Complexity miniproject proposal on "Stochastic modeling of time-domain mass spectrometry data"

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Background

We are working on a long-term project developing stochastic models for FTICR mass spectrometry experiments. The models being developed are founded on theoretical physics and chemistry and they are structured in such a way that relevant parameters can be formally inferred from experimental data using a combination of prior information and likelihood statistics.

Current state of research

So far, we have successfully developed models for the final FTICR output, which is the mass spectrum (MS) itself. Being aware that the MS is a synthetic representation of various processing steps, each of which might introduce specific biases, we have now turned to the fundamental problem of modeling the FTICR's raw time-domain data. The latter represent a noisy convolution of periodic functions with possibly several thousand characteristic frequencies representing the specific mass signatures of different types of ions.

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Miniproject goals

The first aim of this miniproject is that of developing the periodic convolution stochastic model taking into account the physics of interacting ion types, such as the Coloumbic forces causing their mutual repulsions, which are responsible for most of the noise in the data. Second, this miniproject aims at exploring the identifiability of the coefficients of the convolution model using both simulated and available experimental data.

Scope for PhD research

This raw time domain data structure also is common to other mass spectrometry techniques such as nuclear magnetic resonance (NMR), which finds clinical applications for instance in magnetic resonance imaging (MRI) and functional magnetic resonance imaging (fMRI). From this persepctive, the research theme of this miniproject has high potential of being generalised and expanded into a full-fledged PhD research project.

References

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