

A resilient feature extractor in SAXS images

6th Round Table on Deep Learning @ DESY

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Story begins with... Helmholtz Imaging HelpDesk

HelpDesk

The Helmholtz Imaging HelpDesk is the primary gateway for all imaging-related requests in Helmholtz and beyond.



ET

Feature extraction with AE - smartPhase

Ticket#562563 - created 27/01/2023

Dear Helmholtz Imaging Team,

I have a request for help regarding one of my current projects, the inversion of experimental X-ray scattering images using normalizing flows. While the inversion on simulated data is a challenge by itself, the bigger challenge is the inversion of experimental scattering images since artifacts like parasitic scattering, slit scattering, beamstop and detector background is a huge domain shift for the neural network. The parasitic scattering is usually a gaussian blob around the main beam and some photon impacts around that. Slit scattering is a streak that is also around the main beam, while the beamstop covers the main beam (and the other effects) with a stripe so there is no signal. The detector background is in this case an offset with a bit of structure to it. You can find a visual representation of the effects in the appendix. Currently I am perturbing the simulated training dataset with these artifacts but in the future this will not be feasible since we do not know the artifacts beforehand and there is no time to model them during the experiment.

That is why I would like to collaborate with you to come up with a robust feature extractor which can extract features from both simulated and experimental data with unknown artifacts. The features will then be used for inference of the main neural network responsible for inversion. One idea would be to implement a self-supervised algorithm/model using an inpainting task but I am open for suggestions. Furthermore, we are planning to use a similar approach for other modalities like X-ray holography in our HIP project "Smart Phase"

Do you think we can start a collaboration on this project?

Best Regards,
Erik Thiesenhusen

1 ATTACHED FILES

150_3_annotated.png

1.5 MB

set to internal

reply

reply all

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split

Ticket

GROUP *
HI Collaboration

OWNER
Engin Eren

STATE *
closed

PRIORITY *
2 normal

TAGS
+ Add Tag

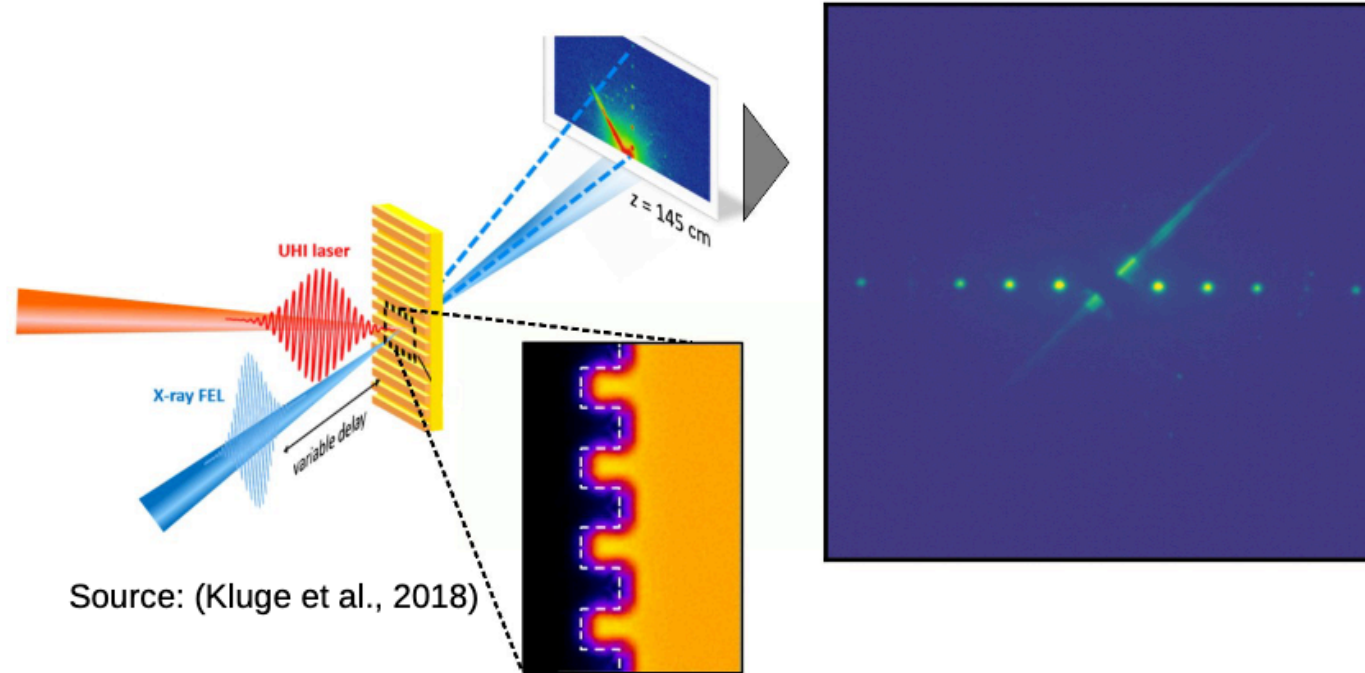
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Experiment

- Goal: understanding laser-solid and laser-plasma interactions + Ion Acceleration
- Simulations for interactions exist → need verification

