WEPV022

SAMPLE ALIGNMENT IN NEUTRON SCATTERING EXPERIMENTS USING DEEP NEURAL NETWORK

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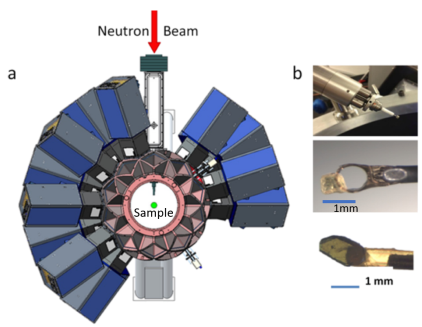
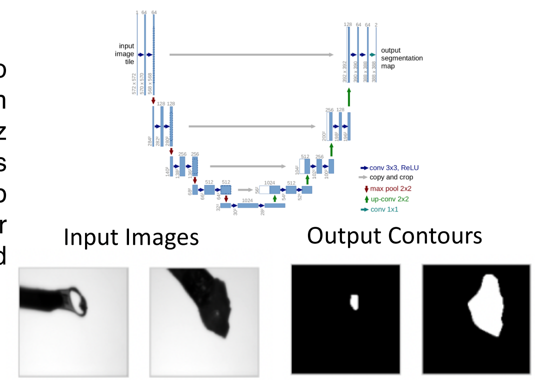
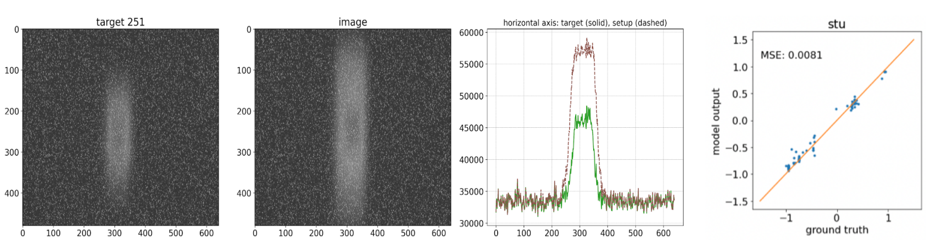


At present the US Government operates two premier neutron scattering user centers; one at Oak Ridge National Laboratory and one at the NIST Center for Neutron Research. These large scale facilities offer flagship research capabilities to academia and industry that serve a broad and growing user community which necessitates their improved operational efficiency and capacity.

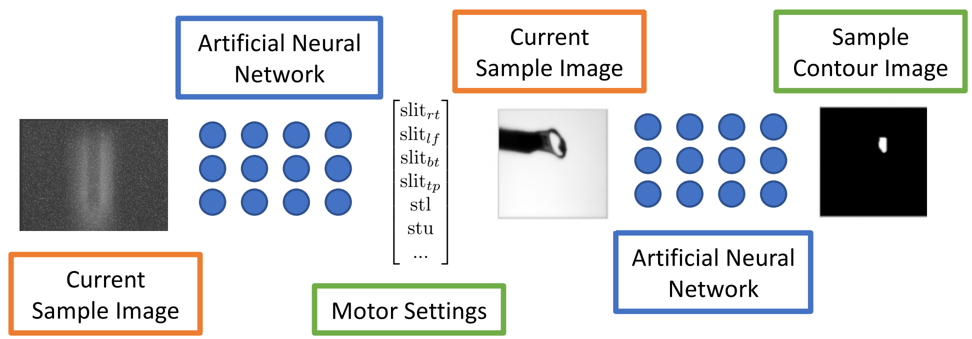
We utilized a U-net architecture to predict sample contours from diagnostic image in the Topaz experiment. The blue boxes represent multichannel feature map while the white boxes are their copies. The gray arrows correspond to the operations from left to right.



We used convolutional neural networks to predict the motor and other experimental settings for the HB2A beamline. The neural network was trained on data spanning several experimental setups.

