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DSP-Based On-Line NMR Spectroscopy Using an Anti-Hebbian Learning Algorithm*

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Abstract

This paper describes a nuclear magnetic resonance (NMR) system that uses an adaptive algorithm to carry out real-time NMR spectroscopy. The system employs a digital signal processor chip to regulate the transmitted and received signal together with spectral analysis of the received signal to determine free induction decay (FID). To implement such a signal-processing routine for detection of the desired signal, an adaptive line enhancer filter that uses an anti-Hebbian learning algorithm is applied to the FID spectra. The results indicate that the adaptive filter can be a reliable technique for on-line spectroscopy study.

Introduction

Spectroscopy is the characterization of chemical contents by studying the absorption and dispersion of their spectra. Nuclear magnetic resonance (NMR) spectroscopy is similar to measurement of the transfer function of a linear system with realizable input and output. When NMR spectroscopy is used this way, the chemical contents can be considered as the transfer function of the system and the NMR spectrum as the output signal.

To measure the transfer function, the proposed system transmits a radio frequency (RF) wave to a sample located in an external magnetic field. The resonance absorption of the RF (NMR spectrum) signal, once detected, can provide information on the validity of the desired signal. To investigate this, an adaptive line enhancer

(ALE) filter applying an anti-Hebbian learning algorithm has been adapted to restrain the unwanted component of the input while passing the desired signal.

Initially, the ALE proposed by Widrow and Stearns [1], which uses least mean square (LMS) algorithm to update the tap weights of the filter, was implemented. Although both the anti-Hebbian and LMS routines provide similar results, the proposed method in this work exhibits a high convergence speed than that of the LMS algorithm.

Theory

Although the main focus of this paper is not to describe NMR theory, one must nevertheless have a modest understanding of the underlying physics of the problem. The reader should refer to references available on this subject [2-3].

As stated earlier, the ALE technique has been applied to analyze free induction decay (FID) spectra. As shown in Fig. 1 ALE is a tapped-delay line filter of some fixed length and whose tap gains may be recursively adjusted by using the proposed algorithm in this work. The delay components, with sufficient length, cause a simple phase shift between the desired signal and the input signal. According to the learning

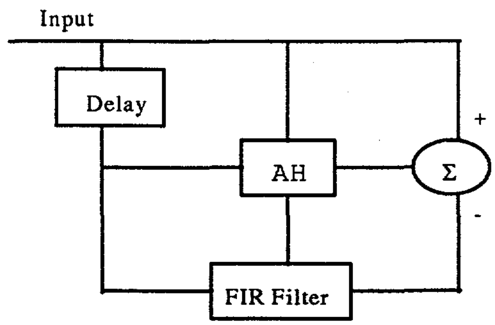

Fig. 1. Adaptive line enhancer(ALE) (AH is anti-Hebbian algorithm).

algorithm, the adaptive filter uses the error signal to form a transfer function so that the unwanted signals cancel each other at the summing junction. The brief discussion of the related work on anti-Hebbian algorithm may assist in formulating an adaptive scheme for a finite-impulse-response (FIR) digital filter.

Recently, it has been found that a simple linear neuron with an unsupervised constrained Hebbian learning rule using the so-called total least square (TLS) routine can extract the principal component from stationary input data [4]. This approach, known as the modified Hebbian method has been widely used in signal processing and pattern recognition where the weight vector tends to converge to the largest eigenvalue of the input data set. On the other hand, in situations such as signal recovering and optimal curve fitting, the weight vector of the linear neuron should reach the eigenvector associated with the minimum eigenvalue of the input correlation matrix . This consideration has led to development of a modified Hebbian learning rule (known as anti-Hebbian rule) that adaptively extracts the minor component of the input data set [5].

Considering the simple neural unit with inputs $\xi(t)$, weights $\eta(t)$, and output

$$z(t) = \sum_{i=1}^{n} \eta_i(t)\xi_i(t) \qquad (1)$$

the anti-Hebbian algorithm can be expressed as [5]

$$\eta(t+1) = \eta(t) - \mu z(t)\left[\xi(t) + \xi_{n+1}(t)\eta(t)\right] \quad (2)$$

where the anti-Hebbian term $-\mu z(t)\xi(t)$ minimizes the correlation between the weight vector and the input data. Correspondingly, the feedback term, $-\mu z(t)\xi_{n+1}\eta(t)$ remains bounded close to unity [5].