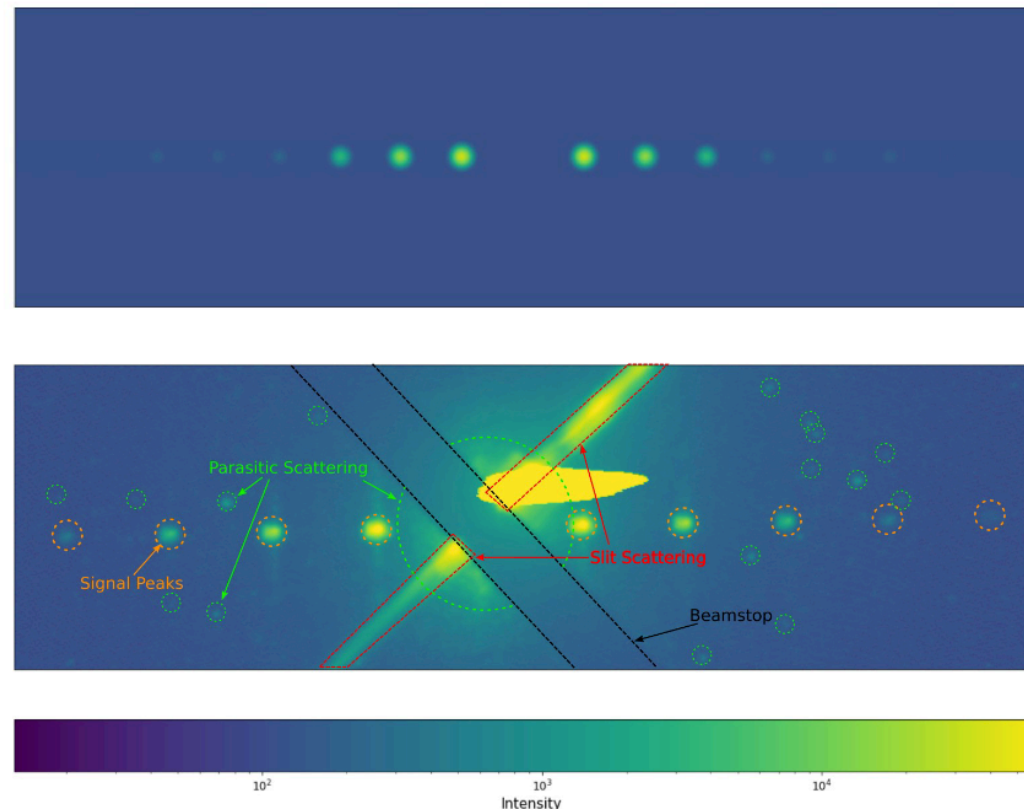


- Sensor only sums up intensity of photons, not phase → phase problem

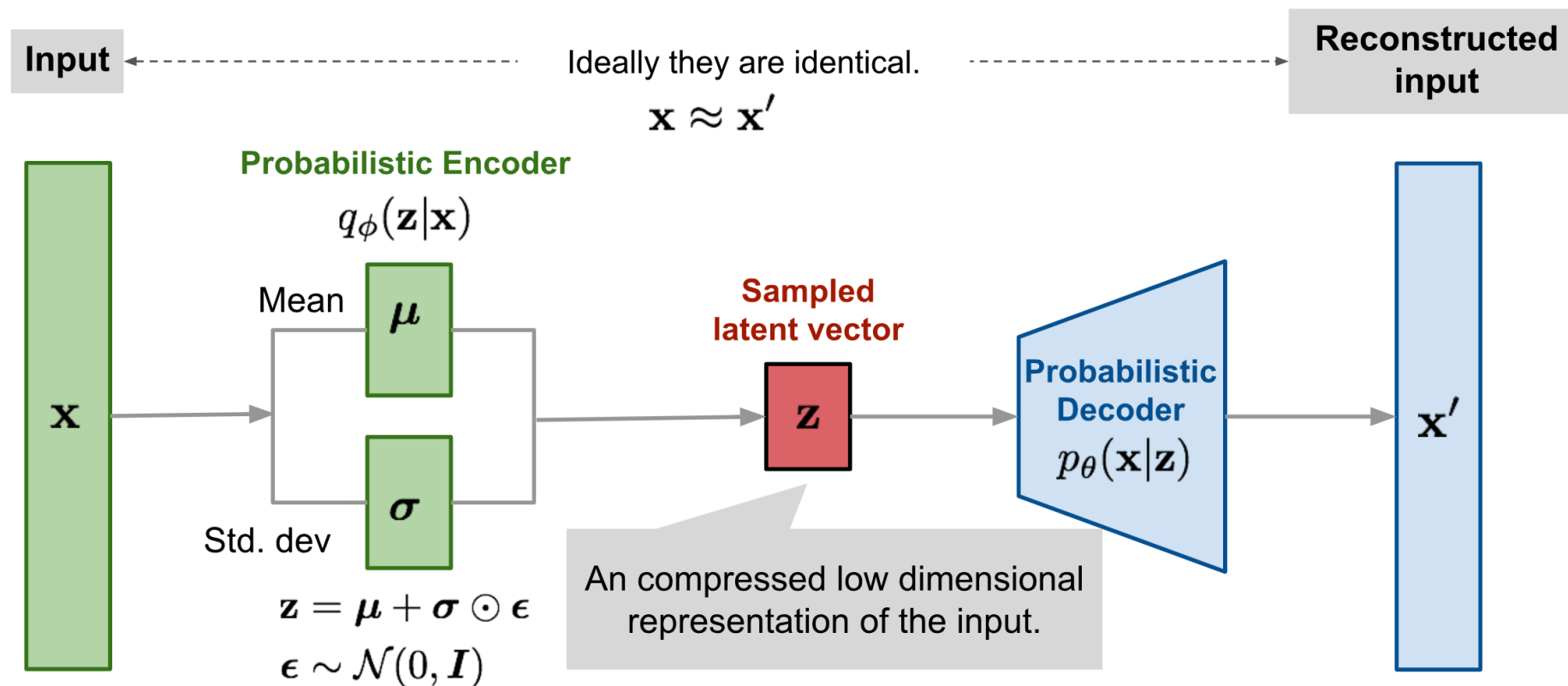


Solution – A robust Feature Extractor

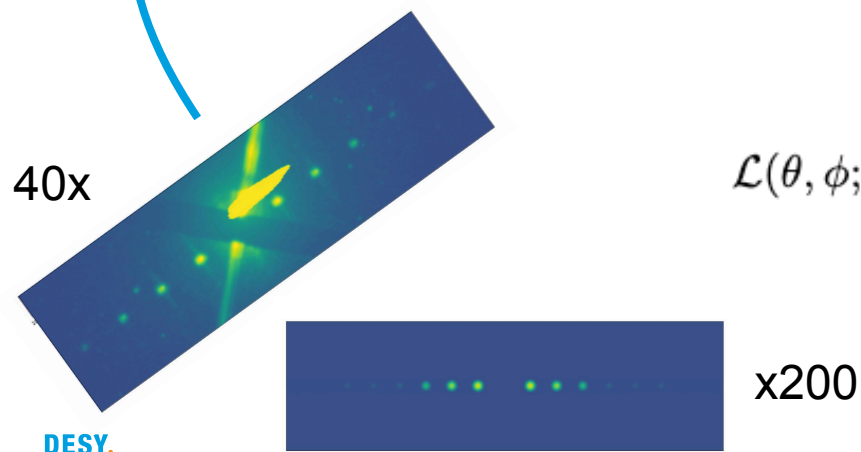
- Need a feature extractor that **works both on simulated and experimental data** (and for different targets)
- Features are used to train cINN
- Additional challenge: **data imbalance** (very few experimental images)
- Available data:
 - **SAXS grating** data both experimental and simulated (LCLS)
 - **SAXS + PCI wire** data; experimental data available, simulated data would need some work (EuXFEL, Hibef)



β -VAE: Learning disentangled representations



Source: <https://lilianweng.github.io/posts/2018-08-12-vae/>



$$\mathcal{L}(\theta, \phi; \mathbf{x}, \mathbf{z}, \beta) = \mathbb{E}_{q_{\phi}(\mathbf{z}|\mathbf{x})}[\log p_{\theta}(\mathbf{x}|\mathbf{z})] - \beta D_{KL}(q_{\phi}(\mathbf{z}|\mathbf{x}) \parallel p(\mathbf{z}))$$