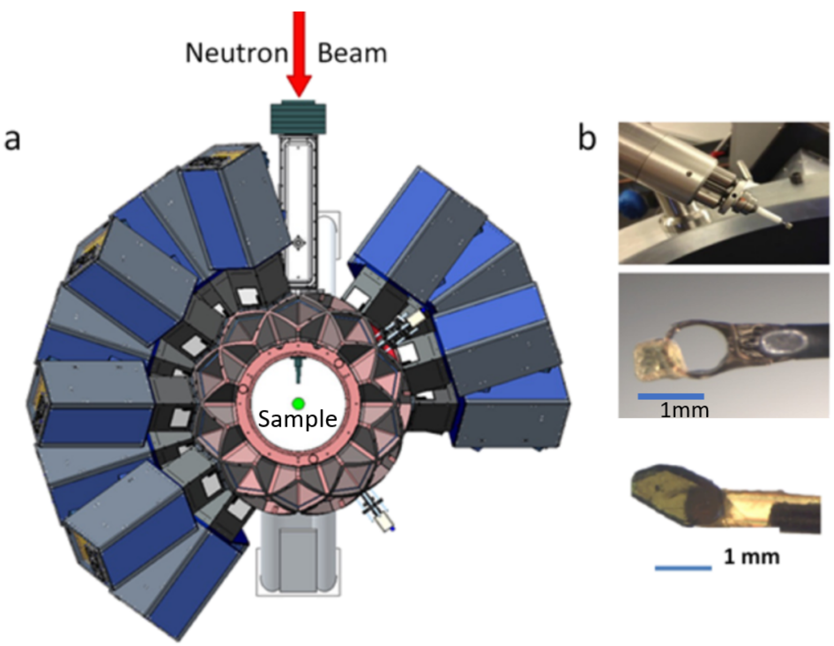


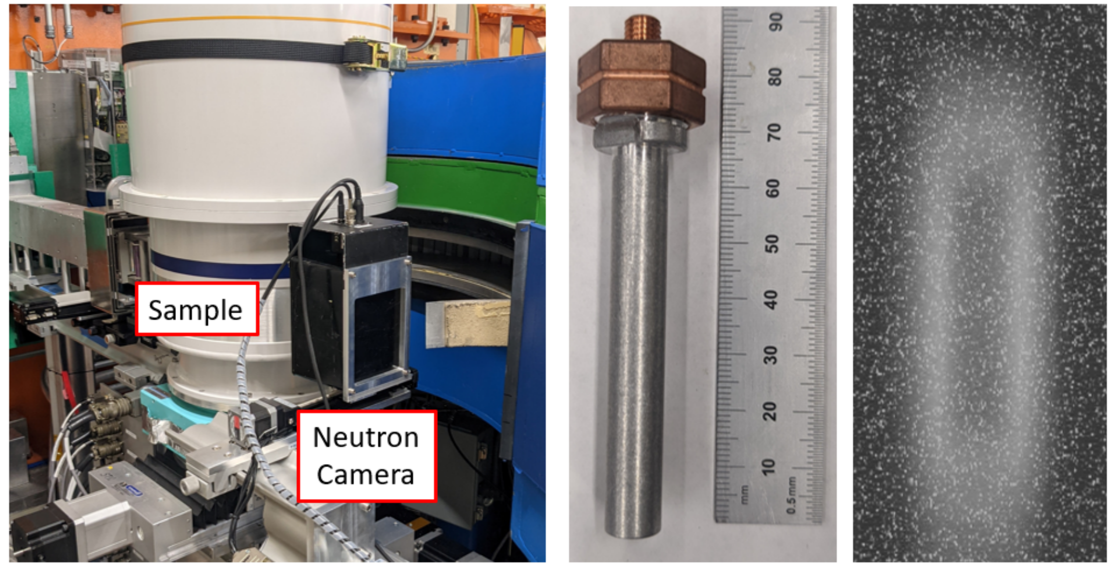
Machine Learning for Sample Alignment



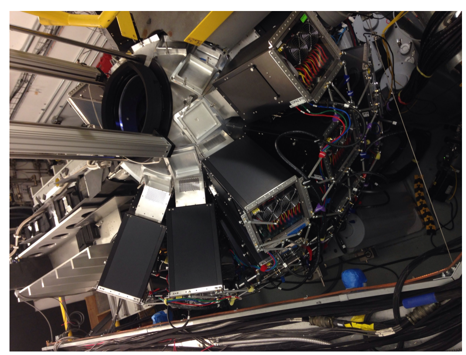
ORNL Beamlines

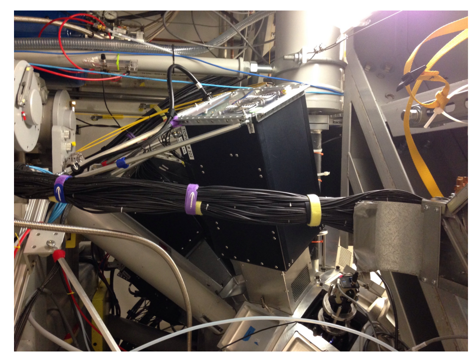
TOPAZ neutron single crystal diffraction instrument. (a) The sample and detector area is shown as viewed from above the instrument. (b) Top image shows the sample goniometer arm. Samples are loaded on pins and attached to the end of the arm. The middle and bottom images show images of the samples attached to sample mounts.





