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LocMAP: A New Localization Method for the Parametric Processing of High Resolution NMR Data

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Abstract

High resolution NMR spectroscopy offers a large number of data points that enable close peaks to be resolved. Data processing algorithms, however, have not yet been able to capitalize on this offering to achieve the highest permissible resolution. Although singular value decomposition (SVD) based methods such as matrix pencil (MPM) are theoretically able to achieve this, their onerous computational cost makes them impractical. In this work, we address this problem and propose a localized MPM method that we refer to as LocMaP, which is capable of delivering the promised high resolution while at the same time taking advantage of the computational efficiency of the FFT. We present the derivation of LocMaP and offer an efficient implementation of it. Evaluation using both Monte Carlo runs and a simulated FID establish the great potential of the proposed method.

Keywords: Matrix Pencil; Parameter Estimation; high resolution; NMR Spectroscopy; FFT; SVD.

1. Introduction

Data processing of high resolution NMR spectra has been, and still is, largely dominated by the Discrete Fourier Transform (DFT) through its efficient implementation using the Fast Fourier

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