

A117 Examination of Statistical Methods for Analysis of Highly Similar Absorbance Spectra From Textile Fibers

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The goal of this presentation is to report on the evaluation of statistical methods for comparison of textile fibers with highly similar UV-visible absorption profiles.

This presentation will impact the forensic science community by providing information on the use of standard statistical techniques for performing comparison of highly similar microspectrophotometry data from textile fibers.

Discriminating clearly dissimilar absorbance spectra from questioned and known sources is straightforward; however, analyzing two fibers with nearly identical absorbance profiles can prove challenging. The goal of this research is to apply established statistical tests to highly similar absorbance spectra with the intent of evaluating the spectral match at a defined significance level. The nonparametric permutation test, Hotelling's T² test and Student's ttest were examined. The Parametric tests were applied to reduced dimensionality data preprocessed by principal components analysis (PCA).

An outside company was contracted to dye two 10 gram swatches of spun nylon 6.6 fabric. One swatch was vat dyed with Acid Blue 25 (M1); the other with Acid Blue 41 (M2). Absorption measurements were collected over the range of 400-725 nm with a microspectrophotometer. Samples of M1 were taken from three different areas (A1, A3, and A5), corresponding to the top left corner, center, and bottom right corner, respectively. Three individual threads (T1 - T3) were cut from both the vertical (D1) and horizontal (D2) directions of M1 in each of the three areas for a total of eighteen threads. After cutting all threads to 1cm lengths, five individual fibers were pulled from each thread (F1 - F5). Fifteen measurements were collected along the length of a single fiber. The spectra along each fiber were collected sequentially, while the order in which each fiber was examined was determined by random numbers drawn from a uniform distribution.

Pairwise comparisons of all fibers from M1 were performed by the nonparametric permutation hypothesis test, returning 100 p-values for each pairwise comparison. An average of 87% of all pairwise comparisons resulted in discriminations at α =0.05. This approach is not dependent upon a normal distribution of the comparative figures of merit. In parametric tests, any deviation from the assumed distribution may shift the actual size of the Type I error; however, in contrast, the actual α level of the permutation test automatically holds because when the null is true, all test statistics are exchangeable, having the identical distribution.¹ The high percent discrimination of fibers from M1 raises questions regarding the sensitivity of the statistical test, given the intended purpose, and possible sources of uncontrolled error in the experiments.

The nonparametric permutation method results were compared with those from the parametric Hotelling's T² test and Student's t-test. PCA was performed on normalized spectra from A5 of M1 to reduce the dimensionality of the data. Typically, greater than 99% of the variance was contained in the first principal component (PC1) for all comparisons. The large fraction of the variance contained in PC1 demonstrates the high spectral similarity. Student's t-test performed on the scores from PC1 allowed accepting the null hypothesis (i.e., the spectra were not discriminated by the test) in all of the five pairwise comparisons at α = 0.05. Results from the Hotelling's T² test on scores from PC1 and PC2 accepted the null hypothesis in two out of five (40%) pairwise comparisons.

To further test the methods, samples from different materials M1 and M2 were analyzed. PCA of highly similar spectra from the two sources contained 98.6% of the variance in PC1 and 99.92% of the variance in PC1 and PC2. The Student's t-test on scores from PC1 accepted the null hypothesis at α =0.05 (i.e., two fibers containing different dyes with highly similar spectra were not differentiated), while the Hotelling's T² test on scores from both PC1 and PC2 rejected the null hypothesis at the same significance level.

Further studies are focused on defining a statistical approach that can be applied to casework samples while maintaining Type I and Type II errors at reasonable levels.

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Reference:

¹ McIntee E, Viglino E, Kumor S, Rinke C, Ni L, Sigman ME. Nonparametric permutation test for discrimination of float glass samples based on LIBS spectra." Journal of Chemometrics 2010;24:312-319.

Spectroscopy, Fiber Analysis, Hypothesis Testing