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PCA on Transposed Data Matrices for Wood FTIR-ATR Spectra Analysis: Application to Archaeological Woods

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Abstract

We applied principal component analysis to the transposed data matrix (PCAt) of FTIR spectra to determine the effects of storage condition on archeological wood composition. Sixty FTIR-ATR spectra were taken from three pine wood cores (one from a living tree and two from archaeological wood) to characterize within and between samples variability. The PCAt of all samples (*n*=60) extracted four PCs related to differences in carbohydrate, lignin and resin acid compounds. The PCAt of l core separately showed that these differences could also be recognized from individual wood cores. Our results suggest that this application is a novel and promising tool for wood characterization.

Introduction

Fourier Transformed Infrared spectroscopy is widely used because it is fast, easy to use and requires minimum sample preparations [1]. It is a non-destructive technique, which is important due to the limited availability of cultural heritage materials. The absorption of an infrared beam by a sample induces molecular bonds vibrations that are recorded as spectra [2].

Studies of wood combining FTIR and PCA successfully allowed molecular differentiation between earlywood and latewood, and between softwood and hardwood [3]. Furthermore, PCA and FTIR have been used to classify woods according to environmental factors (climate and soil properties) [3, 4, 5]. Even though PCA is widely used on FTIR data, the application of PCA to the transposed data matrix (PCAt) of wood spectra remains at this time novel. Using the direct data matrices, the components are computed according to the variation of the absorbance frequency relative to each band in the samples, while the transposed data matrices the factors are computed according to the intensity of the absorbance relative to the whole spectrum. The PCAt applied on combined (spectra from several wood cores) or individual (spectra from a single core) data allows for the assessment of differences in wood chemistry between different trees or between different rings in a given tree, respectively [6]. The former is useful in studying wood type (botanical source on genus/species level) and the latter is aimed to eventually become a provenancing tool (by tracking ring-related variability of different living and archaeological woods). The aim of this study is to explore the use of PCAt to analyze FTIR spectra.

Materials & Methods

The samples used in this study were collected in Spain: a *Pinus nigra* living tree wood core sampled in Sierra de Cazorla, and two archeological wood cores (*Pinus* sp.), obtained from a beam wood of the cathedral of Segovia and from the Magdalena shipwreck in the Bay of Viveiro.

The infrared analytical technique was developed using a Varian 670-IR spectrometer (Varian Inc., Santa Clara, CA). For each sample we recorded 20 spectra from individual tree rings (10 in the recent rings and another 10 in the old rings).

The transposed matrix was used to get details from the spectra through principal component analysis. In the PCAt the samples are considered as input variables instead of the absorption bands in traditional PCA. The transposed matrices PCA is not applied to reduce the space of samples but to obtain information on the nature of the samples. In this particular case, the components' scores characterize the spectral bands. Two PCAt were performed, one on the whole set of samples analysed and another on spectra from individual wood cores. The PCAt were executed using the varimax rotation. This statistical test was done using SPSS 20.

Results

PC1 and PC2 (figure 1a) are related to the polysaccharides with infrared bands related to O-H and C-O bonds vibration in carbohydrate compounds. PC3 (figure 1b) presents a typical resin acid signal according the C-H stretching and the C=O bonds vibrations; whereas PC6 shows a signal for C-H in and/or out of plan vibration for guaiacyl rings. The loading plots below display differences between the three samples related to each extracted factor.

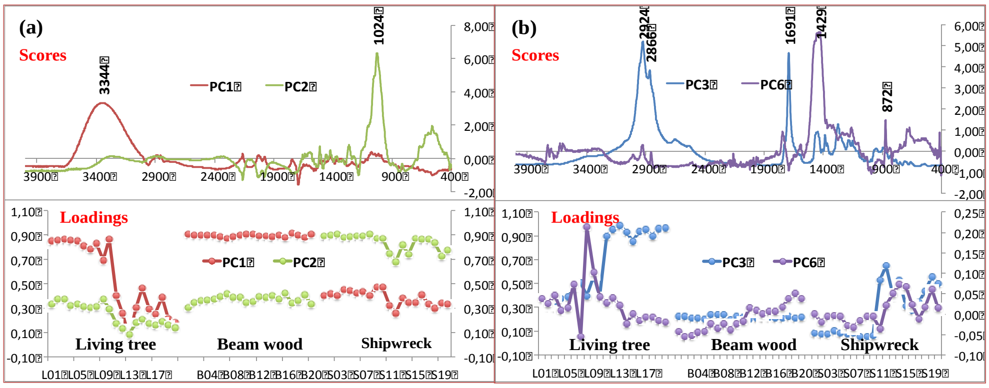

Fig.1: Component scores and loadings plot of the extracted factors (PC1, PC2, PC3 and PC6). PCAt on all samples (n=60).

The factors extracted from the spectra of each sample related to the resin acid, polysaccharide and lignin compounds are shown respectively in figure 2a, 2b and 2c with specific infrared bands. The loading plots related to the extracted factors show the evolution the compounds within each sample according to the component.

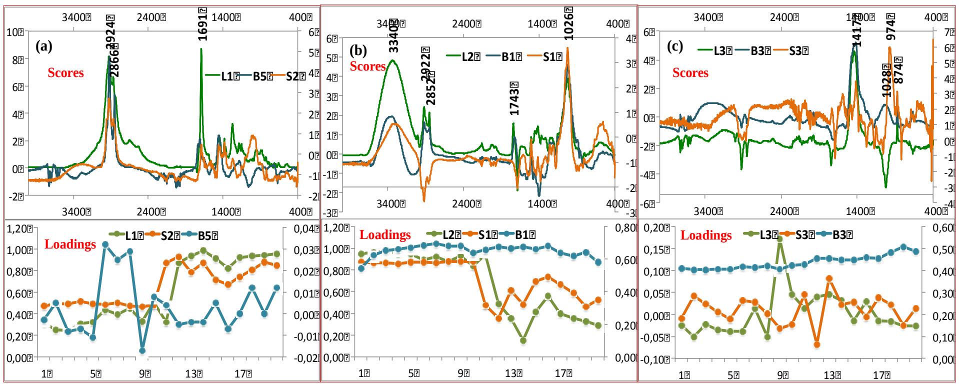

Fig.2: Component scores and loadings plot after individual PCAt: L for living tree (n=20), B: beam wood (n=20), S: shipwreck (n=20); the numbers are related to the order of the extracted factor.

Conclusions

Wood FTIR spectra are known to be complex due to the diverse composition of lignocellulosic materials in general, but this work shows that PCAt is a useful multivariate method to rapidly extract the relevant information of the variability in wood chemistry from FTIR spectra. PCAt applied to single samples spectra allows to know how the wood chemistry changes within the core, while the PCAt on the combined data provides a better understanding that allows comparing between several samples. Our results suggest that combining FTIR-PCAt may eventually become a useful tool for wood provenance.

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