Acc. Chem. Res. **2003,** *36,* 276−283

Wavelet: A New Trend in Chemistry

XUE-GUANG SHAO,[†]
ALEXANDER KAI-MAN LEUNG,[‡] AND
FOO-TIM CHAU*[,§]

Department of Chemistry, University of Science and Technology of China, Hefei, Anhui, 230026, P. R. China, Analytical and Advisory Services, Government Laboratory, Ho Man Tin Government Offices, Kowloon, Hong Kong, P. R. China, and Department of Applied Biology and Chemical Technology, The Hong Kong Polytechnic University, Kowloon, Hong Kong, P. R. China

Received June 26, 2001 (Revised Manuscript Received May 7, 2002)

ABSTRACT

Since 1989, wavelet transform (WT) has attracted much interest of chemists working on signal and image processing, and the WT-based techniques have been successfully applied to the chemical signal processing. This approach has been demonstrated as fast in computation with localization and having quick decay properties, in contrast to the popular methods existing, especially to the fast Fourier transform. More than 370 papers have been published up to the year 2002 which covered applications of WT in various fields of chemistry, including analytical chemistry, chemical physics, and quantum chemistry. In this paper, we report on applications of WT to data compression, data smoothing and denoising, baseline and background correction, resolution of multicomponent overlapping signals, regression and classification, and analytical images processing in analytical chemistry. Through this report we wish to induce greater interest of chemists in WT and to obtain greater benefits from using the WT-based techniques.

1. Introduction

Traditionally, the mathematical technique Fourier transform (FT) plays a very important role in chemistry. It is commonly used in analytical instruments and in computational chemistry for signal processing.[1] Recently, a trend has evolved to more vigorously introduce new mathematical techniques to the chemical studies on signal processing. Over the past decade, a new technique known as wavelet transform (WT) has been successfully employed in various fields of chemistry for signal processing.[2,3] It has been proved to be fast enough in computations and universal in applications, contrary to the popular methods existing, especially to the fast Fourier transform (FFT). More than 370 papers were published within the period from 1989 to early 2002. In these studies, WT was employed mainly for signal processing in various fields of analytical chemistry, including flow injection analysis (FIA), high-performance liquid chromatography (HPLC), capillary electrophoresis (CE), infrared spectrometry (IR), ultraviolet−visible spectrometry (UV−Vis), mass spectrometry (MS), nuclear magnetic resonance spectrometry (NMR), electroanalytical chemistry, and X-ray diffraction. It has also been successfully employed in solving certain problems in quantum chemistry and chemical physics.

The theory of WT was extensively developed in the 1980s. WT became a popular issue in chemistry and in the other fields of science after publication of the important papers by Daubechies[4] (1988) and Mallat[5] (1989), in which the compactly supported orthonormal wavelets and the fast calculation algorithm were proposed. In 1992 and later, several excellent reference books on WT were published.[6−8] In recent years, applications of WT to various fields of chemistry have been introduced by different workers.[9−12]

In this paper, a brief introduction to the theory and algorithms of WT is given, and applications in the field of chemistry are reviewed to draw chemists' greater attention to WT and to gain more benefits from using this technique.

2. Theory and Algorithms

2.1. Wavelet Transform. Wavelet is defined as the dilation and translation of the basis function $\psi(t)$, i.e.

$$\psi_{a,b}(t) = \frac{1}{\sqrt{|a|}}\psi\left(\frac{t-b}{a}\right), \qquad (a,b \in R,\ a \neq 0) \qquad (1)$$

where a and b are, respectively, the scale (dilation) and position (translation) parameters. If a and b are discretized with $a = a_0^j$ and $b = kb_0a_0^j$ ($j,k \in Z$, $a_0 \neq 0$), respectively, eq 1 becomes

$$\psi_{j,k}(t) = a_0^{-j/2}\psi(a_0^{-j}t - kb_0) \qquad (2)$$

The wavelet defined by eq 2 is called discrete wavelet, where $a_0 = 2$ and $b_0 = 1$ are generally used. From the definition, one can tell that the wavelet is a family of functions derived from a basic function $\psi(t)$. Figure 1

Xueguang Shao was born in Shandong province, P. R. China, in 1963. He received his Ph.D. in Chemistry from University of Science and Technology of China (USTC) and Kyoto Institute of Technology (KIT), Japan, in 1992. He is now a Professor of Chemistry at the Department of Chemistry, University of Science and Technology of China, Hefei, P. R. China. His research interests are development of chemometrical methods for chemical studies, including analytical signal processing and molecular simulation.

Alexander Kai-Man Leung was born in Hong Kong, in 1971. He received his Ph.D. in Chemistry from The Hong Kong Polytechnic University, Hong Kong in 1998. He is now a Chemical Analyst at the Government Laboratory. His research interests include applications of chemometrical techniques in analytical chemistry and chemical analysis of traditional Chinese medicines.

Foo-tim Chau was born in Guangdong province, P. R. China, in 1948. He received his Ph.D. in Chemistry from University of British Columbia (UBC), Canada in 1977. He is now a Professor of Chemistry at the Department of Applied Biology and Chemical Technology, The Hong Kong Polytechnic University, Hong Kong. His research interests are development of chemometrical methods for signal processing and chemical analysis of herbal medicines, as well as simulation of photoelectron and molecular spectra using computational chemistry and spectroscopic theory.

* Corresponding author. Address: Department of Applied Biology and Chemical Technology, The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong, P. R. China. Tel.: (852) 2766 5603. Fax: (852) 2364 9932. E-mail: bcftchau@inet.polyu.edu.hk.

[†] University of Science and Technology of China.

[‡] Ho Man Tin Government Offices.

[§] The Hong Kong Polytechnic University.

