

A BAYESIAN SOLUTION TO JOINTLY REMOVE THE BASELINE AND INCREASE THE RESOLUTION OF MASS SPECTROMETRY DATA

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There have been recent advances in different Mass spectrometry technics: 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 technic has his advantages and drawbacks. There is no all purpose perfect system. Data, signals and images coming out of these systems have many limitations: baseline, drift, noise, low resolution, limited dynamics, etc. We can always improve these data by further processing (post-processing) if we can model these imperfections either in deterministic or probabilistic ways. The main tools are inverse problems and the Bayesian inference frameworks. In this tutorial presentation, through the deconvolution example, first the basics of the Bayesian inference are presented. Then, a hierarchical prior model and a data generative model are assembled to handle both the background elimination and the resolution improvement. A few simulation examples show the difficulties and the improvements we can obtain.

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