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Research Article

Gas Chromatography Data Classification Based on Complex Coefficients of an Autoregressive Model

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Abstract
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Abstract

This paper introduces autoregressive (AR) modeling as a novel method to classify outputs from gas chromatography (GC). The inverse Fourier transformation was applied to the original sensor data, and then an AR model was applied to transform data to generate AR model complex coefficients. This series of coefficients effectively contains a compressed version of all of the information in the original GC signal output. We applied this method to chromatograms resulting from proliferating bacteria species grown in culture. Three types of neural networks were used to classify the AR coefficients: backward propagating neural network (BPNN), radial basis function-principal component analysis (RBF-PCA) approach, and radial basis function-partial least squares regression (RBF-PLSR) approach. This exploratory study demonstrates the feasibility of using complex root coefficient patterns to distinguish various classes of experimental data, such as those from the different bacteria species. This cognition approach also proved to be robust and potentially useful for freeing us from time alignment of GC signals.