Global Spectral Deconvolution (GSD) of 1D-NMR Spectra

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A typical experimental NMR spectrum comprises a) spectral peaks arising from the transitions of the studied spin system(s), b) satellite peaks from the very same spin system(s) isotopomers, c) solvent peaks due to the employed solvent, d) impurity peaks due to undesired chemical components of the sample, e) folded-over peaks from outside the spectral window, f) baseline distortions due to the acquisition dead-time or undesirable broad solid-state signals, and g) spikes due to interfering RF signals from the instrument or from the broader environment. For both quantitative and qualitative analysis, it is desirable to decompose the spectrum into the individual components. In particular, one would like to reduce it automatically to an editable peaks list which matches all the recognizable peaks in the experimental spectrum, leaving out any baseline drift and noise. The peaks in such a peak list, each described in a parametric form, can be then subject to automatic and/or manual editing (filtering). For example, one can recognize automatically spikes (anomalously narrow peaks), solid impurities (very broad peaks), folded-over peaks (anomalous phase), and possibly even rotation sidebands and isotopomer satellites.

Several partial approaches to generate such peaks list have been developed in the past, including parametric Linear Prediction [1] and the Filter Diagonalization Method[2] (FDM). As opposed to those methods, based on the direct analysis of the FID, in this work we present a new approach which works directly on the frequency domain and makes use of novel methods for spectral resolution enhancement (Resolution Booster[3] and automatic peak detection. This process can be carried out either by using a fast algorithm based on the knowledge of the first and second derivatives of the data and on limited, local fitting, or by employing a substantially slower massive fitting method to be used when highly accurate values are needed.
We will show several real-life examples of GSD as implemented in Mnova software .[4] Current limitations and restrictions, as well as the future potential and perspectives of this approach will be also presented

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