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Localised High Resolution Spectral Estimator for Resolving Superimposed Peaks in NMR Signals

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Abstract

Nuclear magnetic resonance (NMR) spectroscopy is the prime technique for studying molecular and biomolecular structure as well as dynamics. The time domain NMR signal can be ideally modelled as the sum of damped complex exponentials in additive Gaussian noise. The spectrum of the signal may contain regions having overlapping peaks. In order to understand the underlying chemical structure, these peaks need to be detected and resolved. In this paper, we propose the Localised Capon Estimator (LoCapE) for resolving closely spaced peaks in the NMR spectrum when the actual number of peaks is unknown. The novel method is able to efficiently retrieve the correct number of components and obtain high resolution spectral estimates in the selected regions of the spectrum. LoCapE is tested with simulated and actual proton NMR spectra to verify its performance.

Keywords: Capon; spectral estimation; peak detection; nuclear magnetic resonance spectroscopy; coupling constant.

1. Introduction

Nuclear magnetic resonance (NMR) spectroscopy is a powerful tool for the study of molecular and biomolecular structure and dynamics, [1, 2]. The acquired discrete time domain signal obtained from the NMR spectrometer, which is referred to as the free induction decay (FID), can

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