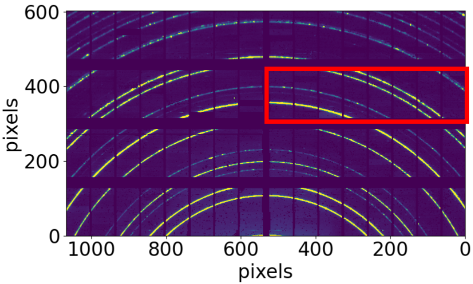
- Hen Egg-White (HEW) Lysozyme.
- AGIPD detector at EuXFEL SPB/SFX.
- Web interface shows optimization progress ⇒ **interpretability**.
- **Quality metrics** also available.
- Optimizes clear science-based metrics ⇒ **context-aware**.

Automated multi-modular geometry tuning

Multi-modular geometry tuning

- Misalignment on module positions.
  - Manual alignment: requires lots of time.
  - Powder diffraction data are often the starting point for techniques requiring high-precision.
  - Powder diffraction-based methods require many parameters and often manual tuning.
- Let's start with powder diffraction: can we improve and *automate* it?





Multi-modular geometry tuning

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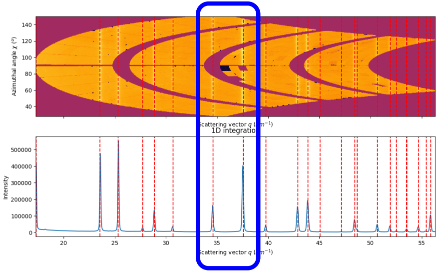
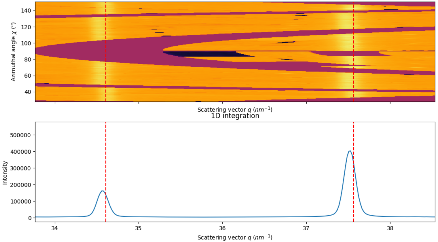


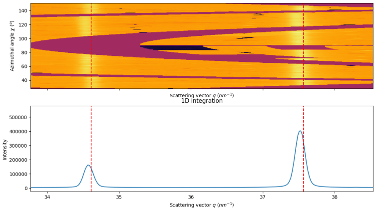


An information-theoretical approach

- Optimizes the *mutual information* between radial distance and azimuthal angle $\rightarrow$ measures independence $\Rightarrow$ **context-aware** and **interpretable**.
- Pre-processing includes background subtraction and polar coordinate transformation.
- Only first step in a long pipeline due to the limited experimental method resolution.
- Validation tools available $\Rightarrow$ quality metrics.

Before inter-module tuning

Tuning only detector-sample distance



Minimize $MI(r, \phi)$

After inter-module tuning

Additionally, inter-module separation tuning

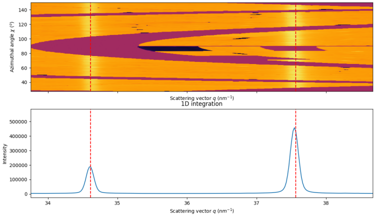
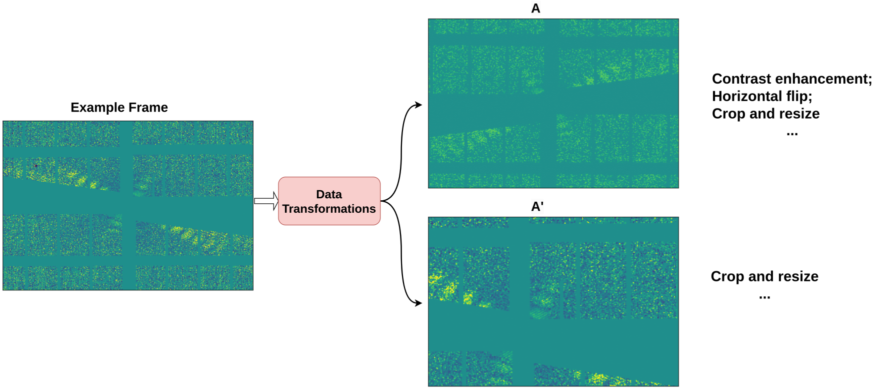


Image clustering

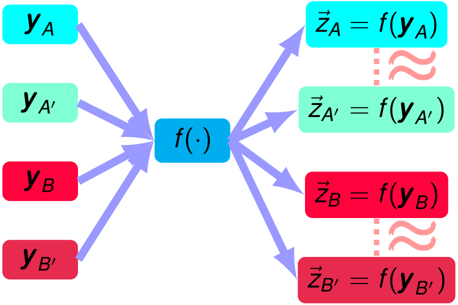
How do we Google data?