The HB2A powder neutron diffraction instrument. The sample and detector area is shown on the left, with the neutron camera behind the sample. Middle shows a standard sample holder that the powder sample is loaded into, with the scale shown in millimeters. An example of a neutron image is shown on the right, with the powder appearing as a shadow-like image in the white beam.



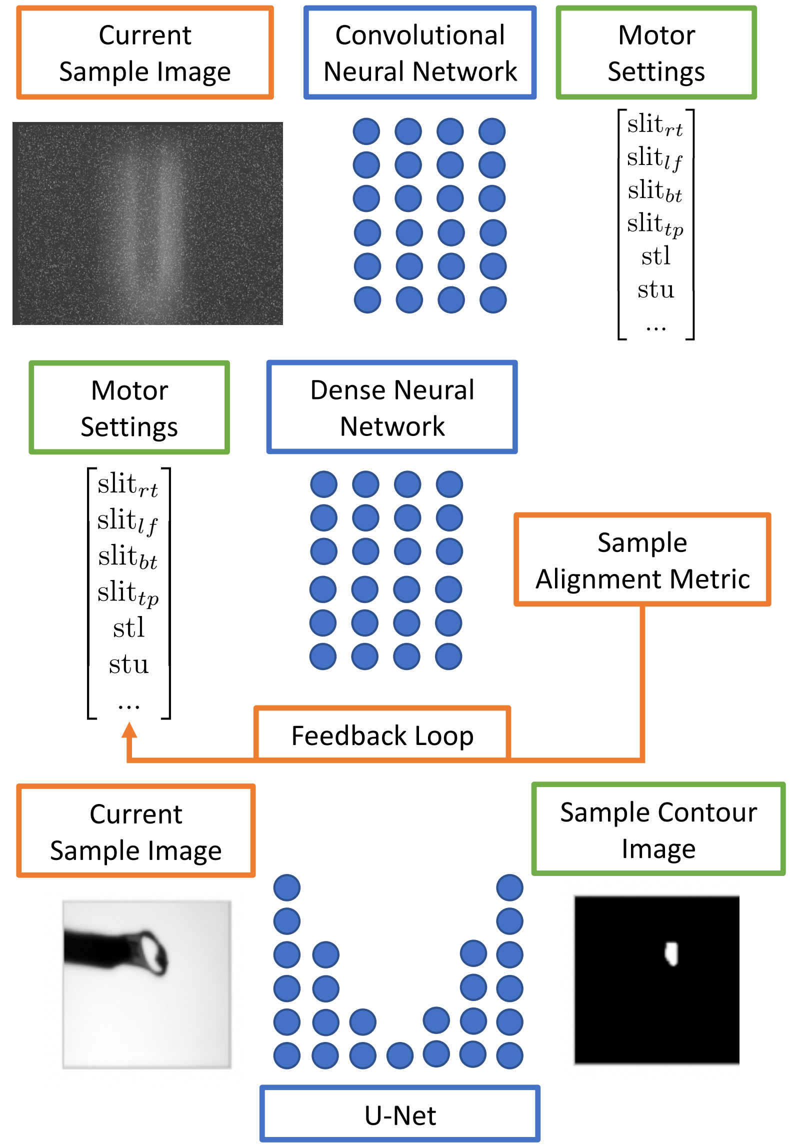


Automation of sample alignment

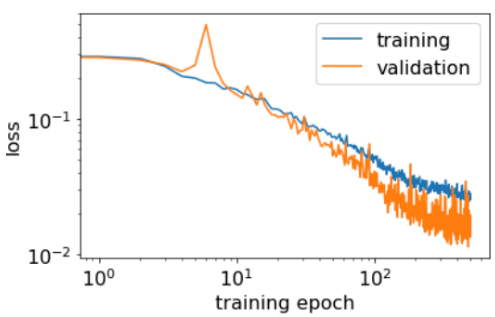
- Convolutional neural networks for feed-forward alignment
  - Use surrogate model to compute motor setting offsets from fully aligned configuration
  - Apply offsets to the experiment

