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Projected Regression Methods for Inverting Fredholm Integrals: Formalism and Application to Analytical Continuation LOUIS-FRANCOIS ARSENAULT, RICHARD NEUBERG, LAUREN A. HANNAH, ANDREW J. MIL-LIS, Columbia Univ — We present a machine learning-based statistical regression approach to the inversion of Fredholm integrals of the first kind by studying an important example for the quantum materials community, the analytical continuation problem of quantum many-body physics. It involves reconstructing the frequency dependence of physical excitation spectra from data obtained at specific points in the complex frequency plane. The approach provides a natural regularization in cases where the inverse of the Fredholm kernel is ill-conditioned and yields robust error metrics. The stability of the forward problem permits the construction of a large database of input-output pairs. Machine learning methods applied to this database generate approximate solutions which are projected onto the subspace of functions satisfying relevant constraints. We show that for low input noise the method performs as well or better than Maximum Entropy (MaxEnt) under standard error metrics, and is substantially more robust to noise. We expect the methodology to be similarly effective for any problem involving a formally ill-conditioned inversion, provided that the forward problem can be efficiently solved.

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