10.1021/ar990163w CCC: $25.00
Published on Web 02/07/2003

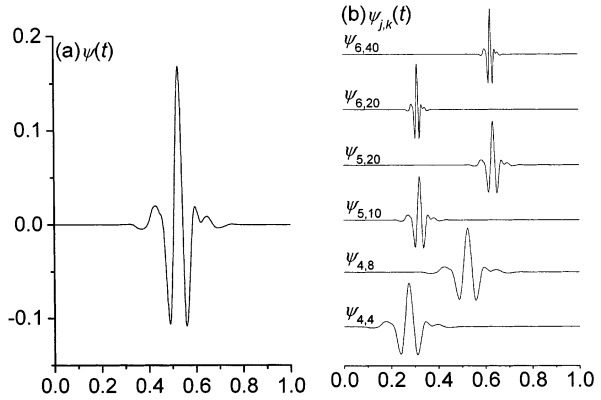

FIGURE 1. An example of the Symmlet wavelet basis function (a) and its derived wavelet (b).

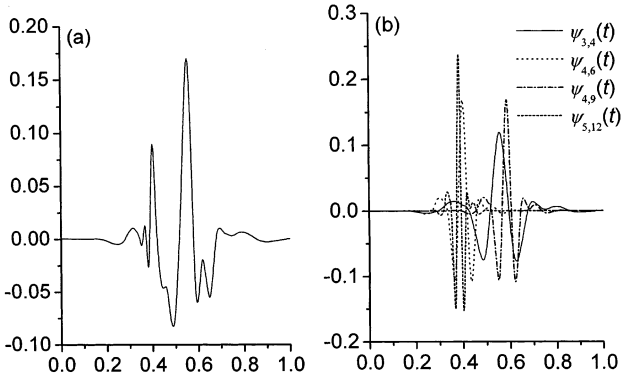

FIGURE 2. A simulated signal (see text for detail) (a) and the wavelet functions that represent the signal (b).

shows an example of the Symmlet wavelets with each function being defined by a specific pair of integer (j, k).

In some respects, the wavelet transform resembles the well-known Fourier transform in which the sine and cosine are the analyzing functions, while the analyzing function of the WT is a family of functions, i.e., the wavelet. The continuous and discrete wavelet transform (CWT and DWT) of a function $f(t)$ or a signal are given, respectively, by

$$W_f(a,b) = \int_{-\infty}^{+\infty} f(t)\overline{\psi_{a,b}(t)}\,\mathrm{d}t \tag{3}$$

and

$$C_f(j,k) = \int_{-\infty}^{+\infty} f(t)\overline{\psi_{j,k}(t)}\,\mathrm{d}t \tag{4}$$

It can been seen that the only difference between the definition of the WT and Fourier transform is the analyzing function. Therefore, the underlying philosophy of WT is a projection of the function or signal to be analyzed onto the wavelet. The basic idea of WT is to represent any function or signal as a superposition of wavelets. For example, the signal as shown in Figure 2a is generated by the four wavelet functions $\psi_{3,4}(t)$, $\psi_{4,6}(t)$, $\psi_{4,9}(t)$, and $\psi_{5,12}(t)$ (Figure 2b), with the corresponding coefficients having values of

$$C_f(3,4) = 1.0; \quad C_f(4,6) = 0.3; \quad C_f(4,9) = -0.5; \quad C_f(5,12) = -0.2.$$

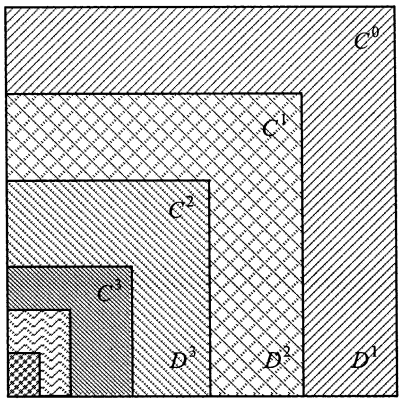

FIGURE 3. A diagram showing the underlying principle of the MRSD.

In this way, the signal can be represented by these four wavelet functions as

$$\psi_{3,4}(t) + 0.3\psi_{4,6}(t) - 0.5\psi_{4,9}(t) - 0.2\psi_{5,12}(t)$$

In general, any function or signal $f(t)$ can be represented by a combination of the wavelet functions in the original domain with the coefficients $\{C_f(i,j)\}$ as

$$f(t) = \sum_{j=-\infty}^{+\infty}\sum_{k=-\infty}^{+\infty} C_f(j,k)\psi_{j,k}(t) \tag{5}$$

2.2. Multiresolution Signal Decomposition (MRSD) Algorithm. Different algorithms have been proposed to carry out WT. Coifman et al.[13] developed the automatic decomposition method which accelerates the development of the wavelet theory. Grossman and Morlet[14] proposed the CWT, which allowed decomposition of a signal into contributions from both the space and the scale domains, based on two separate processes, namely, translation and dilation. Mallat[5] introduced the algorithm of multiresolution signal decomposition (MRSD), which is the one widely used in chemical signal processing and is described below.

MRSD can be viewed as a recursive operation of projection, which is graphically illustrated by Figure 3. Let the whole area of the largest square represent the full information of the original signal C^0. It can be decomposed by WT into two parts D^1 (the area shaded with slash) and C^1 (the whole area of the second largest square). D^1 is the projection of C^0 on the first scale wavelet at the resolution level $j = 1$. C^1 can be further decomposed by WT into two parts of D^2 (the area shaded with cross) and C^2 (the whole area of the third largest square). D^2 is the projection of the C^1 on the second scale wavelet ($j = 2$). The procedure is repeated until a desired scale J is reached. In this way, the pieces of information represented by C^j and D^j are different and correspond to the low frequency and the high-frequency part of C^{j-1}. They are orthogonal to one another.