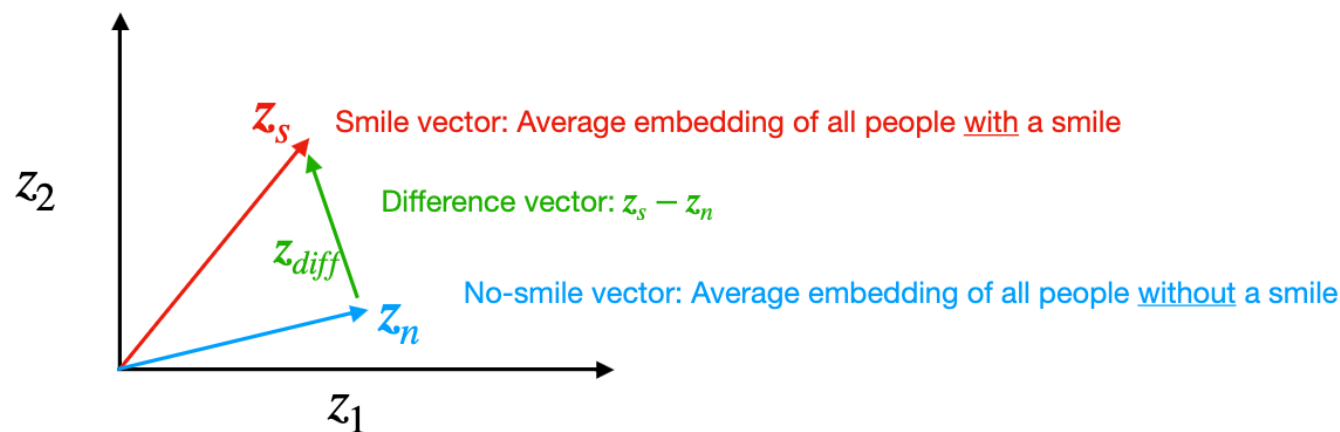
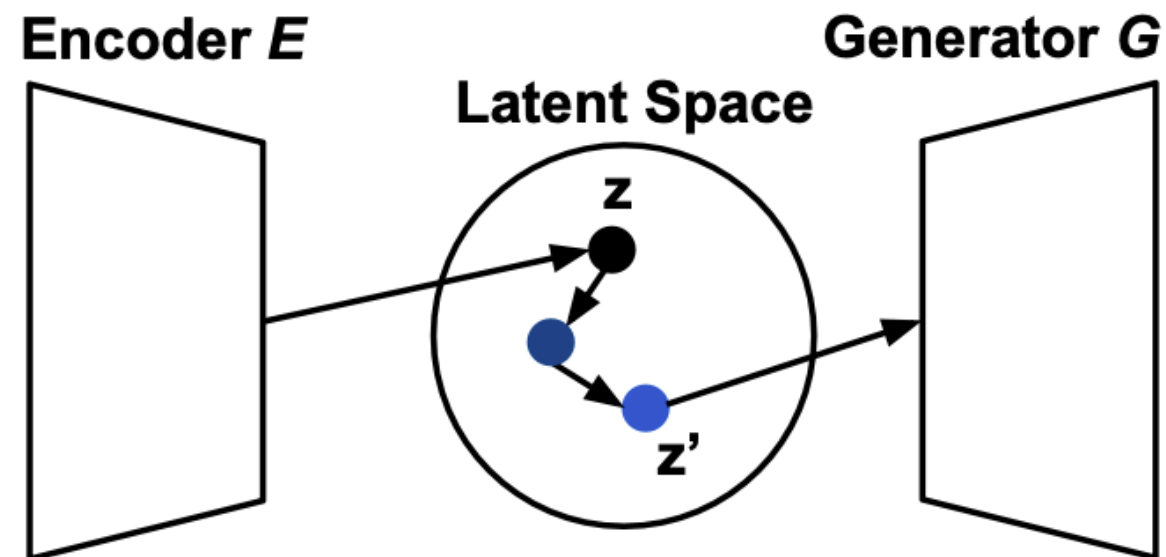
a stronger constraint on the latent bottleneck and results more disentangled latent representations \mathbf{z}

β -VAE: Latent Space Manipulation

Moving in the latent space...

