

# Machine Learning at the EuXFEL

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European XFEL

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# Machine Learning workshop @ the EuXFEL

- Why organize a workshop?
  - New emerging technologies from ML must be adopted for science at the EuXFEL.
  - Data amount is increasing over the time.
  - The EuXFEL can benefit from automation of data analysis.


# Machine Learning workshop @ the EuXFEL

## Artificial Intelligence workshop at EuXFEL ZOOM VIDEO CONFERENCE

Tuesday 8 Jun 2021, 08:45 → 18:00 Europe/Berlin

Arman Davtyan (Eur XFEL (European XFEL)), Danilo Enoque Ferreira de Lima (Eur XFEL (European XFEL)), Luca Gelisio (European XFEL), Steve Aplin (European XFEL)

**Description** Online workshop hosted by the European XFEL to discuss the latest development in Artificial Intelligence applied to photon science.


**Registration**  You are registered for this event. [Check details](#)

**08:45 → 09:00 Welcome** 15m

**Speaker:** Robert Feidenhansl (European XFEL)

**09:00 → 09:25 Classification of diffraction patterns in single particle imaging experiments using a convolutional neural network** 25m

**Speaker:** Alexandr Ignatenko (Deutsches Elektronen-Synchrotron DESY)

 Ignatenko\_EuXFEL\_...

**09:25 → 09:50 Improving the quality of the spectroscopic analysis by supervised machine learning** 25m

**Speaker:** Alexander Guda (Southern Federal University)

**09:50 → 10:15 ML applications within automated data analysis pipelines for MX at Diamond - current state and future plans** 25m

# Machine Learning workshop @ the EuXFEL

- Workshop on June 8<sup>th</sup> with lots of contributions from the photon science community.

- <https://indico.desy.de/event/30321/>

- 14 speakers.

- Up to 160 participants.

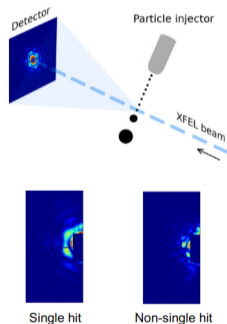
- Supervised / unsupervised / reinforcement learning.

- Different domains and goals:

- ▶ From mining SPI data to orbit optimization.
- ▶ From automation of analysis to reconstruction of XFEL pulses.
- ▶ From object detection to phase retrieval.
- ▶ From automation of beamline operations to theory-guided networks.

# Application of supervised learning

- Supervised ML using CNNs to identify multiple hit diffraction patterns.



Model	Number of selected single hits	Intersection with manual selection	IoU with manual selection, %	Precision, %	Recall, %	F <sub>1</sub> -score, %
YOLOv2, color, linear	1185	597	38	50	60	55
EM	1085	574	34	53	48	50

Ground truth: manual selection

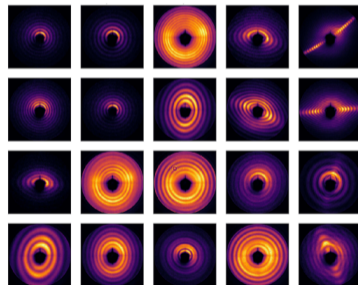
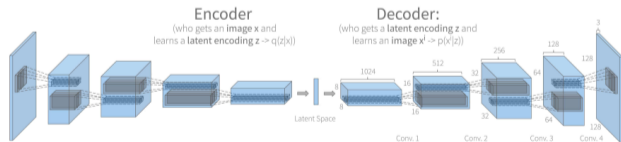
IoU(2 human raters) = 40%

[A. Ignatenko et al 2021 Mach. Learn.: Sci. Technol. 2 025014](#)

(From A. Ignatenko)

# Clustering images

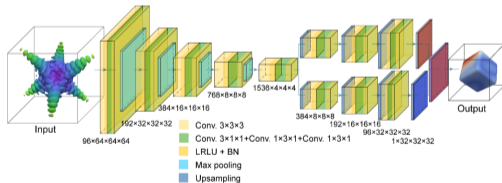
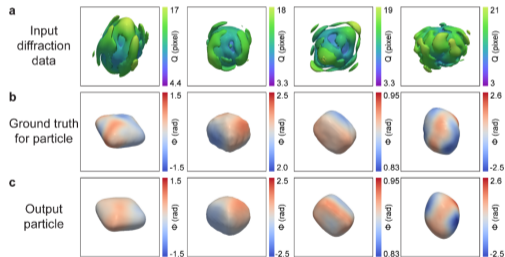
- Identify main qualitative features in images with the latent space of a Variational Auto-Encoder.



