# PATTERN RECOGNITION METHODS FOR THE CLASSIFICATION OF TRACE EVIDENCE TEXTILE FIBERS FROM UV/VISIBLE AND FLUORESCENCE SPECTRA

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## Abstract

Identification of patterns in analytical chemical data and interpretation of observed differences is a frequent task for forensic chemists. A fiber examiner might perform UV/visible microspectrophotometry on known and questioned fibers to evaluate possible associations between source and location. Multivariate statistics enable confirmation of statistical validity of discrimination between different polymer classes and dyed textile fibers, visualization of significant differences between groups of spectra discrimination, and tracking of spectral changes with environmental changes. The fibers and associated spectra in the database, in combination with validated computer programs, represent an extensible tool for fiber comparisons in casework and should also be of value in quality control and training of analysts. In this paper, the application of linear discriminant analysis to a data base of over 5,000 UV/visible absorbance and fluorescence spectra is described.

## Introduction

Questioned and known fibers are often first compared using optical microscopy.[1,2] Polarized light microscopy (PLM)[3] or Fourier transform infrared spectroscopy[4] can be used to determine the generic fiber type (polyester, acrylic, nylon, cotton, *etc*.). These techniques are

nondestructive, maintain the integrity of the original sample, prevent sample contamination, minimize sample handling, and decrease overall analysis time. Visible, ultraviolet (UV)/visible, and fluorescence microspectrophotometry (MSP) also offers direct, relatively inexpensive, and informative means of characterizing dyed fibers. If spectra of the known and questioned fibers match, the hypothesis that the fibers originate from a common source should not be rejected.

UV/visible transmission microspectrophotometry has been used to study single cotton fibers dyed with vat dyes such as indigo and indigo derivatives.[5] Because dye(s) are often the major source of fluorescence on dyed fibers, fluorescence spectra present additional opportunities for fiber discrimination. Macrae et al.[6] reported an increase in discriminating power for fiber comparisons when using UV/fluorescence compared to using white light bright field comparison microscopy. Carroll[7] claims that differences in fluorescence are consistently correlated with the manufacturer, thus suggesting increased discrimination from the use of fluorescence measurements. Cantrell et al.[8] reported fluorescence microscopy of 3025 textile fibers collected from movie theater seats.

Discriminating power was introduced into discussions of trace evidence comparison in the late 1960's to early 1970's.[9-11] Given an analytical technique used to discriminate between two different groups of objects, what is the probability that two randomly chosen objects selected from a combined population will match one another? Discriminating power of a technique is often evaluated by comparing how well two items can be differentiated from one another compared to how well two objects might be expected to match by chance.[14] Roux et al.[12] calculated discriminating power as the ratio of the number of discriminated pairs of samples to the total number of possible pairs in a study on the evidential value of ballpoint pen inks.

Experimental variability in analytical results "limits the ability to differentiate samples that are, in fact, different and from different sources".[13] Multivariate statistics offers an interpretative methodology for discerning significant differences among patterns. Multivariate statistics have been applied to identification of homicides *vs*. suicides and the prediction of homicide/perpetrator relationships[14-16], forensic discrimination of automotive paint samples[17], copy toners[18,19], and counterfeit coins.[20] Additional applications include forensic discrimination of UV/visible spectra from soil[21], classification of prepaid cards by multivariate analysis of X-ray fluorescence data[22], modeling of color properties of a white pigment[23], sex determination by patella measurements[24], and discrimination of ball-point pen inks based on UV/visible spectra.[25] The present paper describes linear discriminant analysis (LDA) for evaluating discrimination of UV/visible absorbance and fluorescence MSP for analysis of textile fibers.

## Methods and Materials

Samples of commercially dyed cotton, polyester (polyethylene terephthalate), acrylics (at least 85 % acrylonitrile), and nylon 6,6 were obtained from commercial sources. Fibers of 11 different colors are included, with blue, brown, and green being the largest color groups. Micro tweezers and a razor blade were used to obtain single fibers from each piece of fabric. Samples were positioned on a microscope slide using micro tweezers. Spectral grade Permount® (Fisher Scientific, Fair Lawn, NJ) was used to mount fibers on glass slides with glass cover slips.