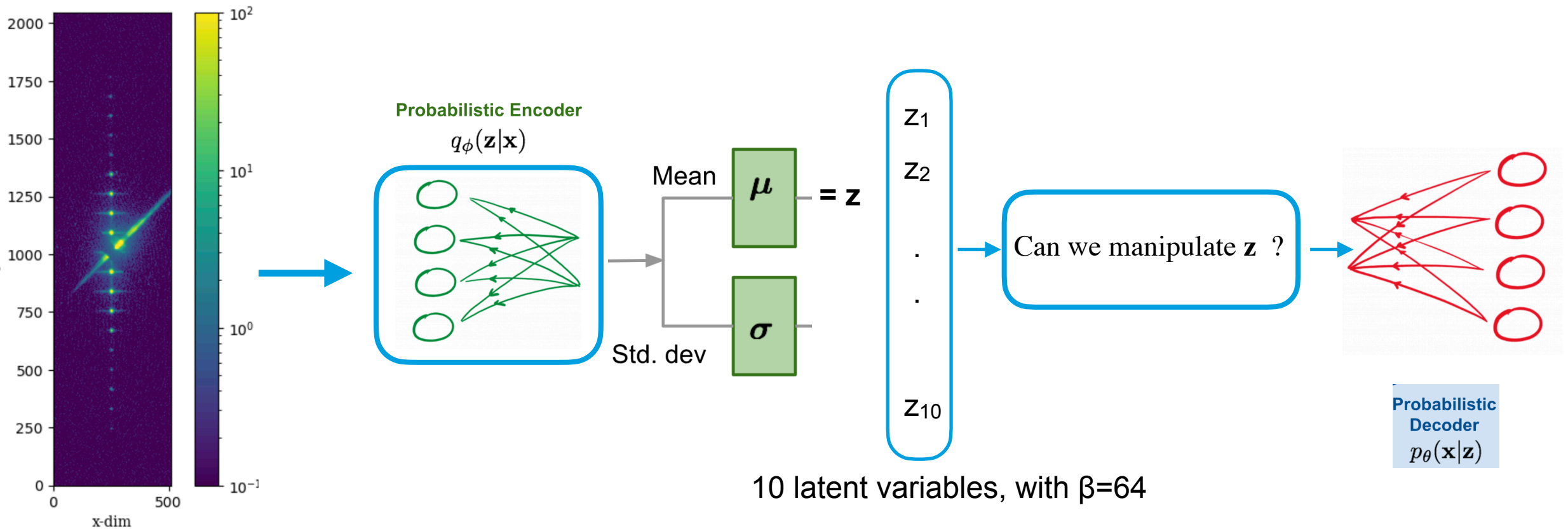


← unsmiling smiling →



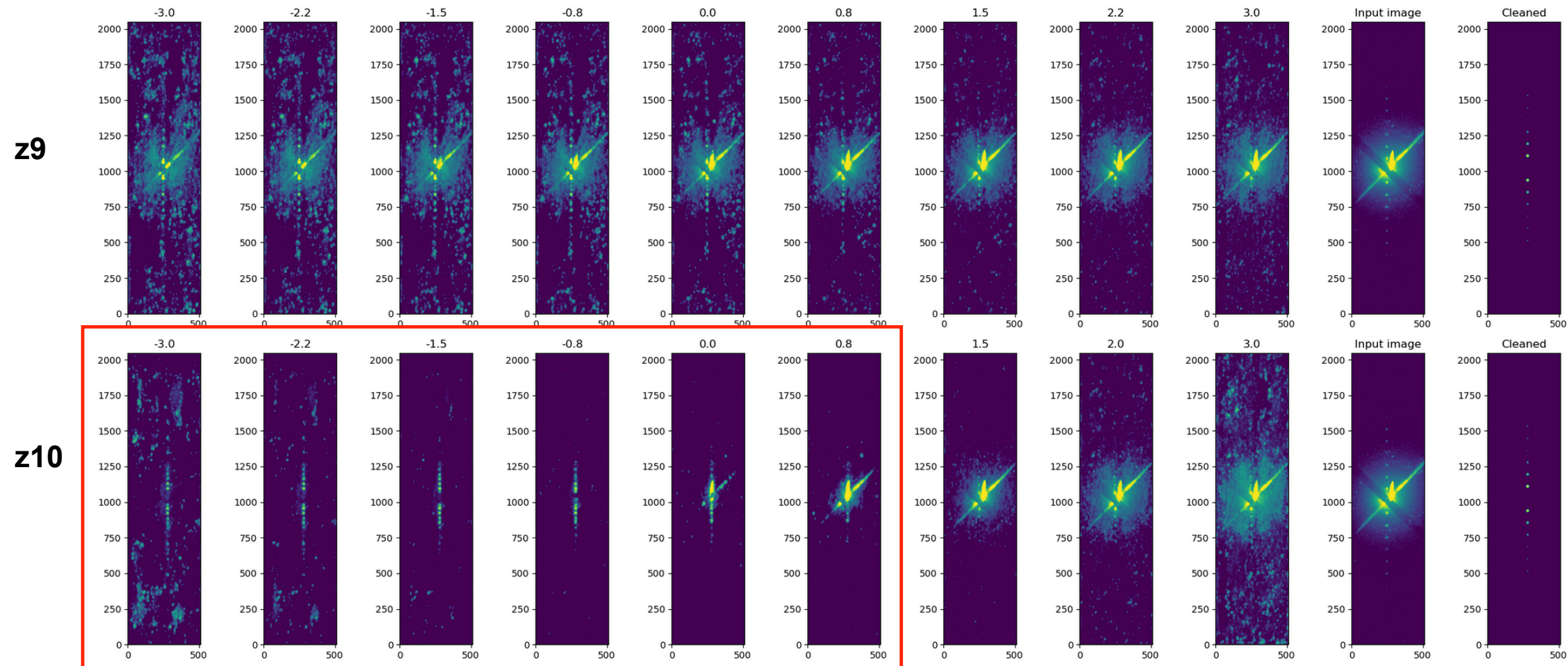
β -VAE: Results

Inference



Latent Space Traversal

Changing 1 variable while keeping others fixed !!!

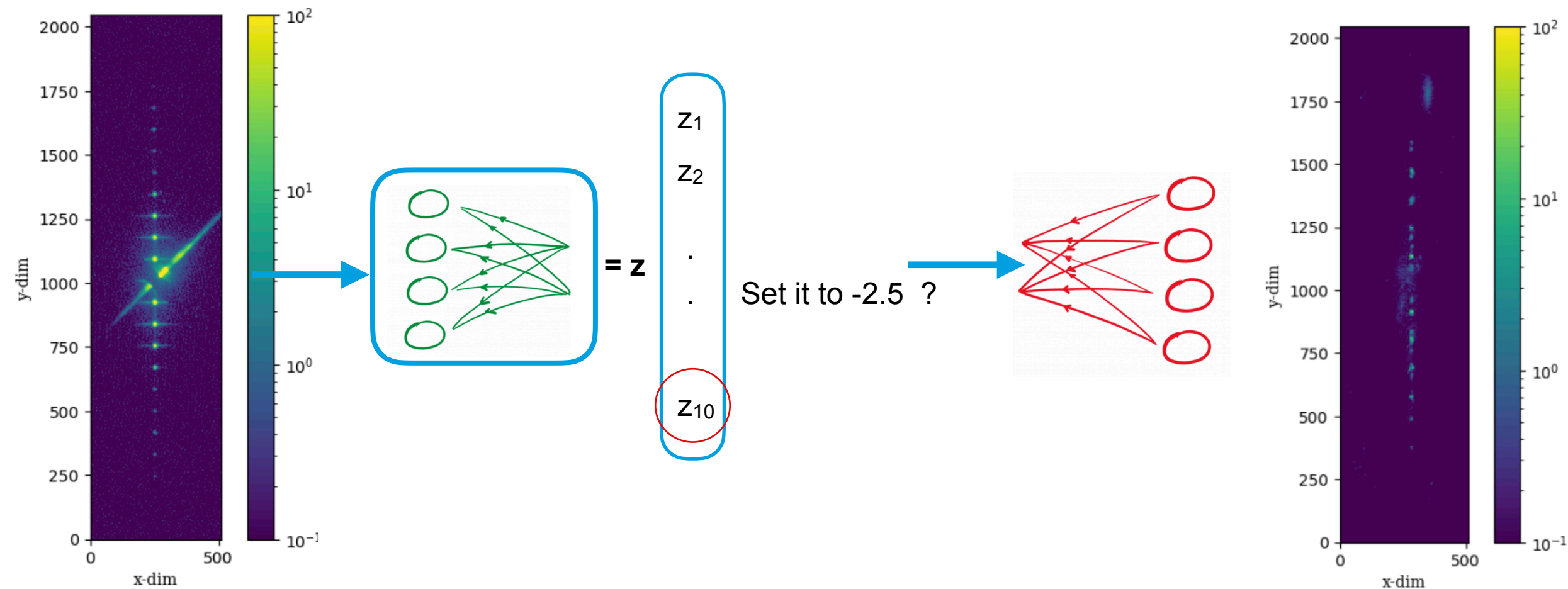


Glimpse of disentanglement ??

Manipulation

Encoding the image and manipulating the z

Original

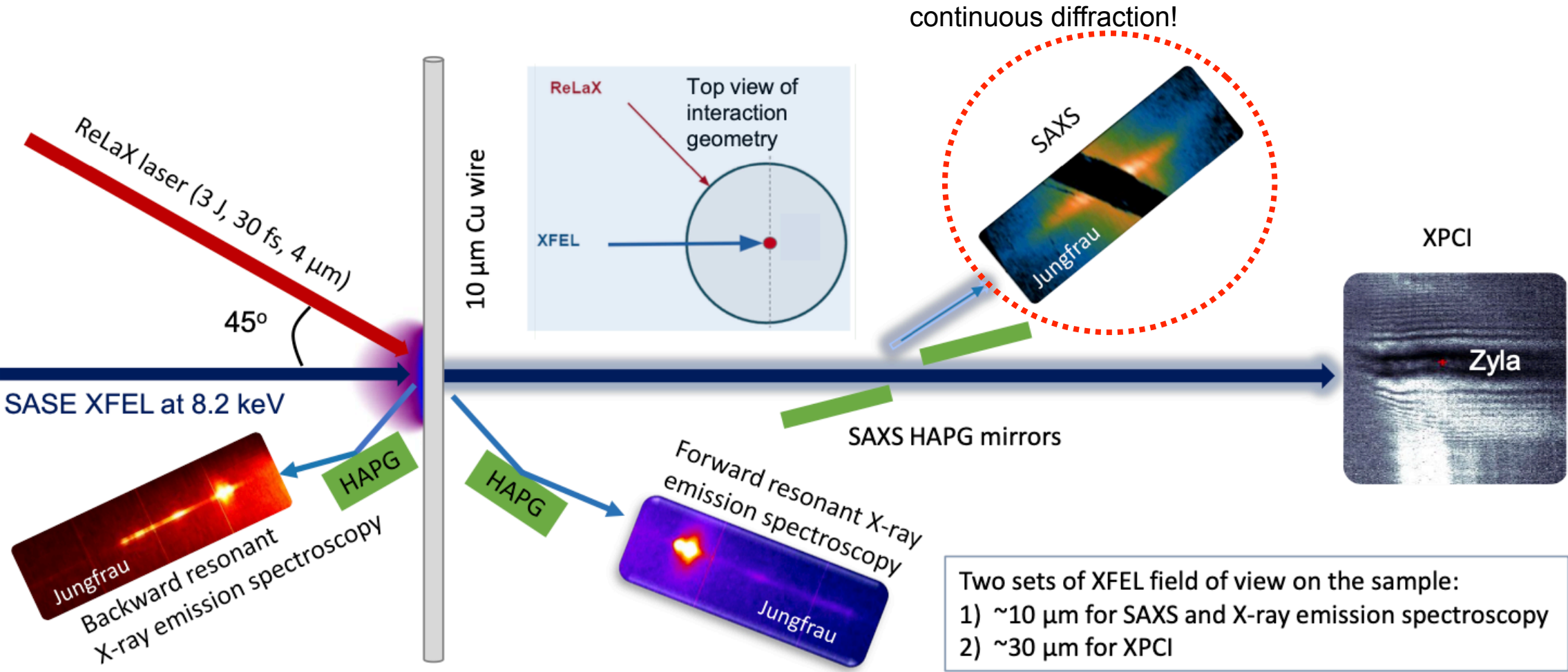


Some artefacts are gone! But.. preservation of the signal quality is not achieved

