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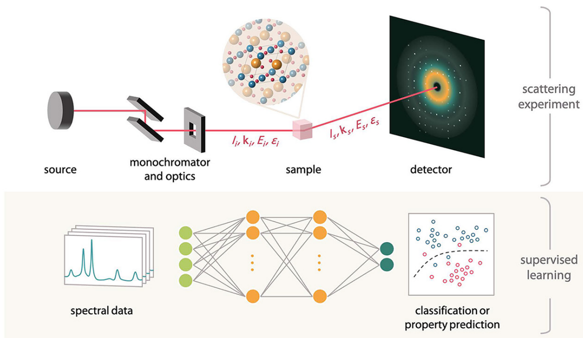
Increasingly, researchers are applying machine learning techniques to scattering experiments to extract useful information from noisy, high-dimensional data.



Neutron and X-ray scattering are techniques to measure the structural and dynamical properties of materials. One limitation in the field is that scattering data tends to be noisy and high-dimensional, meaning researchers must spend a significant amount of time – often months – buried in analysis.

“Scattering experiments have a time constraint called ‘beamtime,’ meaning that each researcher gets roughly one week to do measurements, since there are more users than resources available,” said author Mingda Li. “So we have to plan everything wisely during the week, and noise becomes a natural consequence.”

In a review, Chen et al. discuss how machine learning is a promising and powerful tool to gain new knowledge and physical insights from neutron and X-ray scattering data. In recent years, machine learning has been increasingly applied by researchers to overcome the barriers of limited beamtime and potential bias from conventional analysis.

While machine learning has the potential to advance the collection, analysis and interpretation of data, the most dominant application thus far has been to solve the inverse scattering problem. Training machine learning models using large-scale simulations addresses this bottleneck and leads to greater efficiency in terms of analysis.

In addition, the authors note that machine learning is easier to implement within some sub-classes of scattering techniques compared to others, which may lack reliable training data.

“X-ray absorption and small-angle scattering are relatively straightforward since they have analytical fitting models used to generate massive amount of training data, while for defect structure and quantum materials, there are still many open problems,” said Li. “The most important step is to clarify what are the key issues that should be solved for each type of scattering.”

Source: “Machine learning on neutron and x-ray scattering and spectroscopies,” by Zhantao Chen, Nina Andrejevic, Nathan C. Drucker, Thanh Nguyen, R. Patrick Xian, Tess Smidt, Yao Wang, Ralph Ernstorfer, Alan Tennant, Maria Chan, and Mingda Li, *Chemical Physics Reviews* (2021). The article can be accessed at http://doi.org/10.1063/5.0049111.

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