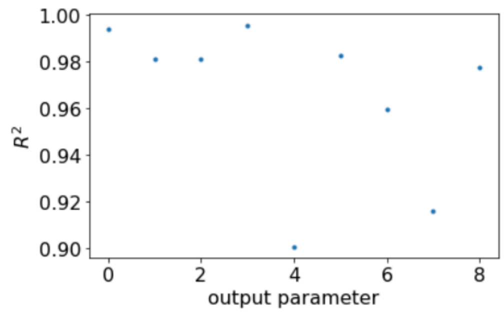
- Neural networks for feedback based alignment
  - Neural network computes alignment error from sample image
  - Optimize motor positions to minimize alignment error

- Identification of sample center of mass.
  - Manually contour the sample in images
  - Predict the sample contour using a u-net
  - Compute sample center of mass from predicted contour

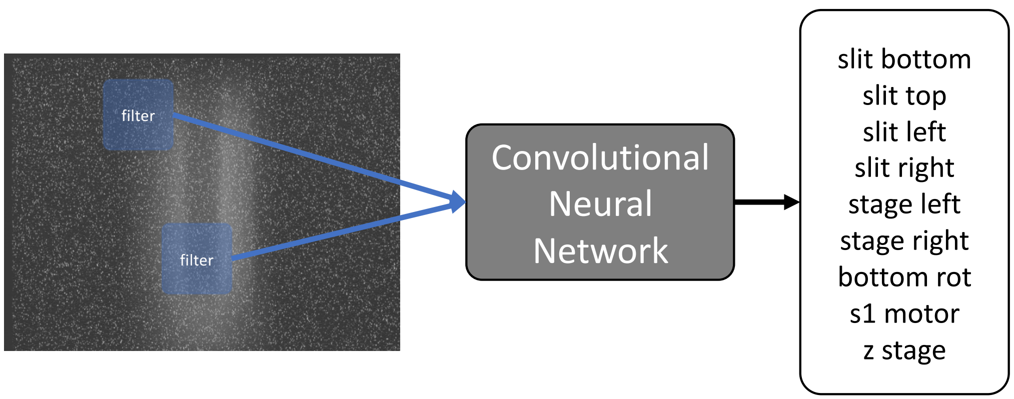


HB2A surrogate model

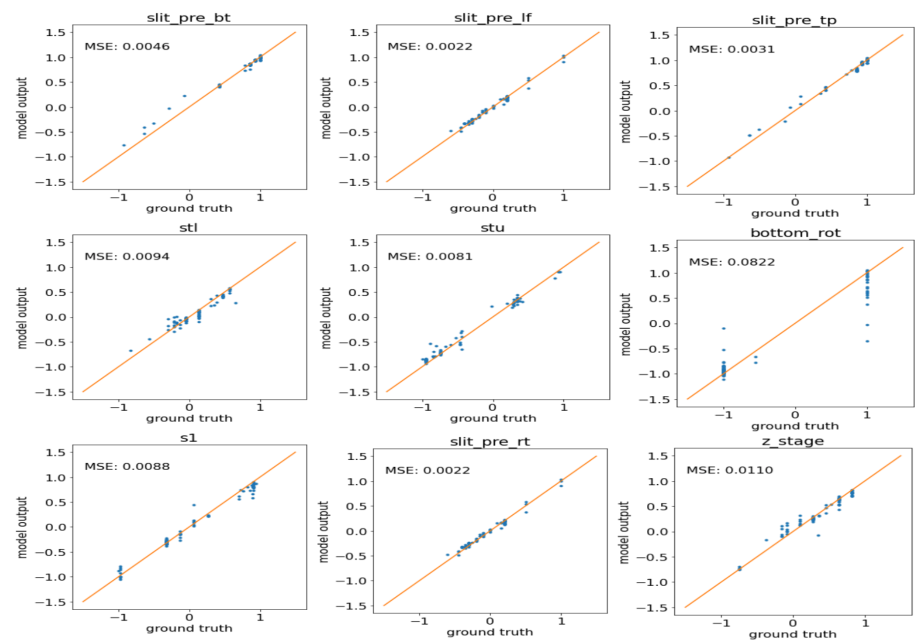




Left: Training an validation loss function at each epoch. Right: the coefficient of determination R^2 for each of the 9 motor parameters