Equations for computing the signal decomposition and reconstruction (inverse transform) to get back the original signal can be found in the work by Mallat.[5] The procedure is depicted by Figure 4, where C^j and D^j are called, respectively, the discrete approximation and the discrete

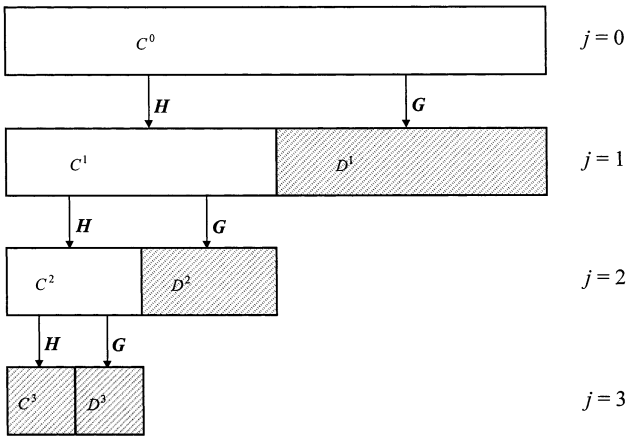

FIGURE 4. A diagram showing the operation of the MRSD method. The slanting line represents the coefficients to be stored.

detail, H and G are discrete filters for the transformation process. The lengths of vectors C^j and D^j are the same and are half of that of C^{j-1}. Algorithms with improved performance and wavelet packets transform (WPT) have also been developed based on that of the MRSD algorithm.[3,15]

3. Applications of Wavelet Transform in Chemistry

Among the papers published between 1989 and 2002,[16] ca. 75% are related to applications of WT in analytical chemistry, basically in spectroscopy, chromatography, and electroanalytical chemistry. WT has been utilized for data compression, data smoothing and denoising, baseline correction, resolution of multicomponent overlapping signals, and processing of analytical images. The remaining 25% of papers are related to quantum chemistry, chemical physics, etc.

3.1. Signal Compression. Modern analytical instruments produce more accurate and multidimensional measurements than in the past, thus allowing acquisition of more abundant information on the samples analyzed. This is, however, possible only with higher storage capacities of the instruments, especially when a database library is needed, e.g., from the field of infrared spectroscopy (IR), mass spectroscopy (MS), nuclear magnetic resonance spectroscopy (NMR), etc.[17−20] Therefore, data compression techniques have been developed and extensively used in the archive of analytical data.

The general procedure of the WT-assisted signal compression can be summarized as follows:

(1) Apply a WT treatment to the original signal and obtain the wavelet coefficients $w = \{C^J,D^J,D^{J-1},...,D^1\}$ using the MRSD algorithm (see Figure 4).

(2) Suppress small coefficients in w, which are considered as too small to contain useful information on the signal by thresholding methods and to store the suppressed vector w_{store}. The number of wavelet coefficients to be stored is going to be determined by the threshold value, which results from a preset compression ratio.

(3) The original signal can be reconstructed, when needed, by applying the inverse transform to the stored vector w_{store}.

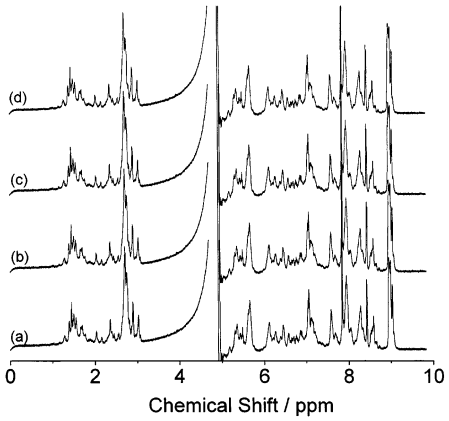

FIGURE 5. A measured NMR spectrum (a) and the reconstructed spectra from the 2048 (b), 1024 (c), and 512 (d) coefficients.[20]

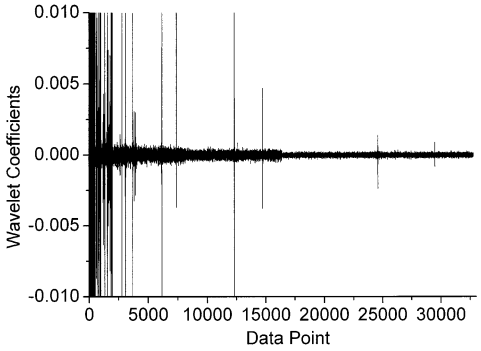

FIGURE 6. Wavelet coefficients corresponding to the NMR spectrum in Figure 5.[20]

Figure 5a gives an NMR spectrum of a biological molecule with 32 768 data points.[20] The wavelet coefficients $w = \{C^J,D^J,D^{J-1},...,D^1\}$ obtained by applying WT to the spectrum with the Symmlet wavelet filters and $J = 9$ are shown in Figure 6. For an easier orientation, data points which are outside the range of ± 0.01 are clipped. It was found out that almost all the coefficients in $\{D^9,D^8,...,D^1\}$ (32704 points) are very small compared to the coefficients in $\{C^9\}$ (64 points). There are only 126 coefficients with absolute values larger than 0.01 in $\{D^9,D^8,...,D^1\}$. Therefore, the main information on the spectrum should be sufficiently represented by 190 wavelet coefficients only. Spectra shown in panels b, c, and d of Figure 5 are reconstructed from 2048, 1024, and 512 wavelet coefficients, respectively, and it can easily be noticed that there is almost no difference among them. The RMSE (root-mean-square error) of the curves shown in panels b, c, and d of Figure 5 with panel a equals to 1.3642×10^{-4}, 1.6977×10^{-4}, and 2.7769×10^{-4}, respectively.[20]

WT is a very efficient method of compression of individual signals, but the set of signals can be compressed to the highest degree by principal component analysis (PCA). Principal components, maximizing description of data variance, are constructed as a linear combination of the original features and have global properties. Application of FFT to simultaneous compression of a set of signals usually offers no advantages at all, due to the fact that compression is less efficient, compared to PCA, and the constructed features are also global. Only compression of

a set of signals in the wavelet domain, although less efficient than PCA, offers features with local properties that can be of great interest for further data processing.

