A New Adaptive Subband Decomposition Approach for Automatic Analysis of NMR Data *

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Abstract

This paper presents a non-iterative, fast, and almost automated time-data analysis method for NMR spectroscopy, based on a new adaptive implementation of high resolution methods used in spectral subbands. It is intended to avoid the choice of the decimation factor (or the width of the spectral windows) which, in the case of a uniform decomposition, strongly conditions the estimation results, and to diminish the computational burden. It is achieved through successive decimation/estimation stages each followed by a test procedure in order to decide whether or not the process should continue. The proposed 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 method proposed 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 Fourier transform (FT) at low signal-to-noise ratio (SNR). The effectiveness of the method is demonstrated by analyzing a simulation signal and raw carbon-13 experimental data.

Key words: Time-data analysis; Linear prediction; High-order Yule-Walker estimation; 13C NMR; Adaptive subband decomposition; Spectral flatness.

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