The collection of about 500 dyed textile fibers was used to generate a reference data set of 24,150 UV-visible absorbance spectra and fluorescence spectra for evaluating discrimination of different MSP approaches. Spectra were obtained using a Quantum Detection Instrument (QDI) 1000 MSP (CRAIC Technologies, Altadena, CA) using GRAMS/AI 7.00 software (Thermo

Galactic, Salem, NH). The MSP was operated in transmission (xenon source) and fluorescence (mercury source) modes using a 15× collecting objective. UV/visible spectra of textile fibers were produced by ratioing fiber spectra against a reference spectrum and taking an average of 100 scans over the spectral range of 200-850 nm at a bandwidth of 10 nm. The integration time for the charged coupled device detector was set to ~4 ms in transmission mode and to 200 ms in fluorescence mode. Fluorescence was produced using excitation wavelengths of 365, 405, 436, and 546 nm.

All data processing was performed on the spectra, saved as comma separated variable (CSV) files. Absorbance spectra were truncated to range from 330 nm (the lower UV/visible cut-off for use of Permount® on glass slides) to 850 nm. Fluorescence spectra were truncated at a lower wavelength cutoff appropriate for the excitation cube in use (390, 444, 470, and 581 nm for 365, 405, 436, and 546 nm excitation, respectively). The lowest intensity in all spectra set to zero by subtracting the lowest non-zero spectral intensity found in each spectrum. Each absorbance spectrum was normalized to reduce systematic variations (e.g., variations in dyeing) by dividing spectral intensities by the sum of spectral intensities across the spectrum; fluorescence spectra were not normalized. All data treatment (including PCA, LDA, and associated graphics) was performed using a program, *Fiber Spectrum Explorer*, written in *MatLab* (The MathWorks, Inc., Natick, MA).

## Results and Discussion

To use multivariate statistics, multiple replicate spectra must be obtained from each individual fiber. Replicate spectra assess experimental variability and facilitate detection of unrepresentative spectra. The 10 replicate spectra taken of each of 483 fibers for our study are a

minimally acceptable number for these purposes. LDA calculates the ratio of variation between the averages of replicate spectra for different fibers compared to the variation within groups of replicate spectra of the same fiber. The first source of variation is the signal the fiber examiner is trying to detect, i.e., whether the fibers have different spectral signatures; the second source is sampling and measurement uncertainty. If the ratio of between- to within-group variation is not larger than that which could have occurred by chance, differences between spectra can not be said to be real. LDA applied to forensic data is described by Morgan and Bartick.[26]

Brown fibers are one of the three largest color groups in our database. For this presentation, brown acrylic fibers (17 fibers) were selected as representative of this large group. Figure 1 shows the projections of the 170 spectra into the space of the first three canonical variates (or discriminant axes), displaying 89.5% of the between-to-within group variation in the data. The three-dimensional projection can be rotated, but it is not possible to find a view from which no overlap of groups is apparent. However, not all the systematic differences (between-to-within group variation) are seen in these two projections (more than 10% is not seen in Figure 5). Leave one-out cross validation[26] correctly classified 147 of the 170 spectra, for a classification accuracy of 86.47%. Classification results displaying the discriminating power of UV/visible MSP for the 17 groups of brown acrylic fibers are shown in the confusion matrix in Table 1.

Comparisons of classification accuracy for UV/visible and fluorescence MSP over about 500 fibers and 25,000 spectra are summarized in Table 2. Entries marked ‘x’ are sets for which LDA was not performed because of the small number of fiber groups. In columns for absorbance, and for fluorescence at each of the four excitation wavelengths, the number of correctly classified spectra (based on leave-one-out cross validation) is listed.

**Figure 1.** Projection of all brown acrylic absorbance spectra into the space of the first three canonical variates, displaying 89.5% of the between-to-within group variation in the spectra. A 95% confidence region is plotted around each group of ten replicate spectra for each of the 17 different fibers (numbered 1-17).