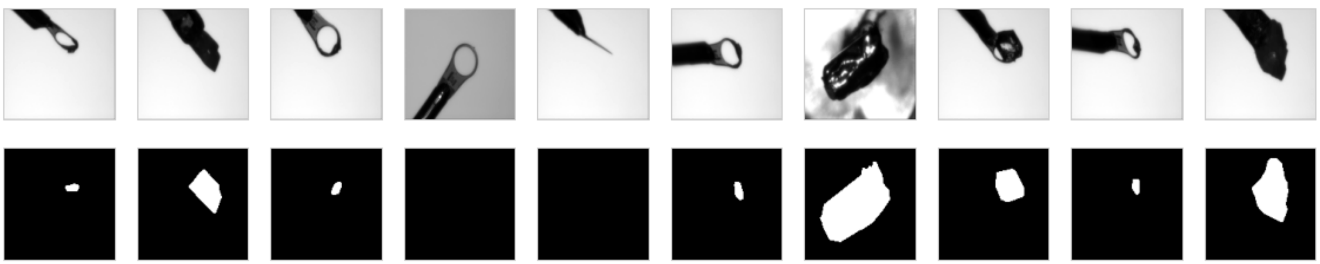


Test of the CNN surrogate performance in the test dataset. Each plot title corresponds to a different instrument motor that can control sample position and beam size. On the x-axis we have the data from the experiment, y-axis represents the model prediction.

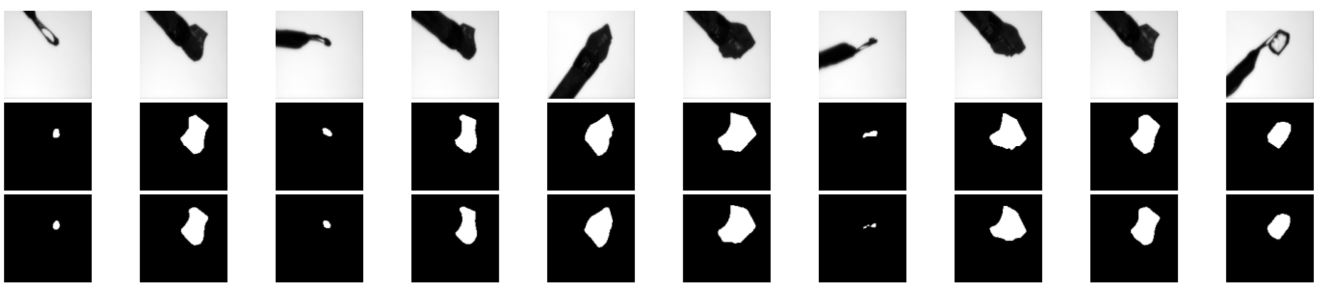


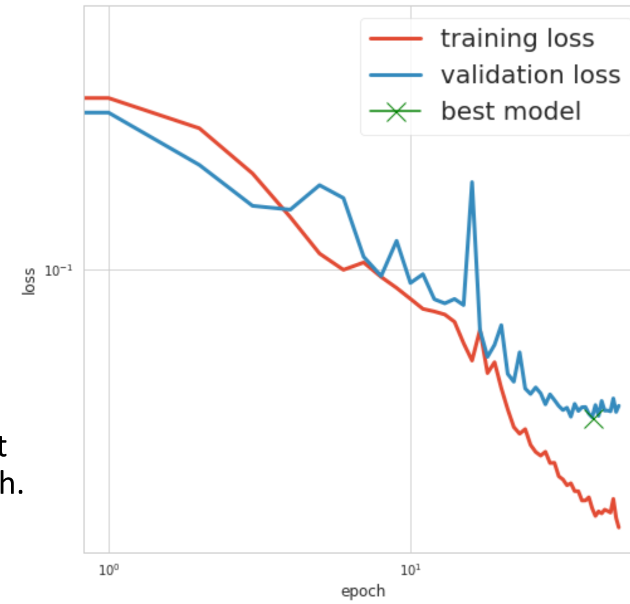
U-Net Predictions of Sample

Examples images obtained from the experiment. The lower plots show binary image masks created around the sample. For images with no sample the mask is empty.



Test model performance for some random images in the test dataset. Top row are the test image (ground truth), middle row: the test image label, and bottom row are the predicted test binary by the U-net algorithm. The predicted test image is visually identical to the ground truth.





Learning curve. Training and validation loss at each epoch