By letting

$$z(t) = w^t(t)x(t-\Delta)-x(t) = e(t) \qquad (3)$$

the anti-Hebbian algorithm for the adaptive line enhancer can be written as

$$w(t+1)=w(t)-\mu e(t)[x(t-\Delta)+x(t)w(t)] \quad (4)$$

where w(t) represents the weights of the filter, and t is the weight number. The parameter μ is a constant that controls stability and rate of convergence. If eq. 4 is stable, then w_i converges to the solution of the Wiener-Hopf matrix equation [6]. Therefore,

$$\lim_{t\to\infty} E[w_i(t)] = w^0(t) \qquad (5)$$

where the Wiener-Hopf matrix solution is

$$R * w^0 = P \qquad (6)$$

and $R = \Phi(t) = E(x(t)*x(t)^t)$ is the autocorrelation matrix, and P is a column vector with elements $\Phi(t + \Delta)$. The mean square error can be shown by the covariance matrix of the weight vector as [6]

$$\lim_{t\to\infty} \operatorname{cov}[w_i(t) - w^0(t)] = \mu e_{min} \qquad (7)$$

$$e_{min} = \Phi(0) - \sum_{n=0}^{t-1} w^0(n) * \Phi(n+\Delta) \qquad (8)$$

Equation 8 reveals that the minimum value of e depends on the energy of the primary signal, the optimal weight vector, and the autocorrelation of the input signal.

Design Considerations and Simulation Results

The underlying principles in constructing an NMR spectrometer are briefly described here. The basis of any NMR system is the pulse controller used to measure the frequency of a nuclear resonance with sufficient accuracy. In principle, NMR spectroscopy involves generation of two RF pulses; the architecture in the appendix shows this operation. The system consists of two blocks of first-in/first-out (FIFO) memory and two blocks of read only memory (ROM) where the wave information is stored.

Memory blocks 1 and 2 are assigned to produce two pulses with sufficient delay. Parameters such as period, delay, and width of the pulse can be adjusted to be directly proportional to the frequency of the timer clock TCLK on

the TMS320C30 [7].

As shown in Fig. 2, the first pulse initiates a gated sinusoid by allowing ROM #1 to flash its data to a 12 bits digital-analog converter (D/A) chip.

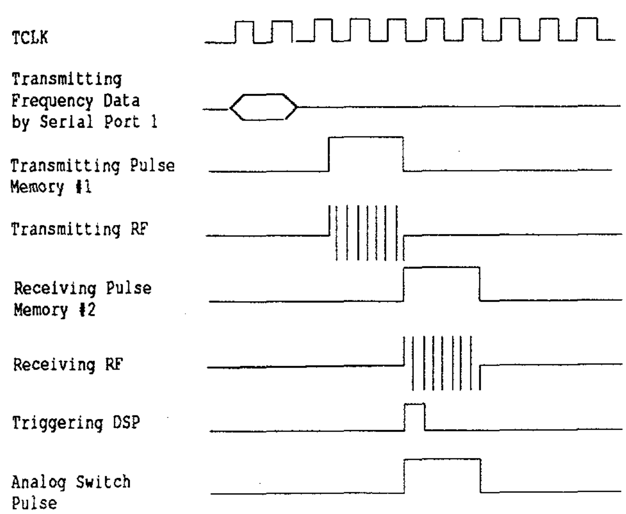

Fig. 2. Timing diagram of NMR controller

The frequency of the waveform is selected by a frequency-control unit. Serial port 1 of the C30 processor loads the frequency information into a 64-bit shift register. The contents of the shift register control the frequency of the sinusoidal output. Phase can be adjusted by a 2 bit phase-control register; the contents of this register is added to a phase accumulator that shifts the phase in 90° increments. The frequency and phase are chosen to be equivalent to the Larmor frequency (ω) of the nuclei. Figure 3 is the flow diagram of the algorithm when performing a pulse NMR technique with the TMS320C30.

