Machine Learning to Quantify XRF Measurements

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In X-ray fluorescence (XRF), a sample is excited with X-rays, and the resulting characteristic radiation is detected to detect elements quantitatively and qualitatively. Quantification is traditionally done in several steps:

1. Normalization of the data
2. Determination of the existing elements
3. Fit of the measured spectrum
4. Calculation of concentrations with fundamental parameters / MC simulations / standard based

The problem with standard based procedures is the availability of corresponding standards. The problem with the calculations is that the measured intensities for XRF measurements are matrix-dependent. Calculations must, therefore, be performed iteratively (= time consuming) in order to determine the chemical composition.

First experiments with gold samples have shown the feasibility of machine learning based quantification in principle. A large number of compositions were simulated (> 10000) and analyzed with a deep learning network. For first experiments, an ANN (Artificial Neural Network) with 3 hidden layers and 33x33x33 neurons was used. This network learned the mapping of spectra to concentrations using supervised learning by multidimensional regression. The input layer was formed by the normalized spectrum, and the output layer directly yielded the searched values. The applicability for real samples was shown by measurements on certified reference materials.

The results and a comparison with genetic algorithm driven quantification will be discussed.

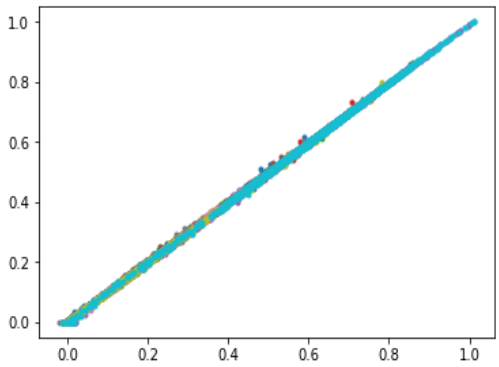

Fig.1: Nominal and actual normalized values for Au, Ag, Ni, Cu and Zn in a gold alloy (MC simulation).