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Deep Neural Networks for XFEL pulse monitoring through emission spectra

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With the high brilliance and ultrashort pulses of X-ray Free Electron Lasers, Serial Femtosecond Crystallography (SFX) achieved atomic-resolution for micro and nano protein crystals. Throughout the data collection the beam is prone to fluctuations caused by the self-amplified spontaneous emission process which generates the beam and is intrinsically a stochastic phenomenon. These fluctuations affect photon energy, pulse duration, and intensity of the beam. Although monitoring tools exist to track the beam, uncertainties in each SFX measurement always remain, due to unknowns such as beam focus and sample position, which are critical but hard to estimate. Using X-ray emission spectroscopy alongside deep neural networks (DNNs) we can estimate beam parameters from emission spectra. By training our model on plasma simulations from a protein crystal, we aim to predict photon energies ranging from 6 to 12 keV, fluences from 5*102 to 5*105 J/cm2 , and pulse durations from 3 to 30 fs. By calculating the saliency maps from the spectras in our test dataset we aim to identify spectral regions most informative to the DNN model, which might allow us to better interpret the model's output and validate its performance for future real time monitoring on experimental data.

Primary authors: AGELII, Harald (Uppsala University); BELLISARIO, Alfredo (Uppsala University); CALEMAN, Carl (Uppsala University; Center for Free-Electron Laser Science CFEL); TIMNEANU, Nicusor (Uppsala University); CARDOCH, Sebastian (Uppsala University)

Presenter: BELLISARIO, Alfredo (Uppsala University)

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