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

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Introduction

- Recycling is becoming increasingly important for environmental, economic, and political reasons.
- We use Prompt Gamma Neutron Activation Analysis (PGNAA) with a High Purity Germanium (HPGe) detector for non-destructive spectral analysis.
- We propose a regression-based approach using Maximum Log-Likelihood estimation to determine continuous alloy mixing ratios from short-time ($\sim 1\,s$) measurements with low counting statistics.

Method

Generating material mixtures

We use long-time (>2 h) measurements of copper and aluminium and simulate mixtures as linear combinations of reference spectra, preserving statistical properties:

$$\mathrm{Mix}(\lambda) = \lambda \mathrm{Cu} + (1-\lambda)\mathrm{Al}, \quad \lambda \in [0,1]$$

Data generation

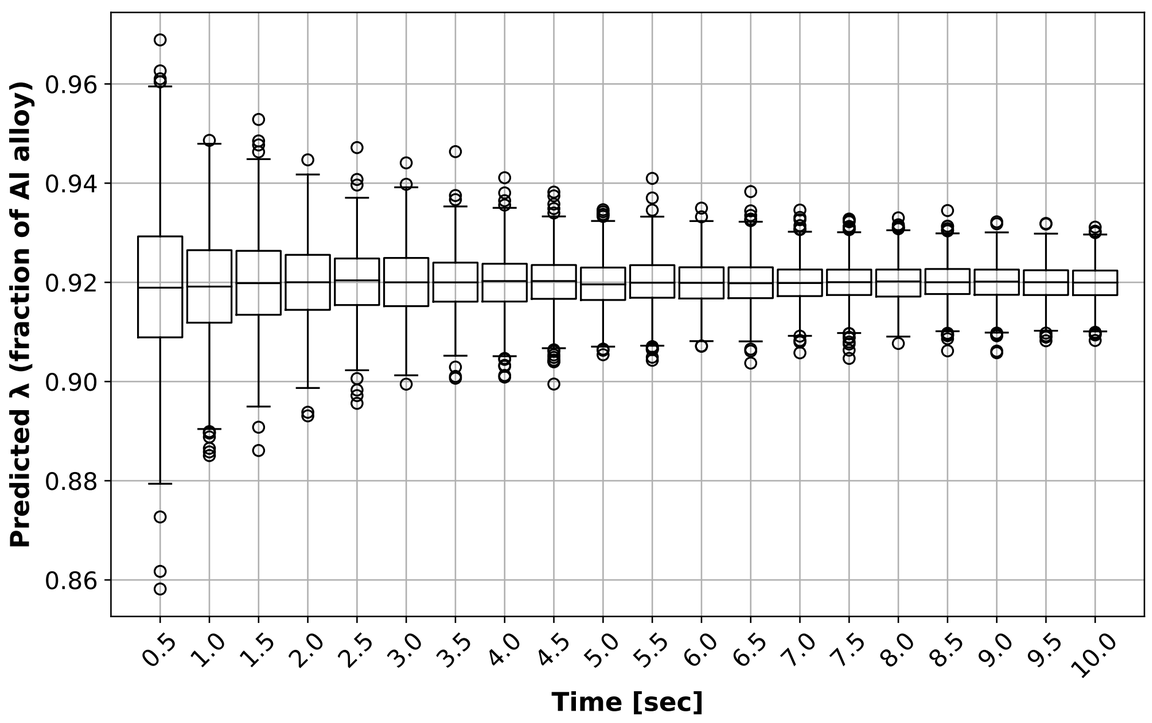
Apply $L1$ normalization to the reference spectrum and sample short-time measurements (e.g., 1 s) from the resulting distribution.

Data classification

The maximum log-likelihood method assigns the short-time measurement to the most fitting distribution of a fully measured spectrum. The parameter λ from the short-time measurement s is estimated by maximizing the log-likelihood function:

$$\arg\max_{\lambda\in[0,1]} \ell(\lambda) = \arg\max_{\lambda\in[0,1]} \log p(s \mid \mathrm{Mix}(\lambda))$$

Result



Predicted aluminium alloy fraction for simulated short-time Al–Cu mixtures ($\lambda = 0.92$). Boxplots show 1000 predictions per acquisition time, with increasing accuracy for longer measurements.

Conclusion

- A regression-based PGNAA framework using Maximum Log-Likelihood estimation enables online quantitative determination of continuous alloy mixture ratios.
- Reliable predictions are achieved despite high noise levels in short-time measurements, with 98 % of predictions deviating by less than 2 % at a $1.5\,s$ acquisition time.
- The method provides a foundation for precise, non-destructive real-time monitoring of heterogeneous metal flows in alloy recycling.

FRN

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