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Real-time Optimization of Nuclear Magnetic Resonance Experiments

Y.-Q. Song[a], Yiqiao Tang[a], M. D. Hürlimann[a], D. G. Cory[b]

[a]*Schlumberger-Doll Research, Cambridge, MA 02139, USA*
[b]*Institute for Quantum Computing, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada*
Department of Chemistry, University of Waterloo, Waterloo, ON, Canada, N2L 3G1
Perimeter Institute for Theoretical Physics, Waterloo, ON, Canada, N2L 2Y5
Canadian Institute for Advanced Research, Toronto, Ontario, Canada, M5G 1Z8

Abstract

Nuclear Magnetic Resonance (NMR) experiments are typically performed with predetermined pulse sequences and acquisition parameters, and are oftentimes sub-optimal for individual samples under investigation. Here we explore a class of real-time optimization methods that conducts stochastic analyses on the acquired data and in turn updates and optimizes the subsequent measurements. We show superiority of the method to static approaches, both in the efficiency and quality of data acquisition, for a wide range of experiments.

Keywords:
NMR, real-time optimization, stochastic analysis

1. Introduction

NMR measurements, despite ample applications in numerous disciplines, are known to be slow. One of the reasons for the slowness is the need for a polarization time that allows the nuclear magnetization to regain the thermal equilibrium. Furthermore for multi-dimensional experiments, many acquisitions are often required to boost SNR (signal to noise ratio) and to vary the pulse parameters to assure sensitivity over the entire parameter space of interest. The prolonged measurement time has limited the application of NMR in a number of practical uses. Any method to accelerate the experimental procedure, such as compressed sensing [1, 2] or spatial multiplexing [3], are highly desired.

Another challenge in many NMR experiments is that the quantities of interest, such as T_1, T_2, diffusion coefficient, J-coupling, and dipole coupling, can span a large numerical range, often of several orders of magnitude. Due to the substantial variance, a fit-for-all-purpose pulse sequence does not exist. Taking as an example the T_1 measurement with the inversion recovery pulse sequence; for a sample of an expected T_1 of 1 s, a good list of encoding times between the 180° and 90° pulse covers the range from 0.1 to a few seconds. Yet this time list is inappropriate for a sample of an expected T_1 in the proximity of 0.01 s. Accordingly, a standard protocol in NMR laboratories for an unknown sample covers encoding times from 1 ms to 10 s. For a given sample, this conventional approach is unavoidably sub-optimal and results in redundant measurements. The issue aggravates in time-constrained applications, such as MRI and subsurface geo-explorations [4], where data quality and measurement efficiency often run into conflict.

The NMR literature is rife with reports on real-time optimization methods. In spectrum domain, automation of NMR data acquisition, along with concurrent analysis and optimization, was attempted in multidimensional spectroscopy measurements with reduced dimensionality techniques [5, 6] and in protein structure determination with a probabilistic pseudo-energetic model [7]. In time domain, past work has been focusing on using non-linear least squares fit [8, 9] or its derivative with Tikhonov regularization [10] to determine experimental precision on-the-fly and accordingly evaluate stopping points; in those examples, however, the NMR measurement parameters (such as the (t_1, t_2) list in a 2D experiment) were not adaptively adjusted for individual samples.

In this paper, we present a time-domain method that optimizes NMR measurements on-the-fly for individual samples under study. More specifically, we utilize a stochastic optimization protocol that conducts a statistical analysis on the acquired data in real-time, and based on the results optimizes the subsequent acquisitions [11]. The new method automatically tailors the acquisition program to a specific sample, optimizing measurement quality while minimizing operator interference and biases.

2. A statistical perspective

The goal of an NMR measurement is to determine NMR quantities of a sample within a definitive margin of error, permitted by the instrument noise limit and allowed experiment time. Ideally, every data acquisition expands,

*Corresponding author
Email address:* ysong@slb.com (Y.-Q. Song)