SAXS + Wire @ European XFEL

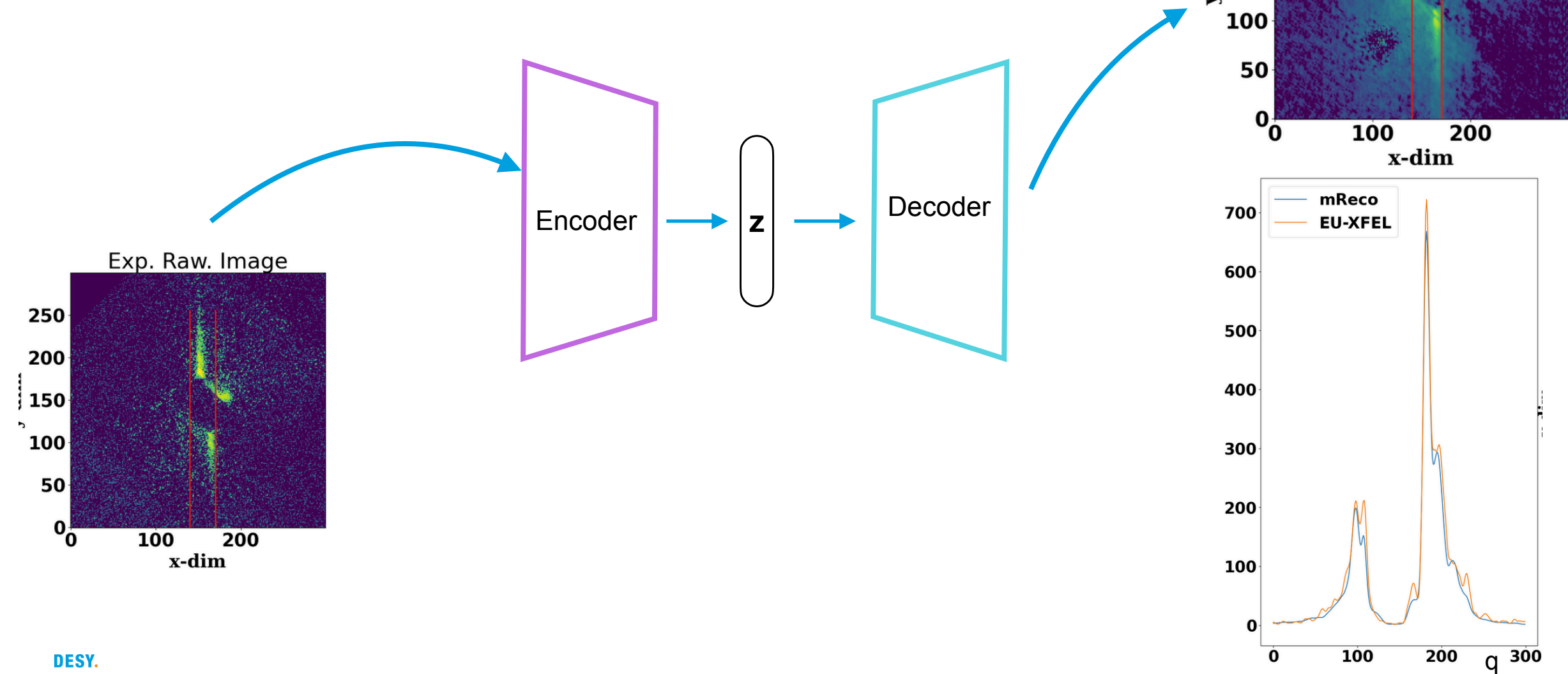
10- μm Cu Wire

(© Lingen Huang)



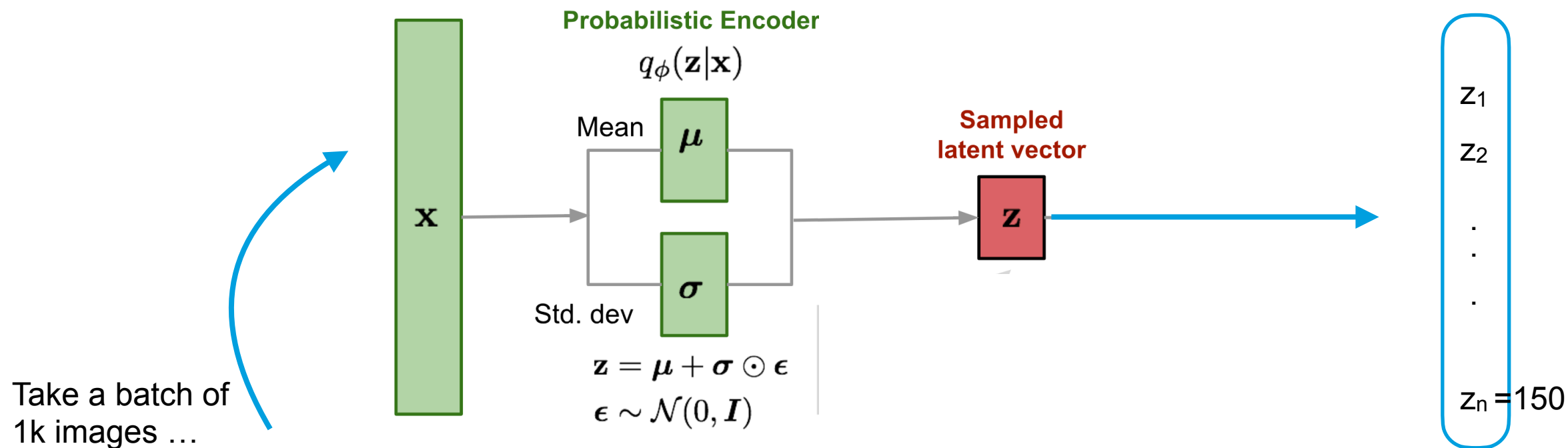
β -VAE: Reconstruction quality

- Training is performed solely with 27k cold-shot data: $z=150$, $\beta = 64$
- Simulation is not yet available

