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Noise Suppression of NMR Spectrum by Shifted Harr Wavelet Transform

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Abstract: The noise suppression of time domain NMR data by discrete wavelet transform with high order Daubechies wavelet coefficients exhibits severe peak distortion and incomplete noise suppression near real signal. However, the fact that even a shift averaged Harr wavelet transform with a set of Daubechies wavelet coefficients (1/2, -1/2) can be used as a new and excellent tool to distinguish real peaks from the noise contaminated NMR signal is introduced. New algorithms of shift averaged Harr wavelet were developed and quantitatively evaluated in terms of threshold and signal to noise ratio (SNR).

INTRODUCTION

The fourier transform (FT) method is one of the most widely used mathematical tool in the conversion of time domain multinuclear multidimensional NMR signals or free induction decay into a frequency domain spectrum. After introduction of wavelet transform by Morlet and his coworkers in 1984,[1,2] many applications of wavelet transform have been received a great attention in many different areas, including image compression, noise suppression of image, signal processing, computer graphics, and pattern recognition.

Some efforts have been made in the analysis of spectral lines and possible applications to NMR spectroscopy[3,4]. The wavelet transform was successfully achieved in the extraction of dynamic behavior in NMR signal at the beginning with discrete wavelet transform (DWT) method[5]. For the convenience, orthogonal wavelet transform that can easily return to original domain has been used to eliminate noise signal in image processing and other signals in processing areas. As a general orthogonal wavelet transform method of DWT, Daubechies developed useful wavelet transform method in which an operational matrix is applied to the data to make a wavelet coefficients and multiply a transverse matrix of previously used ma-

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trix to return to original domain, in 1988.[6] Mallat developed a fast algorithm that can be used with orthogonal wavelet transform.[7]

The terminology of "discrete" used in DWT is from the "discretized from CWT". There are three types of discretized wavelet transform.[8] The first type of DWT is given by following Eq. (1)

$$W(m,n) = a_o^{-\frac{m}{2}} \int x(t)\Psi(a_o^{-m}t - nb_o)dt \qquad (1)$$

Where the parameters *a*, *b* are discretized to $a = a_o^m$ and $b = nb_o a_o^m$ with sampling intervals a_o, b_o and integers *m*, *n*. Even though a discretization is made, $x(t)$ and $\Psi(a_o^{-m}t)$ are still continuous for time domain. The second type of DWT is given by the following Eq. (2).

$$W(m,n) = a_0^{-\frac{m}{2}} \sum_k x(k)\Psi(a_o^{-m}k - nb_o) \qquad (2)$$

The Eq. (2) is a time discretization of (1) with $t=kT$ and the sampling interval $T=1$. And this is similar to the discrete fourier series where both time and frequency are discrete. The third type of DWT is given by the following Eq. (3).

$$W(m,n) = 2^{-\frac{m}{2}} \sum_k x(k)\Psi(2^{-m}k - n) \qquad (3)$$

Here the discrete wavelet $\Psi(k)$ can be a sampled version of continuous counterpart. The Eq. (3) is derived from the Eq. (2) when $\Psi(k)$ is a discretization of $\Psi(t)$, and a_o and b_o are fixed to 2 and 1. Discrete wavelet transform generally refers to the third type of Eq. (3). Signals distinguished from the noisy time domain data in a wavelet space can be more efficiently treated. Therefore, the efficiency of noise elimination increases when a proper noise elimination step is applied in a wavelet space.

Using a simple DWT with a set of Daubechies wavelet coefficients(1/2, -1/2), Harr wavelet in combination with shift averaging of NMR data, a new NMR data processing method were developed as extension of our previous work.[9] The most interesting and characteristic of this method is the great improvement of S/N ratio with fast processing time and high resolution. For the purpose of noise elimination, three steps of operation such as wavelet transform, noise elimination in wavelet space, and inverse wavelet transform are basically required.[10] Therefore, forward and backward (inverse) wavelet transform must be considered simultaneously. In order to avoid the serious peak distortion and incomplete noise suppression near real NMR peak, the subsequent shift signal averaging methods were adopted in this current work. Theoretical background of wavelet transforms, detail methods of noise elimination, new algorithms of shifted averaged Harr wavelet, and results were quantitatively discussed in terms of threshold and signal to noise ratio(SNR).

