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High-resolution MR spectroscopy via adaptive sub-band decomposition

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Abstract

For several years, the possibility of using non-iterative high-resolution (HR) spectral estimators instead of Fourier transform (FT) has received considerable attention in the NMR literature. Different approaches have been proposed, including maximum entropy methods, linear prediction (LP) methods, and state space methods. When used in good conditions, all these HR estimators present several advantages over the FT in terms of resolution and detection, and what is more, they yield directly the relevant parameters. However, limitations of these methods appear when attempting to process measured signals made of numerous data samples (over 10,000) and/or containing a lot of resonances. Indeed, the computation cost becomes prohibitive in this case. As a reaction, last years, there was a renewed interest for parametric Frequency Selective (FS) approaches, a concept initially proposed in 1988 with the LP-ZOOM approach. Several new FS methods have been proposed which possess two features that make them efficient with high-complexity signals: high robustness against out-of-band interferences and low computational burden. Nevertheless, in practice, it is often desirable to perform a systematic analysis of the whole spectral band. In this case, without a priori information, the problem remains of how to select the spectral sub-bands, their width and location. Now this choice is of primary concern because it strongly conditions the estimation results.

After some recalls about the main parametric FS approaches and their advantages over full-band approaches, the present work describes a fast, and almost automated time-data analysis method for NMR spectroscopy, based on an adaptive implementation of certain HR methods usable in spectral sub-bands. Originally designed as an improvement of the SVD-based High-Order Yule-Walker method in Sub-Bands, and intended to avoid the choice of the decimation factor and to reduce the computational complexity, the adaptive decomposition is achieved through successive decimation/estimation stages each followed by a test procedure to decide whether

or not the process should continue. The test is based on a local spectral flatness measure of the estimation residuals. This stop-criterion involves an a posteriori validation of the estimation, thus the proposed strategy allows one to obtain a better detection rate at a lower complexity comparatively to other stopping rules, while preserving a reasonable estimation variance. Moreover, the reliability of the fitting algorithms considered is improved, by decreasing the influence of the model order and the number of false detections. Finally, the method is more efficient than FT at low signal-to-noise ratio. The choice of the fitting algorithm is discussed and the effectiveness of the strategy is demonstrated by analyzing some simulation signals and several sets of one-dimensional NMR experimental data.

Key words: Time-data analysis, High-resolution methods, Linear prediction, High-order Yule-Walker estimation, ARMA modeling, ^{13}C NMR, Damped exponentials, Adaptive sub-band decomposition, Spectral flatness
PACS:

1 Introduction

A free induction decay (FID) or NMR signal (generally an average signal raising out of multiple measurements of the same experiment) is commonly modeled as a superposition of M damped complex exponentials in noise:

$$\begin{aligned} y(n) &= \sum_{k=1}^M A_k e^{(-\alpha_k + j2\pi f_k)n + j\phi_k} + e(n) \\ &= x(n) + e(n) \end{aligned} \quad (1)$$

for $n = 0, \dots, N - 1$. A_k is the amplitude, f_k the frequency, α_k the damping factor and ϕ_k the phase of each of the M components. N is the total number of observations. Note that the sampling period has been included in α_k and f_k for simplicity. The error term $e(n)$ is representative of measurement noise. It is usually assumed to be white noise. Anyhow, it will be seen later that it is possible to deal with colored noise of moving-average (MA) type. The preceding equation may be written in a more compact form:

$$y(n) = \sum_{k=1}^M h_k z_k^n + e(n) \quad (2)$$

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