Application of Wavelet Transform in Improving Resolution of Two-Dimensional Infrared Correlation Spectroscopy

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Abstract. FTIR is a great improvement in IR spectroscopy, and two-dimensional infrared (2D IR) correlation spectroscopy well advances its capabilities. But for complicated mixture systems, such as traditional Chinese medicines, the spectra are rather similar and these methods fall short. To improve the resolution of 2D IR spectrum, and make it possible to distinguish complicated mixture systems, the application of wavelet transform to 2D IR was explored in this paper. After performing decomposition, processing, and reconstruction of the set of dynamic spectra, the resolution of the synchronous 2D IR correlation spectrum was improved obviously. More peaks appeared and the peaks became quite clear and separate. Four Coptis samples of aged 1-4 could be distinguished with this approach. Using wavelet transform, 2D IR would become more powerful in analysis and discrimination.

1 Introduction

Wavelet analysis has been a powerful analytical tool in many scientific and practical fields, such as quantum mechanics, signal analysis, image processing and so on. The main reason is that wavelet analysis has many particular characteristics. For example, it can analyze signals at different scales or resolutions, which is called multiresolution. And it also can localize signals in both frequency and time domains. Compared to Fourier analysis, which uses endless basic functions sine and cosine, wavelet analysis uses basic functions that are only nonzero in limited space or time. Therefore, wavelets can well express the signals that have non-stationary variations [1]. In Fourier translation infrared (FTIR) spectra, sharp peaks always exist, so in some ways, it would be better to process with wavelets than other methods.

FTIR really enhances the capabilities of IR spectroscopy. Signal noise ratio (SNR) is improved, so are the resolution and the speed of scan. However, no matter what have been done, the end point of a technique could never be reached. Some things are always waiting for study. For FTIR, the resolution is still expected to be enhanced so that more information could be obtained from the spectra. In recent years, a new tech-

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nology called two-dimensional (2D) correlation spectroscopy [2] attracts more and more people. Here, the 2D concept is some different from the one in nuclear magnetic resonance (NMR). It is called generalized two-dimension. It can base on many kinds of perturbations, like temperature, concentration, pressure, magnetic field, electric field, etc. [3]. This technology has been use in various fields, such as FTIR spectroscopy, fluorescence spectroscopy, and Raman spectroscopy and so on [4][5]. When used in FTIR, it is called 2D IR. Though 2D IR well improves the resolution of the IR spectrum, and was used to discriminate rather similar complicated mixture systems like traditional Chinese medicine [4], that is not enough. Sometimes the IR spectra of different samples are almost the same as each other, even in high resolution 2D correlation spectra. To distinguish these kinds of samples, it still requires enhancing the resolution.

As we know, Coptis is a common traditional Chinese medicine, and it is a kind of broadspectrum antimicrobials. Its effective components are Coptisine, Berberine, Epiberberine, Palmatine, and some other alkaloids. Different ages of Coptis have discrepancies in their functions. So it is very important to distinguish them. But the spectra of different ages Coptis are rather similar, it’s difficult to distinguish them directly.

This paper is concerned with the application of wavelet transform to 2D IR, wish to enhance the performances of 2D correlation spectrum, and explore the possibility to distinguish the much similar complex compounds like Coptis.

1.1 Wavelet Transform

Wavelet transform is the development of Fourier transform with the following general definition:

\[ W_{a,b}(f(t), \Psi) = \frac{1}{\sqrt{a}} \int_{-\infty}^{\infty} f(t) \Psi\left(\frac{t-b}{a}\right) dt \]  \hspace{1cm} (1)

Where \( a, b \in \mathbb{R} \) with \( a \neq 0 \), \( f \) is the signal function, \( \Psi \) is the basic wavelet function. The parameter \( a \) is the dilation factor while \( b \) is the translation factor. An intuitive physical explanation of equation (1) is very simple: \( W \) is the ‘energy’ of \( f(t) \) of scale \( a \) at \( t=b \) [5]. Because of localized vibration, \( \Psi \) looks just like a window function. This makes it possible to decompose a signal in given time domain or space domain. Hence, wavelet transform in some sense is the same as the linear combination of wavelets of different scales and different locations.

Using wavelet transform, signals can be decomposed into several levels. At each level, two sets of coefficients are obtained. One is for approximation coefficients and the other is for detail coefficients. The decomposition can be show in Fig.1. Original signal \( S0 \) is decomposed in to two parts, one is the approximation \( A1 \), the other is the detail \( D1 \). Then, \( A1 \) can be taken to decompose. In this way, original can be decomposed into specified levels.

After decomposition, the approximation and detail coefficients can be processed according to special need, such as signal denoising, image compression and so on. At last, to obtain the processed signal, reconstruction with the coefficients is needed. This is also called inverse wavelet transform [7], see equation (2).