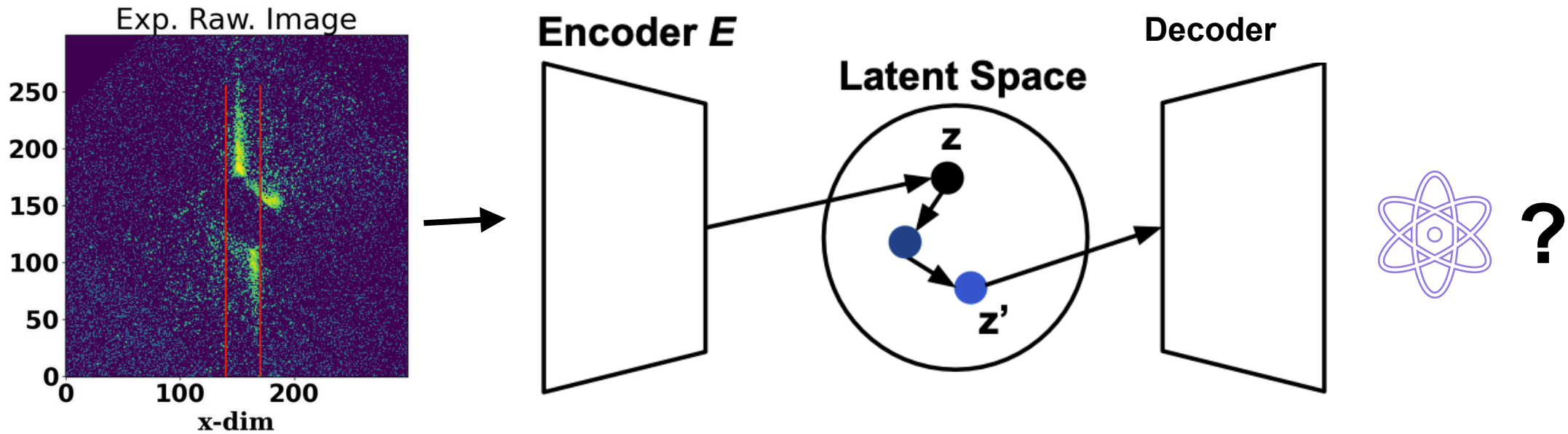


β -VAE: Get the Latent Space

After training the β -VAE, need to construct the latent space



β -VAE: Manipulation



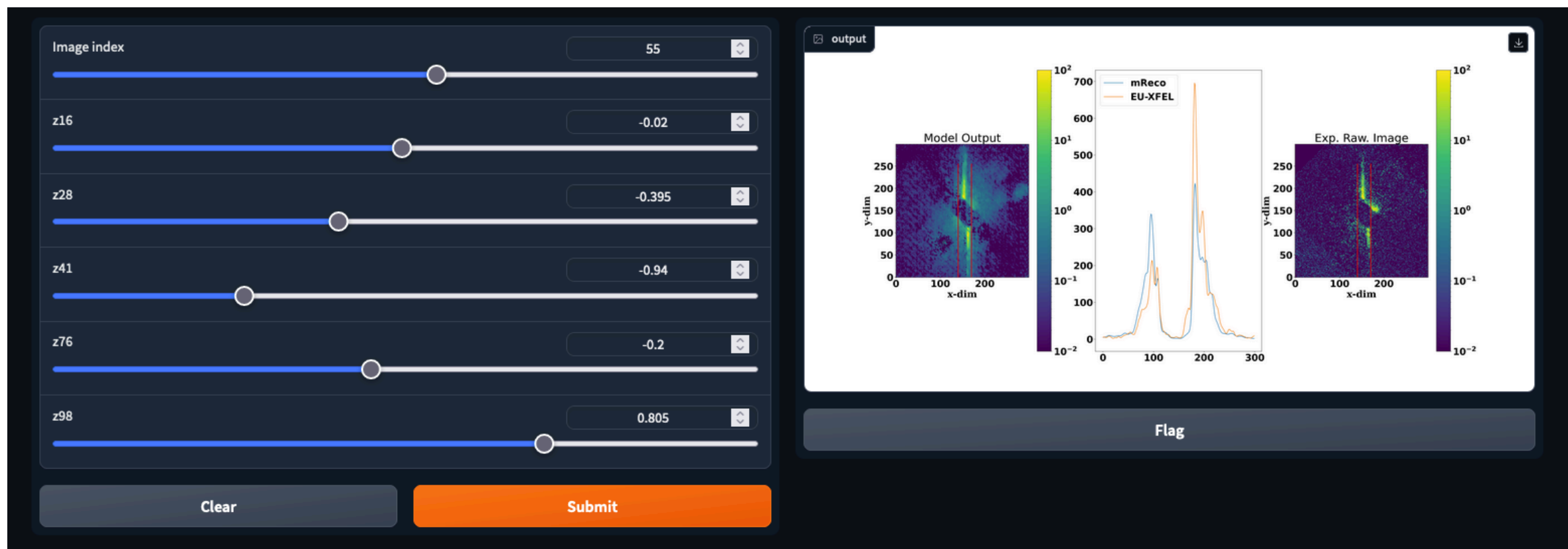
How can we move in our z in the direction of no-artefact space ?

β -VAE: Latent Space Manipulation

Running on local URL: <http://127.0.0.1:7860>

Running on public URL: <https://47787e1c13e6fa8a69.gradio.live>

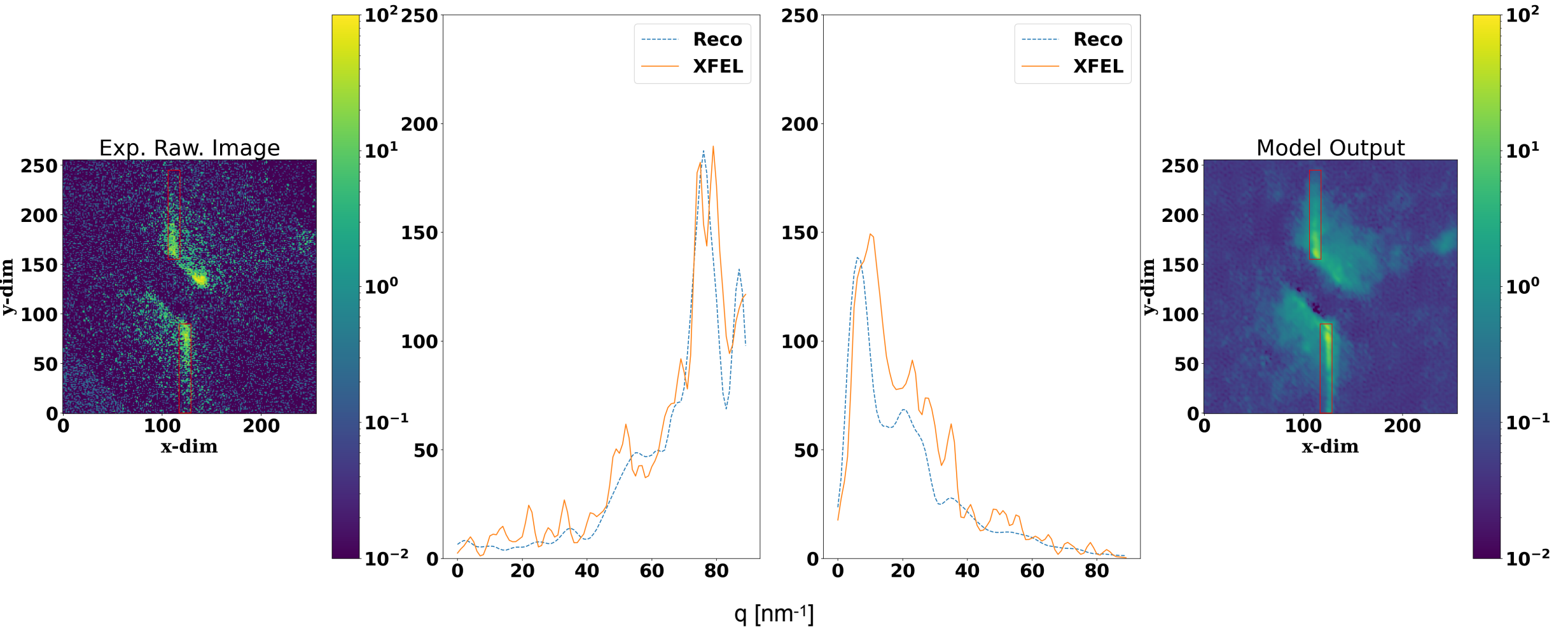
This share link expires in 72 hours. For free permanent hosting and GPU upgrades, [spaces](#))