CODING of WAVELET TRANSFORM and EXPERIMENTS

Specially designed orthogonal or biorthogonal wavelet transforms easily going back to the original domain can be simply applied to the noise elimination method. However, nonorthogonal wavelet transform carrying a complex inversion mechanism similar to equations are generally complicate and not easy to apply for noise elimination. Detail computational procedure and noise suppression methods are described in detail as follow.

All C/C++ codes are programmed on SGI Octane workstation. ^{1}H coupled ^{13}C-NMR data of the alanine was used as a test data. Sample purchased from Cambridge Isotope Co. was prepared by dissolving ^{13}C labeled alanine in D_2O solvent. All NMR spectra were recoded on a Varian Mercury 300 spectrometer with 64 k data points. This data was converted into HyNMR^{TM}(Hanyang NMR, multidimensional NMR data processor) data format and was processed with currently developed methods for wavelet transform and noise reduction procedure.

Procedure of the Shifted Signal Averaging and Harr Wavelet Transform

Harr wavelet transforms were coded with pyramidal algorithm and Daubechies filter coefficients (1/2,-1/2) to suppress noises by utilizing a threshold method. Because of asymmetric shape of the Daubechies wavelet, the baseline of the reconstructed signals after the application of threshold in the wavelet space is always distorted.

For the purpose of the correction of this distortion and incomplete suppression of noise near real signal, a shifted signal averaging with certain shifted data set were accomplished prior to wavelet transform. The method is shown in Figure 1. The procedure of noise suppression with the shift averaged Harr wavelet transform starts from the generation of NMR signal sets by shift averaged data point for noise-containing original NMR signal. After the Harr wavelet transform for each NMR signal set, noises are suppressed by a certain hard threshold value. Noise suppressed NMR signals in frequency domain are then back by inverse Harr wavelet transform. The final noise suppressed NMR signal without distortion in baseline and peak shape is finally generated by the back-shift signal averaging.

RESULT and DISCUSSION

Noise reductions have been attempted to NMR data with currently developed DWT method implemented with a set of Daubechies filter coefficients (1/2, -1/2). Harr wavelet itself gives

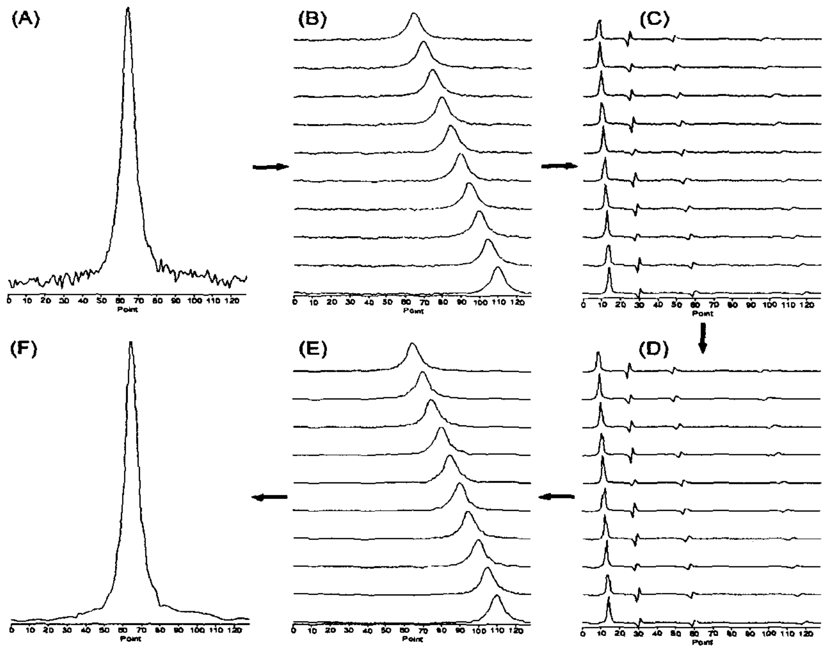

Fig.1. The procedure of noise suppression by the shift averaged Harr wavelet transform. (A) The noise-containing original NMR signal, (B) NMR signal sets generated by shift averaged 200 data point, (C) After Harr wavelet transform for each NMR signal set, (D) Noises are suppressed by a certain threshold value, (E) The final Noise suppressed NMR signal in frequency domain by Inverse Harr wavelet transform. (F) The final noise-suppressed NMR signal with no baseline distortion by the back-shifted signal averaging.