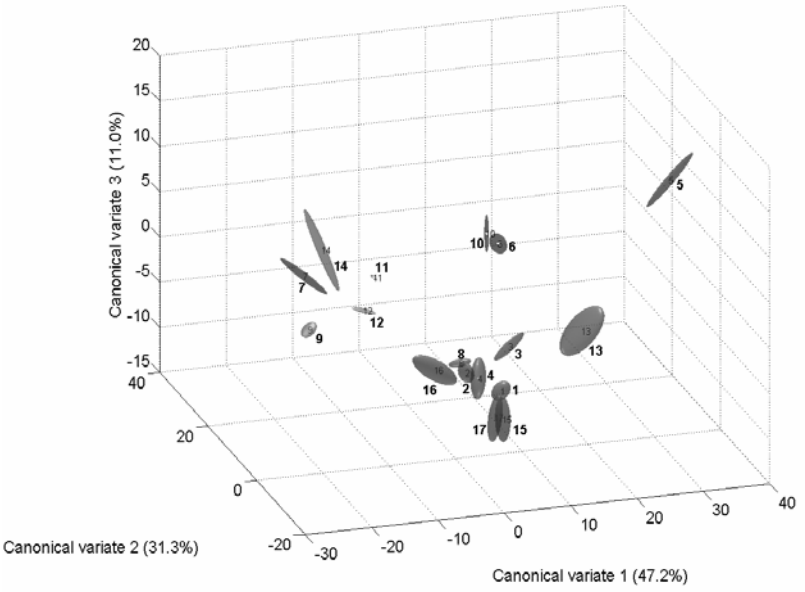


**Table 1.** Confusion matrix displaying the LDA leave-one-out cross-validated classification results for the brown acrylic fiber absorbance spectra.

| Group | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | Totals |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **1** | 7 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | **10** |
| **2** | 3 | 6 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | **10** |
| **3** | 0 | 0 | 10 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | **10** |
| **4** | 0 | 0 | 0 | 10 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | **10** |
| **5** | 0 | 0 | 0 | 0 | 9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | **10** |
| **6** | 0 | 0 | 0 | 0 | 0 | 10 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | **10** |
| **7** | 0 | 0 | 0 | 0 | 0 | 0 | 10 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | **10** |
| **8** | 1 | 5 | 0 | 0 | 0 | 0 | 0 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | **10** |
| **9** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | **10** |
| **10** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 10 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | **10** |
| **11** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 10 | 0 | 0 | 0 | 0 | 0 | 0 | **10** |
| **12** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 10 | 0 | 0 | 0 | 0 | 0 | **10** |
| **13** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 9 | 0 | 0 | 0 | 0 | **10** |
| **14** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 10 | 0 | 0 | 0 | **10** |
| **15** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 7 | 0 | 3 | **10** |
| **16** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | 0 | 0 | 8 | 0 | **10** |
| **17** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | 0 | 8 | **10** |
| **Totals** | **11** | **14** | **10** | **10** | **9** | **10** | **10** | **7** | **9** | **10** | **10** | **10** | **12** | **10** | **9** | **8** | **11** | **170** |

Classification accuracy = 147/170 = 86.47 %
Classification error = 23/170 = 13.53 %
Proportional chance accuracy = 10.0/170 = 5.88 %

