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Nonlinear Identification of NMR Spin Systems by Adaptive Filtering

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In this paper, we present two new methods for identifying NMR spin systems. These methods are based on nonlinear adaptive filtering. The spin system is assumed to be time-invariant with memory. The first method uses a truncated discrete Volterra series to describe the nonlinear relationship between excitation (input) and system response (output). First-, second-, and third-order kernels of this series are estimated employing the least mean square (LMS) algorithm. Three parallel filters can then model the NMR spin system so that its output is no more than simple sum of three convolution products between combinations of the input signal and filters coefficients. It is also shown that the contribution of the Volterra second-order term to the total system response is neglected compared with the contributions of the first- and the third-order terms. In the second identification method, the output signal is related to the input signal through a recursive nonlinear difference equation with constant coefficients. The LMS algorithm is used again to estimate the equation coefficients. The two methods are validated with a simulated NMR system model based on Bloch equations. The results and the performances of these methods are analyzed and compared. It is shown that our methods permit a simple identification of NMR spin systems. The field of applications of this study is promising in the optimization of NMR signal detection, especially in the cases of low signal-to-noise ratios where optimum signal filtering and analysis must be performed.

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Key Words: **NMR; system identification; nonlinear adaptive filtering; Volterra series; recursive nonlinear filter.**

1. INTRODUCTION

Due to the nonlinear characteristics of the NMR spin system, there is no general way to deduce the system response $y(t)$ to an arbitrarily shaped excitation pulse $x(t)$. A variety of methods have been proposed to solve the problem. Hoult (*1*) used perturbation theory and linear system analysis to obtain an analytical solution for the Bloch equations. In his arguments and calculations, concerning the case where a strong gradient is applied to the object, he assumed that the transfer function of the system was flat over the spectral bandwidth of the excitation signal. If this is not the case, the method cannot be applied directly.

Other methods, using a functional expansion, like the Volterra series, to describe the relation between excitation and the nonlinear behavior of the system have appeared (*2, 3*). The system response can, in principle, be written as

$$y(t) = \sum_{p=0}^{\infty} \int_0^{\infty} \cdots \int_0^{\infty} h_p(\tau_1, \ldots, \tau_p) \times x(t-\tau_1) \ldots x(t-\tau_p) d\tau_1 \ldots d\tau_p. \quad [1]$$

The p-dimensional time functions $h_p(\tau_1, \tau_2, \ldots, \tau_p)$ are called Volterra kernels and describe the system characteristics. Since the Volterra series of Eq. [1] does not lead to orthogonal expansion, the estimation of Volterra kernels from a given excitation–response data set is far from trivial (*3, 4*).

Blümich and Ziessow (*2*) proposed an expansion of the nonlinear system response into a functional integral series with heuristic ansatz for the Volterra kernels. They deduced that the NMR system is equivalent to two parallel linear bandpass filters with memory followed by a nonlinear system without memory. This system can represent a nonlinear infinite impulse response filter (IIR) which depends on the excitation nature.

Kaulisch *et al.* (*3*) used the fact that the Volterra series can be orthogonalized in a Wiener series if the excitation is a Gaussian white noise of zero mean and he calculated the Wiener kernels employing a cross-correlation technique. All of his calculations were conducted on complex stochastic excitation.

In the search for optimum NMR signal detection and processing, it can be of great value to introduce the nonlinear characteristics of NMR spin systems. In fact, when the signal-to-noise ratio is low, optimum filters are necessary to extract the NMR signal. Actually, most of the NMR signal processing systems employ linear filters. Increasing excitation levels may produce distorted spectrum resulting from linear processing of a nonlinear spin response. So, in order to optimize NMR signal detection and analysis, it is useful to consider nonlinear filters. The implementation of such filters requires knowledge of the nonlinear behavior of the system. Moreover, more accurate signal spectral analysis can be conducted if one could identify, in a practical manner, the system under investigation.

In this paper, we propose two new methods for the identi-

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fication of NMR spin systems. These methods are based on nonlinear adaptive filtering techniques. In the first method, the input–output relationship of the NMR system is described by a truncated discrete Volterra series. The first three kernels of this series are estimated. The contribution of each term of the Volterra series to the total system response is illustrated. It is shown that the second-order contribution is neglected. In the second identification method, we use a recursive nonlinear infinite impulse response filter to model the NMR spin system. In this latter case, system identification is equivalent to the estimation of the IIR filter coefficients.

The validity of the two methods is demonstrated with simulated NMR signals. The advantages and the limits of each method are analyzed. Our future work will validate these identification approaches on real NMR signals.

2. NMR SIMULATED SIGNALS

2-1. Simulation Method

Many articles concerning the computer simulation of NMR images have been published (*5–9*). The basic idea of simulation is to solve numerically the Bloch equations, in the rotating frame, for each point (voxel) in the object, at each sample in time during the pulse sequence. This method is valid for describing the time evolution of spin systems. In our paper, we are limited to NMR signal simulation in the case of uncoupled spins (*5–9*).

Our simulation program starts by defining an object (1D, 2D, or 3D) using a special computer function that creates a box, a sphere, a cylinder, or any shape given by mathematical expression. This object is spatially sampled, with respect to Shannon's sampling theorem, into small volumes (voxels) with defined dimensions, local magnetization vector, proton density, and longitudinal and transversal relaxation times (T_1 and T_2). Static magnetic field inhomgeneities and chemical shifts can be included in the object definition.

The effect of a rectangular RF pulse on a local magnetization vector is described by a rotation matrix operator with the knowledge that relaxation is neglected during the excitation period (*5–10*). This operator can also take into account the presence of magnetic field gradients. RF pulses, with varying B_1 field, are modeled by dividing the waveform of the pulse into finite samples in time (small rectangular pulses with different intensities). Each sample is described by its rotation matrix. These matrix operators are applied successively to the magnetic moment, so that the set is quite similar to the application of one pulse with amplitude modulation. Any amplitude modulated RF pulse can be simulated by this technique. Four different types of RF pulses are currently available: rectangular, Gaussian-modulated, sinc-modulated, and random noise modulated pulses. Each of them is defined by its duration, central frequency, spectral bandwidth, phase, and flip angle. In our identification methods (see Sections 4, 5, and 6), a 90° sinc-modulated RF pulse of 1 ms is used as an excitation signal.

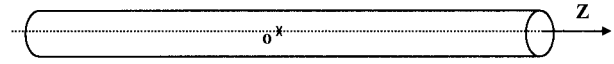


FIG. 1. A 1D cylindrical homogeneous object 25 cm in length. The longitudinal and the transversal relaxation times are, respectively, $T_1 = 100$ ms, $T_2 = 10$ ms for all the object voxels.

Relaxation operators are applied to calculate the results of the relaxation processes (T_1 and T_2) and the changes in the phase of the magnetization, due to applied magnetic field gradients, local magnetic field inhomogeneities, and chemical shifts.

All of the routines of signal simulation are written in C language using the LINUX operating system. The simulation generates a signal (free induction decay, FID) by summing the transverse magnetization of all of the object points at discrete time intervals determined by the sampling rate. This simulated signal is detected in the rotating frame of reference. In our simulations, the input and the output signals are normalized with respect to their maximum amplitudes.

2-2. Examples of Simulated Signals

We consider, for simplicity, a 1D finite cylindrical homogeneous object of axis OZ (Fig. 1). The transversal and the longitudinal relaxation times, T_2 and T_1, are, respectively, 10 and 100 ms, for all the object voxels. This object is placed in a 0.1-T static magnetic field. We neglect the effect of local magnetic field inhomogeneities and chemical shifts.

As an illustration of the simulated (FID) signals, let us take the case where a strong linear field gradient (2.5 mT/m) is applied along the cylinder axis during a RF excitation pulse (*1*). We calculate the FID in unswitched gradient, i.e., the gradient is still applied during the signal sampling period (*1, 10*). Figure 2a shows the system response (FID) to a 1-ms RF rectangular pulse of 4.25 MHz (Larmor frequency at 0.1 T) with a flip angle of 90°. It can be seen that the form of the response approaches the shape of the RF excitation pulse. This result confirms the early work of Hoult and Mansfield and Morris (*1, 10*). In Fig. 2b, we plotted the FID resulting from the application of a 90° sinc-modulated RF pulse of 1 ms. This latter FID is used as a reference signal in our identification schemes (see Sections 4, 5, and 6).