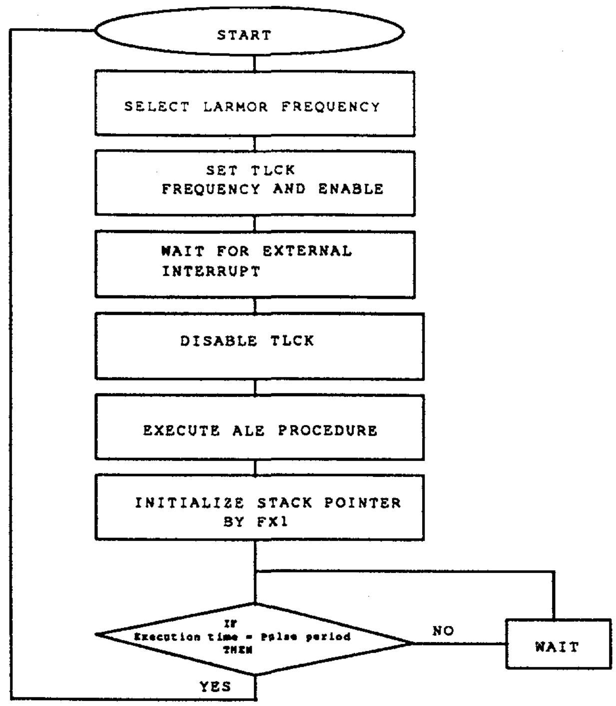

Fig. 3. A flow diagram to Illustrate a pulse NMR technique with TMS320C30.

A computer simulation was carried out to demonstrate the detection of water in a composite spectra by applying the ALE procedure. Data were collected from a series of off-line laboratory experiments. The FID spectrum of the input signal and the final result are shown in Fig. 4. It is clear that the system removed the unwanted background noise and kept the desired signal at 450 Hz.

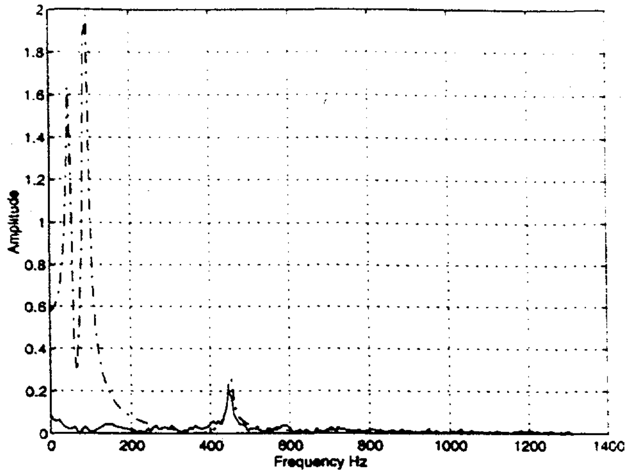

Fig. 4. Spectrum of composite signal (dashed line)and spectrum of the desired signal(solid line), after passing through ALE.

In conjunction, a computer simulation was implemented to compare the anti-Hebbian and LMS (a conventional approach to update the ALE weight vector) algorithms. For this purpose, a parameter defined as

$$Tran = \sum_{i=0}^{n} w_i(t) * w_i^T(t) \qquad (9)$$

was used as the index of convergence rate where n is the size of the weight vector. The simulation scheme is shown in Fig. 5, where the coefficient of adaptive filter converges to w^0 by allowing the known FIR filter coefficients to be

$w^0 = [0.9, 0.4, 0.5, 0.32, 0.21, 0.14]$.

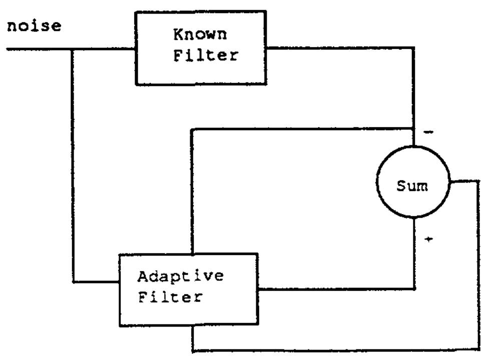

Fig. 5. An adaptive filter to estimate w^0

As shown in Fig. 6, the adaptive filter that uses the proposed algorithm updates the filter coefficients quicker than does the LMS method.