- How can we make data findable as soon as we collect it?
- **Concept**: *Change* the data *view* and enforce their similarity.

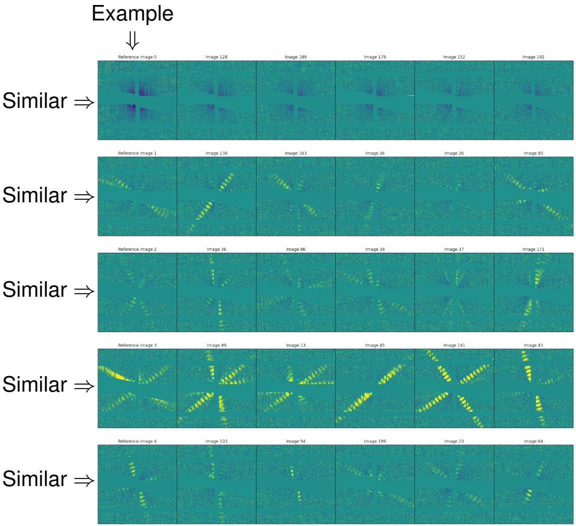


Creating a similarity metric

- *Equivalent views* → variations to ignore, based on the science ⇒ **context-aware**.



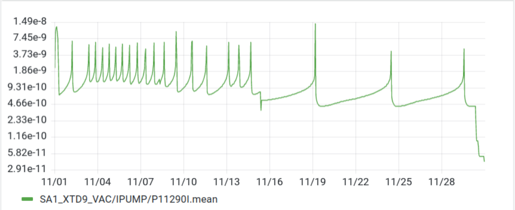
In *Automated phase transition discovery*: Sun, Y., Brockhauser, S., Hegedüs, P. , Plückthun, C., Gelisio, L., Ferreira de Lima, D. E., Sci. Rep., (2023).



Predictive Maintenance

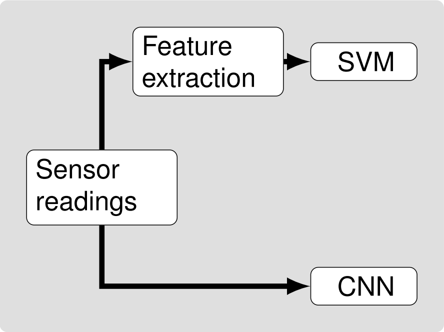
Predictive Maintenance: ion vacuum pump use-case

- Faults may lead to loss of beam time.
- Important to detect them early.
- Difficulty: complex system makes it hard for humans to monitor everything.
- Example: Ion pump faults have lead to significant downtime.
- Detection mechanism: frequent surges in pressure level.



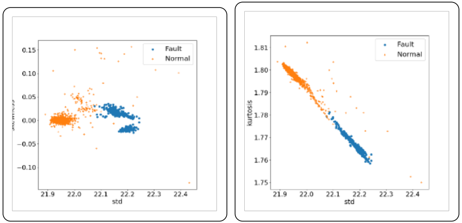
(Amna Majid)

How can we detect it?



Method	Accuracy [%]	Precision	Recall
SVM	99.98	1.00	0.96
CNN	99.95	0.99	0.99

(Amna Majid)



- Two methods researched with similar performance.
- SVM makes a linear cut in the feature space of peak characteristics → easy **interpretation** and based on **context**.
- CNN uses all information.
- Prefer interpretable method!
- Web interface for monitoring ⇒ **quality control**.

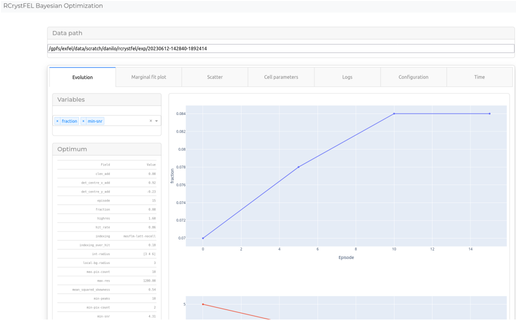
Summary

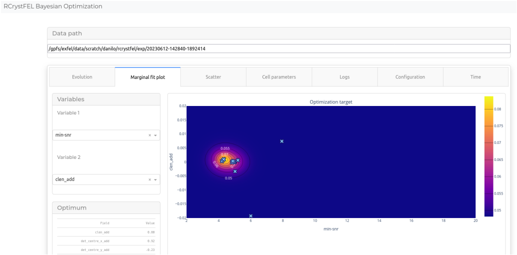
- Several approaches to enhance automation at the EuXFEL.
- **Interpretability**, **context-awareness** and **quality control** are seen as assets to guide towards adequate solutions.
- Control system allows for integration and deployable methods.
  - Interface design is simple, but highlights those characteristics to guide users.
  - Aim for a holistic approach to integrate those features in all applications.


