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Physics-informed input representations for SANS patterns classification

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Small Angle Neutron Scattering (SANS) is a vital technique for probing the structural properties of materials at the nanoscale. This makes it indispensable for studying nanometer-sized physical systems. Traditionally, SANS data analysis relies on mathematical models, but the advent of Machine Learning has offered new tools for data analysis. Recent work (Robledo, et al., 2024) shows that Convolutional Neural Networks (CNNs) can predict material structure from 2D SANS images with high accuracy across diverse datasets.

However, the computational cost and extensive data requirements of deep learning models pose challenges, particularly when dealing with smaller datasets. To address this, we propose a physics-informed input representation utilizing the Fourier transform in polar coordinates, which aligns naturally with the circular symmetry often observed in isotropic materials.

Our results, based on synthetic SANS patterns, show that this input representation can be effectively classified with a simpler shallow neural network, achieving performance comparable to deep CNNs. Moreover, when applied to CNNs, the physics-informed input encoding further enhances model accuracy. We evaluate the network's performance with real experimental data, exploring the robustness of our method.

In conclusion, we develop a more efficient data analysis procedure that incorporates domain-specific knowledge and facilitates faster and more robust SANS model recommendations for smaller datasets.

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