rectangular form of signal, but shifted signal averaging with 200 data points was good enough to suppress unwanted noises in NMR spectrum. High order Daubechies filter coefficients(4,8,12,16) give serious distortion of baseline resulting incomplete noise suppression near the real gaussian type NMR signal. However, the simplest DWT form, Harr wavelet in combination with shifted signal averaging give rise to good results as shown in Figure 2.

The comparisons of noise containing experimental, and noise suppressed spectra with increasing hard threshold value of 50,000, 100,000, 150,000, 200,000 for the ^{13}C-NMR spectrum show that the higher SNR value can be obtained within certain threshold value, but too big value of threshold can rather give small SNR value and peak distortion. This means that the graphical plotting between threshold and SNR value can have hyperbolic form giving maximum SNR at certain threshold value.

The qualitative comparisons of NMR signal resulting from the shift averaged Harr wavelet methods and window function including exponential multiplication, gaussian window function

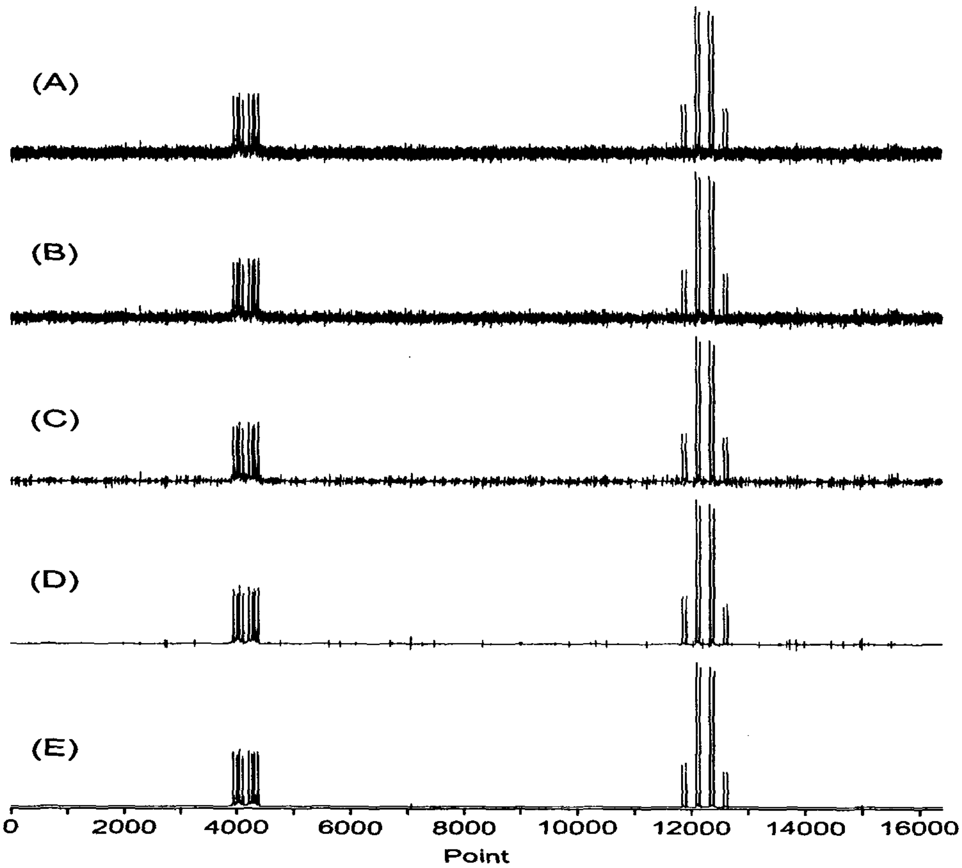

Fig.2. The ^{13}C-NMR spectrum of ^{13}C-labeled alanine with proton decoupling by Harr wavelet and 200 shift averaged data sets with uniform threshold values for each data set. (A) Signal averaged ^{13}C-NMR spectrum with four number of acquisition. (B) Noise eliminated spectrum with hard threshold 50000, (C) Noise eliminated spectrum with hard threshold 100000, (D) Noise eliminated spectrum with hard threshold 150000, and (E) Noise eliminated spectrum with hard threshold 200000