Thank you!

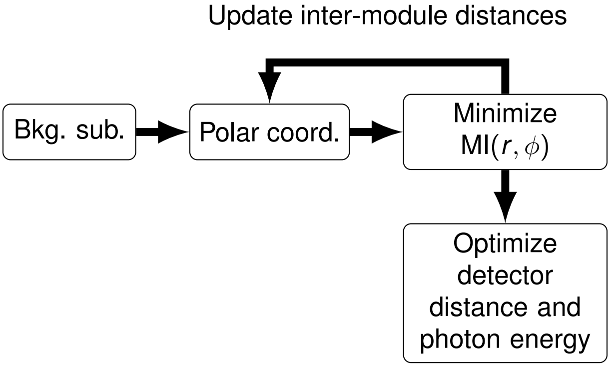
Additional material

Interpretability in a Web interface



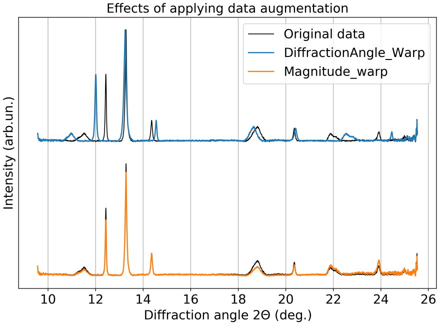


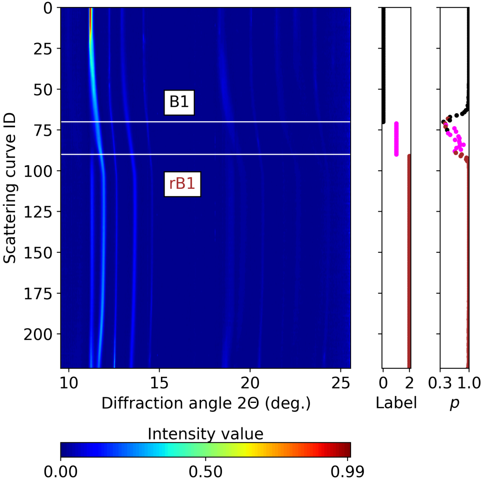
Multi-modular geometry tuning: concept



Googling phase transitions

- Ignore all changes in the spectra, *but* phase transitions.
- Learn to map irrelevant variations into the same $\vec{z}$.

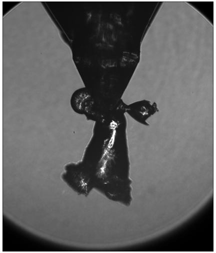




Sun, Y., Brockhauser, S., Hegedüs, P. , Plückthun, C., Gelisio, L., Ferreira de Lima, D.E., Sci. Rep., (2023).

Protecting detectors from damage

- Ice can form on the tip of nozzles, and scatter X-rays that can destroy detector pixels.
- **Idea:** Use computer vision techniques to detect:
  - jet instabilities, reducing beamtimes efficiency;
  - ice formation.
- Information can be used to alert operators or even intervene.



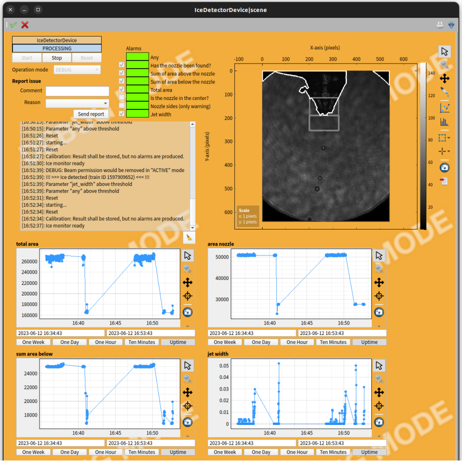
Protecting detectors from damage

Experiment's side camera.

