

MXAimbot: ML based sample centering for macro-molecular crystallography

MXAimbot is a neural network based tool, designed to automate the task of centering samples for macro-molecular X-ray crystallography experiments before exposing the sample to the beam.

MXAimbot uses a convolutional neural network (CNN) trained on a few thousands images from an industrial vision camera pointed at the sample to predict suitable crystal centering for subsequent data collection.

The motivation for this project is that the machine vision automated sample positioning allows X-ray laboratories and synchrotron beamlines to offer a more efficient alternative for the *manual centering*, which is time consuming and difficult to automate with conventional image analysis, and for the X-ray *mesh scan centering*, which can introduce radiation damage to the crystal. MXAimbot can be used to improve results of standard LUCID loop centering for fully automated data collection in fragment-screening campaigns. No need for sample rotation should be an additional advantage.

In the short term, the project aims at providing suggested centerings to users which they may reject if they are not satisfied. In the long term the project aims to be able to operate fully without supervision, processing whole batteries of samples without a human present.

A few original approaches and CNN architectures were tested by the authors in [1,2]. They were using X-ray data resulting from mesh scans and not relying on manual annotations. Finally for a current production a more simple method inspired by a DeepCentering approach [3] from SPring-8, has been adopted. The original training dataset was manually annotated with bounding-boxes around each crystal and the new CNN architecture is using the annotated data. MXAimbot can be used by other systems via a REST API. The next step for the project is including MXAimbot into MXCuBE3 - the common data acquisition framework at several European synchrotron facilities. This allows collection of anonymised datasets from the sample vision camera in the BioMAX beamline at the MAX IV synchrotron which can be further used for training and optimisation of CNNs and later be seamlessly included as an additional option in the MXCuBE3 data collection pipeline.

To the authors knowledge CNNs have been implemented for crystal centering at least at two synchrotron facilities including MAX IV. So far the CNN approach has shown outstanding results in automatically positioning crystals. Work is currently underway to test and statistically compare the model predictions to the manual centerings by real users with the goal of integrating MXAimbot into the FragMAX [4] - fragment screening facility at the MAX IV synchrotron.

[1] SCHURMANN, Jonathan; LINDHÉ, Isak. Crystal Centering Using Deep Learning. LU-CS-EX 2019-25, 2019.

[2] SCHURMANN, Jonathan; LINDHÉ, Isak et al. Crystal centering using deep learning in X-ray crystallography. Asilomar Conference on Signals, Systems, and Computers, 2019, 978-983. doi: 10.1109/IEEECONF44664.2019.9048793

[3] ITO, Sho; UENO, Go; YAMAMOTO, Masaki. DeepCentering: fully automated crystal centering using deep learning for macromolecular crystallography. Journal of synchrotron radiation, 2019, 26.4: 1361-1366. doi: 10.1107/S160057751900434X

[4] LIMA, Gustavo MA, et al. FragMAX: the fragment-screening platform at the MAX IV Laboratory. Acta Crystallographica Section D: Structural Biology, 2020, 76.8: 771-777. doi: 10.1107/S205979832000889X