**Table 2.** Classification accuracy for all fiber types and colors.

| *Color* | *Fiber Type* | *Groups* | *Absorbance* | *FE 365* | *FE 405* | *FE 436* | *FE 546* |
|---|---|---|---|---|---|---|---|
| Black | Acrylic | 6 | 60 | 55 | 57 | 52 | 59 |
| | Cotton | 8 | 73 | 67 | 63 | 59 | 68 |
| | Nylon 6,6 | 13 | 122 | 78 | 77 | 67 | 73 |
| | Polyester | 14 | 102 | 93 | 100 | 86 | 77 |
| Blue | Acrylic | 30 | 274 | 229 | 263 | 269 | 271 |
| | Cotton | 21 | 160 | 121 | 127 | 122 | 115 |
| | Nylon 6,6 | 26 | 230 | 163 | 170 | 162 | 216 |
| | Polyester | 19 | 140 | 157 | 159 | 158 | 156 |
| Brown | Acrylic | 17 | 147 | 126 | 152 | 142 | 147 |
| | Cotton | 22 | 134 | 150 | 174 | 168 | 159 |
| | Nylon 6,6 | 16 | 100 | 92 | 78 | 70 | 75 |
| | Polyester | 39 | 173 | 261 | 295 | 277 | 291 |
| Green | Acrylic | 16 | 150 | 133 | 147 | 152 | 150 |
| | Cotton | 23 | 177 | 140 | 174 | 157 | 112 |
| | Nylon 6,6 | 15 | 133 | 103 | 80 | 90 | 97 |
| | Polyester | 19 | 113 | 143 | 158 | 157 | 151 |
| Grey | Acrylic | 5 | 50 | 50 | 48 | 50 | 50 |
| | Cotton | 7 | 60 | 58 | 60 | 60 | 48 |
| | Nylon 6,6 | 8 | 60 | 41 | 53 | 54 | 31 |
| | Polyester | 6 | 39 | 51 | 52 | 58 | 54 |
| Orange | Acrylic | 3 | 30 | 30 | 30 | 30 | 30 |
| | Cotton | 4 | 40 | 40 | 40 | 40 | 40 |
| | Nylon 6,6 | 7 | 66 | 46 | 56 | 55 | 45 |
| | Polyester | 3 | 30 | 30 | 30 | 30 | 30 |
| Pink | Acrylic | 6 | 60 | 57 | 58 | 60 | 60 |
| | Cotton | 8 | 53 | 49 | 64 | 56 | 38 |
| | Nylon 6,6 | 2 | 20 | 20 | 20 | 20 | 19 |
| | Polyester | 2 | 18 | 20 | 20 | 20 | 20 |
| Purple | Acrylic | 10 | 87 | 93 | 99 | 98 | 96 |
| | Cotton | 9 | 73 | 73 | 81 | 81 | 77 |
| | Nylon 6,6 | 7 | 70 | 58 | 55 | 46 | 54 |
| | Polyester | 1 | x | x | x | x | x |
| Red | Acrylic | 16 | 159 | 144 | 154 | 151 | 154 |
| | Cotton | 8 | 71 | 62 | 66 | 68 | 74 |
| | Nylon 6,6 | 12 | 108 | 84 | 76 | 75 | 82 |
| | Polyester | 10 | 90 | 73 | 82 | 78 | 94 |
| White | Acrylic | 11 | 71 | 75 | 83 | 81 | 68 |
| | Cotton | 2 | 19 | 16 | 13 | 14 | 13 |
| | Nylon 6,6 | 4 | 24 | 33 | 35 | 39 | 38 |
| | Polyester | 7 | 64 | 57 | 60 | 65 | 58 |
| Yellow | Acrylic | 5 | 49 | 50 | 50 | 50 | 48 |
| | Cotton | 13 | 73 | 84 | 77 | 84 | 71 |
| | Nylon 6,6 | 1 | x | x | x | x | x |
| | Polyester | 4 | 39 | 40 | 38 | 40 | 29 |
| *Total Spectra* | | 4830 | 3811 | 3545 | 3774 | 3691 | 3638 |
| *% Classification Accuracy* | | | 78.90 | 73.40 | 78.14 | 76.42 | 75.32 |

Trends are difficult to spot, but some effects are suggested. For the dyed acrylic fibers, UV/visible and fluorescence MSP at the 405 nm excitation wavelength have the highest discriminating power, while excitation at 436 and 545 had slightly lower discriminating power. For the dyed cotton fibers, UV/visible MSP and fluorescence MSP at the 405 nm excitation wavelength have the highest discriminating power. Excitation at 436 had slightly lower discriminating power. For the dyed nylon 6,6 fibers, UV/visible MSP had the highest discriminating power; fluorescence had lower discriminating power. For the dyed polyester fibers, fluorescence at the higher three excitation wavelengths had the highest discriminating power and UV/visible MSP had a much lower discriminating power. In terms of discriminating power for different colored fibers, UV/visible MSP typically has the highest discriminating power. Consistent with the overall average trend in Table 1, discriminating power tends to be higher at the 405 and 436 fluorescence excitation wavelengths. It should be mentioned that white fibers in our database have not been dyed with fluorescent brighteners and discrimination of white acrylic and cotton fibers was poor. However, discriminating power with white polyester using absorbance or fluorescence, and with fluorescence data taken for white nylon 6,6, was high.

## Conclusions

Multivariate statistical methods provide tools for handling high dimensional spectral data and for assessing the uniqueness of a particular fiber relative to other fibers with which it is to be compared. Identification of which analyses produce the most discriminating data insures that the limited time and resources available in forensic laboratories are appropriately applied. Multivariate statistics is of great utility in exploring relationships among groups of spectra, in

visualizing differences between groups of spectra, and in assessing quantitatively the discriminating power of different spectroscopic techniques.

Statistics should not be used by themselves to support a hypothesis of common origin for different fibers; in our case, classification results can be interpreted with knowledge of the dyes present on each fiber. Both UV/visible and fluorescence spectra provide discriminating information, depending on the particular dyed textile fibers under comparisons. UV/visible microspectrophotometry, by itself, was the best single discriminating technique. The discriminating power of fluorescence MSP approaches that of UV/visible MSP, and appears to add considerable discrimination beyond that provided by absorbance measurements. For colored fibers, the excitation wavelengths 405 and 436 provide the best discriminating power. Which fluorescence excitation wavelength is most discriminating depends of the dyes present on the fiber. A further caveat is that the dye producing the major color of the fiber may not always be the component that produces discrimination among similar fluorescence spectra.

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