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Recommendation system for small angle neutron scattering models based on machine learning from Monte Carlo virtual experiments

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We present a classification model consisting of an ensemble of Convolution Neural Networks (CNNs) to recommend the small angle scattering (SAS) model from the inspection of two-dimensional images generated by the position sensitive detector in small angle neutron scattering experiments. This recommendation system ranks the highest scores in the SoftMax layer of the ensemble and can provide 5 models with an accuracy of 99% that the correct model is found between the selected ones. We describe the training procedure on 260.000 images generated by means of Monte Carlo simulations. This database was generated from virtual experiments of the KWS-1 instrument at FRM-II, Garching, in Germany, in which the instrument configuration was varied between 12 setups and the SAS model of the sample was varied between 46 different models (database available in Zenodo). We also interpret the results obtained by means of explainable Artificial intelligence algorithms and discuss the possibilities of using generative adversarial networks to bring experimental features into simulated data.

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Sitzung Einordnung: Mounting Posters, Beer and light Dinner

Track Klassifizierung: Instrumentation & Data Management