Transverse and Longitudinal Relaxation Time Distribution from Spin- echo Experiments Using Hopfield Neural Network

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Abstract: *The Hopfield neural network is proposed in this work to invert transverse and longitudinal relaxation time decay curve from spin-echo experiments. Simulated and experimental data were used to test the performance of this approach. The inverse Laplace transform, commonly used to address this problem, is used as the initial guess for the network. The probability density function can be used in a large variety of problems involving multiple sclerosis diagnostics or Portland cement studies, which will be discussed in the present work.*

Resumo: *A Rede neural de Hopfield é proposta neste trabalho para inversão da curva de decaimento do tempo de relaxação transversal e longitudinal a partir de experimentos de eco de spin. Dados simulados e experimentais serão usados para testar o desempenho do método. A transformada inversa de Laplace, geralmente selecionada para tratar este tipo de problema, é utilizada como valor inicial para a rede. A função densidade de probabilidade pode ser usada em diversos problemas, tais como, em diagnósticos de esclerose múltipla ou análise de cimento Portand, problemas a serem discutidos no presente trabalho.*

Introduction

Spatial inhomogeneity of the magnetic field causes individual precession frequency of the nuclear magnetization at each infinitesimal volume element. Spins interaction induces a rapid decay of the free induction signal,[1] which is avoided by multiple refocusing pulses. The resultant train of spin-echoes is denoted by the spin-echo experiment and can be used to calculate transverse longitudinal relaxation times by, for example, fitting the data to exponential functions. Nevertheless, we have used spin-echo data to recover the probability density function. This consists of an ill-conditioned inverse problem, and particular methods are required.[2,3,4] In the Hadamard sense,[5] the inverse problem is characterized by a solution that does not exist, is not unique or is not continuous. In this work, the Hopfield neural network will be applied to simulated and experimental data. During the inversion procedure, the multiple solution character of the problem and the ill-conditioned nature of the matrices will be emphasized.

Theoretical Background

The longitudinal, T_1, and transverse, T_2, relaxation times concept was established by Bloch in 1946 with the gyroscopic motion description.[6] Using this macroscopic model one can study the behavior of the spins when a magnetic field is applied. In the same volume element there is no variation of intensity, and the spatial inhomogeneity of the field has to be considered.[1] This will cause the neighboring elements to have slightly different intensity of the applied field, and the magnetization equation has to be considered as a sum of multiple T_2 components[7,8] :

(1) $$M_{xy} = \sum P(\lambda_i)\exp(-t\lambda_i)$$

with $\lambda_i = 1/T_2^{(i)}$ being the rate constant for each process and $P(\lambda_i)$ its corresponding probability. In the continuum limit for the transverse relaxation time and for the probability density function $f(\lambda)=P(\lambda)/\Delta\lambda$, one has[9]:

(2) $$g(t) = \int_a^b K(t,\lambda) f(\lambda) d\lambda$$

where *g(t)* is the spin-echo data and $K(t,\lambda)=\exp(-t\lambda)$. Equation (2) is also denoted as a Fredholm integral equation of first kind.[10,11]

For the longitudinal relaxation time, the kernel of the magnetization equation is represented by

(3) $$g(t) = (1-\exp(-t\lambda))$$

As in the transverse relaxation problem, spins interactions and the inhomogeneity of the magnetic field should be considered. In this sense, equation 3 can be rewritten[1] as:

$$g(t) = \int (1-\exp(-t\lambda)) f(\lambda) d\lambda$$, or,

(4) $$1 - g(t) = \int \exp(-t\lambda) f(\lambda) d\lambda$$

in which $\lambda=1/T_1^{(i)}$, $f(\lambda)$ the distribution function of the longitudinal relaxation time and *g*(t) the signal intensities.

Methodology

Calculation of density probability function, $f(\lambda)$, from the decay curve g(t) characterizes a set of problems denoted by ill-conditioned inverse problems, and requires special techniques for its solution.[2,3,4] In our work, the Hopfield recurrent neural network[4,12] was chosen. The Hopfield neural network consist of one recurrent layer network with fully connected neurons. The information in the network is propagated by the state activation of neurons, u_i, which is calculated by a weighted sum of all its inputs.[10,11,13] The activation function, $\phi(u_i(t))$ is chosen as an increasing function conform to the nervous impulse model.[4,12]

In a neural network approach, an energy function is defined,

(5) $$E = \frac{1}{2}\sum_{j=1}^{m}((\sum_{i=1}^{n} K_{ij} f_i) - g_j)^2$$

with $f_i=\phi(u_i(t))$, *n* the number of points used to represent (2) and *m*, the number of available experimental data.

The convergence criteria is established by imposing the condition,

(6) $$\frac{du_i}{dt} = -\frac{\partial E}{\partial f_i}$$

and the stable state, **f**, that minimizes $\|\mathbf{Kf}-\mathbf{g}\|_2^2$ is reached.