Simultaneous compression of *m* signals with the aid of DWT can be described as follows:

(1) Decompose *m* signals with the selected filter and organized wavelet coefficients in the matrix form, **W**.

(2) Calculate variance vector, elements thereof representing variance of wavelets coefficients in individual columns of matrix **W**.

(3) Compress matrix **W** to the columns associated with these coefficients, for which the highest variance is observed.

Successful applications of WT and WPT in data sets compression can be found in the literatures.[18,19]

Although WT is an efficient data compression technique, its performance can further be enhanced, if it is combined with the other relevant compression techniques. New models based on WT were proposed for data compression, such as the wavelet neural network (WNN)[21] and the recurrent neural network (RNN).[22] Preprocessing of the data sets by WT and WPT before using them in the other chemometrical methods (such as WFA, KNN, and SIMCA) was also studied. All the results obtained point out to the fact that WT and WPT are both preprocessors of high performance, yielding features with local properties.

3.2. Signal Denoising. Denoising is a problem of interest in all fields of science and technology, and a large number of filtering methods (such as Fourier filtering method, Savitzky−Golay smoothing method, and Kalman filtering method) have been developed.[23]

The philosophy underlying denoising with aid of WT is generally considered as resembling the traditional Fourier filtering, in which the high-frequency components are cut off by the low-pass filters. However, in the Fourier filtering the assumption is made that the frequency components of the signal are present mainly at low frequencies and those of the noise at high frequencies. This assumption is fulfilled for stationary signals, although not in the case of unstationary signals. Unstationary signals can have the high-frequency components as well and require decomposition in local basis, such as wavelet basis.

The general procedure of denoising with wavelet analysis is summarized as follows:

(1) Apply WT to a noisy signal f_{noisy} and obtain wavelet coefficients, *w*.

(2) Suppress these elements in *w*, which are considered as attributing noise by the thresholding methods of denoising.

(3) Apply the inverse transform to the suppressed *w*, to obtain the denoised signal f_{denoised}.

Two different approaches for suppression of the elements in *w* are generally used in wavelet denoising, i.e., hard thresholding (simply setting all wavelet coefficients below a certain threshold to zero) and soft thresholding (reducing values of all wavelet coefficients toward zero by the threshold value). Various methods are used to estimate the threshold and to perform the thresholding,[18,23,24] such as the simple hard and soft thresholding, SURE, VISU, HYBRID, MINMAX, etc.

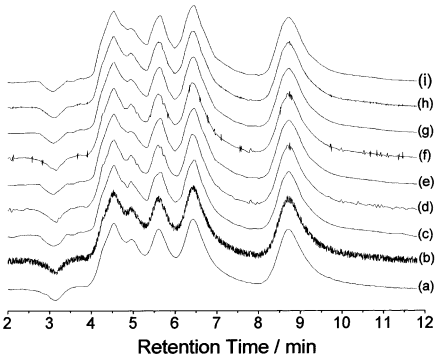

FIGURE 7. A comparison of the various thresholding methods in wavelet denoising of a signal with random noise.[3] (a) A smoothed chromatogram, (b) signal a with 10% of random noise, and the denoised signals by (c) hard thresholding with the threshold being 2.0% of the maximal wavelet coefficients, (d) SURE, (e) VISU with hard thresholding, (f) MINMAX, (g) soft thresholding with the threshold being 1.0% of the maximal wavelet coefficients, (h) HYBRID, and (i) VISU with soft thresholding.

Figure 7 offers a comparison of the data denoised by several thresholding methods, including the Daubechies wavelet. The plot shown in Figure 7a is a smoothed chromatogram, and to the plot given in Figure 7b, random noise was added. The curves shown in Figure 7c−i characterize the effect of application of the various denoising methods. From Figure 7 it can be seen that almost all the results are similar, and except for the plots given in Figure 7d,f, for which some artifacts are observed.

To improve signal denoising, i.e, to reduce such artifacts, Coifman and Donoho[25] developed a translation-invariant denoising method, able to average out the mismatch between the signal and the analyzing wavelet.

The WT technique has been shown as a very powerful denoising tool for unstationary signals. So far, it has been applied to denoising IR spectra,[26] chromatograms,[27] capillary electrophoresis signals,[28] near-infrared diffusive reflectance spectra,[29] oscillographic chronopotentiometric signals,[30] deconvolution voltammetry signal,[31] and also many other data sets. On-line denoising of instrumental signals using an on-line WT technique,[32] application of WPT to denoising,[33] and usage of the WT denoising as a preprocessor of the other chemometrical methods have been studied.[4,5] Techniques for denoising in the instrumentation software packages and for removing the noise in very sharp peaks were also developed.[34]

3.3. Baseline/Background Correction. Baseline drift is a very common problem in analytical chemistry. In many cases, the baseline drift in analytical signals is just like the noise which often causes difficulties with the further data processing. However, the baseline is different in properties from the noise in the sense that the frequency of the drifting baseline is always considerably lower than that of the signals to be analyzed. According to the theory of wavelet decomposition, the baseline component in an

analytical signal should be easy to separate from drifting signals.

