Interpretable Machine Learning at European XFEL

Danilo Ferreira de Lima[1] Oleksii Turkot[1] Thomas Michelat[1] Egor Sobolev[1] Fabio Dall'Antonia[1] Šarlota Birnšteinová[1] Tim Berberich[1] Luca Gelisio[1] with many collaborators from DA, CTRL, SPB/SFX, THE at the European XFEL, and CFEL at DESY

[1]European X-Ray Free Electron Laser

Machine Learning at the EuXFEL

Solutions must conform to:

- *interpretability* → what do the results mean?
- *explainability* → science-aware methods?
- *quality control* → conditions for operation?

How to achieve it?

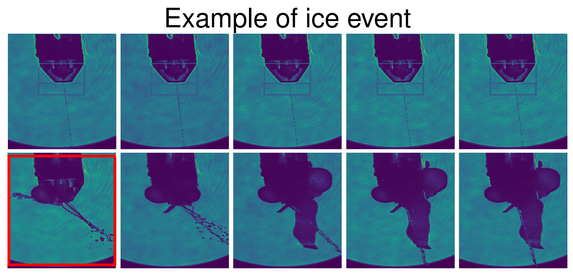
- Clarify how the method works.
- Shape methods based on scientific content.
- Estimate uncertainties and data quality.

Use-case: Prevent damage on imagers

deployed

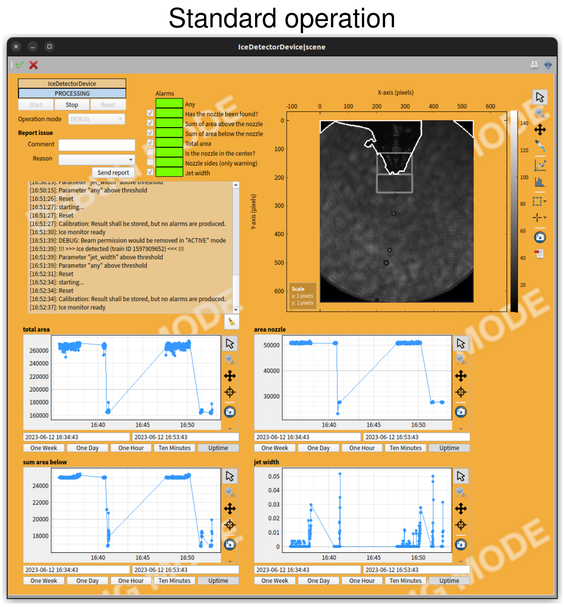
- Ice can form on the tip of sample delivery nozzles, and scatter X-rays that can damage detector pixels.
- Using computer vision techniques we detect:
  - ► jet instabilities to improve beamtime efficiency;
  - ► ice formation to prevent detector damage.
- Warns beamline operator and/or automatically stops beam delivery.

Example of ice event

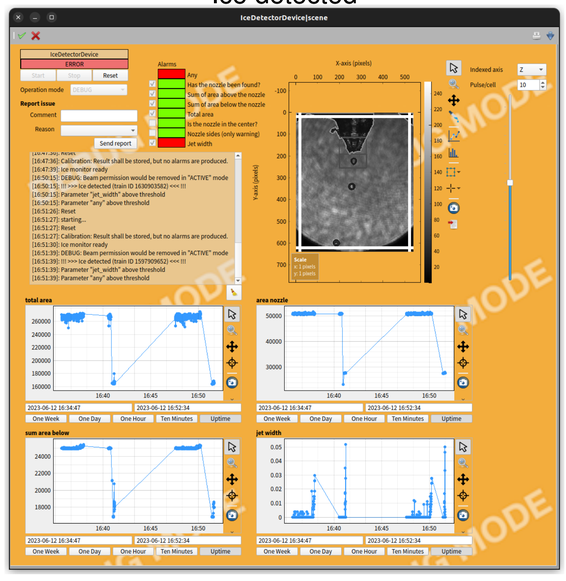


Two consecutive frames separated by 100 ms.

Standard operation



Ice detected



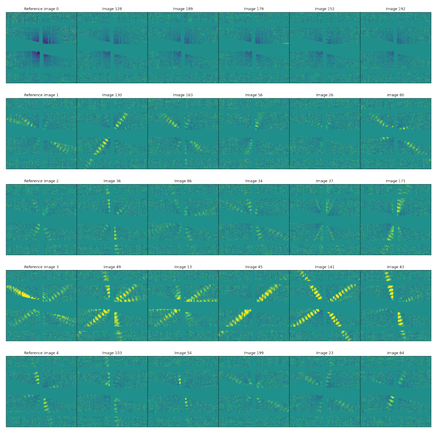
Use-case: How do we search data?

validated

- How can we identify different kinds of data as we collect it?
- **Idea**: *Change* the data *view* and enforce their similarity.
- See, e. g., Ref. [1].
- *Equivalent views* ⇒ variations to ignore.