3. IDENTIFICATION BY ADAPTIVE VOLTERRA FILTERING

3-1. Volterra Series Expansion for Nonlinear Systems

Let $x(n)$ and $y(n)$ represent the input and the output, respectively, of a discrete-time and causal nonlinear system with memory. The relationship between input and output can be, generally, expressed as

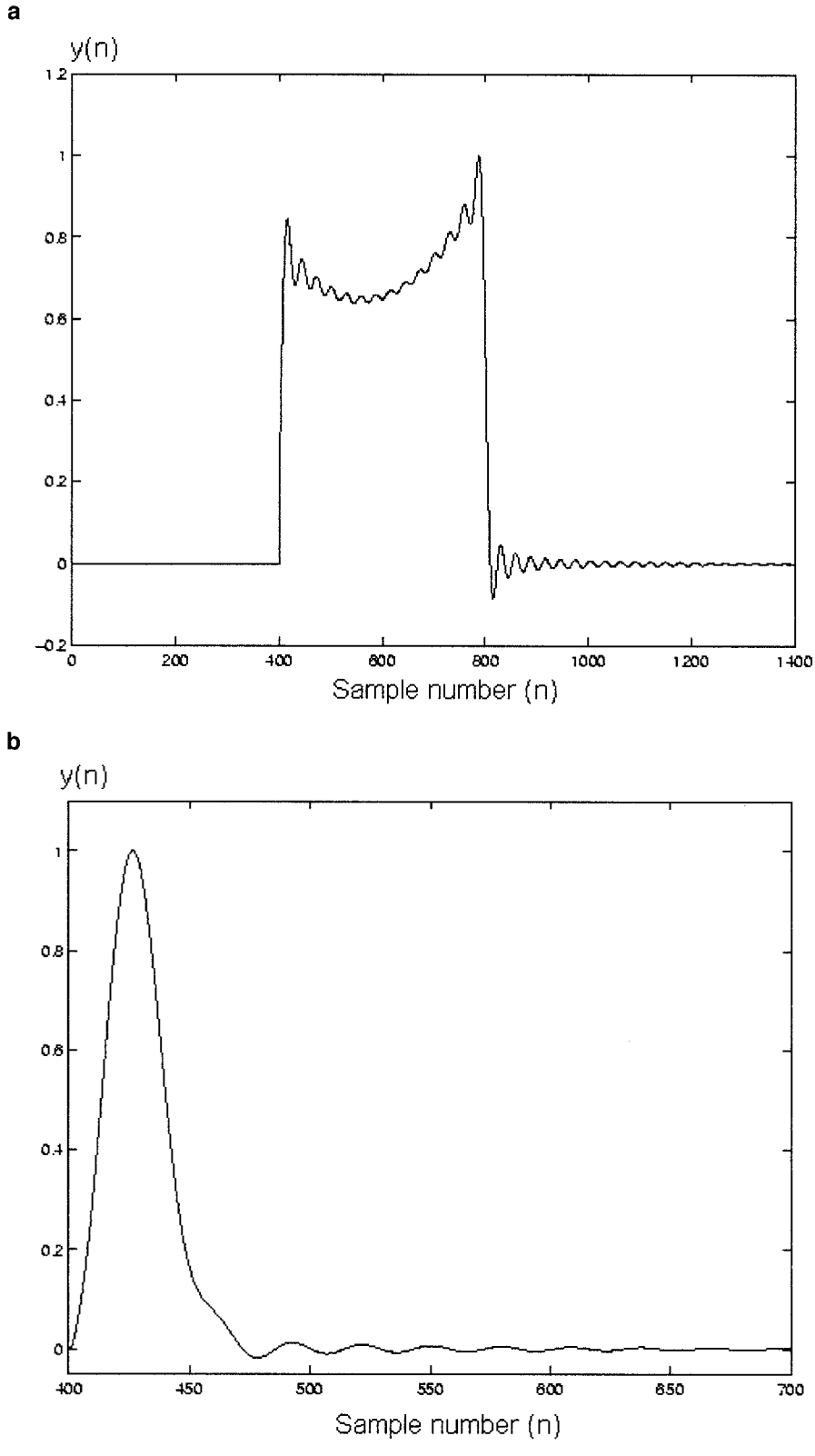


FIG. 2. Simulated FIDs signals $y(n)$ in response to a 90° rectangular RF pulse of 1 ms (a) and to a 90° sinc RF pulse of 1 ms (b). On the X-axis, 400 samples = 1 ms.

$$y(n) = f[x(n), x(n-1), \ldots, x(n-N+1)], \quad [2]$$

where (n) is the sample number and N is the memory length of the system. The direct identification approach of a system is to determine the function f that minimizes some suitable defined error between a desired output sequence $y(n)$ and the actual output sequence $\hat{y}(n)$. However, for nonlinear systems, this approach leads generally to equations that cannot be solved in any practical manner, which is the case for NMR spin systems.

A solution for this problem is to consider a polynomial approximation to the function appearing in Eq. [2] so that the system under investigation can be easily characterized and analyzed.

Consider the input–output relationship of Eq. [2]. We assumed that the function f is sufficiently regular in the neighborhood of the origin. In this case f admits a discrete Volterra series expansion which converges in a suitable neighborhood of the origin (*11*). By truncating this series to a finite number of terms, we obtain an approximation of the input–output relationship of the form

$$\begin{aligned}\hat{y}(n) = &\sum_{m_1=0}^{N-1} \hat{h}_1(m_1)\, x(n-m_1) + \sum_{m_1=0}^{N-1}\sum_{m_2=0}^{N-1} \hat{h}_2(m_1, m_2) \\ &\times x(n-m_1)\, x(n-m_2) + \ldots \\ &+ \sum_{m_1=0}^{N-1}\sum_{m_2=0}^{N-1} \ldots \sum_{m_p=0}^{N-1} \hat{h}_p(m_1, m_2, \ldots, m_p) \\ &\times x(n-m_1)\, x(n-m_2) \ldots x(n-m_p). \end{aligned} \quad [3]$$

In this equation, $\hat{h}_p(m_1, m_2, \ldots, m_p)$ is the pth-order discrete Volterra kernel of the system. System identification is equivalent to the choice of these kernels which in turn characterize the system behavior. We can have the desired degree of accuracy by a suitable choice of the order p as well as system memory length N.

We assume, in the next section, that the Volterra kernels are symmetric, i.e., $h_p(m_1, m_2, \ldots, m_p)$ is left unchanged for any of the possible $(p!)^2$ permutations of the indices $m_1, m_2, \ldots, m_p$ (*12*). This does not entail any loss of generality, but the complexity of Eq. [3] is reduced, especially in the case of high-order kernels ($p \geq 3$), and consequently the calculation time is considerably reduced.

3-2. System Identification by Second-Order Volterra Series

For calculation simplicity and without loss of generality, let us consider, for the first time, a second-order ($p = 2$) Volterra series expansion. The choice of the memory length N will be discussed latter. Our goal now is to identify the first- and the second-order kernels employing adaptive filtering techniques.

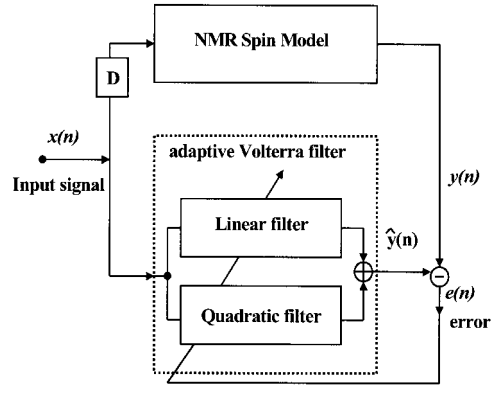


FIG. 3. Block diagram of second-order nonlinear adaptive identification. D is a delay element.

