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Combination of Independent Component Analysis and modelisations for the identification of metabonomic biomarker in 1H-NMR spectroscopy

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Abstract.
The metabolism is the set of chemical reactions that occur in a living organism in order to maintain life. These processes product and transform small molecules called Metabolites.

A recent scientific platform, named Metabonomics, studies the development of biological reactions consecutive to a contact with a physio-pathological stimulus, through changes in the metabolites. The ^{1}H-NMR spectroscopy is used to describe the composition of the metabolites in form of spectra. Biologists can then confirm the presence of a biological reaction by the alteration of specific spectral regions (biomarkers) in regards to spectra obtained in physiological situations.

However, this process supposed the preliminary identification in an experimental database of biomarkers or spectral regions, to examine because of their changes in case of the biological response. Traditionally, this identification is realised, with some limitations, by examination of the 2 first components from a Principal Component Analysis.

This talk proposes a new methodology for the identification of metabonomics biomarker. In a first step, Independent Component Analysis (ICA) is substituted to PCA in order to obtain more relevant and interpretable components. A second step proposes several models allowing to identify biomarkers from the obtained components and to predict the profile of a spectrum in a chosen condition.