Automatic Fitting Of Gaussian Peaks Using Abductive Machine Learning

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Summary

Analytical techniques have been used for many years for fitting Gaussian peaks in nuclear spectroscopy. However, the complexity of the approach warrants looking for machine-learning alternatives where intensive computations are required only once (during training), while actual analysis on individual spectra is greatly simplified and quickened. This should allow the use of simple portable systems for fast and automated analysis of large numbers of spectra, particularly in situations where accuracy may be traded for speed and simplicity. This paper proposes the use of abductive networks machine learning for this purpose. The Abductory Induction Mechanism (AIM) tool was used to build models for analyzing both single and double Gaussian peaks in the presence of noise depicting statistical uncertainties in collected spectra. AIM networks were synthesized by training on 1000 representative simulated spectra and evaluated on 500 new spectra. A classifier network determines the multiplicity of single/double peaks with an accuracy of 5.8%. With statistical uncertainties corresponding to a peak count of 100, average percentage absolute errors for the height, position, and width of single peaks are 4.9, 2.9, and 4.2%, respectively. For double peaks, these average errors are within 7.0, 3.1, and 5.9%, respectively. Models have been developed which account for the effect of a linear background on a single peak. Performance is compared with a neural network application and with an analytical curve-fitting routine, and the new technique is applied to actual data of an alpha spectrum.

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