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BAYESIAN SOLUTIONS FOR DATA, SIGNAL AND IMAGE PROCESSING IN MASS SPECTROMETRY

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In the last three decades, there have been recent advances in different techniques of mass spectrometry: time-of-flight (TOF), matrix assisted laser desorption/ionization (MALDI), orbitraps, quadrupoles, ion traps, gas chromatography-mass spectrometry (GCIMS), Fourier transform ion cyclotron resonance (FT-ICR), etc. Each technique has its advantages and drawbacks; there is no all-purpose perfect system. The results coming out of these systems have many limitations such as baseline, drift, noise, low resolution, etc. We can always improve these results by further processing if we can model these imperfections, either in a deterministic or probabilistic way. The main tools are inverse problems and the Bayesian inference frameworks. In this tutorial presentation, a few of these inverse problems are presented and an overview of the methods to handle them is given. The Bayesian inference approach is a very useful approach to handle these problems as it gives the possibility to account both for soft prior modeling of the signals and images as well as for the uncertainly associated to the measurement process. It also gives the necessary tools to estimate the hyper parameters and the remaining uncertainties in the proposed solution. To illustrate this, we take the deconvolution problem which is one of the main inverse problems in mass spectrometry and go through the different regularization and Bayesian inference methods and compare their relative performances. In particular, prior models such as Bernouilli-Gaussian, Bernouilli-Gamma, Laplace, Student's t-test and hierarchical mixture models are used in a Bayesian approach for simple or blind deconvolution problems.

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