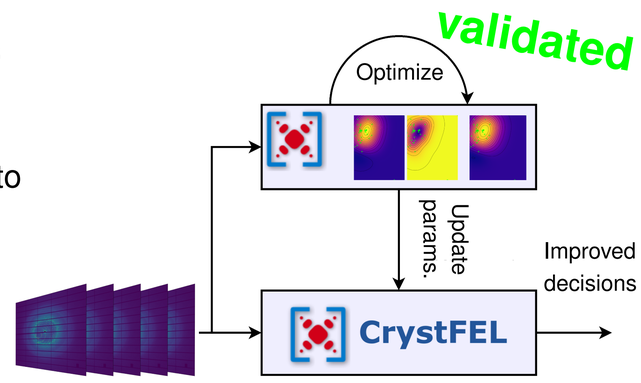
Example ⇓

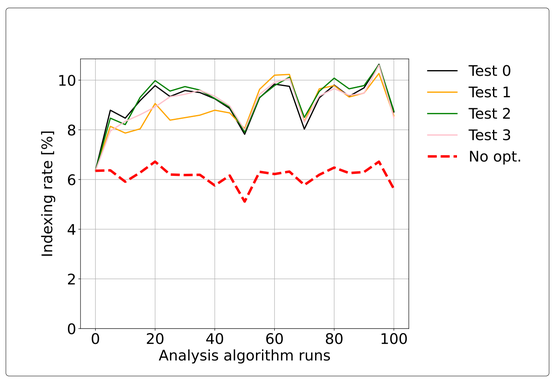
Similar ⇒

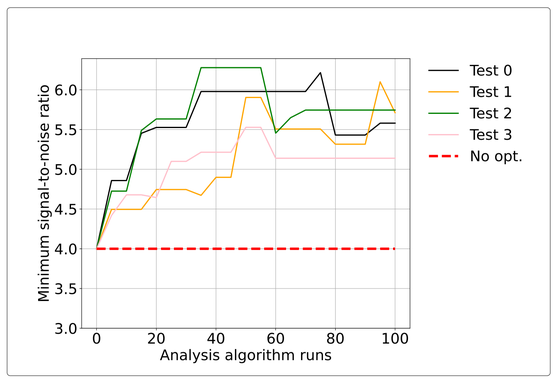


Use-case: Streamlining data analysis using ML

- Typically data analysis pipelines have parameters.
- **Idea:** Simplify data analysis for non-experts – tune parameters to maximize a *metric*
- Metric: indexed frames fraction.
- *Online*: fast feedback, higher success chances.
- *Offline*: improved scientific findings.





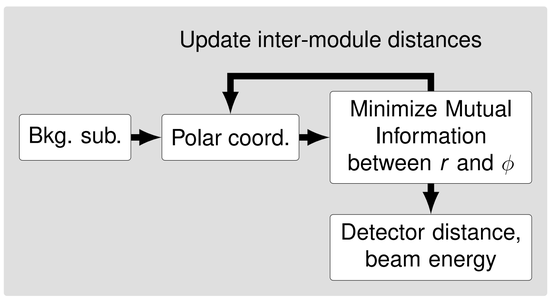


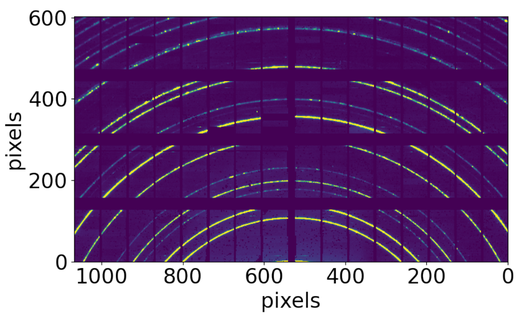
- Hen Egg-White (HEW) Lysozyme with the AGIPD detector at EuXFEL SPB/SFX.

Use-case: Multi-modular geometry tuning

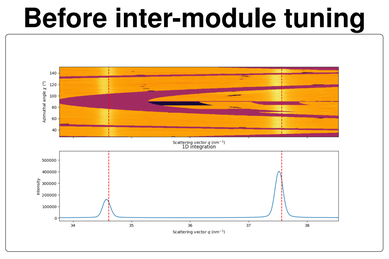
deployed

- Misalignment of module positions.
  - ► Manual alignment: requires lots of time.
  - ► Powder diffraction-based existing toold require many parameters and often manual tuning.
- **Idea**: use *independence* between r and θ to *automate* geometry tuning in powder diffraction.



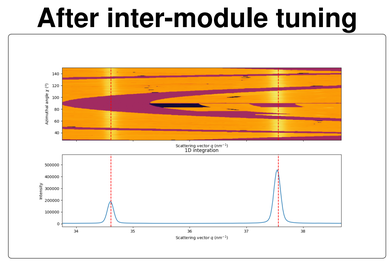


Before inter-module tuning



Impose independence between r and ϕ

After inter-module tuning



Summary

- Several approaches to enhance automation at the EuXFEL being researched and developed.
- Control system allows for integration and deployable methods.
- Interpretability, explainability and quality control assets to guide towards adequate solutions.
- Aim for a holistic approach to integrate those features in all applications.

Related posters

Electron-photon correlations: towards x-ray pulse diagnostics at MHz repetition rate, F. Bishara
Automated SFX data analysis, O. Turkot
Automation of facility sub-systems, S. Birnsteinova
Experiment overview and automated data analysis with DAMNIT, T. Michelat
Enhancing spectral and temporal diagnostics at European XFEL, D. Ferreira de Lima

References

[1] Yue Sun et al. "Application of self-supervised approaches to the classification of X-ray diffraction spectra during phase transitions". In: *Scientific Reports* 13 (June 2023).