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Wavelet-based spectral analysis

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ABSTRACT

Wavelets are a topic of pure mathematics. But over the past decade, they have shown great promise and are now being adapted for a vast number of signal-processing applications. One of the main advantages of wavelet analysis is the amount of information that can be extracted from a signal. It has demonstrated unprecedented success in terms of asymptotic optimality, spatial adaptivity and computational efficiency. Applications of wavelet transform and wavelet-packet transform in spectral analysis from 2002 to 2013 are reviewed in this article, clearly stating that wavelet methods significantly outperform other traditional methods of signal processing.

Contents

1. Introduction

Signal processing incorporates all aspects of operations on or analysis of analog and digitized signals, representing time-varying or spatially varying physical quantities. In the past decade, this field has unambiguously become a burgeoning area of research and design.

Wavelet Transform (WT) is one of the recent techniques for processing signals. It is defined as mathematical functions that cut up data into different frequency components, and then study each component with a resolution matched to its scale [1]. Wavelet signal processing is different from other signal-processing methods because of the unique properties of wavelets (i.e., wavelets can be symmetric or asymmetric, sharp or smooth, regular or irregular). It can represent signals sparsely, capture the transient features of signals, and enable signal analysis at multiple resolutions. Interest in wavelets and their potential application has resulted in an explosion of papers in life sciences and physical sciences.

The goal of this review is to comment on all outstanding and state-of-the-art articles of wavelet-based spectral analysis published in the period 2002–13 in the context of developments and challenges yet to be addressed.

2. Theoretical background

Given a time-varying signal, f(t), WT consists of computing coefficients, which are inner products of the signal and a family of wavelets. In other words, WT decomposes a signal into localized contributions (details and approximations) labeled by a scale and a position parameter. The spatial localization of wavelets makes them more suited to present a large class of signals [i.e., spectra can be represented by far fewer wavelets than sinusoids obtained from Fourier Transform (FT)]. WT is categorized into continuous wavelet tools and discrete wavelet tools. Usually, continuous wavelet tools are used for signal analysis, such as self-similarity analysis and time-frequency analysis. However, discrete wavelet tools are employed for both signal analysis and signal processing, such as noise

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reduction, data compression, and peak detection. A more detailed introduction to the theory and potential application of WT is available in books [2–4].

Generally, the Continuous Wavelet Transform (CWT) of a signal, f (t), can be written as:

$$W_f(\tau,s)=\frac{1}{\sqrt{|s|}}\int_{-\infty}^{+\infty} f(t)\Psi\left(\frac{t-\tau}{s}\right)dt$$

where τ and s are the so-called translation (or time location) factor and the scaling (or dilation) factor, respectively. Factor $|s|^{-1/2}$ is for energy normalization across the different scales, whereas $\Psi_{\tau,s}(t)$ can be obtained by dilations and translations of a single function Ψ(t), the so-called "mother wavelet", as follows:

$$\Psi_{\tau,s}(t)=\frac{1}{\sqrt{|s|}}\Psi\left(\frac{t-\tau}{s}\right).$$

Thus, the original signal can be exactly reconstructed from the wavelet coefficients by Inverse Wavelet Transform (IWT):

$$f(t)=\frac{1}{C_\Psi}\int_0^{\infty}\int_{-\infty}^{+\infty} W_f(\tau,s)\Psi_{\tau,s}(t)d\tau\frac{ds}{s^2}$$

where C_Ψ is defined as:

$$C_\Psi=\int_0^{\infty}\frac{|\Psi(\omega)|^2}{\omega}d\omega$$

and Ψ(ω) is the FT of the mother wavelet.

If $s=s_0^j$ and $\tau=k\tau_0 s_0^j\,(j,k\in Z, s_0\neq 0)$, the wavelet can be re-written as:

$$\Psi_{j,k}(t)=s_0^{-j/2}\Psi\left(s_0^{-j}t-k\tau_0\right)$$

This is used in the computation of Discrete Wavelet Transform (DWT), where $s_0 = 2$ and $\tau_0 = 1$ (dyadic dilations and translations) are generally used. DWT is very useful in compressing data, because it does not change the amount of data (the total number of coefficients is equal to that of data points of the original signal), but the relevant information is often stored in only very few coefficients.

The basic idea of wavelet analysis is that of multi-resolution signal decomposition introduced by Mallat (i.e., the simultaneous appearance of a signal on multiple scales to study its various features) [5]. This algorithm consists of a series of successive decompositions of the signal (with length 2^n) into two components: "detail coefficients D_j" and "approximation coefficients A_j", both with a reduced size of 2^{n-j}, where j is the decomposition level. At each level, the input signal is decomposed by high-pass filters to record the high-frequency components and low-pass filters to extract the low-frequency components for the next scale. The procedure is repeated with sets of high-pass and low-pass filters until at a prescribed level j is reached ($j \leq n$).