In this sense, the time evolution of the neurons is given by:

(7) $$\frac{du_i}{dt} = \sum_{n}^{j=1} T_{ij} f_j + I_i$$

with,

$$T_{ij} = -\sum_{n}^{l=1} K_{li} K_{lj} = T_{ji} \qquad I_i = \sum_{n}^{j=1} K_{ji} g_j$$

This equation has to be integrated until an establishment of the equilibrium is reached[14], which corresponds to a solution **f** of the problem. The multiple solution character of the ill-posed problem can be observed along the integration procedure. If the output error is within experimental error, the experimentalist can decide on the right solution, based, for example, on the relative areas and position of the components.

Results and Discussion

T_2 Relaxation Time Distribution

The Laplace transform of the probability density function, equation 2, is used to represent the signal intensity, *g(t)*, measured at echoes time, *t*. These data of the T_2 decay curve[7,15] were generated by the bi-exponential function:

(8) $$g(t) = 850 * \exp(-t/120) + 150 * \exp(-t/30)$$

These simulated data is shown in Figure (1). The system of differential equations, Eq. 7, requires an initial condition to be solved. In this sense, the **f** function for initial guess was calculated by the analytical inverse Laplace transform[13,16,17],

(9) $$f(\lambda) = \lim_{k\to\infty} \sum_{i=1}^{2} \frac{(-1)^{2k}}{k!} \alpha_i^k A_i \exp(-\alpha_i \frac{k}{y}) \left(\frac{k}{y}\right)^{k+1}$$

The constants A_i and α_i are respectively the amplitudes and rate constants used in equation (8) and y the inverse of the transverse relaxation time. Numerical integration of the direct problem, with k=30 in equation 9 was performed[14] recovering the synthetic data with seven significant figures. The matrices of $\mathbf{Kf} = \mathbf{g}$ problem were calculated in a rectangular representation with *n*=32 and 16 data points.

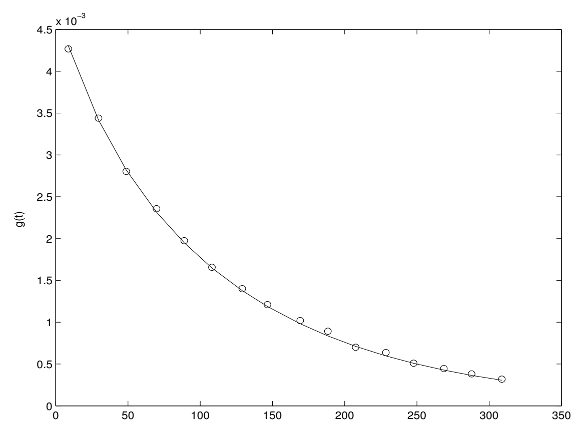

Figure 1. Bi-exponential T_2 decay curve.

In the representation procedure of equation 2, the size of the sub-spaces involved in the problem is established, since $K \in R^{mxn}$, $f \in R^n$ and $g \in R^m$.[3,12] This base size gives a residual error of eight significant figures in comparison with the data given by Equation 8. Figure 2 shows the distribution function obtained in the inversion of the simulated data. Integration of equation (7) was stopped at a point in which the residual error,

(10) $$\left\|\mathbf{Kf} - \mathbf{g}\right\|_2^2$$

reached a desired tolerance.

Errors of about 20% were considered in the initial guess. The neural network results are still in reasonable agreement with the Eq. 9 function, presenting the transverse relaxation time distribution with two peaks in the same positions. At 30% of error in the initial guess, the smallest peak in the probability density function is slightly changed. Another analysis was made including 20% of error in the simulated data of the T_2 decay curve. In this case, although the solution presents negative numbers, the two peaks in the right position were also recovered.

This inversion procedure of the experimental T_2 decay data can be used in multiple sclerosis diagnostics.[13] As multiple sclerosis (MS) lesions have intrinsic increased transverse relaxation times in comparison with the surrounding white matter, this experiment can distinguish MS lesions from the normal white matter using these T_2 relaxation properties.

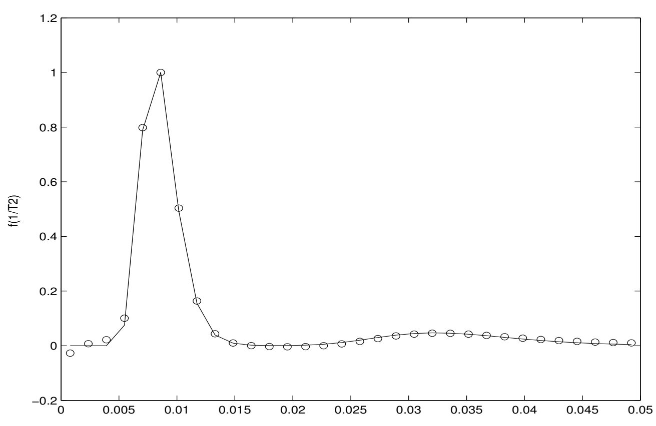

Figure 2. State of the neurons (bullet) and density function of Eq. 9 (line). Simulated data was used.