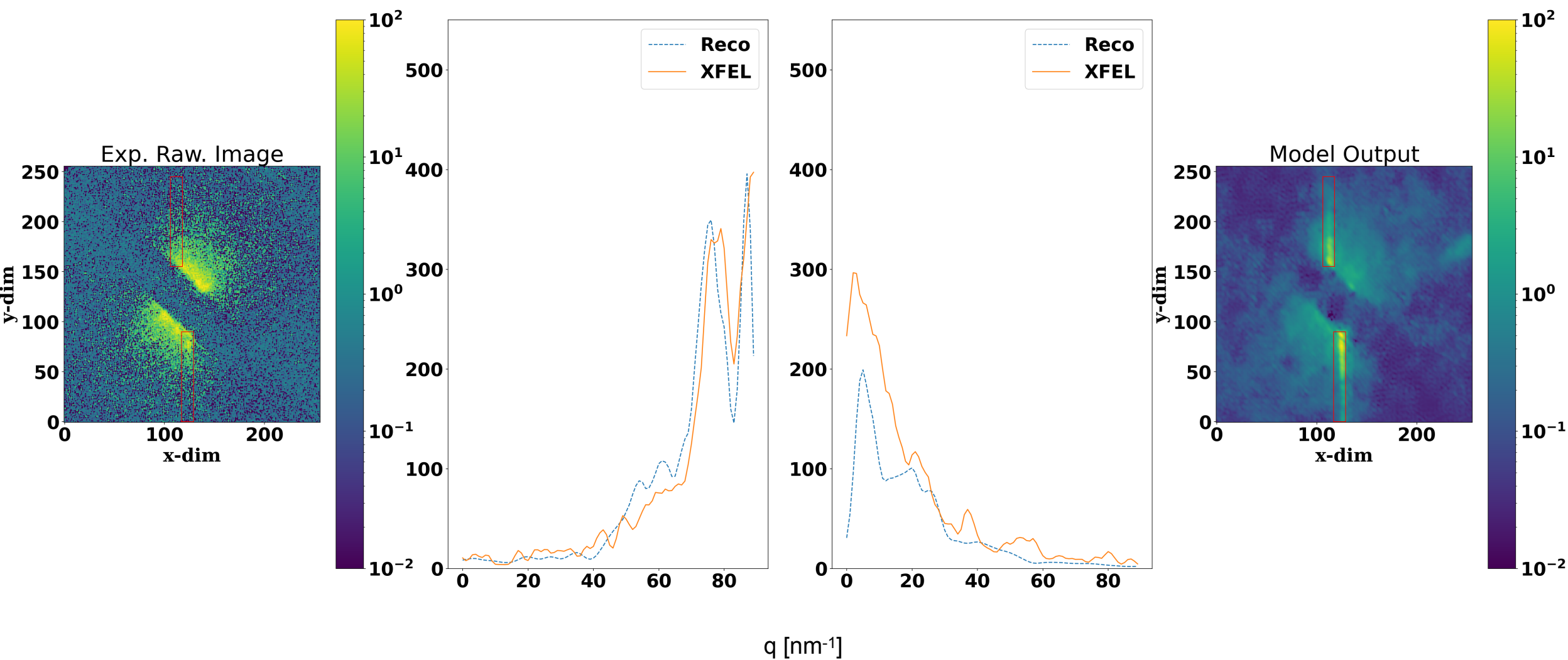
Default values these z's are: -0.02007344365119934 -0.3955821394920349 -0.6009646058082581 -0.5929316282272339 0.8053598403930664

Default values these z's are: -0.02007344365119934 -0.3955821394920349 -0.6009646058082581 -0.5929316282272339 0.8053598403930664

β -VAE: Latent Space Manipulation



β -VAE: Latent Space Manipulation



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ac technology operating at MHz repetition rate. Distributing the ration of three undulators. The High Energy Density (HED) scientific ium, is a new, unique platform for experiments combining hard X-ray conditions of pressure, temperature or electric field using the FEL, cal lasers, or pulsed magnets.

solved X-ray Scattering, is accommodated by the versatile MID aturing different detector configurations and a multi-purpose quenching, stopped-flow devices, or rapid evaporational cooling.

e exoplanets, of new extreme-pressure phases and solid-density high magnetic fields. The first user experiment took place in May ies, such as focusing, spectrometers, monochromators, sample target chamber, a diamond anvil cell platform, the RE.LA.X and DiPOLE rimental data is taken from the sharp3129 user beamtime performed aser with relativistic intensity higher than 10²⁰ W/cm² to

s small angle X-ray scattering (SAXS), X-ray phase contrast imaging nge of multi-scale spatio-temporal processes resulting from hot m femtoseconds to hundreds of picoseconds, enabling us to examine the

10 nm resolution during pre- and intra-short-laser-pulse wire

y recombination, which can be revealed by resonant XES up to 10 ps. 1 μm resolution during hydrodynamic time scales, as measured by time-

runs spanning from 435 to 621. These particular , we acquired around 500 preshots. Subsequently, we preprocess these ep learning models. For details on the preprocessing workflow, you

Exploring Artifact Removal Methods via Deep Learning in the context of SAXS Images

Engin Eren, Philipp Heuser, Erik Thiessenhusen, Lingen Huang

October 18, 2023

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More information

Beta-VAE with EuXFEL wire data

The project consists of two main parts, each responsible for a specific task.

Part 1: Creating Training Data

To create the training data, follow these steps:

```
python flowXFELwire.py run --outputF 'demo.hdf5'
```

**METAFLOW**

XfelWireFlow/1691064082765476/start/1
Task Metadata

Task Created On	2023-08-03 02:01:22 PM
Task Finished On	2023-08-03 02:01:30 PM
Task Duration	0:00:07
Tags	python_version:3.10.9, user:eren, runtime:dev, metaflow_
User	eren

Task Info

Task Metadata

Flow Parameters

Artifacts

DAG

Part 2: Starting Training

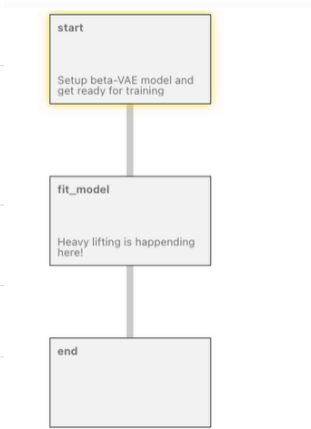
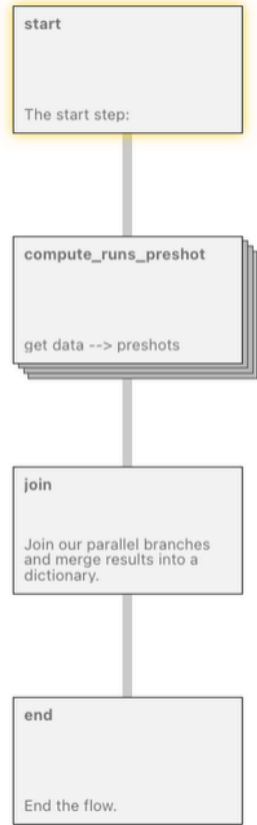
To start the training process, you need to modify the `flowXFELwire.py` file as follows:

```
if __name__ == "__main__":  
    #XfelWireFlow()  
    bvaeFlow()
```

now you can run

```
python fflowXFELwire.py run --tagg TEST --max_iters 100
```

Parameters used here:




