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Deep Learning-Driven GISAXS Data Processing for Nanostructure Characterization

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Grazing-incidence small-angle X-ray scattering (GISAXS) has emerged as a uniquely powerful technique for elucidating surface and near-surface morphologies over length scales from roughly 1 nm to 1 µm. Yet, extracting quantitative structural parameters from GISAXS data requires solving an inverse problem: one must assume a structural model, simulate its scattering response, and iteratively refine model parameters through curve-fitting routines. This process can extend over hours or days per dataset, demands expert intuition to select and constrain models, and may converge to local minima, limiting throughput and reproducibility.

Recent developments in machine learning (ML) and deep neural networks present a promising alternative, capable of learning direct mappings between observed scattering patterns and underlying structural descriptors without explicit model fitting. In domains such as X-ray crystallography phase retrieval and transmission small-angle scattering, ML has demonstrated rapid classification, denoising, and parameter extraction capabilities. However, applications to two-dimensional GISAXS inversion are still in its infancy. A major enabling factor in GISAXS lies in the ability to generate large, labeled training datasets via forward simulations based on first-principles physics. By sampling broad parameter spaces of particle geometries, interparticle spacings, disorder metrics, and experimental artifacts, one can train supervised learning models to generalize to real experimental data, potentially delivering real-time analysis.

Here, we present a dual-branch convolutional neural network (CNN) framework designed to fully automate GISAXS data inversion, simultaneously retrieving (1) the particle size distribution, as a discretized probability density function representing particle dimensions (form factor), and (2) interparticle correlation parameters, namely average center-to-center distance and positional disorder (structure factor). Our approach integrates physics-based simulation, data preprocessing, and modern deep learning architectures to achieve millisecond-scale inference on standard computing hardware.

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