B151 Comparisons of Multivariate Preprocessing for Forensic Discrimination of Fibers by UV/Visible Microspectrophotometry

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The goal of this presentation is to present research studies to validate the forensic comparison advantages of first derivative preprocessing for comparison of Ultraviolet/Visible (UV/Vis) spectra of fibers. The effects of first derivative processing will be demonstrated with clear examples of improved discrimination between selected fibers and by improved classification accuracies using multivariate statistics.

This presentation will impact the forensic science community by illustrating how performing multivariate statistics on derivative spectra can improve discrimination of cotton fibers over other methods of spectral preprocessing for forensic comparisons. Significant increases in discrimination of fibers with mostly flat spectra with small changes in absorbance are possible using derivative spectra. Direct-dyed cotton fibers are one class of fibers that would seemingly benefit significantly from utilizing derivative spectra since these fibers tend to have distinctively low changes in absorbance. Although no single method of preprocessing is best for all types of spectra, the analyst must show caution when selecting cases in which derivatives should be used.

Determining which analytical method will have the highest discrimination power for trace evidence examinations is important to forensic laboratories in terms of allocation of time and resources. The importance of statistical methods for evaluation of trace evidence analysis in forensic science has also been of recent focus.[1]

Color plays a critical role when analyzing natural fibers such as cotton in forensic investigations. UV/Vis Microspectrophotometry (MSP) is a non-destructive technique capable of providing objective color measurements on fibers in the form of absorption or transmission spectra; however, forensic fiber examinations can be hindered by spectra with little detail or points of comparison. Wiggins originally suggested that derivative preprocessing can enhance comparisons in UV/Vis spectra regard of cotton fibers.[2,3] Although derivative preprocessing has been used for many years in analytical chemistry for the various applications described, it has not been widely utilized in forensic applications.[3,4]

To validate this suggestion, multivariate classification on spectra of reactive, direct, and vat-dyed cotton fibers has been performed. These spectra were preprocessed using multiple methods including baseline correction, normalization, and first and second derivatives. Principal Component Analysis (PCA) followed by linear discriminant analysis (LDA) was employed to estimate classification accuracy.[5] Direct-dyed fibers exhibited almost featureless and low-absorbing spectra compared to those of reactive and vat-dyed fibers. As a result, classification accuracies for direct-dyed fibers were lower than those calculated for reactive and vat-dyed fibers. The results of this study show that derivative spectra can significantly enhance classification accuracy when analyzing spectra with only subtle features such as those seen with direct-dyed cotton fibers. No single method was best for all classes of fibers in the study and the shapes and intensities of the curves are important when determining if derivative calculations are auspicious.

The generality of this conclusion was confirmed using UV/Vis spectra from more than 400 dyed textile samples of cotton, acrylic, nylon 6,6, and polyester. All spectra were subjected to first derivative preprocessing and classified using PCA/LDA. Leave-one-out cross validation was used to test the discrimination of fiber spectra in each color and polymer group. The high discriminating power of UV/Vis spectra for fibers was further validated by correct classification for 89.50% with this diverse group of spectra from four different textile classes.

References:

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