Chapter XI
A Method of Estimation for Magnetic Resonance Spectroscopy Using Complex-Valued Neural Networks

Naoyuki Morita
Kochi Gakuen College, Japan

ABSTRACT

The author proposes an automatic estimation method for nuclear magnetic resonance (NMR) spectra of the metabolites in the living body by magnetic resonance spectroscopy (MRS) without human intervention or complicated calculations. In the method, the problem of NMR spectrum estimation is transformed into the estimation of the parameters of a mathematical model of the NMR signal. To estimate these parameters, Morita designed a complex-valued Hopfield neural network, noting that NMR signals are essentially complex-valued. In addition, we devised a technique called "sequential extension of section (SES)" that takes into account the decay state of the NMR signal. Morita evaluated the performance of his method using simulations and shows that the estimation precision on the spectrum improves when SES is used in combination the neural network, and that SES has an ability to avoid the local minimum solution on Hopfield neural networks.

INTRODUCTION

Magnetic resonance spectroscopy (MRS) is used to determine the quantity of metabolites, such as creatine phosphate (PCr) and adenocine triphosphate (ATP), in the living body by collecting their nuclear magnetic resonance (NMR) spectra. In the field of MRS, the frequency spectrum of metabolites is usually obtained by applying the fast Fourier transform (FFT) (Cooley & Tukey, 1965) to the NMR signal collected from the living

body. Then, quantification of the metabolites is carried out by estimating the area under each spectral peak using a curve fitting procedure (Maddams, 1980; Mierisová & Ala-Korpel, 2001; Sijens et al., 1998), as described in the **BACKGROUND** section. However, this method is not suitable for processing large quantities of data because human intervention is necessary. In this chapter, an automatic spectral estimation method, which we developed in order to process large quantities of data without human intervention, is presented.

This chapter is organized as follows: **BACKGROUND** reviews MRS and some conventional estimation methods of NMR spectra, and briefly outlines our method. **MATHEMATICAL MODEL OF THE NMR SIGNAL AND ESTIMATION OF SPECTRA** first, gives an overview of NMR phenomenon and NMR signal, next, presents a mathematical model of the NMR signal; and finally, describes our approach to spectral estimation. **DESIGN OF A COMPLEX-VALUED HOPFIELD NEURAL NETWORK AS A SPECTRAL ESTIMATIOR** describes the design of our complex-valued Hopfield neural network. **SEQUENTIAL EXTENSION OF SECTION (SES)** explains the concept of SES. For performance evaluation of our method, simulations were carried out using sample signals that imitate an actual NMR signal, and the results of those simulations are given in **SIMULATIONS**. The results are evaluated and discussed in **DISCUSSION**. Finally, we give some conclusions and future research directions.

BACKGROUND

Magnetic resonance imaging (MRI) systems, which produce medical images using the nuclear magnetic resonance (NMR) phenomenon, have recently become popular. Additional technological innovations, such as high-speed imaging technologies (Feinberg & Oshio, 1991; Henning, Nauerth, & Fnedburg, 1986; Mansfield, 1977; Melki, Mulkern, Panych, & Joles, 1991; Meyer, Hu, Nishimura, & Macovski, 1992) and imaging of brain function using functional MRI (Belliveau et al., 1991; Kwong et al., 1992; Ogawa, Lee, Nayak, & Glynn, 1990), are also rapidly progressing. Currently, the above-mentioned imaging technologies mainly take advantage of the NMR phenomena of protons. The atomic nuclei used for analyzing metabolism in the living body include proton, phosphorus-31, carbon-13, fluorine-19 and sodium-22. Phosphorus-31 NMR spectroscopy has been widely used for measurement of the living body, because it is able to track the metabolism of energy.

NMR was originally developed and used in the field of analytical chemistry. In that field, NMR spectra are used to analyze the chemical structure of various materials. This is called NMR spectroscopy. In medical imaging, it is also possible to obtain NMR spectra. In this case, the technique is called magnetic resonance spectroscopy (MRS), and it can be used to collect the spectra of metabolites in organs such as the brain, heart, liver and muscle. The difference between NMR spectroscopy and MRS is that in MRS, we collect spectra from the living body in a relatively low magnetic field (usually, about 1.5 Tesla); in NMR spectroscopy, small chemical samples are measured in a high magnetic field.

In MRI systems, the Fourier transform is widely used as a standard tool to produce an image from the measured data and to obtain NMR spectra. In NMR spectroscopy, we can obtain a frequency spectrum by applying the fast Fourier transform (FFT) to the free induction decay (FID) that is observed as a result of the magnetic relaxation phenomenon (Derome, 1987). Here the FID is an NMR signal in the time domain and it is a time series, that is, it can be modeled as a set of sinusoids exponentially damping with time. When the FFT is applied to such a signal, the spectral peaks obtained are of the form called a Lorentz curve (Derome, 1987). If the signal is damped rapidly, the height of the spectral peaks will be decreased and the width of the peaks will increase. This is an inevitable result of applying FFT to FIDs. In addition, the resolution of the spectrum collected in a low magnetic field is much lower than a typical spectrum obtained by NMR spectroscopy. Thus, the spectra by MRS are quite different from those by NMR spectroscopy. That is, the spectral peaks obtained by MRS are spread out and the spectral distribution obtained is very different from the original distribution as shown in Figure 1. Thus, we cannot use a peak height to quantify a metabolite. Instead, we estimate the area under each peak using curve-fitting procedures (Figure 1(d): non-linear least square methods) (Maddams, 1980; Mierisová & Ala-Korpela, 2001; Sijens et al., 1998). However, existing curve-fitting procedures are inadequate for processing large quantities of data because they require human intervention. The aim of us is to devise a method that does not require such a human intervention.

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