

Machine Learning for Inverse Problems in Scattering Physics

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Machine learning (ML) is increasingly being applied to data analysis and discovery in scattering physics, but the lack of standardized tools and frameworks presents ongoing challenges [1]. This talk will explore the current landscape of ML in scattering, focusing primarily on the inverse problem, which is at the core of data analysis and data-driven discovery. I will showcase different approaches to the inverse problem for several experimental techniques, including X-ray and neutron reflectometry [2–5] and grazing-incidence wide-angle X-ray scattering (GIWAXS) [6–8]. I will discuss how advances in computational power, efficient simulations, and modern probabilistic machine learning tools [9, 10] reshape our approach to data analysis [2, 11] and enable novel types of experiments [12]. The particular focus is on approximate Bayesian and post-Bayesian methods that provide an efficient and reliable framework for fast analysis of various scattering techniques.

After the development of electron-spin resonance (ESR) in a scanning tunneling microscope in 2015 [1] a myriad of potential applications appeared, exploiting the extremely high spatial resolution of the STM and high energy resolution of ESR.

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