Figure 3 shows the identification block diagram. The delayed input signal $x(n)$ is applied to the system under investigation which gives the reference signal $y(n)$. The adaptive filter would try to estimate the desired response signal $y(n)$ using a second-order truncated Volterra series expansion in the input signal $x(n)$ as

$$\begin{aligned}\hat{y}(n) = &\sum_{m_1=0}^{N-1} \hat{h}_1(m_1{:}n)\, x(n-m_1) \\ &+ \sum_{m_1=0}^{N-1}\sum_{m_2=m_1}^{N-1} \hat{h}_2(m_1, m_2{:}n)\, x(n-m_1)\, x(n-m_2). \end{aligned} \quad [4]$$

$\hat{h}_1(m_1{:}n)$ and $\hat{h}_2(m_1, m_2{:}n)$ in Eq. [4] are the adaptive filter coefficients at time (n). These coefficients are iteratively updated at each time so as to minimize some function of the quadratic error signal defined as

$$e^2(n) = |y(n) - \hat{y}(n)|^2. \quad [5]$$

For notational simplicity as well as ease of performance analysis, it is usual to rewrite the expression of $\hat{y}(n)$ in another form using vector notations[3] (*12*).

$$\hat{y}(n) = \hat{H}_1^{\mathrm{T}}(n)\, X_1(n) + \hat{H}_2^{\mathrm{T}}(n)\, X_2(n), \quad [6]$$

where $\hat{H}_1(n)$ is the coefficient vector of the first-order kernel (linear filter) and $\hat{H}_2(n)$ is the coefficient vector of the second-order kernel (quadratic filter) at time (n):

[2] ! Denotes the factorial function.

[3] $[.]^{\mathrm{T}}$ denotes matrix transpose.

$$\hat{H}_1(n) = [\hat{h}_1(0{:}n),\ \hat{h}_1(1{:}n),\ \ldots,\ \hat{h}_1(N-1{:}n)]^{\mathrm{T}} \quad [7]$$

$$\hat{H}_2(n) = [\hat{h}_2(0,\ 0{:}n),\ \hat{h}_2(0,\ 1{:}n),\ \ldots,\ \hat{h}_2(0,\ N-1{:}n),\ \hat{h}_2(1,\ 1{:}n),\ \ldots,\ \hat{h}_2(N-1,\ N-1{:}n)]^{\mathrm{T}}. \quad [8]$$

$X_1(n)$ and $X_2(n)$ are the input vectors to the adaptive filter at time (n). They are defined as

$$X_1(n) = [x(n),\ x(n-1),\ \ldots,\ x(n-N+1)]^{\mathrm{T}} \quad [9]$$

$$X_2(n) = [x^2(n),\ x(n)x(n-1),\ \ldots,\ x(n)x(n-N+1),\ x^2(n-1),\ x(n-1)x(n-2),\ \ldots\ x^2(n-N+1)]^{\mathrm{T}}. \quad [10]$$

At each time (n), optimum coefficients are determined using a least mean squares algorithm (LMS). This recursive algorithm permits one to calculate new coefficients at time $(n+1)$. The initial coefficients values at $(n=0)$ are forced to zero. The nonlinear adaptive filter is then defined by three recursive equations (*12, 13*):

$$e(n) = y(n) - \hat{H}_1^{\mathrm{T}}(n)\,X_1(n) - \hat{H}_2^{\mathrm{T}}(n)\,X_2(n) \quad [11]$$

$$\hat{H}_1(n+1) = \hat{H}_1(n) + \delta_1 X_1(n) e(n) \quad [12]$$

$$\hat{H}_2(n+1) = \hat{H}_2(n) + \delta_2 X_2(n) e(n). \quad [13]$$

In these equations, δ_1 and δ_2 are positive constant factors (called adaptive gains) that control the stability of the adaptive filter and its rate of convergence. If we define σ_x^2 as an input signal power, it could be shown that the stability of the adaptive filter can be assured if δ_1 and δ_2 satisfy (*13*)

$$0 < \delta_1 < \frac{2}{N\sigma_x^2} \quad [14]$$

$$0 < \delta_2 < \frac{2}{(N\sigma_x^2)^2}. \quad [15]$$

In the next section, we will use the adaptive Volterra filter to model the NMR nonlinear system.

4. NMR SYSTEM IDENTIFICATION BY SECOND-ORDER VOLTERRA ADAPTIVE FILTERING

The recursive algorithm needs some attentions in the choice of its parameters like the adaptive filter order N (the memory length) and the adaptive gains (δ_1 and δ_2). These parameters control, in addition to the stability, the accuracy of the results during the convergence of the algorithm.

4-1. Choice of δ_1 and δ_2 for NMR Signals

In NMR, the input signal $x(n)$ and the output signal, $y(n)$ of the system are, in general, nonstationary. The stability of the adaptive filter depends largely on σ_x^2, i.e., it depends on δ_1 and δ_2 (see Eqs. [14] and [15]). When using fixed values for δ_1 and δ_2, instability appears for impulsive input signals. To prevent this phenomenon, we consider variable δ_1 and δ_2 of the form

$$\delta_1(n) = \frac{\beta_1}{N\sigma_x^2(n)} \quad [16]$$

$$\delta_2(n) = \frac{\beta_2}{(N\sigma_x^2(n))^2}. \quad [17]$$

β_1 and β_2 are small positive constant factors. $\sigma_x^2(n)$ is an estimation of the input signal power at time (n). The most direct estimation of $\sigma_x^2(n)$ is given by (*13*)

$$\sigma_x^2(n) = \sigma_0 + \frac{1}{N_0}\sum_{i=0}^{N_0-1} x^2(n-i), \quad [18]$$

where σ_0 is a positive constant which avoids division by zero. The parameter N_0, time observation window, is the period during which the signal could be considered stationary.

4-2. Identification Results

The adaptive identification algorithm is programmed using MATLAB. As an illustration of the identification results, let us consider the object described in Fig. 1. The input signal $x(n)$ is a 90° sinc pulse of 1 ms. The correspondent output signal $y(n)$ is the one shown in Fig. 2b. The convergence of the algorithm is obtained rapidly with a suitable choice of the parameters β_1, β_2, N_0, and σ_0. For example, $\beta_1 = 0.25$, $\beta_2 = 0.0025$, $\sigma_0 = 0.08$, and $N_0 = 20$ are chosen, in the case of $N = 64$, to assure convergence and to have a minimum residual mean-square error (MSE). We introduce a delay element (D) in the identification block diagram (Fig. 3) for convergence rapidity and results enhancement (*14*). The value of D depends on the filter order N and on the model to estimate. For $N = 64$ the delay element is of 200 samples. An estimation of the first- and the second-order kernels is then obtained. These kernels are plotted in Figs. 4a and 4b for two values of the filter order ($N = 64$ and 128). In the two cases, the first-order kernel is a FID-like function, which is a well-known result (*2, 4*). The real and the imaginary parts of the Fourier transform of this kernel are proportional, respectively, to the absorption and the dispersion components (see Fig. 5).

4-3. Choice of the Filter Order N

After convergence of the adaptive algorithm, the two resulting kernels are the best description of the NMR model in the sense of the mean-square error. In this case, only the

