

## Tips for training

1. Prepare simulation datasets, e.g. for STO 13.6mrad PACBED, simulate 1-120 nm, tilt 0-4 mrad.
2. Run code **main\_PACBED\_XXX\_dataprep\_XXX.m** to generate big training datasets for neural network training. Note that code modification is typically needed for specific application.
3. Above code will dump image sum output files, run **main\_get\_image\_sum.m** to generate mean image used for the training.
4. Replace **ImageDatastore.m** and **Trainer.m** in Matlab folders with the modified code provided in **/Func** folder, remove underline first. The m file is specifically for Matlab2017a version.  
Target folder copy to (**ImageDatastore.m**): .../MATLAB\_R2017a/toolbox/matlab/datastoreio/+matlab/+io/+datastore/@ImageDatastore/ImageDatastore.m  
Target folder copy to (**Trainer.m**): .../MATLAB\_R2017a/toolbox/nnet/cnn/+nnet/+internal/+cnn/Trainer.m
5. For shift and rotation CNN training, comment on the random rotate code portion (line 399-410) in the modified **ImageDatastore.m**.
6. Setup parameters in **main\_PACBED\_XXX\_transfer\_training\_XXX.m**, run code, answer questions and input filename of averaged image as request.
7. The network training may takes hours to finish. Beware of cooling and UPS backup. Intermediate result will be dumped after each epoch is done.

Workstation used to generate data and train PACBED neural networks:

1. Titan X Pascal
2. i7-6800K with 128GB DDR4 memory
3. 3TB SSD drive

If you find this software package is useful, please cite:

Weizong Xu, James M. LeBeau, A Deep Convolutional Neural Network to Analyze Position Averaged Convergent Beam Electron Diffraction Patterns, arXiv: 1708.00855, 2017.

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