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Uncommon multivariate statistical methods for environmental studies: A review

Mauro Mecozzi [a,*], Mabel Beatriz Tudino [b], Maria Grazia Finoia [c], Marcelo Enrique Conti [d]

[a] Italian National Institute for Environmental Protection and Research, Laboratory of Chemometrics and Environmental Applications, Via di Castel Romano 100, 00128 Rome, Italy
[b] INQUIMAE, Departamento de Química Inorgánica, Analítica y Química Física, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Buenos Aires, Argentina
[c] Italian National Institute for Environmental Protection and Research, Via Vitaliano Brancati 60, 00166 Rome, Italy
[d] Department of Management, Sapienza University of Rome, Via del Castro Laurenziano 9, 00161 Rome, Italy

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ABSTRACT

In this paper we describe the characteristics and the applications of the multivariate methods for spectroscopic and chromatographic techniques independent component analysis (ICA) and two-dimensional correlation spectroscopy (2DCOS) focused to their use in environmental studies. In our opinion, these methods are important because they allow to characterize environmental samples with different aims and scopes from those generally obtained by means of more common multivariate methods such as principal component analysis (PCA) and partial least squares (PLS). The new insights of these methods in recent environmental studies are reviewed and debated.

Contents

1. Introduction

In analytical chemistry, principal component analysis (PCA) and partial least squares analysis (PLS) are multivariate statistic techniques widely applied as methods for quantitative analysis

* Corresponding author. Tel.: +39 0650073287.
E-mail addresses: mauro.mecozzi@isprambiente.it, mauromecozzi2004@libero.it (M. Mecozzi).

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and for the discrimination and differentiation of multivariate data samples [1–3] by means of specific chemometric software [1,4,5].

As far as environmental studies concern, PCA has been applied to study the distribution of hydrocarbons [6,7] and heavy metals in marine sediments [8], to support the identification of baseline levels of heavy metals in marine and terrestrial organisms [9–14], to study the different driving force involved in the mechanisms of organic matter degradation in East Siberian and Laptev seas [15] and to determine physiological cell states in environmental water quality control by FTIR spectroscopy [16].

With the same aim, PLS has been applied to support vibrational spectroscopy in the assessment of environmental quality of soils and sediments [17,18], to improve the analytical accuracy in the determination of total carbohydrate contents in seawater [19] and to support the simultaneous determination of ten polycyclic aromatic hydrocarbons in natural water by fluorescence spectroscopy [20].

Being well known and widely applied, PCA and PLS applications in environmental studies are practically unlimited and for this reason we do not include the discussion of their uses in this review.

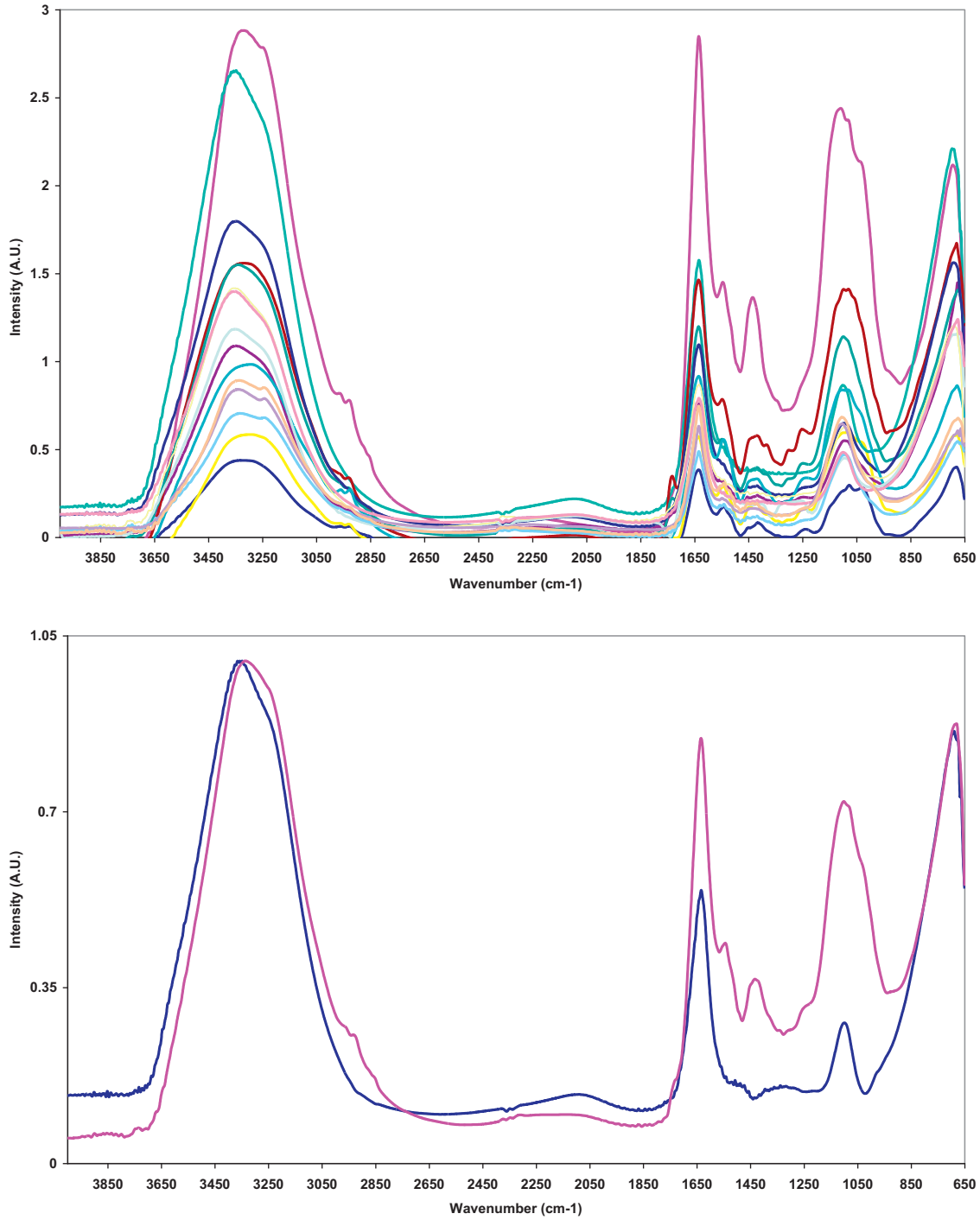

Fig. 1. Example of ICA application by means of the MILCA algorithm to a FTIR spectral data set of samples of marine organic matter during the process of evolution (followed for 21 days). The bottom plot reporting two spectra (i.e., two ICs) only shows that the whole process of organic matter aggregation is described by the formation of amino acids (the blue spectrum) and a complex mixture of compounds (the pink spectrum) where polysaccharides proteins high polymerized are present [31]. (For interpretation of the reference to color in this figure legend, the reader is referred to the web version of this article.)