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UNSUPERVISED CONTRIBUTION ANALYSIS: REVEALING AND RESOLVING OBJECTS

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Chromatography, in particularly High-Performance Liquid Chromatography (HPLC), its 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 analysing real and complex samples, it is frequent to observe signal distortions related with analytes co-eluiton, spectral interference and column lack of selectivity. Is it possible to be aware of this situation and circumvent these problems? In this work we propose Unsupervised Contribution Analysis (UCA) to address these situations, were 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 studys [1,2] we suggested how to retrieve independent component contributions in spectroscopic (synchronous fluorescence and 1H-NMR) 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 its 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 a) independent contributions, b) their specific chromatogram and c) respective contributions using same approach, specially 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.

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