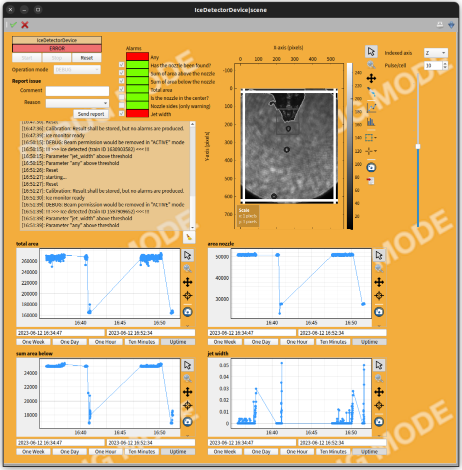
Two consecutive frames are separated by 0.1 s.

Software deployed

Standard operation

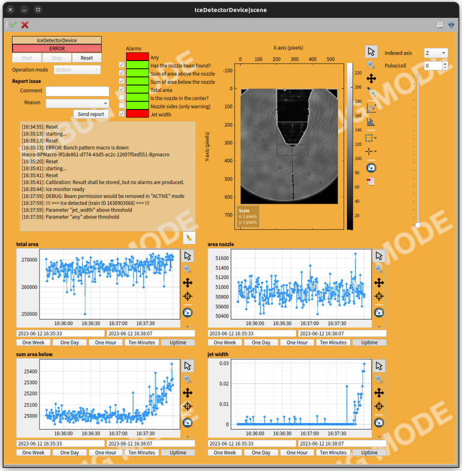


Ice detected



age. Human monitoring slow.

Drive control system responsibly



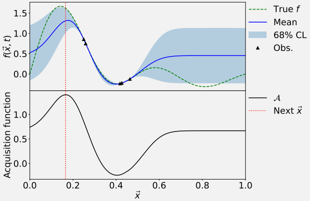
- Ice formation may lead to detector damage. Human monitoring slow.
- *Interpretability*: Interface informs on alarm source and low-quality data.
- Operators are still in control: we only guide them on request.

Baysian Optimization: How does it work?

Initially run analysis ($\times n$) and store:

Parameter	Objective
$\vec{x}_1$	$f(\vec{x}_1, \mathcal{D}(t=1))$
⋮	⋮
$\vec{x}_n$	$f(\vec{x}_n, \mathcal{D}(t=1))$

Fit $\hat{f}(\vec{x}, t)$ including uncertainty and calculate $\mathcal{A}$



$$\vec{x}_{n+1} = \arg\max_{\vec{x}} \mathcal{A}(\vec{x}, t=1)$$

Run analysis at $\vec{x}_{n+1}$ and store:

Parameter	Objective
$\vec{x}_1$	$f(\vec{x}_1, \mathcal{D}(t=1))$
⋮	⋮
$\vec{x}_{n+1}$	$f(\vec{x}_{n+1}, \mathcal{D}(t=2))$

⋮

Dynamic Bayesian optimization.

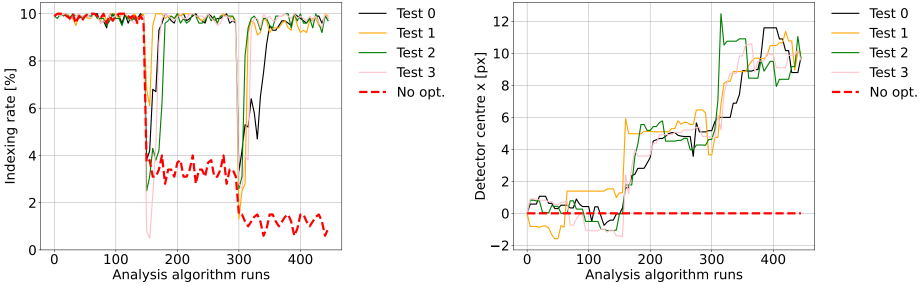
- A Gaussian process is used to fit the objective function f

$$C(\vec{x}_1, t_1, \vec{x}_2, t_2 | S, \vec{L}, T, \sigma) = S^2\, \mathrm{e}^{-\frac{(\vec{x}_1 - \vec{x}_2)^2}{2\,\vec{L}^2}}\, \mathrm{e}^{-\frac{(t_1 - t_2)^2}{2\,T^2}} + \sigma^2$$

- The acquisition function is defined as

$$\mathcal{A}(\vec{x}) = \bar{f}(\vec{x}, t = \mathrm{current}) + \sqrt{\beta}\, \delta f(\vec{x}, t = \mathrm{current})$$

Bayesian Optimization: Simulating a detector shift



- Hen Egg-White (HEW) Lysozyme.
- Simulated AGIPD data, X-ray beam pointing shifting twice.

Enforce self-consistency mapping

Idea: different views of the data containing the same information must be understood as the same.