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Automated Selection for Physical Models of Small-Angle Neutron Scattering

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To characterize the structures and properties of samples in the analysis of experimental data of Small-Angle Neutron Scattering (SANS), a physical model must be selected corresponding to each sample for iterative fitting. However, the conventional method of model selection is primarily based on manual experience, which has a high threshold for analysis and low accuracy. Furthermore, the automated selection of physical models based on standard neural networks face challenges such as the lack of local image features, large intra-class differences, and small inter-class differences. This paper proposes a Bimodal Feature Fusion Convolutional Neural Network (BFF-CNN) model to mitigate these issues. Initially, a physically informed Fourier-Bessel Transform (FBT) is deployed to extract global structural information from scattering images. Then, the original and FBT-transformed images are fed into two subnetworks for feature extraction and fusion, enhancing the overall feature representation capability of the neural network. A Restricted Softmax (R-Softmax) loss function is implemented, adding a penalty term to the original Softmax loss function for limiting the probability of input samples being assigned to incorrect classes. This alleviates the vanishing gradient problem when the Softmax loss approaches zero, thereby improving the convergence speed. Experimental results obtained using a self-built SANS image dataset show that the BFF-CNN significantly improves the prediction accuracy and average recall as compared to models such as the Residual Network (ResNet)-18 and PMG. Using the joint learning strategy of R-Softmax and center loss functions, the prediction accuracy and recall has improved by 5.4 and 10.5 percentage points, respectively, as compared to the case using only the Softmax loss function, demonstrating good classification performance for SANS data.

Significance

The proposed method can recommend physics-based models for small-angle neutron scattering (SANS) data fitting, significantly improving analysis efficiency, lowering technical barriers, and shortening experimental cycles

References

Experiment context, if any

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