

Restore High-Resolution Nuclear Magnetic Resonance Spectra from Inhomogeneous Magnetic Fields Using a Neural Network

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ABSTRACT: High-resolution nuclear magnetic resonance (NMR) spectroscopy is a powerful analytical tool with wide applications. However, the conventional shim technique may not guarantee the homogeneity of the magnetic field when the experimental conditions are unfavorable. In this study, we proposed a data postprocessing method called Restore High-resolution Unet (RH-Unet), which uses a convolutional neural network to restore distorted NMR spectra that have been acquired in inhomogeneous magnetic fields. The method generates feature-label pairs from single peak regions and ideal Lorentzian line shapes and trains a RH-Unet model to map low-resolution spectra to high-resolution spectra. The method was applied to different samples and showed superior performance than the reference deconvolution method incorporated in Bruker Topspin software. The proposed method provides a simple and fast way to obtain high-resolution NMR spectra in inhomogeneous fields that can facilitate the application of NMR spectroscopy in various fields.



INTRODUCTION

High-resolution nuclear magnetic resonance (NMR) spectroscopy is a powerful analytical tool for studying molecular structure, conformation, composition, and dynamics at the level of atoms. It provides detailed information about chemical shifts, *J*-coupling, and relaxation rates and has been widely used in chemical analysis, structural biology, and life sciences.^{1–3} The spectral resolution and signal-to-noise ratio are crucial criteria for the quality of the NMR spectra. With the continuous development of NMR equipment hardware (e.g., a stronger superconducting magnet⁴ and a cryogenic probe⁵) and experimental techniques (e.g., cross-polarization⁶ and hyperpolarization⁷), sensitivity has been greatly improved in modern NMR spectroscopy. On the other hand, the resolution of NMR spectra is also highly valued. Various techniques have been developed to improve the resolution of spectra, such as various decoupling techniques^{8,9} and TROSY.¹⁰ However, ultimately, the resolution of the NMR spectra is determined by the uniformity of the magnetic field. The more uniform the magnetic field, the higher the NMR resolution. The resolution of modern NMR spectrometers is usually up to 0.1 Hz, which requires that the magnetic field uniformity must reach 1 part in 10⁶. Therefore, before performing NMR experiments, operators should carefully optimize the magnetic field by adjusting the current of the shim circuits.

The development of advanced magnets and the implementation of advanced magnetic shimming and deuterium locking techniques have greatly improved the homogeneity of the magnetic field in NMR experiments. However, under some

experimental conditions, the magnetic field may still suffer from spatial inhomogeneity or temporal instability, such as measurements on biological tissues with intrinsic magnetic susceptibility variations. Shimming is sometimes difficult to avoid these magnetic field inhomogeneities in some NMR equipment, even for homogeneous samples.¹¹ In addition, slight disturbance or unsatisfactory shimming can also reduce the homogeneity of the magnetic field. Magnetic field inhomogeneity is a common issue in NMR experiments. If the magnetic field cannot meet the requirements after automatic shimming before sampling, it must take a lot of time to shimming manually or accept poor spectral quality, which results in missing information about *J*-coupling and overlapped peaks and makes it challenging to extract useful information from spectra. Therefore, it is necessary to develop corresponding methods to obtain higher-resolution NMR spectra under inhomogeneous magnetic field conditions.

There are several techniques that have been proposed to achieve this goal.¹² Chen et al. reviewed three types of experimental techniques that can measure high-resolution NMR spectra free from the influence of inhomogeneous

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High Resolution NMR Edwin D. Becker, 2012-12-02 High Resolution NMR Theory and Chemical Applications discusses the principles and theory of nuclear magnetic resonance and how this concept is used in the chemical sciences. This book is written at an intermediate level with mathematics used to augment verbal descriptions of the phenomena. This text pays attention to developing and interrelating four approaches: the steady state energy levels, the rotating vector picture, the density matrix, and the product operator formalism. The style of this book is based on the assumption that the reader has an acquaintance with the general principles of quantum mechanics but no extensive background in quantum theory or proficiency in mathematics is required. This book begins with a description of the basic physics together with a brief account of the historical development of the field. It looks at the study of NMR in liquids including high resolution NMR in the solid state and the principles of NMR imaging and localized spectroscopy. This book is intended to assist chemistry graduate students, advanced undergraduate students, or researchers to understand NMR at a fundamental level. This text also provides illustrations of the applications of NMR to the determination of the structure of small organic molecules and macromolecules including proteins.

High-resolution NMR Techniques in Organic Chemistry T. Claridge, 1999-12-24 From the initial observation of proton magnetic resonance in water and in paraffin, the discipline of nuclear magnetic resonance has seen unparalleled growth as an analytical method. Modern NMR spectroscopy is a highly developed yet still evolving subject which finds application in chemistry, biology, medicine, materials science, and geology. In this book, emphasis is on the more recently developed methods of solution state NMR applicable to chemical research which are chosen for their wide applicability and robustness. These have in many cases already become established techniques in NMR laboratories in both academic and industrial establishments. A considerable amount of information and guidance is given on the implementation and execution of the techniques described in this book.

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