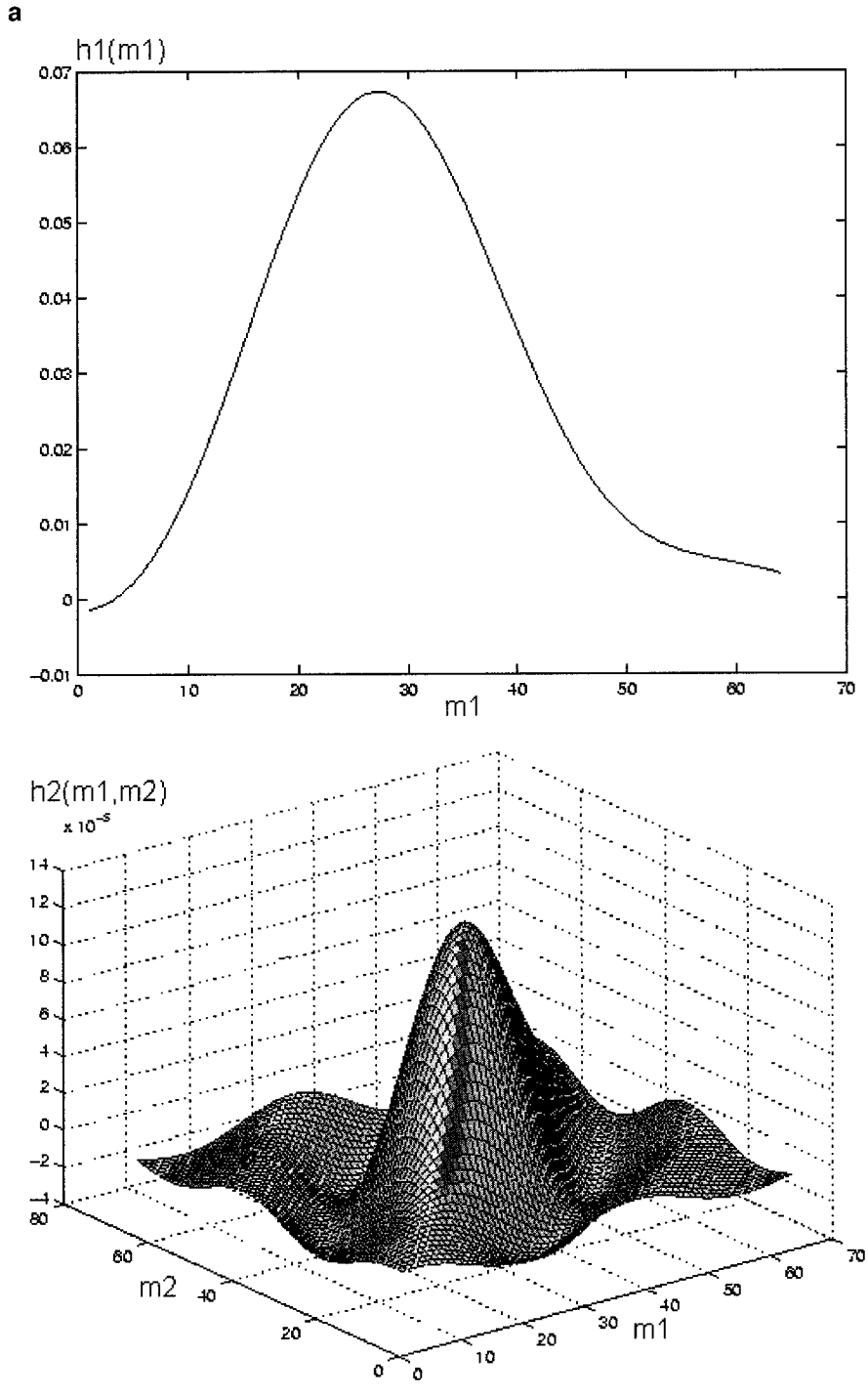
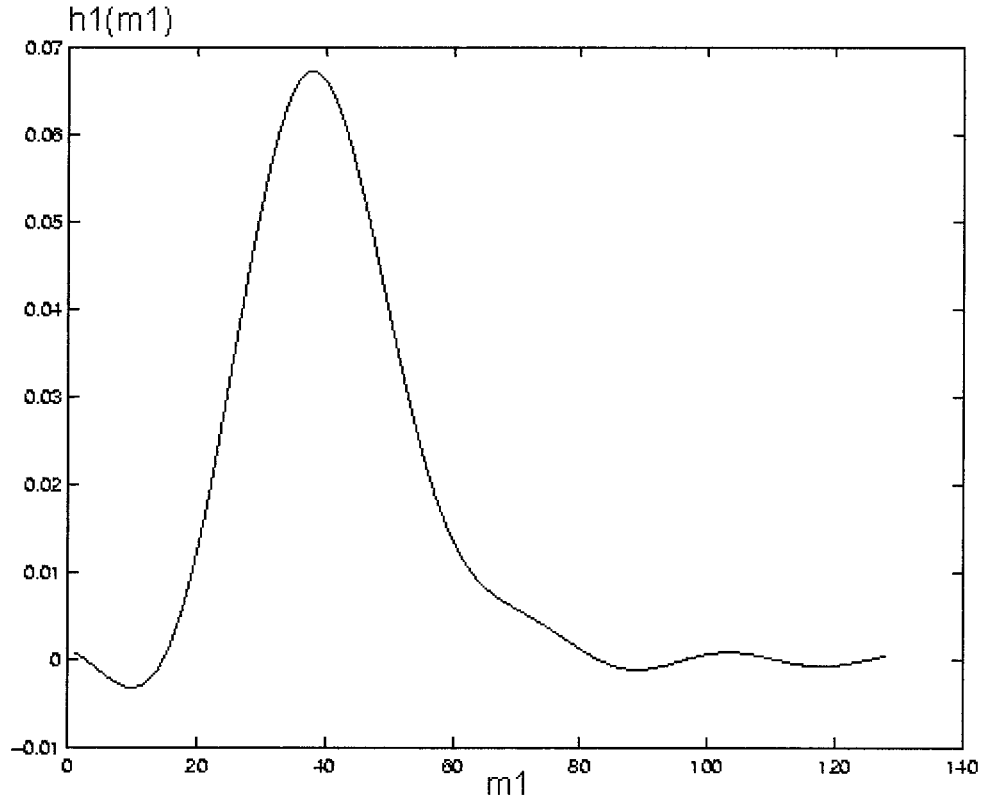


FIG. 4. (a) The first- and the second-order kernels, $h_1(m_1)$ and $h_2(m_1, m_2)$, for $N = 64$. (b) The first- and the second-order kernels, $h_1(m_1)$ and $h_2(m_1, m_2)$, for $N = 128$.

filter order N controls the accuracy of results. This parameter is chosen to minimize the residual MSE after convergence. We show in Fig. 6 the variation of the minimum residual MSE, averaged over the last 100 samples, as a function of N. We observe that for N larger than 64 the residual mean-square error is practically unchanged. The filter order should be greater than the effective transversal relaxation time T_2^* divided by the sampling period T_e:

$$N > \frac{T_2^*}{T_e}. \qquad [19]$$

b



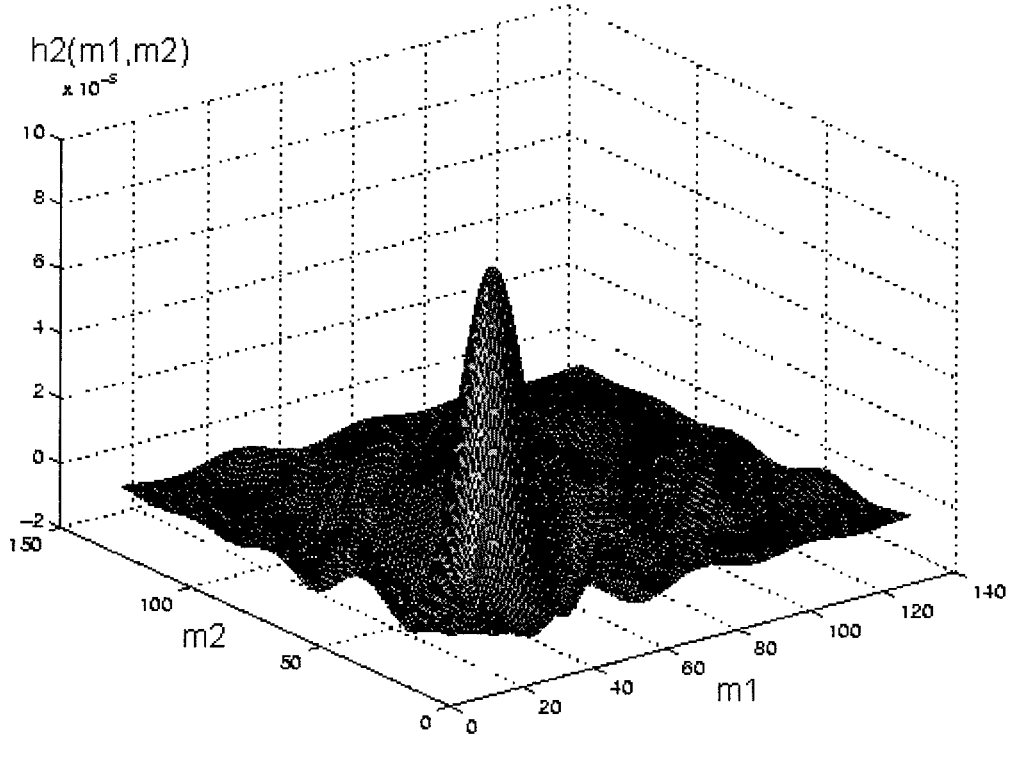


FIG. 4—*Continued*

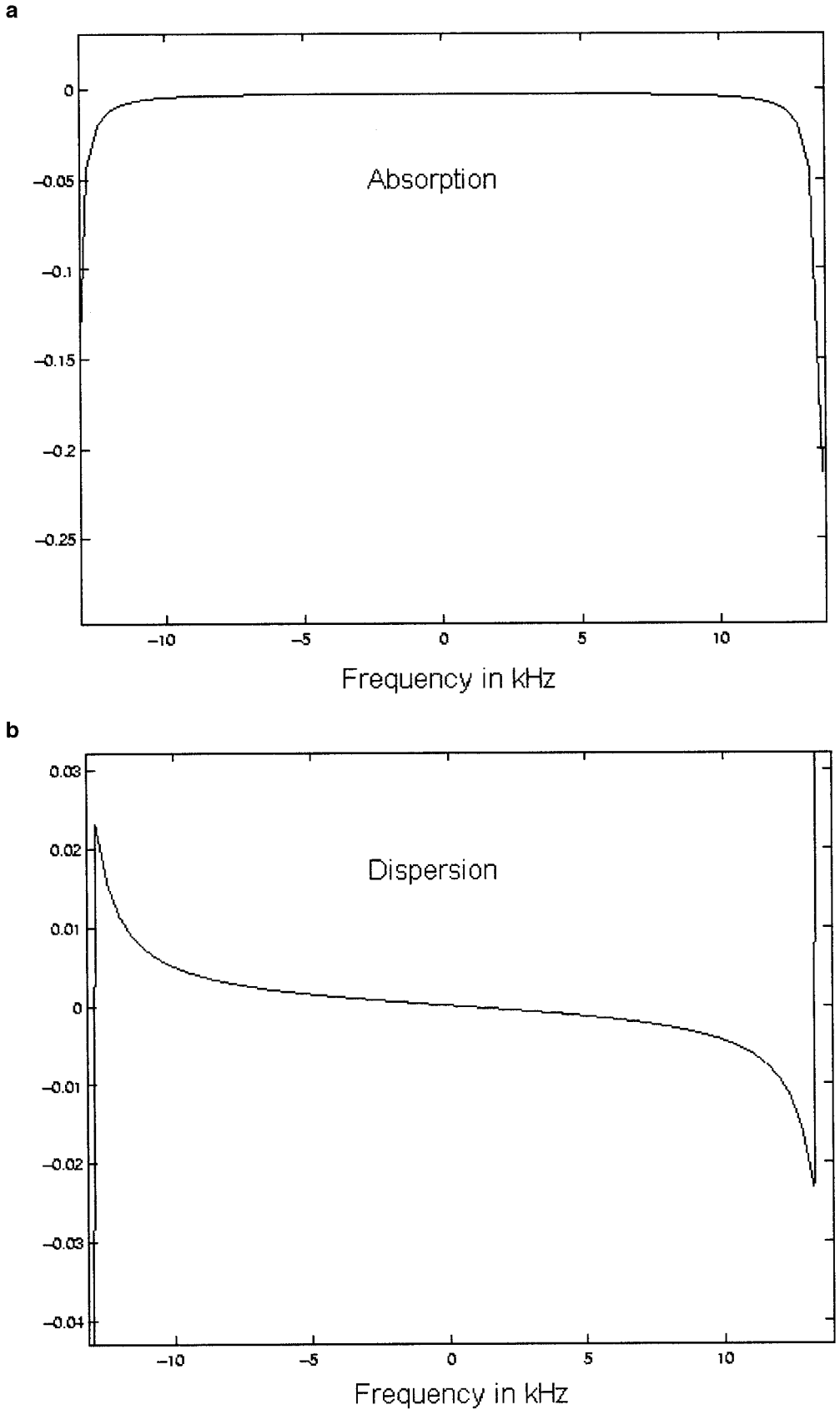


FIG. 5. The real (absorption) and the imaginary (dispersion) parts of the Fourier transform of the first-order kernel for $N = 64$.

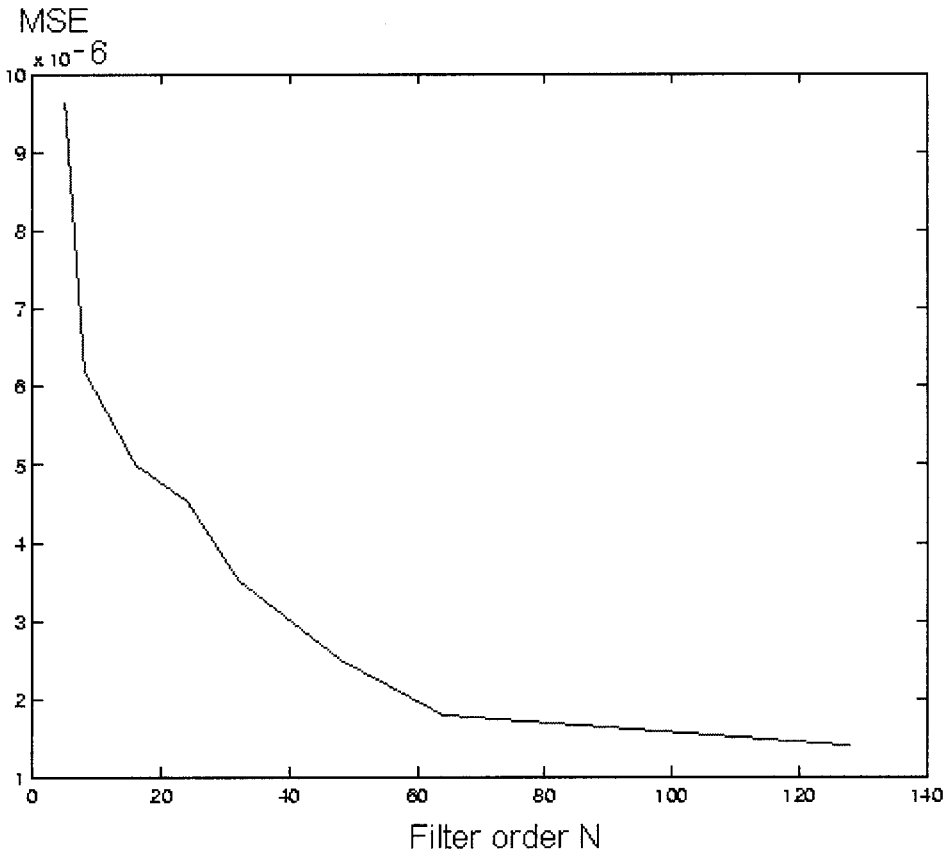


FIG. 6. The residual mean-square error (MSE) as a function of the filter order N.

This result assumes that the period of the input signal is greater than four times T_2^*. Once noncorrelated experimental noise is present, the accuracy of the results is expected to improve with N increasing beyond 64.

4-4. Discussion

We show that the NMR system can be modeled by a linear filter in parallel with a quadratic filter with no feedback as that of Blümich and Ziessow's model (*2*). This model is tested by applying an excitation signal $x(n)$ (a 90° sinc RF pulse of 1 ms) to the filters system input. The resulting output signal for $N = 64$ is shown together with the reference signal $y(n)$ in Fig. 7. The best accuracy can be obtained for higher filter orders.

It is important to evaluate here the contribution of each filter, i.e., the linear part and the quadratic part. The results are presented in Fig. 8. We can see that the contribution of the second-order filter, in the system response, is small with respect to the contribution of the linear filter. In fact, in NMR, since the response changes sign when the RF excitation is changed in sign, the response is an odd function of the excitation, and all even-order responses of Volterra series disappear (*4*). However, in our identification, the truncation of the Volterra series leads to some contribution of the second order in the system response. In order to emphasize this fact and to have more accurate results, we extend our development to the third order.

