A Maximum Log-Likelihood Regression Approach for Quantitative Mixture Prediction in PGNAA Spectroscopy

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Scrap recycling is a vital source of sustainable raw materials, yet real-time analysis of heterogeneous metal flows remains a significant challenge. While Prompt Gamma Neutron Activation Analysis (PGNAA) offers a non-destructive method for elemental analysis, traditional categorical classification models are limited by their inability to resolve intermediate material compositions. In this work, we present a novel regression-based approach for PGNAA spectroscopy that enables, for the first time, the quantitative determination of arbitrary mixture ratios in metal alloys.

Our framework utilizes a probability-distribution-based sampling method to generate synthetic datasets from reference long-term spectra. These mixtures are modeled as linear combinations of reference alloys, defined by a single mixing parameter λ. We employ a Maximum Log-Likelihood method to estimate λ from noisy, short-term measurements.

The results demonstrate high prediction accuracy despite the inherent statistical noise of rapid acquisition times. At a measurement time of only 1.5 s, 98% of the predictions for Aluminium-copper mixtures deviate by less than 2% from the true fraction. Furthermore, the approach proves robust across various alloy combinations, maintaining a median prediction close to the preset fraction. This work represents an important step toward precise, non-destructive online analysis of heterogeneous metal flows and provides a technical foundation for future real-time monitoring of alloy compositions.