First application of the method involved separation of the drifting baseline from a chromatogram acquired via gradient elution.[35] In this work, an experimental signal (C^0) was decomposed into the discrete details D^j and the discrete approximations C^j by using an improved MRSD algorithm. It was found that there is one discrete approximation (C^8) resembling the drifting baseline. The baseline was removed by $C^0 - f \times C^8$ (f is a factor and $f =$ 0.93 was utilized).

Considering the importance of the removal of the baseline from a chromatogram, it is even more important to separate the background from the experimental spectrum of the extended X-ray absorption fine structure (EXAFS) because no useful information can be obtained from the raw spectra. Two approaches were proposed for this purpose, one following the above procedures and another one based on the MRSD algorithm.[36]

Furthermore, a WT-based method for the removal of the background of 2-D analytical data sets (such as HPLC-DAD[37]), application of WT to the background removal from NMR spectra,[38,39] and application of WT to NIR spectral data to deal with nonconstant background for multivariate calibration[40] were also reported.

However, application of the WT in baseline/background removal can only be performed in the limited cases because the properties of the baseline or background are different in various analytical signals. For example, for processing of spectroscopic signals, a time-frequency approach would be more suitable than the time-scale analysis tool (i.e., the WT).[41]

3.4. Peak Detection and Resolution Enhancement. Both peak detection and resolution enhancement are universal problems in analytical chemistry. Mathematical techniques are badly needed by analytical chemists in order to resolve overlapping chromatograms, low-resolution spectra etc. Usually, such problems are solved by using linear or nonlinear regression analysis, curve-fitting techniques, derivative techniques, neural networks, and factor analysis. Owing to the favorable characteristics of WT, applications of the multiresolution technique to resolution enhancement and peak detection in analytical signals were widely studied.[42−45]

The derivative technique is a powerful method, generally used to resolve overlapping analytical signals because it offers higher resolution of the differential data, compared to original data. Although the technique proved very useful in data analysis, it has a major drawback in increasing the noise level in calculations of the higher-order derivative. Therefore, a method, which utilizes WT for the approximate derivative calculations, was proposed.[42] This method can enhance the signal-to-noise ratios for calculations of the higher order derivatives, and at the same time, it retains all major properties of the conventional methods. An approximate first-derivative of an analytical signal can be expressed as the difference between the two scale coefficients C^{j-1}, which are generated from any two Daubechies wavelet functions at different scale. The higher order approximate derivatives can also be obtained from the previous order derivative.

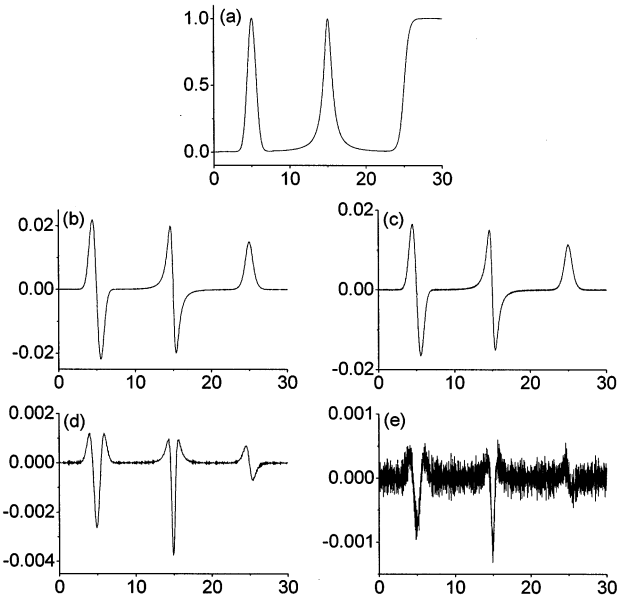

FIGURE 8. A simulated signal (a) and its first derivative (b and c), as well as the second derivative (d and e) obtained by the WT method and by conventional method, respectively.

Figure 8 furnishes a comparison between the results obtained by the WT method and by a conventional method from a simulated signal, which is generated by the Gaussian, Lorentzian and Sigmoid functions with an added white noise. The noise level equals to 0.0002 (SNR equals to 2500). It is evident that the signal-to-noise value for the results obtained by WT is much better than that obtained by the conventional method.

Another method for estimation of an approximate derivative based on CWT with the Haar wavelet was also proposed.[43] Owing to the characteristics of the Haar wavelet function, the approximate nth derivative of an analytical signal can be obtained by applying WT n times to the signal. The results obtained by employing the four methods (i.e., the conventional numerical differentiation, the Fourier transform, the Savitzky-Golay, and the WT method) were compared with the CWT approach. It was demonstrated that all the results are closely similar for signals not contaminated with noise. But for noisy signals, the CWT method is superior to the three remaining ones. Figure 9 shows the approximate first and second derivative of the photoacoustic spectrum of $Pr(Gly)_3Cl_3 \cdot 3H_2O$, obtained using the CWT method. It can easily be seen that the results are satisfactory.[43]

Various resolution methods have been reported for resolution of multicomponent overlapping analytical signals, such as Fourier self-deconvolution (FSD), Fourier derivation (FD), and factor analysis. Since WT can easily be used to decompose a signal into components having different frequencies, the resolved signals should be retrievable by WT decomposition of overlapping signals.

Two approaches were proposed for resolution of overlapping signals, using the WT decomposition and

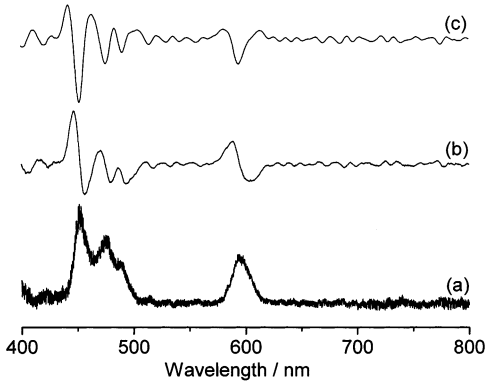

FIGURE 9. The photoacoustic spectrum of $Pr(Gly)_3Cl_3 \cdot 3H_2O$ (a) and its first derivative (b) and second derivative (c) obtained by the CWT method.[43]

reconstruction procedures. The first approach includes the following two steps:[44]

(1) Use WT to decompose an overlapping signal to its components (approximations and details). The component at a different wavelet scale will be in a different frequency.

