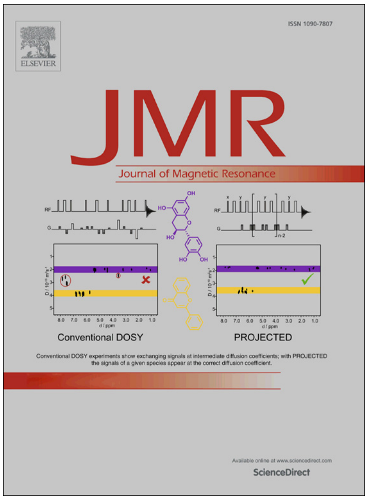

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The Inversion of 2D NMR Relaxometry Data Using L1 Regularization

Xiaolong Zhou[1], Guanqun Su[1], Lijia Wang[1], Shengdong Nie[1*], Xinmin Ge[2]

[1] Institute of Medical Imaging Engineering, University of Shanghai for Science and Technology, Shanghai 200093, China

[2] School of Geosciences in China University of Petroleum. Qingdao 266580, Shandong Province, China

Abstract: NMR relaxometry has been used as a powerful tool to study molecular dynamics. Many algorithms have been developed for the inversion of 2D NMR relaxometry data. Unlike traditional algorithms implementing L2 regularization, high order Tikhonov regularization or iterative regularization, L1 penalty term is involved to constrain the sparsity of resultant spectra in this paper. Then fast iterative shrinkage-thresholding algorithm (FISTA) is proposed to solve the L1 regularization problem. The effectiveness, noise vulnerability and practical utility of the proposed algorithm are analyzed by simulations and experiments. The results demonstrate that the proposed algorithm has a more excellent capability to reveal narrow peaks than traditional inversion algorithms. The L1 regularization implemented by our algorithm can be a useful complementary to the existing algorithms.

Keywords: Low-field NMR; 2D inversion; FISTA; 2D spectra

1. Introduction

Relaxation time measured by NMR is reported to correlate with many material characteristics like viscosity, crystallinity, concentration, and even length of polymer chain [1]. Hence NMR relaxometry, the measurement of relaxation time, has been becoming a powerful approach to explore structures of the mixture. The traditional 1D T_2 or T_1 relaxometry analysis is rapid, non-invasive and non-destructive. It can be implemented by a low cost, compact low-field NMR equipment. However, when 1D relaxometry analysis is used for the complex mixtures, the peaks of different components are prone to overlap together, resulting in the misinterpretation of the spectra. This is the major obstacle of 1D relaxometry. Herein, the 2D relaxometry, the measurement of both T_2 and T_1 at a single experiment, is proposed to outcome this obstacle.

Original sampling signals from NMR equipment are too intricate to understand. These signals can be transformed into understandable and valuable spectra by inversion, which is a helpful and essential technology. Comparing to 1D inversion, 2D inversion need solve two main difficult problems. First, the data used by 2D inversion is much larger than that used in 1D case. Consequently, the 2D inversion problem, without data compressing, could not be handled properly by common computers. Second, the ill-posedness of the 2D inversion problem characterized by instability and non-uniqueness is more serious. As a result, the 2D spectra will be severely contaminated by noise when applying direct least squares fitting. To circumvent these problems, various approaches have been proposed.

In general, there are two kinds of algorithms for the inversion of 2D NMR relaxometry: iterative algorithms and explicit regularization algorithms. The iterative algorithms regularize the 2D inversion problem using proper stopping criterions. As the iteration goes, the fitting residual decreases and the influence of noise increases. When the iteration converges, a resultant spectrum with little fitting residual (even zero fitting residual is possible) is produced. But this spectrum is always bad to interpret because it is contaminated by noise seriously. Early iterations often produce

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*Corresponding author：Shengdong Nie, professor of University of Shanghai for Science and Technology, Tel: +86-021-55271172, E-mail: nsd4647@163.com