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Machine Learning for automatic selection of a nanoparticle analytical model for Small Angle X-Ray Scattering data analysis

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Small-angle X-ray scattering (SAXS) is widely used to analyse the shape and size of nanoparticles in solution. A multitude of models describing the SAXS intensity resulting from nanoparticles of various shapes have been developed by the scientific community and are used for data analysis. Choosing the optimal model is a crucial step in data analysis that can be difficult and time-consuming. We propose an algorithm based on machine learning which instantly selects the best model to describe SAXS data. The different algorithms compared are trained and evaluated on a simulated database, consisting of 90,000 scattering spectra from 9 nanoparticle models, that realistically simulates various instrumental configurations.

Deploying a universal solution for automatic nanoparticle model selection is a challenge that raises a number of issues. The diversity of SAXS instruments and their flexibility means that the algorithm must be robust to unseen instrument configurations or to high noise levels. We highlight the poor transferability of classification rules learned on one instrumental configuration to another configuration. We show that training on several instrumental configurations makes it possible to generalise the algorithm, with no degradation in performance compared with configuration-specific training.
Our classification algorithm is then validated on a real data set obtained by performing SAXS experiments on nanoparticles for each of the instrumental configurations, which have been characterised by transmission electron microscopy. Although this data set is very limited, it allows us to estimate the transferability of the classification rules learned from simulated data to real data.
Finally, the use of deep learning automatically leading to poor explainability of results, the issue of user confidence is raised. Thus, there is a need for safeguards to guarantee the detection of outliers data and bad predictions. We propose a method based on deep contrastive learning to implement a prediction confidence indicator and an outlier data detector.

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