D20 Soft Classification by Combined Target Factor Analysis and Bayesian Decision Theory

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The goal of this presentation is to inform attendees of a new chemometric soft classification method that can be applied to forensic problems.

This presentation will impact the forensic science community by providing information on a soft classification method that is designed to work in the presence of unspecified background interferences and provide the user with probabilities of correct class assignment.

There are analytical problems in forensic science where individualization is not currently possible; however, the analyst may benefit from assigning an analyte to one or more possible classes. This is especially true for mass produced items that do not involve DNA analysis. When analysis of the item of interest is free from significant background interference, existing classification methods (i.e., linear discriminant analysis, partial least squares discriminant analysis, etc.) may be applicable. However, when there is significant background interference, classical discriminant analysis methods may fail, especially when the background signature is unspecified and possibly unknown. Fire debris analysis is one example of this type of problem. The analyst's goal is to determine if ignitable liquid residue is present and, if so, assign the residue to a class under the American Society of Testing and Materials (ASTM) Standard Method E1618.[1] Pyrolysis product contributions may be large and by coincidence, some pyrolysis products may be the same as ignitable liquid components. In these cases, visual pattern recognition will become more challenging as the ignitable liquid signature decreases and the background signature increases. A new method of addressing this problem is examined by combining Bayesian soft classification with target factor analysis (TFA). The method will be described and test results from the analysis of fire debris data will be presented.

The method relies on analysis of the average mass spectrum across the chromatographic profile (i.e., the total ion spectrum, TIS) from multiple samples collected from a single fire scene.[2] The multiple TIS are concatenated into a single data matrix and subjected to abstract factor analysis, and target factor rotation. TIS from reference ignitable liquids with assigned ASTM classifications are used as the target factors in TFA. Class-conditional distributions of the correlations between the target and predicted TIS spectra for each ASTM class are represented by kernel functions and analyzed by Bayesian decision theory.[3] The soft classification approach assists in assessing the probability that ignitable liquid residue from a specific ASTM E1618 class is present in a set of samples from a single fire scene, even in the presence of unspecified background contributions from pyrolysis products.[3,4]

The method was tested on: (1) computationally generated data sets; (2) small-scale laboratory burn experiments; and, (3) large-scale experimental burns. In all cases, the correct classification rates exceeded 80%. The method and results will be discussed along with the potential for expanding the method to other forensic applications.

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Fire Debris, Soft Classification, Factor Analysis

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