5. NMR SYSTEM IDENTIFICATION BY THIRD-ORDER VOLTERRA ADAPTIVE FILTERING

When we take into account the third-order kernel in the Volterra series, Eq. [3] becomes

$$\begin{aligned}\hat{y}(n) = &\sum_{m_1=0}^{N-1} \hat{h}_1(m_1{:}n)\, x(n-m_1) \\ &+ \sum_{m_1=0}^{N-1}\sum_{m_2=m_1}^{N-1} \hat{h}_2(m_1, m_2{:}n)\, x(n-m_1)\, x(n-m_2) \\ &+ \sum_{m_1=0}^{N-1}\sum_{m_2=m_1}^{N-1}\sum_{m_3=m_2}^{N-1} \hat{h}_3(m_1, m_2, m_3{:}n) \\ &\times x(n-m_1)\, x(n-m_2)\, x(n-m_3). \qquad [20]\end{aligned}$$

Consequently, the third-order nonlinear adaptive filter is defined by

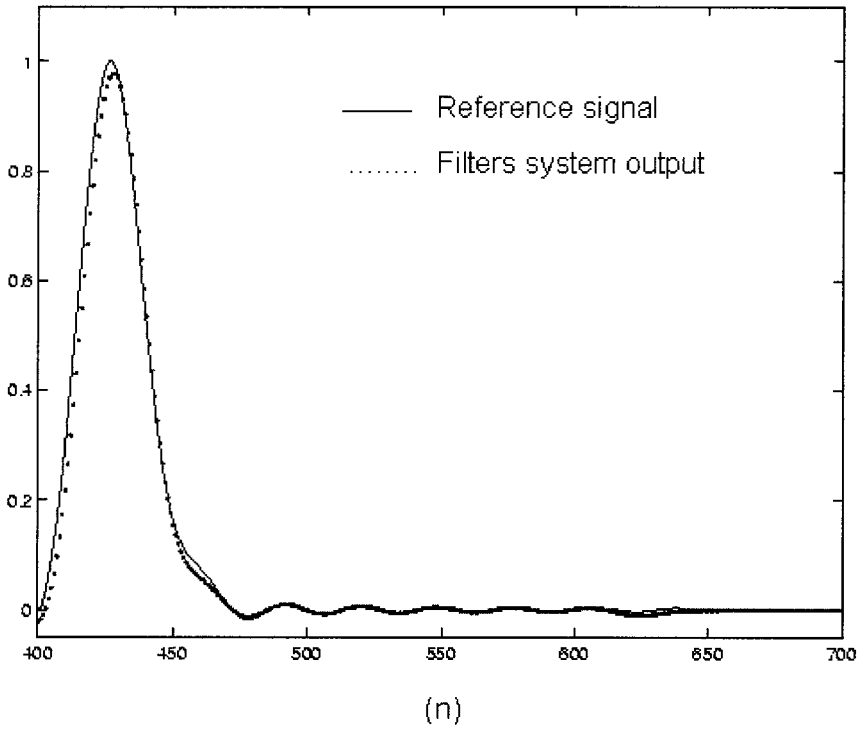


FIG. 7. The reference FID signal and the signal at the output of the filters system (linear and quadratic filters) for a 90° sinc-modulated input signal of 1 ms. The filter order is $N = 64$.

$$e(n) = y(n) - \hat{H}_1^{\mathrm{T}}(n)\,X_1(n) - \hat{H}_2^{\mathrm{T}}(n)\,X_2(n) - \hat{H}_3^{\mathrm{T}}(n)\,X_3(n) \quad [21]$$

$$\hat{H}_3(n+1) = \hat{H}_3(n) + \delta_3 X_3(n) e(n). \quad [22]$$

$\hat{H}_3(n)$ is the coefficient vector of the third-order kernel at time (n) and $X_3(n)$ is the correspondent input vector. $\hat{H}_1(n)$, $\hat{H}_2(n)$, $X_1(n)$, and $X_2(n)$ are defined by Eqs. [7], [8], [9], and [10], respectively. δ_3 is a positive factor that must satisfy $0 < \delta_3 < 2/(N\sigma_x^2)^3$ to assure the stability of the adaptive filter. In practice, we use a variable form for δ_3 which changes with respect to σ_x^2.

For $N = 64$, the convergence of the algorithm is obtained rapidly and we get an estimation of the first three Volterra kernels. In this case, three parallel filters (first, second, and third order) model the NMR spin system. Figure 9 shows the reference signal together with the output of the filters system for the same excitation signal (a 90° sinc RF pulse of 1 ms). The accuracy of the results is improved (compared with Fig. 7). The contributions of the three filters to the total system response are illustrated in Fig. 10. This time, the second-order contribution is very small compared to the first-order and the third-order contributions. The third-order term appears clearly and its maximum contribution is about 6% of the total response of the system. We emphasize the disappearance of even orders in the Volterra series. It is important to notice that the linear approximation of NMR system is good even for large flip angles. However, in the case where the SNR of the NMR signal is low, taking into account the third-order term may permit more accurate signal processing and analysis.

Our model is attractive since the expansion is a linear combination of a nonlinear function of the input signal. The output signal is no more than simple convolution products between combinations of the input signal and the kernels. This fact is important for real implementation of optimum NMR signal detection and processing systems and for future development of accurate spectral analysis and signal estimation. For example, when the NMR signal-to-noise ratio is low, identifying the NMR system in this practical manner may conduct to the optimum matched filter.

6. ADAPTIVE FILTERING IDENTIFICATION USING RECURSIVE NONLINEAR IIR FILTER

The major problem associated with Volterra series representation of nonlinear systems is that, in some cases, a very high filter order (a large number of coefficients) is required to describe the nonlinear model. In such a case, the discrete Volterra series is not the adequate model. Consequently, it is important to search for an alternative model. One such model is the recursive nonlinear IIR filter whose input–output relationship is governed by a recursive nonlinear difference equation with constant coefficients (*12*).

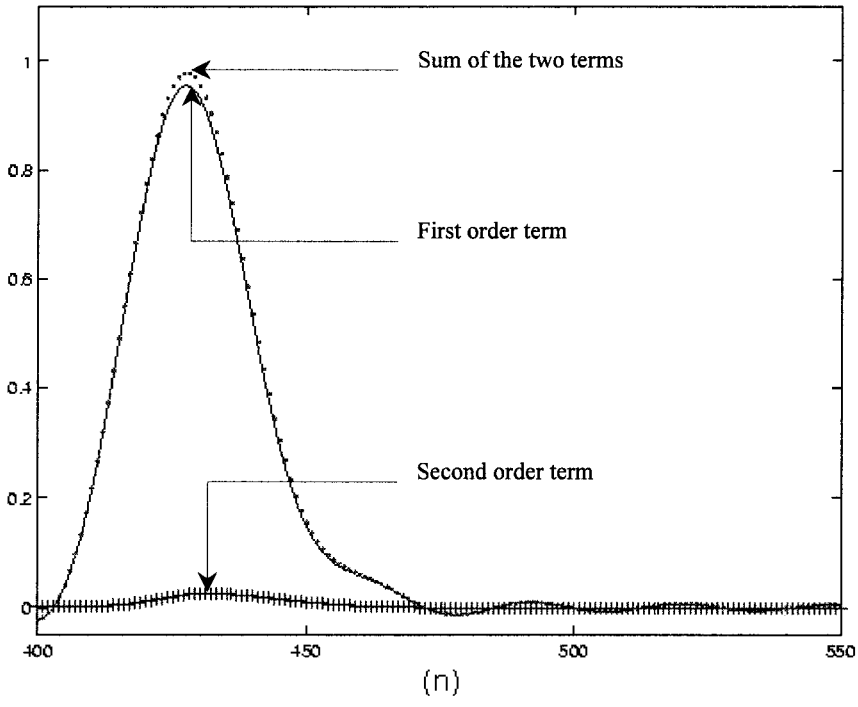


FIG. 8. The contributions of the first- and the second-order terms to the system response. The second-order term forms less than 2% of the total response.

6-1. Recursive Nonlinear Systems

The simplest of nonlinear recursive systems is the one in which the input–output relationship is given by (*12*)

$$y(n) = \sum_{i=1}^{N-1} c(i)y(n-i) + \sum_{i=0}^{N-1}\sum_{j=1}^{N-1} b(i,j)y(n-j)x(n-i) + \sum_{i=0}^{N-1} a(i)x(n-i). \quad [23]$$

This system representation can model nonlinear systems with fewer coefficients, i.e., $a(i)$, $b(i, j)$, and $c(i)$, than the Volterra series representation. The block diagram of a recursive nonlinear system for the case of $N = 2$ is shown in Fig. 11. Here, Z^{-1} represents the unit memory element that simply delays the signal passing through it by one sample. $a(0)$ and $a(1)$ are called forward coefficients and $c(1)$ is the backward coefficient. $b(0, 1)$ and $b(1, 1)$ are the nonlinear coefficients. Equation [23] is then written as

$$y(n) = c(1)y(n-1) + b(0,1)y(n-1)x(n) + b(1,1)y(n-1)x(n-1) + a(0)x(n) + a(1)x(n-1). \quad [24]$$

At each sample (n), the output signal of this recursive system is calculated using the input signal at time (n) and at time $(n - 1)$ but also using the output signal at time $(n - 1)$.

