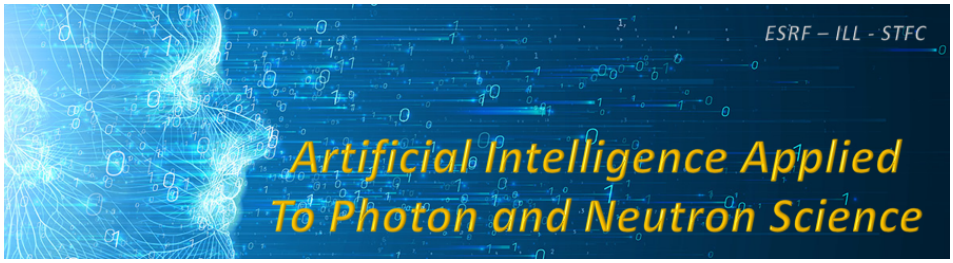

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Deep learning for classifying and sorting diffraction images

Wednesday, 13 November 2019 11:50 (25 minutes)

Intense pulses from free-electron lasers and high-harmonic-generation sources enable diffractive imaging of individual nanoparticles in free-flight with a single short-wavelength laser shot. The size of the data sets necessary for successful structure determination, often up to several million diffraction patterns, represents a significant problem for data analysis. Usually, hand-made algorithms are developed to approximate particular features within the data with the goal to reduce the dataset size and to filter out irrelevant images, but such approaches do not generalize well to other datasets and are very time-consuming.

Recently, we have shown in [1,2] that deep neural networks can be used to classify large amounts of diffraction data if a smaller subset of the data is labeled by a researcher and used for the training of the network. We found that deep neural networks significantly outperform previous attempts for sorting and classifying complex diffraction patterns and can improve post-processing of large amounts of experimental coherent diffraction imaging data.

Going beyond this approach, we here present first results using unsupervised deep neural networks. A combination of training a variant of the variational auto-encoder factorVAE [3] and a traditional clustering algorithm, namely Hierarchical Density-Based Spatial Clustering of Applications with Noise [4] are utilized. This approach allows us to find characteristic classes of patterns within a data set without any a priori knowledge about the recorded data. Our ultimate goal is to reduce the amount of time, a researcher has to spend on sorting and classifying datasets, to an absolute minimum. Our unsupervised approach will play very well as a pre-sorting step with our already published supervised routine. Datasets with several hundreds of GByte should be sortable and classifiable within few days time instead of multiple weeks. In addition, the unsupervised routine is applicable to online-analysis during experiments. A trained VAE can pre-sort diffraction images while recoding them, making it a valuable asset during experiments.

[1] Zimmermann et al. Phys. Rev. E 99, 063309 (2019)
[2] Langbehn et al. Phys. Rev. Lett. 121, 255301 (2018)
[3] Kim, H. & Mnih, A. arXiv:1802.05983 (2018)
[4] McInnes L, Healy J. (ICDMW), IEEE, pp 33-42. 2017

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