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Automated machine learning spectrum unfolding for neutron spectrometry with Bonner spheres

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The unfolding of neutron spectra from Bonner multi-sphere spectrometer (BSS) measurements is an important task in radiation dosimetry. This study investigates the application of an Automated Machine Learning (AutoML) framework for neutron spectrum unfolding. To train and validate the model, a dataset of 5×10^5 synthetic spectra was generated as weighted combinations of four spectral components: thermal, epithermal, fast and high energy. The performance of the developed algorithm was evaluated using a database of 340 experimentally measured spectra. The model was trained and tested on the JINR Multifunctional Information and Computing Complex. The LightAutoML and FEDOT frameworks were used to optimize the model through hyperparameter tuning and ensemble blending of multiple machine learning algorithms, including: L2-regularized linear regression, LightGBM, CatBoost and Random Forest. AutoML results were compared with the developed neural network model. Two spectra representation methods were evaluated: spectra discretization over the energy grid and Legendre polynomial expansion. The uncertainty in spectrum unfolding was estimated using a Monte Carlo approach, where random perturbations were introduced into the input data. To assess the unfolding quality, the following metrics were analyzed: Spearman and Pearson correlation coefficients, cosine similarity, cross-entropy, Wasserstein distance, Kullback–Leibler divergence, maximum mean discrepancy and coefficient of determination (R^2). Based on the developed algorithm, a prototype web application was designed to facilitate spectrum unfolding in practical applications. The research was carried out within the state assignment of Ministry of Science and Higher Education of the Russian Federation (theme No. 124112200072-2).

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