(2) Select a decomposed component by visual inspection at the medium wavelet scale, which represents the resolved information.

Then directly use the selected component for a further study, such as elucidation of the spectra for spectral analysis and the area calculation for quantitative determination.

The second approach is based on the WT decomposition and reconstruction;[45] i.e.,

(1) decompose the analyzed signal to its components and select one or more components, which represent the resolved information,

(2) multiply the selected components by a factor k with a value higher than 1.0, and

(3) construct the analyzed signal by using the reverse transform.

It is evident that the essence of the approach is to increase the resolved information into the overlapping signal.

A successful example on application of the first approach to resolve overlapping analytical signals was published in Analytical Chemistry.[44] Chromatograms of a mixture of samples composed of differentiated concentrations of benzene, methylbenzene and ethylbenzene were investigated. Employing the D^3 component obtained by using the WT decomposition with the Haar wavelet, the three peaks could be well resolved and very good calibration curves with peak areas versus the concentrations were obtained.

Using exactly the same approach, the WPT resolution and quantitative determination of heavily overlapping chromatograms were also studied.[46] It was found that WPT performs better than the WT approaches. Furthermore, this method was also employed for detection of the number of components in overlapping chromatograms.[47] The number of components can easily be determined just by counting the number of the positive peaks in the data resolved by WT processing.

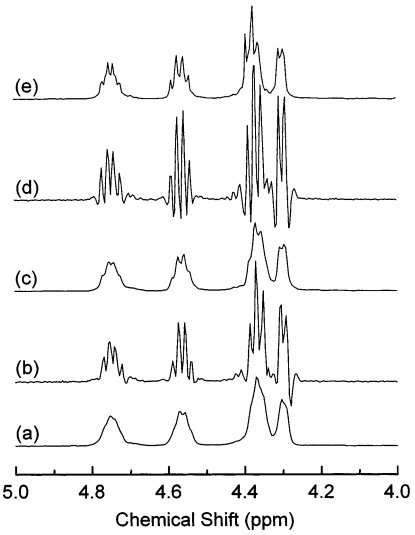

FIGURE 10. A comparison of the experimental NMR spectra and their resolved results. Curves a and c are the experimental spectra with low resolution, curves b and d are the resolved results from a and c, respectively, and curve e is the experimental spectrum with the best resolution.[45]

As a good illustration of the second approach for overlapping signals, resolution of the NMR spectra was studied.[45] Figure 10 shows a part of the results, in which, the curves a, c, and e represent the three experimental spectra of a biological sample with different resolutions and curves b and d are resolved results from curves a and c, respectively, via components D^1 and D^2 with $k = 10$. It can easily be seen that resolution is greatly improved by the wavelet treatment.

Although the procedures above have been successfully used for resolution of overlapping signals in several cases, there are still problems and limitations in practical uses, such as the effects of the wavelet filters and the largest decomposition scale J on the WT transformed result. They have not been proved as a general approach for obtaining any kind of analytical signals. Further studies are still needed.

3.5. Calibration, Regression, and Classification. Several methods for modeling of the high-dimensional spectral data have been proposed, including the principal component regression (PCR) and the partial least square (PLS) method. PLS coupled with the feature selection in the wavelet domain was reported and successfully applied to the analysis of the NIR spectra of polyether polyols, pharmaceutical tablets, and gasoline samples.[48]

For classification and regression, an adaptive wavelet algorithm (AWA) employing the higher multiplicity wavelets was proposed,[12] allowing a procedure to stepwise design the specific filter coefficients by an adaptive iteration. Defining the novel classification criterion function and the regression assessment criterion, classification of the seagrass, *para*-xylene, and butanol samples with aid of the NIR spectra was attained, and the regression studies aiming at quantification of the components in sugar and wheat were performed.[12]

New methods based on WT or WPT were also developed recently. By using the WPT decomposition and reconstruction from selected coefficients, a WPTER (wavelet packet transform for efficient pattern recognition of signals) method was proposed and successfully applied to a data set consisting of X-ray diffractograms on fired tiles subjected to different firing cycles.[49] Discriminant analysis of the ion mobility spectrometry (IMS) was achieved by combining the WT compression and a regularized version of linear discriminant analysis (LDA).[50]

3.6. Analytical Image Processing. A vast number of papers have been published on applications of WT or WPT for image processing. These include denoising, compression, image coding, feature selection, etc. In the field of chemistry, application of WT in an analytical image processing was also reported.[51,52] In these papers, denoising, compression, feature extraction, registration and fusion of the 2-D and 3-D secondary ion mass spectrometry (SIMS) and electron probe microanalysis (EPMA) images were studied, via the 2-D and 3-D wavelet transform.

4. Conclusion

Since 1989, various possibilities of applications of WT to the different fields of chemistry have been investigated. Apart from the studies mentioned in this paper, other papers have reported the applications of WT in chemistry such as, e.g., an online detection of transitions in the time series, fractal structure analysis, protein sequences analysis etc. These studies have proven that the WT-based techniques are very efficient and therefore they can play an important role in the chemical signal processing. The authors hope that this paper will stimulate broader interest in applications of WT. Further investigations on the topics are still proceeding, and the WT techniques are expected to gain popularity among chemists in the future as a widely used approach.