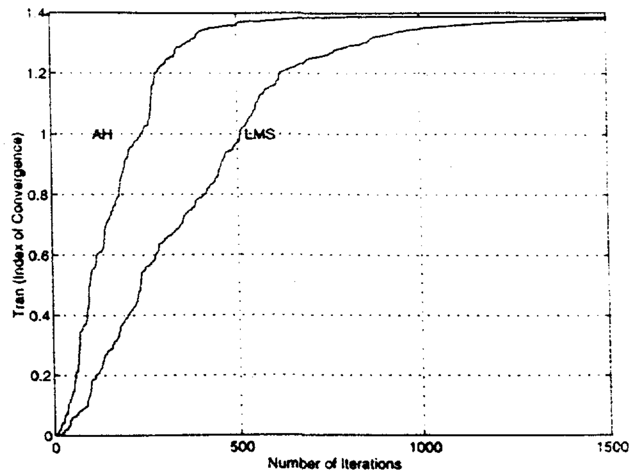

Fig. 6. Convergence rate for AH and LMS algorithm

Conclusions

In this paper, development of an on-line controller based on the TMS320C30 processor has been described for measuring nuclear resonance by an adaptive line enhancer method that uses the proposed algorithm. This approach does not require an external reference signal for detection and observation of the desired signal. Simulation has shown that the proposed learning rule results in faster and smoother convergence. In addition, under the total least square routine, this algorithm provides more accurate estimates than those obtained by LMS algorithm in noisy conditions. The system described here has a high potential for on-line monitoring applications and may contribute greatly to improved process control.

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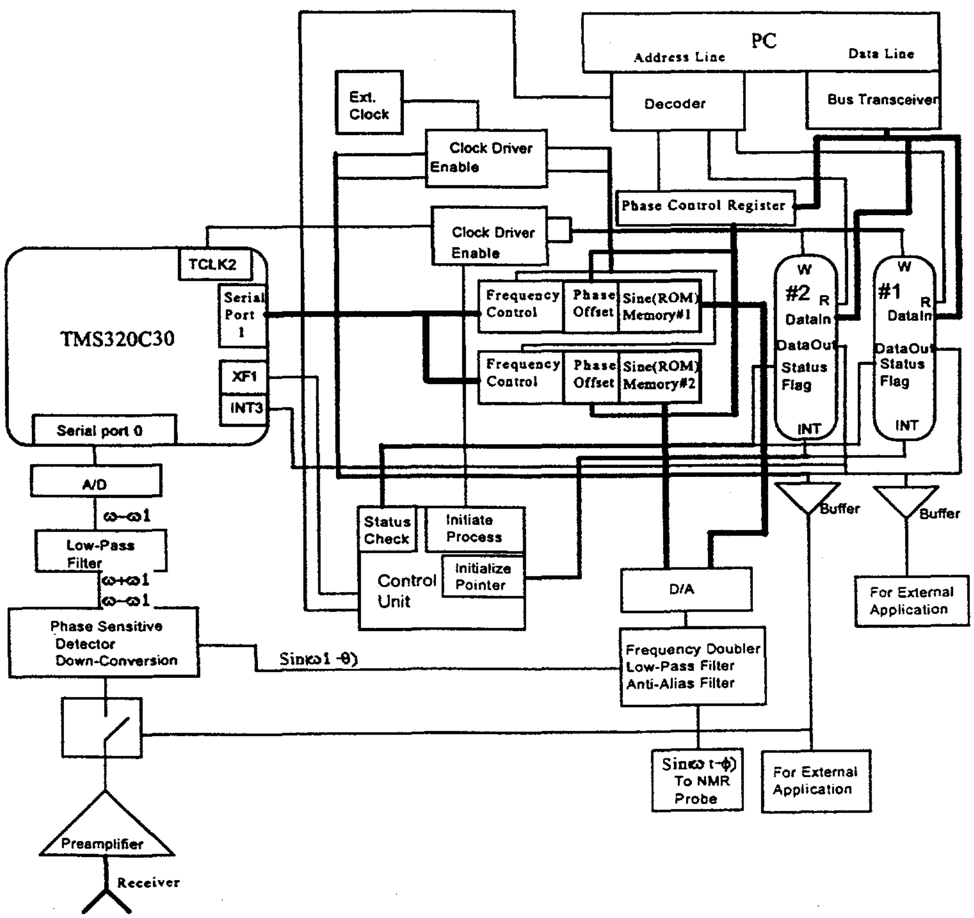

Appendix: Block diagram of NMR controller