6-2. Adaptive Recursive Identification

In this section we would like to identify a NMR spin system with a recursive nonlinear IIR filter. In other words, we will try to calculate the coefficients $a(i)$, $b(i, j)$, and $c(i)$ (the coefficients of the IIR filter) using, once again, an adaptive filtering technique. The identification block diagram is shown in Fig. 12. For a given value of N, the adaptive filter estimates the output signal $\hat{y}(n)$ using the last N values of the input signal $x(n)$ and the last $(N - 1)$ values of the reference signal $y(n)$ (*12, 15*). The coefficients are updated at each sample (n) in order to minimize the quadratic error between $y(n)$ and $\hat{y}(n)$. The recursive nonlinear adaptive filtering algorithm is defined by

$$e(n) = y(n) - \hat{A}^{\mathrm{T}}(n)X(n) - \hat{B}^{\mathrm{T}}(n)XY(n) - \hat{C}^{\mathrm{T}}(n)Y(n) \quad [25]$$

$$\hat{A}(n+1) = \hat{A}_1(n) + \delta_a X(n)e(n) \quad [26]$$

$$\hat{B}(n+1) = \hat{B}(n) + \delta_b XY(n)e(n) \quad [27]$$

$$\hat{C}(n+1) = \hat{C}(n) + \delta_c Y(n)e(n), \quad [28]$$

where $e(n)$ is the calculated error between the actual response $\hat{y}(n)$ and the reference signal $y(n)$, and

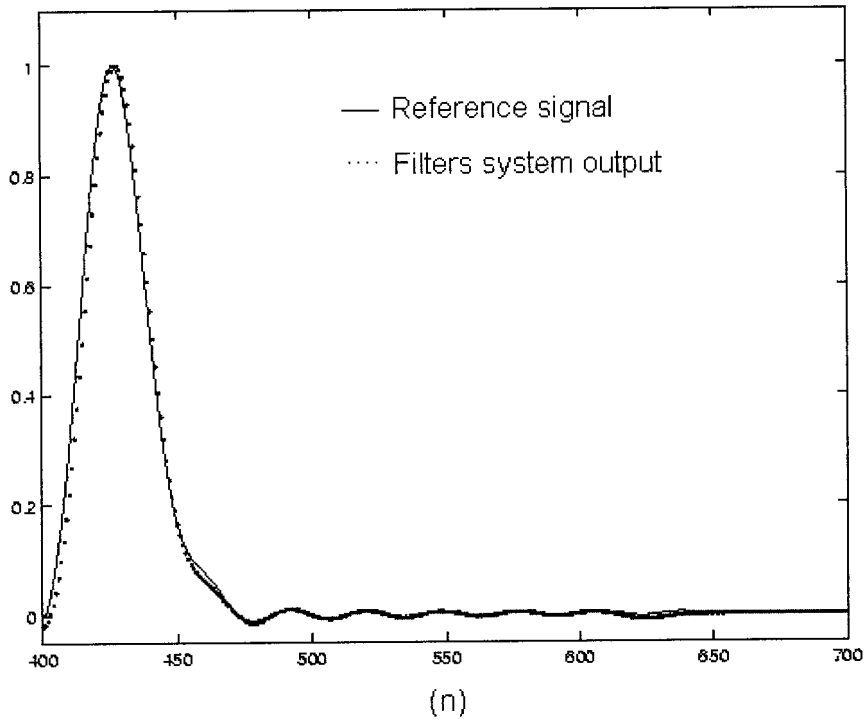


FIG. 9. The reference FID signal and the signal at the output of the filters system (linear, quadratic, and third-order filters) for a 90° sinc-modulated input signal of 1 ms. The filter order is $N = 64$.

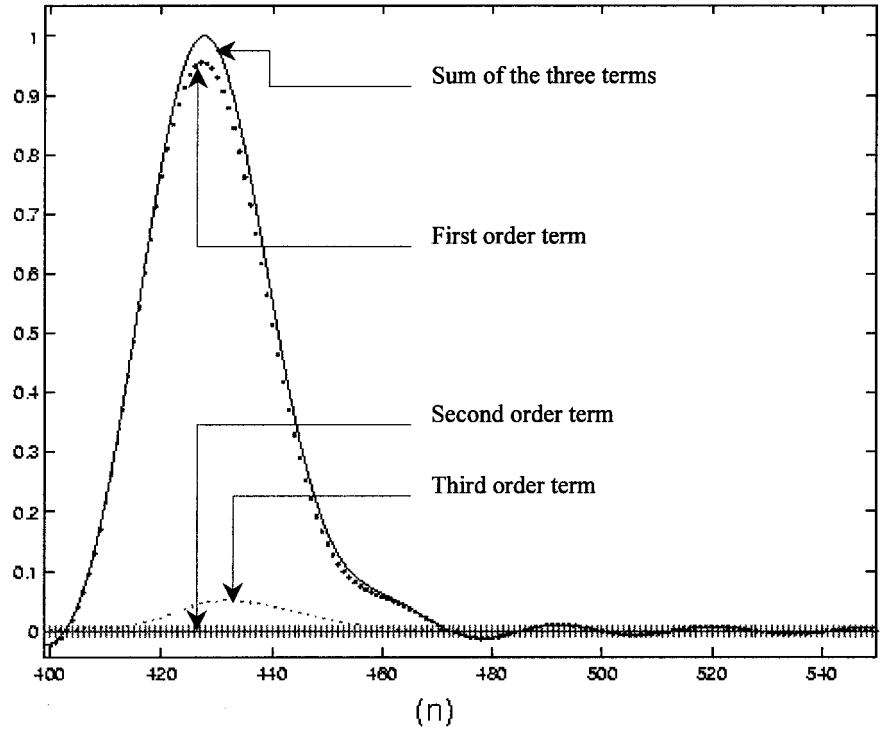


FIG. 10. The contributions of the three filters to the system response. The second-order term is neglected. The third-order term contributes to about 6% of the total response.

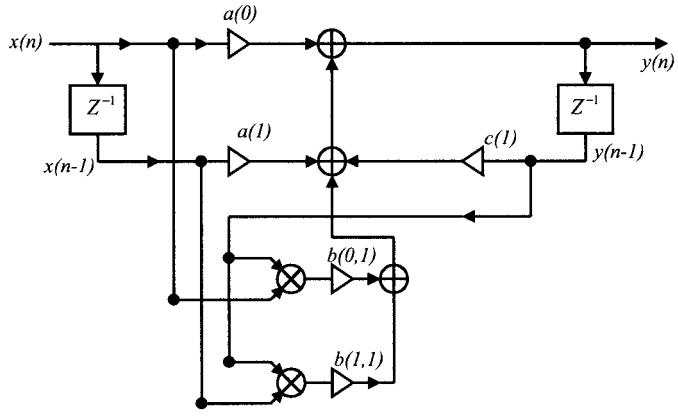


FIG. 11. Block diagram of a recursive nonlinear system of order $N = 2$.

$$\hat{A}(n) = [\hat{a}(0{:}n), \hat{a}(1{:}n), \ldots, \hat{a}(N-1{:}n)] \quad [29]$$

$$\hat{B}(n) = [\hat{b}(0, 1{:}n), \hat{b}(0, 2{:}n), \ldots, \hat{b}(N-1, N-1{:}n)] \quad [30]$$

$$\hat{C}(n) = [\hat{c}(1{:}n), \hat{c}(2{:}n), \ldots, \hat{c}(N-1{:}n)] \quad [31]$$

are the adaptive filter coefficient vectors at time (n). The vectors

$$X(n) = [x(n), x(n-1), \ldots, x(n-N+1)] \quad [32]$$

$$XY(n) = [x(n)y(n-1), x(n)y(n-2), \ldots, x(n-N+1)y(n-N+1)] \quad [33]$$

$$Y(n) = [y(n-1), y(n-2), \ldots, y(n-N+1)] \quad [34]$$

are the input vectors to the adaptive filter. Finally, δ_a, δ_b, and δ_c are the adaptive gains that are calculated at each time (n) to assure the stability of the algorithm.