Thanks are due to Dr. Beata Walczak for critical reading of the manuscript. This work was supported by the University Grants Council (UGC) of Hong Kong SAR via the Area of Excellence project "Chinese Medicine Research and Further Development" (AoE/B-10/01), the BRC of The Hong Kong Polytechnic University (Grant No. 9687), and NSFC (National Natural Science Foundation) of China.

Note after ASAP Posting

This article first appeared on the web on 2/7/2003 with errors in Figure 6 and the text. The correct version was published on 2/14/2003.

References

(1) Glasser, L. Fourier transforms for chemists. *J. Chem. Educ.* **1987**, *64*, A228−A233, A260−A266, A306−313.
(2) Leung, A. K. M.; Chau, F. T.; Gao, J. B. A review on application of wavelet transform techniques in chemical analysis: 1989−1997. *Chemom. Intell. Lab. Syst.* **1998**, *43*, 165−184.
(3) Shao, X. G.; Cai, W. S. Wavelet analysis in analytical chemistry. *Rev. Anal. Chem.* **1998**, *XVII*, 235−285.
(4) Daubechies, I. Orthonormal bases of compactly supported wavelets. *Commun. Pure Appl. Math.* **1988**, *41*, 909−996.
(5) Mallat, S. G. A theory of multiresolution signal decomposition: the wavelet representation. *IEEE Trans. Pattern Anal. Machine Learning* **1989**, *11*, 674−693.
(6) Daubechies, D. *Ten Lectures on Wavelets*; SIAM Press: Philadelphia, 1992.
(7) Chui, C. K. *Wavelets: A Tutorial in Theory and Application*; Academic Press: Boston, 1992.
(8) Chui, C. K. *Wavelets: A Mathematical Tool for Signal Processing*; SIAM Press: Philadelphia, 1997.
(9) Hoch, J. C.; Stern, A. S. *NMR Data Processing*; John Wiley & Sons: New York, 1996.
(10) Felinger, A. *Data Analysis and Signal Processing in Chromatography*; Elsevier Science: Amsterdam, 1998.
(11) Vandeginste, B. G. M.; Massart, D. L.; Buydens, L. M. C.; de Jong, S.; Lewi, P. J.; Smeyers-Verbeke, J. *Handbook of Chemometrics and Qualimetrics: Part B*; Elsevier Science: Amsterdam, 1998.
(12) Walczak, B. *Wavelets in Chemistry*; Elsevier Science: Amsterdam, 2000.
(13) Coifman, R. R.; Wickerhauser, M. V. Entropy-based algorithms for best basis selection. *IEEE Trans. Inf. Theory* **1992**, *38*, 713−719.
(14) Grossman, A.; Morlet, J. Decomposition of Hardy functions into square integrable wavelets of constraint shape. *SIAM J. Math.* **1984**, *15*, 723−736.
(15) Shao, X. G.; Li, W.; Chen, G.; Su, Q. D. On-line analysis of the photoacoustic spectral signal using wavelet transform. *Fresenius J. Anal. Chem.* **1999**, *363*, 215−218.
(16) Leung, A. K. M. Wavelet transform in chemistry (http://fg702−6.abct.polyu.edu. hk/wavelet.html).
(17) Chau, F. T.; Shih, T. M.; Gao, J. B.; Chan, C. K. Infrared spectral compression procedure using the fast wavelet transform method. *Appl. Spectrosc.* **1996**, *50*, 339−348.
(18) Walczak, B.; Massart, D. L. Noise suppression and signal compression using the wavelet packet transform. *Chemom. Intell. Lab. Syst.* **1997**, *36*, 81−94.
(19) Leung, A. K. M.; Chau, F. T.; Gao, J. B.; Shih, T. M. Application of wavelet transform in infrared spectrometry: spectral compression and library search. *Chemom. Intell. Lab. Syst.* **1998**, *43*, 69−88.
(20) Shao, X. G.; Gu, H.; Cai, W. S.; Pan, Z. X. Studies on data compression of 1-D NMR spectra using wavelet transform. *Spectrosc. Spectrosc. Anal.* **1999**, *19*, 139−141.
(21) Liu, W.; Li, J. P.; Xiong, J. H.; Pan, Z. X.; Zhang, M. S. The Compression of IR spectra by using wavelet neural network. *Chin. Sci. Bull.* (English Edition) **1997**, *42*, 822−825.
(22) Li, L. K.; Chau, F. T.; Leung, A. K. M. Compression of ultraviolet−visible spectrum with recurrent neural network. *Chemom. Intell. Lab. Syst.* **2000**, *52*, 135−143.
(23) Barclay, V. J.; Bonner, R. F.; Hamilton, I. P. Application of wavelet transforms to experimental spectra: smoothing, denoising, and data set compression. *Anal. Chem.* **1997**, *69*, 78−90.
(24) Mittermayr, C. R.; Nikolov, S. G.; Hutter, H.; Grasserbauer, M. Wavelet denoising of Gaussian peaks: a comparative study. *Chemom. Intell. Lab. Syst.* **1996**, *34*, 187−202.
(25) Coifman, R. R.; Donoho, D. L. In *Wavelets and Statistics*; Antoniadis, A., Oppenheim, G., Eds.; Springer-Verlag: New York, 1995; pp 103−125.
(26) Alsberg, B. K.; Woodward, A. M.; Winson, M. K.; Rowland, J.; Kell, D. B. Wavelet denoising of infrared spectra. *Analyst* **1997**, *122* (7), 645−652.
(27) Shao, L. M.; Tang, B.; Shao, X. G.; Zhao, G. W.; Liu, S. T. Wavelet transform treatment of noise in high performance liquid chromatography. *Chin. J. Anal. Chem.* **1997**, *25* (1), 15−18.
(28) Wang, L. S.; Yang, X. Y.; Xi, S. F.; Mo, J. Y. Wavelet smoothing and denoising to process capillary electrophoresis signals. *Chem. J. Chin. Univ.* **1999**, *20* (3), 383−386.
(29) Min, S. G.; Xie, X. J.; Zhou, X. Q.; Li, L.; Yan, Y. L. Noise filtering for near infrared diffusive reflectance spectra by wavelet transform. *Chin. J. Anal. Chem.* **1998**, *26* (1), 34−37.
(30) Gu, W. L.; Zhang, S. L.; Zhang, H. Q.; Zheng, J. B. Application of denoising by wavelet transform in the processing of oscillographic chronopotentiometric signal. *Chin. J. Anal. Chem.* **1999**, *27* (2), 220−223.
(31) Lu, X. Q.; Mo, J. Y. Methods of handling discrete data for deconvolution voltammetry (I) wavelet transform smoothing. *Chem. J. Chin. Univ.* **1997**, *18* (1), 49−51.
(32) Shao, X. G.; Hou, S. Q. An on-line wavelet transform for denoising of high performance liquid chromatograms. *Analy. Lett.* **1999**, *32* (12), 2507−2520.
(33) Shao, X. G.; Cai, W. S. A novel algorithm of the wavelet packets transform and its application to de-noising of analytical signals. *Anal. Lett.* **1999**, *32* (4), 743−760.