By doing so, signal f(t) can be written as a limit of successive approximations at different approximation subspaces, while each of the approximations at subspaces is a smoother version of f(t). According to the Mallat's algorithm, in the case of CWT, a signal can be decomposed with wavelets as follows:

$$f(t)=\sum_{k=-\infty}^{\infty} A_{j,k}\varphi_{j,k}(t)+\sum_{j=1}^{n}\sum_{k=-\infty}^{\infty} D_{j,k}\Psi_{j,k}(t)$$

where $\varphi_{j,k}(t)$ and $\Psi_{j,k}(t)$ are called scaling functions and wavelet functions, respectively. $A_{j,k}$ and $D_{j,k}$ are the approximation coefficients and the detail coefficients mentioned in the Mallat's algorithm. At each successive scale (or decomposition level), only high-frequency information (noise) is retained in the details, while the low-frequency information (signal features) is retained in the approximations. The de-noised signal can then be reconstructed with the new estimated wavelet coefficients:

$$f^*(t)=\sum_{k=-\infty}^{\infty} A_{n_{opt},k}\varphi_{j,k}(t)+\sum_{j=1}^{n_{opt}}\sum_{k=-\infty}^{\infty} D^*_{j,k}\Psi_{j,k}(t)$$

where $A_{nopt,k}$ are the approximation coefficients at the optimal decomposition level n_{opt}, and $D^*_{j,k}$ are the detail coefficients retained.

3. Noise removal and resolution enhancement

Noise distortion can occur during spectral signal acquisition and transmission. Unfortunately, most optical instruments are often limited in sensitivity and specificity by noise fringes superimposed on the recorded spectra. To remove unwanted components, WT was investigated for automated implementation of baseline removal. It was noted that, with synthetic data sets designed to exemplify vibrational spectroscopic signals, WT could filter out high-frequency noise but was less successful with high signal-to-noise ratio (SNR) spectra and in congested regions [6]. In addition, the applicability of translation-invariant WT in filtering light signals from spectrophotometers was studied [7]. The main advantages of this technique are a substantial increase in the SNR and preservation of the spectral peak location and width, as compared to Gaussian, Wiener and orthogonal wavelet filters using a fixed threshold. On the other hand, laser-induced breakdown spectroscopy signals could be de-noised by an extension of the Donoho's scheme, which uses a redundant form of WT and an adaptive threshold-estimation method [8]. Adaptive stationary wavelet filtering via variable thresholding offers noise-suppression improvement in parallel with signal preservation, which is superior to that offered by DWT thresholding and Gaussian filtering.

In another study, a methodology based on an improved, second-generation Adaptive Wavelet Transform (AWT) algorithm was presented for Raman spectral denoising and baseline elimination [9]. This methodology uses a spectrally adapted lifting scheme to generate an infinite basis of wavelet filters from a single conventional wavelet, and then finds the optimal one. As a result, it is more efficient than DWT because it enables the custom design of wavelet filters according to the topological characteristics of Raman spectra at hand. CWT was also suitable for removing the variant background of NIR diffuse reflectance spectroscopy in pharmaceutical analysis [10]. Nevertheless, DWT could be successfully used for denoising short-wave NIR reflectance spectra when the preprocessed data were used as the input of the Support Vector Machine (SVM) system, especially when the number of samples was small [11].

A wavelet-based denoising technique was applied to a quantum-cascade laser spectrometer for *in situ* and real-time atmospheric trace-gas measurements [12]. The wavelet digital-filter technique in post-signal processing proved to give better measurement precision and higher detection sensitivity without reducing the fast temporal response, as compared to other commonly used digital-filter techniques (i.e., Kalman filter, Wiener filter and moving average). Because both wavelets and Kalman filters could handle non-stationary signals, a more promising technique based on incorporating both WT and Kalman filter (i.e., a wavelet-based Kalman filter) would be more effectively applied for trace-gas sensors. It was also found that CWT has better space-time resolution and is relatively simpler to perform, as compared to DWT, for the elimination of the fluctuating background in NIR spectra [13]. WT produces better calibration models of NIR single-beam spectra, with improvements in concentration prediction of the order of 30% being realized relative to models based on second-derivative spectra or spectra preprocessed with simple additive and multiplicative scaling correction