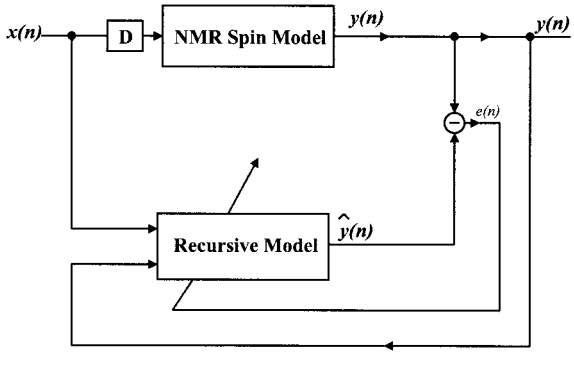


FIG. 12. Block diagram of the identification of NMR system with a recursive nonlinear system. D is a delay element.

6-3. Results of the Recursive Nonlinear Identification

Consider the 1D homogeneous object described on Fig. 1. Let us take, once again, a 90° sinc-modulated pulse of 1 ms. The system response (reference signal) is the one presented on Fig. 2b. The coefficients $a(i)$, $b(i, j)$, and $c(i)$, obtained after convergence, are plotted in Fig. 13 in the case of $N = 24$. These coefficients are the best estimation of the NMR model in the sense of mean square error. Figure 14 shows the reference

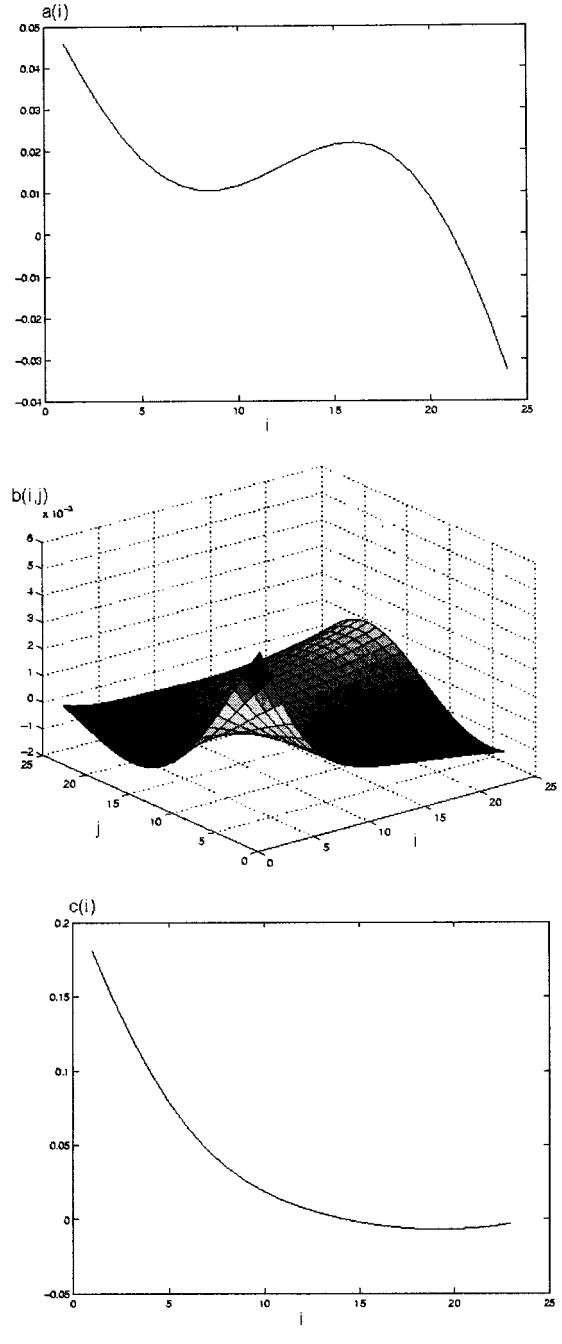


FIG. 13. The coefficients of the recursive nonlinear IIR filter obtained by adaptive filtering for $N = 24$.

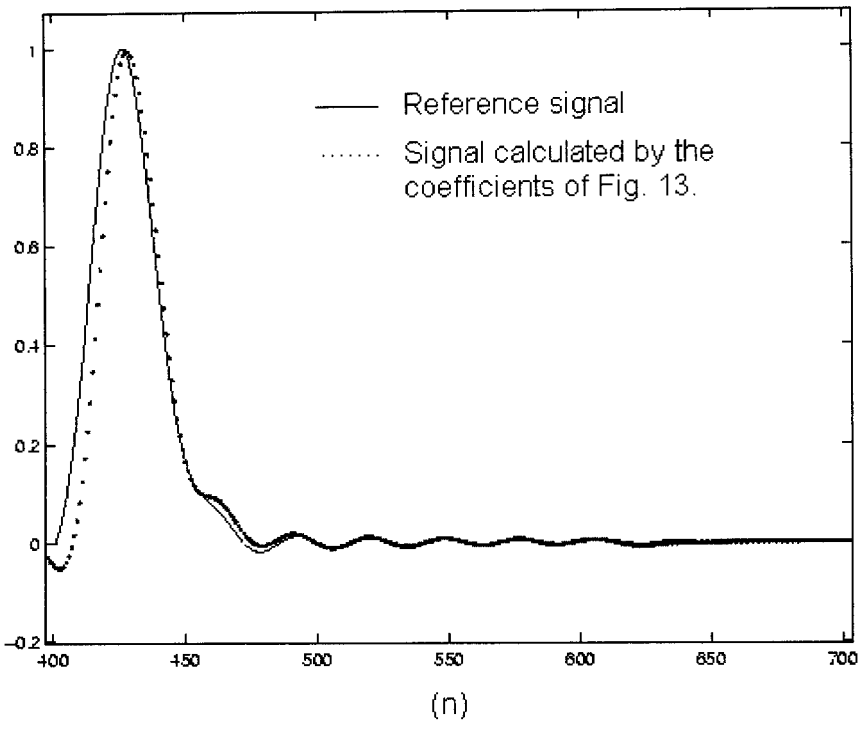


FIG. 14. The reference signal and the signal calculated with the coefficients of Fig. 13. The excitation is a 90° sinc-modulated signal of 1 ms.

signal together with the signal calculated using the coefficients of Fig. 13 (i.e., the signal at the output of the IIR filter). The initial values of this latter signal are forced to zero.

The key advantage of this recursive nonlinear model is that it is possible to represent the NMR systems with relatively fewer coefficients when compared with Volterra system representation. The residual mean-square error—after convergence—for the recursive model of order 24 is smaller than the residual MSE for the Volterra model of order 64. However, the recursive model cannot be reduced to separate convolution products as the Volterra model can. Thus, this recursive model cannot replace entirely the Volterra representation. Each model has its advantages and its specific limits. The issue of which one to use depends on the nature of application. In practice, the Volterra model could be employed in filtering problems where there is a requirement for linear-phase characteristics, especially for the linear part. If there is no requirement for linear-phase, either the Volterra model or the recursive model may be employed. However, if some phase distortion is tolerable, the recursive model is preferable because its implementation involves fewer coefficients, fewer memory requirements, and lower calculation time and complexity.

CONCLUSION

We present, in this paper, two new methods for identifying NMR spin systems employing nonlinear adaptive filtering techniques. The first method is based on discrete Volterra series development of the system response. The first three kernels of this series are estimated using the least mean square algorithm. Three parallel filters modeled the NMR spin system so that its output is no more than simple convolution products between filters coefficients and combinations of the input signal. The contribution, to the total system response, of the second-order term of the Volterra series is shown to be neglected. In the second method, the input–output relationship of the system is described by a recursive nonlinear difference equation with constant coefficients. The LMS algorithm is employed to calculate these coefficients.

Our identification methods can be useful for better time description and nonlinear spectral analysis of NMR signals. They are promising for real implementation of optimum NMR signal detection and processing systems. Our future work will validate these models on real NMR signals.

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