(34) Perrin, C.; Walczak, B.; Massart, D. L. The use of wavelets for signal denoising in capillary electrophoresis. *Anal. Chem.* **2001**, *73*, 4903−4917.
(35) Shao, X. G.; Cai, W. S.; Pan, Z. X. Wavelet transform and its applications in high performance liquid chromatography (HPLC) analysis. *Chemom. Intell. Lab. Syst.* **1999**, *45*, 249−256.
(36) Shao, X. G.; Shao, L. M.; Zhao, G. W. Extraction of extended X-ray absorption fine structure information from the experimental data using the wavelet transform. *Anal. Commun.* **1998**, *35*, 135−137.
(37) Shen, H. L.; Wang, J. H.; Liang, Y. Z.; Pettersson, K.; Josefson, M.; Gottfries, J.; Lee, F. Chemical rank estimation by multiresolution analysis for two-way data in the presence of background. *Chemom. Intell. Lab. Syst.* **1997**, *37*, 261−269.
(38) Barache, D.; Antoine, J. P.; Dereppe, J. M. The continuous wavelet transform, an analysis tool for NMR spectroscopy. *J. Magn. Reson.* **1997**, *128*, 1−11.
(39) Gunther, U. L.; Ludwig, C.; Ruterjans, H. WAVEWAT-Improved solvent suppression in NMR spectra employing wavelet transforms. *J. Magn. Reson.* **2002**, *156*, 19−25.
(40) Tan, H. W.; Brown, S. D. Wavelet analysis applied to removing non-constant, varying spectroscopic background in multivariate calibration. *J. Chemometr.* **2002**, *16*, 228−240.
(41) Antoine, J. P.; Coron, A.; Dereppe, J. M. Water peak suppression: Time-frequency vs time-scale approach. *J. Magn. Reson.* **2000**, *144*, 189−194.
(42) Leung, A. K. M.; Chau, F. T.; Gao, J. B. Wavelet transform: a novel method for derivative calculation in analytical chemistry. *Anal. Chem.* **1998**, *70*, 5222−5229.
(43) Shao, X. G.; Pang, C. Y.; Su, Q. D. A novel method to calculate the approximate derivative photoacoustic spectrum using continuous wavelet transform. *Fresenius J. Anal. Chem.* **2000**, *367*, 525−529.
(44) Shao, X. G.; Cai, W. S.; Sun, P. Y.; Zhang, M. S.; Zhao, G. W. Quantitative determination of the components in overlapping chromatographic peaks using wavelet transform. *Anal. Chem.* **1997**, *69*, 1722−1725.
(45) Shao, X. G.; Gu, H.; Wu, J. H.; Shi, Y. Y. Resolution of the NMR spectrum using wavelet transform. *Appl. Spectrosc.* **2000**, *54*, 731−738.
(46) Shao, X. G.; Cai, W. S. An application of the wavelet packets analysis to resolution of multicomponent overlapping analytical signals. *Chem. J. Chin. Univ.* **1999**, *20* (1), 42−46.
(47) Shao, X. G.; Cai, W. S.; Sun, P. Y. Determination of the component number in overlapping multicomponent chromatogram using wavelet transform. *Chemom. Intell. Lab. Syst.* **1998**, *43*, 147−155.
(48) Jouan-Rimbaud, D.; Walczak, B.; Poppi, R. J.; de Noord, O. E.; Massart, D. L. Application of Wavelet Transform to Extract The Relevant Component from Spectral Data for Multivariate Calibration. *Anal. Chem.* **1997**, *69*, 4317−4323.
(49) Cocchi, M.; Seeber, R.; Ulrici, A. WPTER: wavelet packet transform for efficient pattern recognition of signals. *Chemom. Intell. Lab. Syst.* **2001**, *57*, 97−119.
(50) Mehay, A. W.; Cai, C. S.; Harrington, P. D. Regularized linear discriminant analysis of wavelet compressed ion mobility spectra. *Appl. Spectrosc.* **2002**, *56*, 223−231.
(51) Nikolov, S.; Hutter, H.; Grasserbauer, M. De-noising of SIMS images via wavelet shrinkage. *Chemometr. Intell. Lab. Syst.* **1996**, *34*, 263−273.
(52) Wolkenstein, M. G.; Hutter, H.; Grasserbauer, M. Improvement of SIMS image classification by means of wavelet de-noising. *Fresenius J. Anal. Chem.* **1997**, *357*, 783−788.

AR990163W