T_1 Relaxation Time Distribution

In this work, experimental data of longitudinal relaxation decay curve for Portland cement was considered, and we also used the inverse Laplace transform. Equation 4 was used to deal with the experimental data, and the base size chosen has 128 data points and n=264. The experimental data and the recovered data in the direct problem, $\mathbf{Kf} = \mathbf{g}$, is shown in Figure 3.

The magnetization recovery, determined by the Inversion-Recovery experiment, is an increasing curve. Figure 3 displays the “mirror image” of the experimental data around the x-axis.

The longitudinal relaxation time distribution obtained by the inversion procedure is shown in Figure 4. The inverse Laplace transform was used as the initial guess by the Hopfield neural network. At this point, it is important to note the decreasing energy property of the neural network.

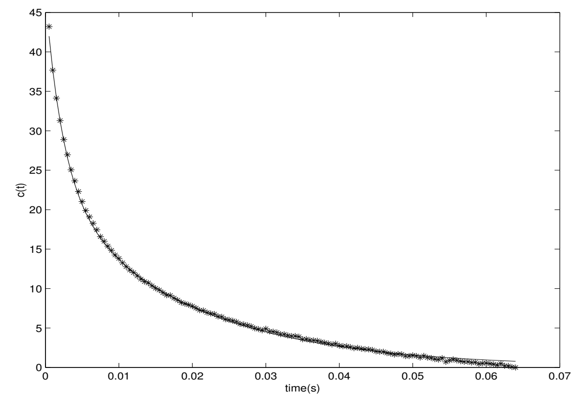

Figure 3. Experimental data (*) and recovered data (full line) in the direct problem.

Since the inverse Laplace transform is given as the initial guess for the network, it will be improved and the neural network results will have a smaller residual error. In Table 1 the residual errors and peak position of each distribution are displayed.

Table 1. Residual errors and peak positions of the distribution functions.

	Inverse Laplace transform	Hopfield neural network
Residual errors $\left\| \mathbf{Kf} - \mathbf{g} \right\|_2^2$	3.185	2.955
Peak position	0.0197	0.0197
T_1(s)	0.0026	0.0031

Another analysis was made considering a null initial guess, which corresponds to $\phi(u_i(t))=0$ for all the neurons.

The distribution function retrieved by the network is similar to the obtained by the network in Figure 4. But, in this case, no information *a priori* is given. The multiple solution character of the inverse problem is also an important consideration.

Although the neural network solution has a smaller residual error; the most appropriate solution has to be determined together with the chemical information of the problem.

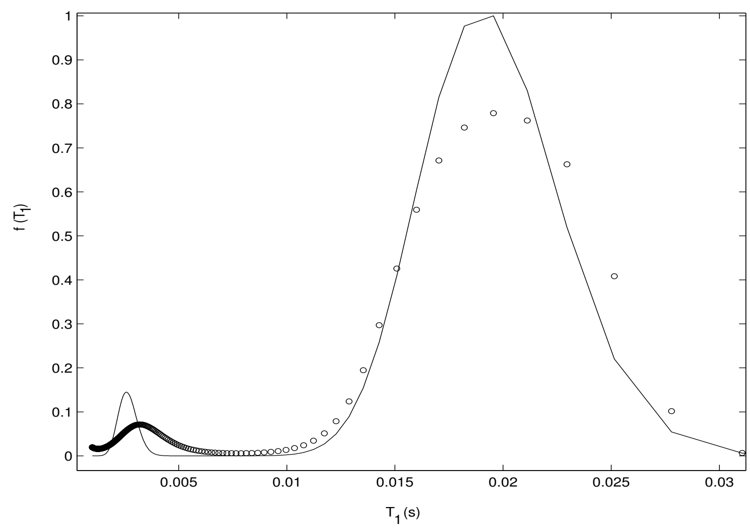

Figure 4. Longitudinal relaxation time distribution obtained by ILT (full line) and the HNN (bullets).

Conclusions

Recovering the transverse and longitudinal relaxation time distribution from spin-echo data is indeed, an ill-posed problem. The results obtained were in excellent agreement with the experimental data in the direct problem, confirming the usefulness of the method. The use of the recurrent neural network is attractive for its efficiency and simplicity. The theory and numerical background requires only elementary concepts. Also, the computer code developed is very short. Except for the integration routine, the code has about 100 lines and is very simple to use.

The inverse Laplace transform as the initial guess proved to be appropriate. The recurrent neural network, due to its property of decreasing energy, improves the initial condition, generating a distribution function with lower residual error.

The methodology used here is not restricted to characterizing MS lesions or Portland cement analysis, but can be used to determine the transverse and longitudinal relaxation time distribution from the spin-echo data in a wide variety of systems.[9,12,13]

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