RIC > Helmholtz Imaging > **xfel-saxs-wire**



xfel-saxs-wire
Project ID: 7809

16 Commits 1 Branch 0 Tags 317 KiB Project Storage

**main README**
Engin Eren authored 4 months ago

main xfel-saxs-wire / + History

README Add LICENSE Add CHANGELOG Add CONTRIBUTING Enab

Add Kubernetes cluster Set up CI/CD Add Wiki Configure Integrations

Name	Last commit
beta-vae_xfelwire	adding pics and DAG
unet_xfelwire	typo
.gitignore	Test2

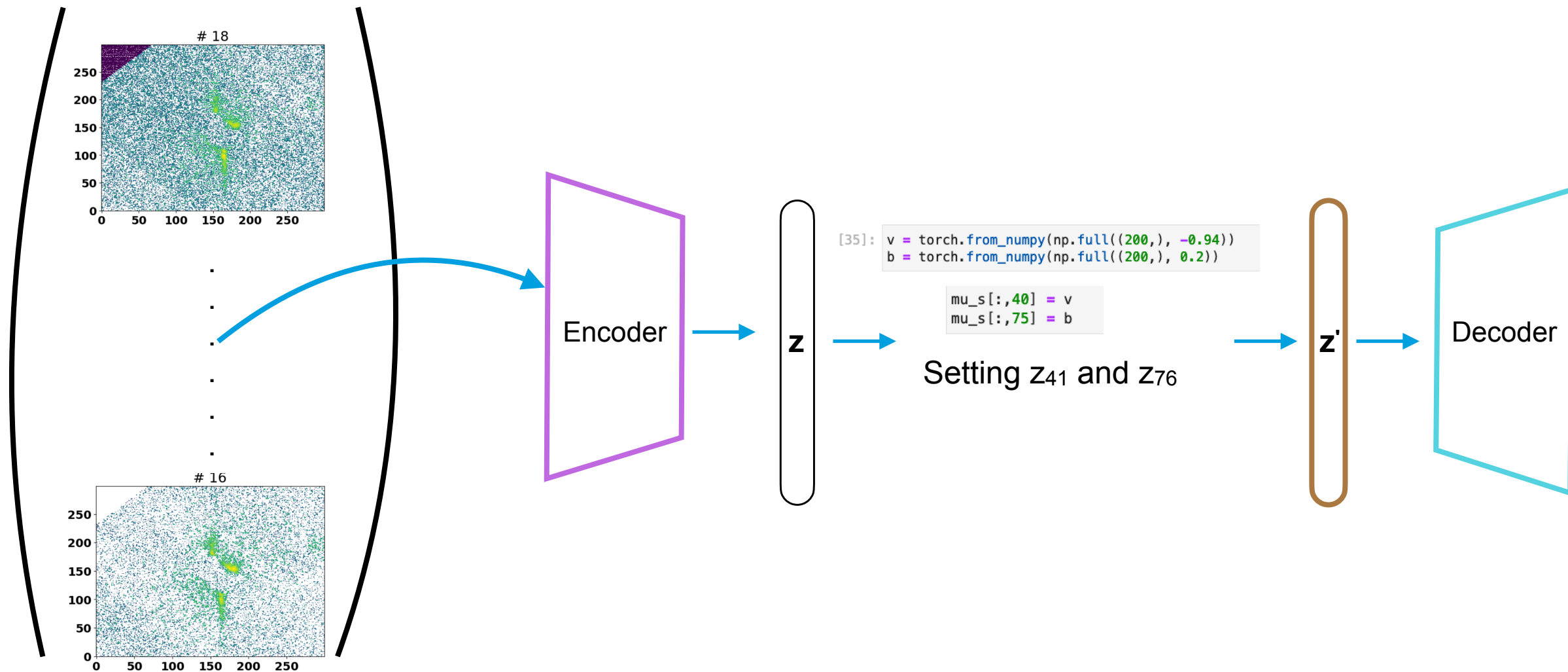
https://gitlab.desy.de/ric/helmholtz_imaging/xfel-saxs-wire

Backup

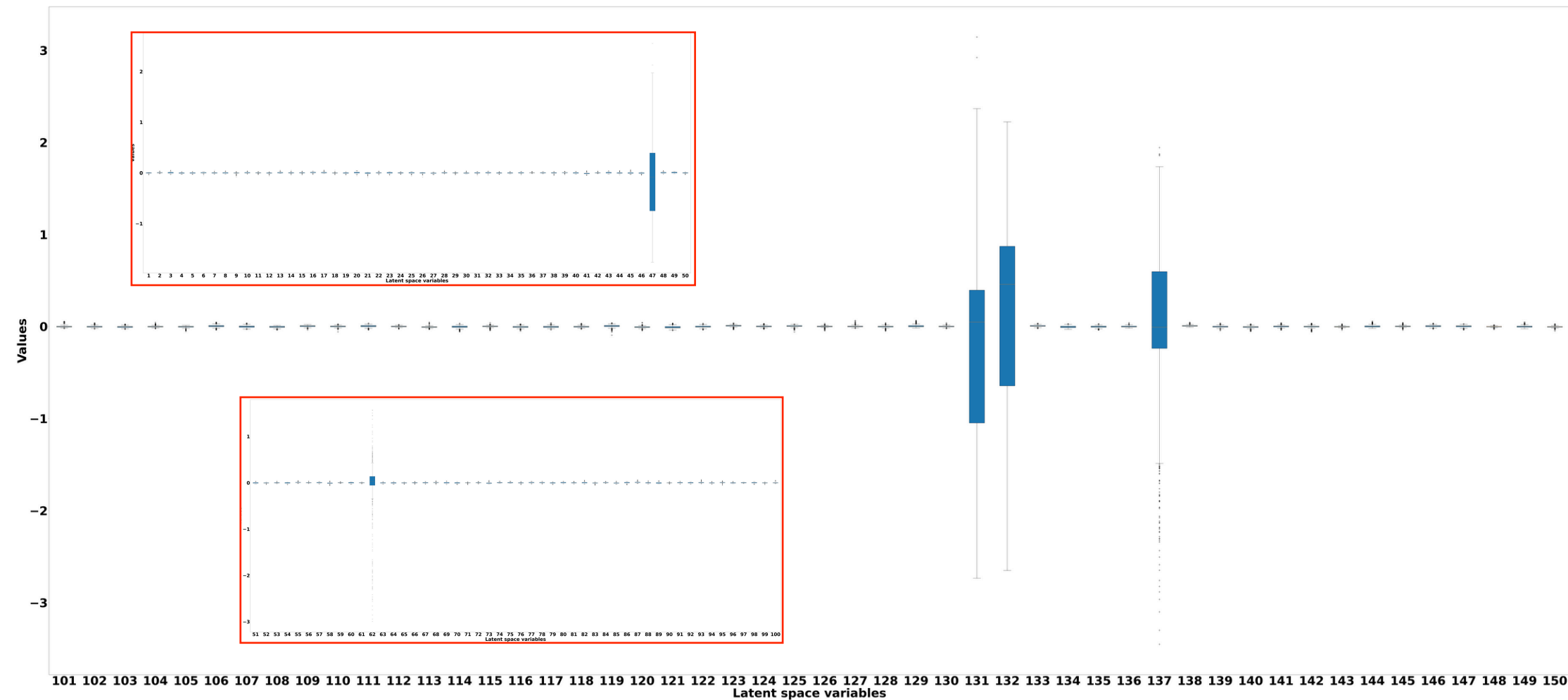
β -VAE: Latent Space Manipulation

Batch-wise

Take a subset of 200 images with obvious artefacts



Distribution of Latent variables



5 latent variables are responsible for artefacts + signal ??