Contribution ID: **47** Type: **Poster**

AI-supported preclassification of GISAXS images: mathematical identity detection by autoencoders

Tuesday 9 April 2024 18:30 (20 minutes)

Due to the high amount of data during a series of GISAXS measurements, automatic binning is helpful for the evaluation by the researcher. This binning supports the confirmation of existing theories or shows outliers where physics and models need to be refined. Such bins represent unique, relevant parameters of the results, also called identity = "collective aspect of the set of characteristics and properties by which a thing is recognizable or known"[1]. In terms of GISAXS images with 1 mio. Pixels, this identity can ideally be reduced to its few relevant physical parameters such as radius, distance, radius, relative scattering and structure type. However due to the indirect measurement method, the high noise and the randomness of individual electron movements, the resulting image can –currently –only visually be analysed. With our research, use AI methods to overcome the missing determinism of the resulting images and to find unique properties for preprocessing and binning [2].

The overall **research question** is: How has a multistage AI-supported process been designed and trained to detect and pre-classify GISAXS images?

In our first attempt, we tried Convolutional Neuronal Networks (CNNs) for simulations to generate predictions of nanostructures of experimental GISAXS data [2]. One of the limitations was that the experimental GISAXS data contained noise while the simulations did not. The work identified two options that exist to close the sim-to-real gap: adding noise to the simulations (data augmentation) or trying to remove the noise from the experimental data (denoising). The approach used in [3] was data augmentation. The limitation of this approach is that we need to make sure that the CNN can generalize the noise and simply learn a few specific instances of the possible noise.

Therefore, we decided to use Autoencoders [4]: Autoencoders (AEs) are self-supervised neuronal networks (NNs) divided into an encoder and a decoder network and are used to learn the identity function for the input. A multitude of architecture variations for the AE architecture exist that are used to either prevent the AE from learning the identity function or enhance the ability to capture the important information and create a richer learning representation. One of these variations is the denoising AE (DAE), which removes the noise in an image during the decoding process by learning the noise identity and storing it in its latent space. In our overall processing pipeline, this is a promising first step to understand and model the noise on GISAXS images better. In later steps towards binning, we will use the knowledge about the noise in the latent space to apply this noise to simulation images for further training steps of NNs.

At the conference, we will present the AE architecture and the encouraging results of artificially created, deterministic images in terms of their noise detection, noise classification and identification.

[1] International Standardization Organisation (ISO), "ISO/IEC 20944-1:2013(en): Information technology —Metadata Registries Interoperability and Bindings (MDR-IB) —Part 1: Framework, common vocabulary, and common provisions for conformance,"2013. [Online]. Available: https://www.iso.org/obp/ui#iso:std:iso-iec:20944:-1:ed-1:v1:en:term:3.21.11.15. [Accessed 13 12 2023].
[2] V. Skwarek, E. Almamedov, S.-J. Wöhnert, S. Dan, A. Rothkirch, M. Schwartzkopf and S. V. Roth, "The role of identities for advanced measurement,"in Gisasx Workshop, Hamburg, 2022.
[3] E. Almamedov, Entwicklung eines Deep Learning Algorithmus zur Bestimmung von morphologischen Identitätsparametern aus GISAXS-Streubildern, Hamburg: Deutsches Elektron Synchrotron & University of

Applied sciences Hamburg (HAW), 2022.
[4] S. Dan, E. Almamedov, M. Schwarzkopf, V. Skwarek, T. Chaves, A. Rothkirch and S. V.Roth, “Application Overview for Autoencoder in GISAXS Data Analysis,”in GISAXS Workshop, Hamburg, 2022.

Primary authors: SCHAEFER, Eric (HAW); SKWAREK, Volker (HAW)

Co-authors: ROTH, Stephan (DESY / KTH); TROPMANN-FRICK, Marina (HAW)

Presenters: SCHAEFER, Eric (HAW); SKWAREK, Volker (HAW)

Session Classification: Posters

Track Classification: MLC