(From J. Zimmermann)

# Phase retrieval

Teach CNNs to do phase retrieval on diffraction images.



(From W. Longlong)

# Workshop survey

How interesting was the Workshop?

Answered: 14

A. The worst ever: 0 (0.00%)

B. It was OK: 7 (50.00%)

C. The best ever: 7 (50.00%)



Are you already using AI for your work?

Answered: 14

A. No, and I'm not planning to: 0 (0.00%)

B. No, but I'm planning to: 6 (42.86%)

C. Yes!: 7 (50.00%)

D. No selection: 1 (7.14%)



Did you meet new potential collaborators?

Answered: 12

A. Yes: 8 (66.67%)

B. No: 4 (33.33%)



If you are not using AI, would you consider using it after the Workshop?

Answered: 9

A. Yes: 9 (100.00%)

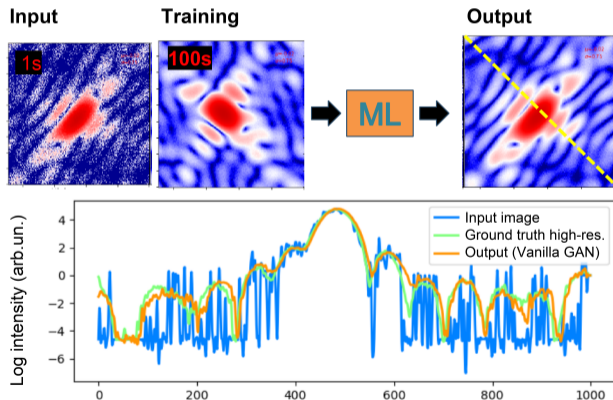
B. No: 0 (0.00%)





# In the EuXFEL data analysis group

Automatic parameter tuning (next presentation), automatic clustering, image quality enhancement.

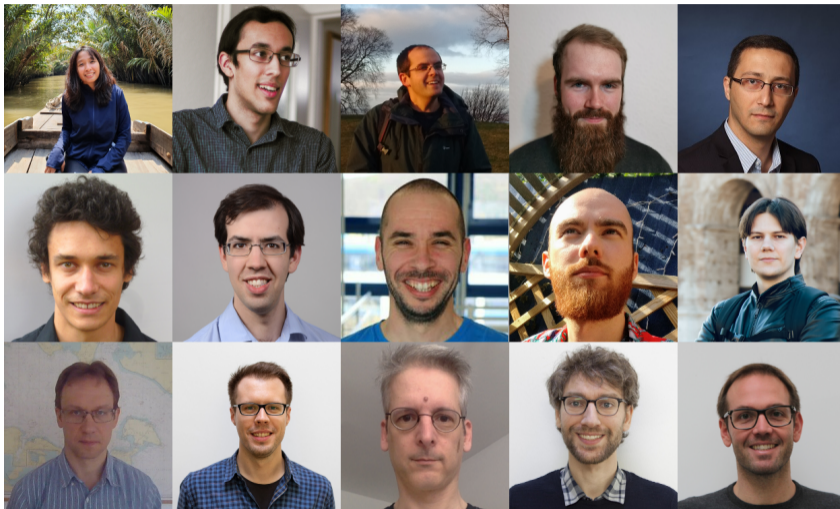


# The Data Analysis group



- 15 people from various places in the world with diverse backgrounds:
- physics, engineering, computer science, chemistry, biology, artificial intelligence, ...

# Thank you for your attention!



Contact us at [da@xfel.eu](mailto:da@xfel.eu)