HIGH-RESOLUTION NMR SPECTROSCOPY BY USING AUTOCORRELATION-BASED METHOD

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1. Introduction: Nuclear magnetic resonance (NMR) spectroscopy is a powerful technique for structural and dynamic studies of molecules. An important step in the NMR spectroscopic analysis of is an accurate estimation of the chemical shift values (or frequencies) of peaks observed in the spectrum. Typically, the NMR measurements or free-induction decay (FID) modeled as a superposition of damped exponentials. The structural information of the underlying molecules lies in the frequency, damping, and amplitude parameters of the FIDs. For analysis, it is important to accurately estimate the frequencies or chemical shits from noisy FID samples. In a typical Fourier-based spectral analysis, the resolution is proportional to the number of measurements. A larger number of measurements requires longer and expensive experimental time. By using the structure of the FIDs, typically, a linear-prediction based method is employed to increase resolution [1]. Recently, we proposed a robust autocorrelation-based frequency estimation method [2] which is based on estimation of signal parameters via rotational invariance technique (ESPRIT). The algorithm is an extension to the classical ESPRIT to estimate the damped-exponentials (code named DEESPRIT). In this work, we would like to showcase an important feature of DEESPRIT. In the NMR spectra of many chemical solutions, the presence of strong peak due to water overshadows the smaller peaks and it is difficult to resolve them using conventional Fourier-based methods. By applying DEESPRIT, we could detect and resolve these peaks with fewer measurements.

2. Results: Below, Fig. (a) shows ^{1}H NMR spectrum of a mixture of amino acids prepared in 95% of H_2O. There is a strong peak at 5 ppm due to water. Figure (b) shows the zoomed in part highlighted by the rectangle. We show that DEESPRIT could resolve peaks by using 39% of the total samples.

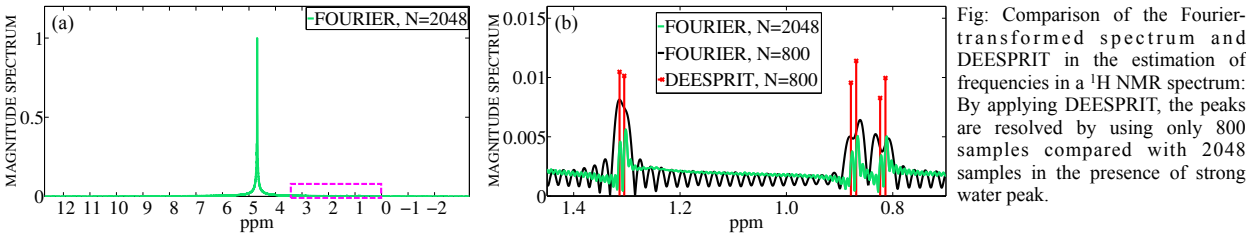

Fig: Comparison of the Fourier-transformed spectrum and DEESPRIT in the estimation of frequencies in a ^{1}H NMR spectrum: By applying DEESPRIT, the peaks are resolved by using only 800 samples compared with 2048 samples in the presence of strong water peak.

References:

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