were also accomplished in Figure 3. The experimental ^{13}C-NMR spectrum of ^{13}C-labeled alanine with number of acquisition 1 and without proton decoupling was used in comparison. The shift averaged Harr wavelet transform with calculated optimal threshold gives same magnitude and shape of signal, but poor noise suppression. However, a uniform threshold 370,000 is applied to each shifted data set, the maximum SNR was obtained. In case of exponential 1Hz window function, serious reduction of the magnitude of peak and smoothing was observed. Gaussian window function with 1Hz also gives less reduction of peak compare to exponential function. Although brief spectral comparison shows that our current new meth-

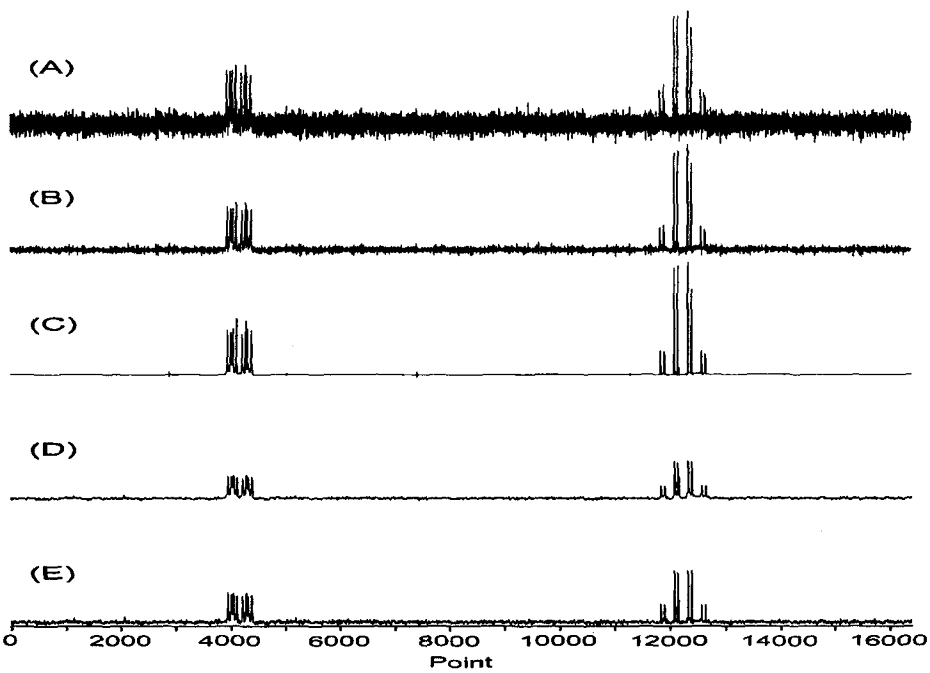

Fig.3 The qualitative comparisons of NMR signal resulting from the shift averaged Harr wavelet methods and window function including exponential multiplication, gaussian window function. (A) Experimental ^{13}C-NMR spectrum of ^{13}C-labeled alanine with number of acquisition 1 and without proton decoupling, (B) The noise eliminated spectrum with calculated optimal threshold applied to each shifted data set, (C) Noise eliminated spectrum with uniform threshold 370000 giving maximum SNR, (D) Noise eliminated spectrum with 1Hz exponential multiplication window function, (E) Noise eliminated spectrum with 1Hz gaussian window function.

ods are promising and applicable to similar noise reduction studies, there are still necessity of quantitative comparison between the current method and MEM, MLM methods in efficiency in terms of the computation time of noise reduction and SNR, peak shape after noise reduction, and further extension toward multidimensional NMR data process.

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