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Unsupervised contribution analysis: Revealing relevant objects

Chromatography, particularly High Performance Liquid Chromatography (HPLC), is probably the most used standard instrumental analytical technique, widespread over all analytical labs around the world, very convenient to perform fast separation and simultaneous quantification of several analytes in several complex samples. Most convenient, reliable and roust detectors are usually related with UV-vis detection such as Diode Array Detectors (DAD). However, when analyzing real and complex samples, it is frequent to observe signal distortions related with analytes co-elution, spectral interference and column lack of selectivity. Is it possible to be aware of these situations and circumvent these problems? In this work we propose Unsupervised Contribution Analysis (UCA) to address these situations; all chromatographic data should be checked in order to find out the real number of independent contributions that are consistent with dataset in study. In a recent study, we suggested how to retrieve independent component contributions in spectroscopic (synchronous fluorescence) analysis of environmental samples. In this work, Independent Component Analysis (ICA) was used in order to retrieve spectral sources and respective component contributions. However, in order to preform ICA, it was necessary to previously determine the number of independent components responsible for data spectra. Using Principal Object Analysis (POA), we showed how it's possible to find out system independent contributions in a robust and reliable manner. With this same concept, we have proved the ability of UCA to determine independent contributions; their specific chromatogram and; respective contributions using same approach, especially when there are evidences for co-elution profiles in (UV/vis)-HPLC and other non-specific instrumental methods. Some examples, practical and theoretical considerations will be addressed in order to maximize the ability of Unsupervised Component Analysis (UCA) to evaluate chromatographic response in complex systems.
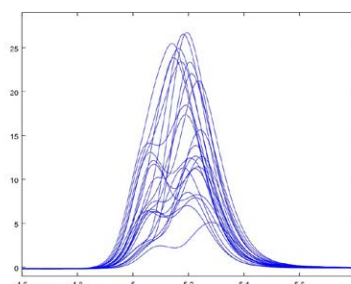
Figure1: HPLC determination of aquatic environmental contaminants by HPLC-DAD (220 nm): examples of separation optimization of ternary mixtures.

Biography

Jorge Costa Pereira has completed his BSc, MSc and PhD at University of Coimbra. His main research work is in the field of Chemical Analytical Control and Environment Quality Control specially related with statistics, analytical method validation and chemometrics. He has published 30 papers in well reputed international journals and is member of the editorial board or Portugaliae Electrochimica Acta.

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