Supporting Information

Innovative Wavelet Protocols in Analysing Elastic Incoherent Neutron Scattering

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I. CONTINUE WAVELET TRANSFORM (CWT)

The continuous wavelet transform (CWT) of $y(t) \in L^2(\mathbb{R})$ is defined as:

$$W_y(\tau, s) = \langle y, \psi_{\tau,s} \rangle = \int_{-\infty}^{\infty} y(t)\psi_{\tau,s}^*(t)dt \quad (1)$$

where <,> is the scalar product in $L^2(\mathbb{R})$ defined as $< f, g >:= \int f(t)g^*(t)\, dt$ and the asteriks denote the complex conjugate and $\psi_{\tau,s}$ is the mother wavelet:

$$\psi_{\tau,s} = \frac{1}{\sqrt{s}}\psi\left(\frac{t-\tau}{s}\right) \quad (2)$$

where $\tau \in \mathbb{R}$ is a translation parameter, whereas $s \in \mathbb{R}^+$ $(s \neq 0)$ is a dilation or scale parameter. The factor $s^{-1/2}$ is a normalization constant such that the energy, i.e., $\|\psi_{\tau,s}\| = \|\psi\| = \langle\psi|\psi\rangle^{1/2} = 1$, the value provided through the square integrability of $\psi_{\tau,s}$ is the same for all scale a. One notices that the scale parameter a rules the dilations of independent variable $(t - \tau)$. In the same way, the factor $s^{-1/2}$ rules the dilation in the values taken by ψ. One notices that the scale parameters rules the dilations of independent variable $(t - \tau)$. In the same way, the factor $s^{-1/2}$ rules the dilation in the values taken by ψ and one is able to decompose a square integrable function $y(t)$ in terms of these dilated-translated wavelets. The CWT measures the variation of x in a neighborhood of the point τ, whose size is proportional to s. If one is interested to reconstruct y from its wavelet transform one makes use of the reconstruction formula:

$$y(t) = \frac{1}{C_\psi}\int_0^{\infty}\int_{-\infty}^{\infty} W_y(\tau, s)\psi_{\tau,s}(t)\frac{d\tau ds}{s^2} \quad (3)$$

where it is now clear why it imposed $C_\psi = \int_0^{\infty}\frac{|\hat{\psi}(\omega)|^2}{|\omega|}d\omega < \infty$.

The CWT can operate at every scale, from that of the original signal up to some maximum scale that one determines. The CWT is also continuous in terms of shifting during computation, the analyzing wavelet is shifted smoothly over the full domain of the analyzed function.

II. DISCRETE WAVELET TRANSFORM (DWT)

However, a huge amount of data are represented by a finite number of values, so it is important to consider a discrete version of the CWT. Generally, the orthogonal (discrete) wavelets are employed because this method associates the wavelets to orthonormal bases of $L^2(\mathbb{R})$. In this case, the wavelet transform is performed only a discrete grid of parameters of dilation and translation, i.e., s and τ take only integral values. Within this framework, an arbitrary signal $y(t)$ of finite energy can be written using an orthonormal wavelet basis:

$$y(t) = \sum_m \sum_n d_n^m \psi_n^m(t), \quad (4)$$

where the coefficient of the expansion are given by:

$$d_n^m = \int_{-\infty}^{\infty} y(t)\, \psi_n^m(t)dt. \quad (5)$$

The orthonormal basis functions are all dilations and translations of a function referred as the analyzing wavelet $\psi(t)$, and they can be expressed in the form:

$$\psi_n^m = 2^{m/2}\psi(2^m t - n), \quad (6)$$

with m and n denoting the dilation and translation indices, respectively. The contribution of the signal at a particular wavelet level m is given by:

$$d_m(t) = \sum_n d_n^m \psi_n^m(t), \quad (7)$$

which provides information on the time behavior of the signal within different scale bands. Additionally, it provides knowledge of their contribution to the total signal energy. In this context, Mallat (1999) developed computationally efficient method to calculate $y(t) = \sum_m \sum_n d_n^m \psi_n^m(t)$ and $d_n^m = \int_{-\infty}^{\infty} y(t)\, \psi_n^m(t)dt$. This method is known as a multiresolution analysis (MRA) [51]. The MRA provides to construct wavelet with different properties and it connects, in an elegant way, wavelets and filter banks. A sequence $\{V_j\}_{j\in\mathbb{Z}}$ of closed subspaces of $L^2(\mathbb{R})$ is a MRA if the following 6 properties are satisfied:

1. $\forall(j,k) \in \mathbb{Z}, \qquad y(t) \in V_j \Leftrightarrow x\left(t - 2^j k\right) \in V_j$ (8)
2. $\forall j \in \mathbb{Z}, \qquad V_{j+1} \in V_j,$ (9)
3. $\forall j \in \mathbb{Z}, \qquad y(t) \in V_j \Leftrightarrow y\left(\frac{t}{2}\right) \in V_{j+1},$ (10)
4. $\lim_{j\to\infty} V_j = \bigcap_{j=-\infty}^{\infty} V_j = \{0\},$ (11)
5. $\lim_{j\to\infty} V_j = \overline{\bigcup_{-\infty}^{\infty} V_j = L^2(\mathbb{R})}$ (12)
6. There exists θ such that $\{\theta(t-n)\}_{n\in\mathbb{Z}}$ is a Riesz basis of V_0. (13)

The space $L^2(\mathbb{R})$ is ordery partitioned and the relationship between adjacent spaces V_j and V_{j+1} is reflected from condition 2) and 3), so the basis of V_j and V_{j+1} differs only on the scale by 2. In order to construct an orthogonal basis is necessary to introduce that a space series W_j satisfies $V_j \oplus W_j \subset V_{j-1}$. By this idea, the function space can be decomposed like

$$V_{0=}W_1 \oplus W_2 \oplus \dots \oplus W_j \oplus\subset V_0 \quad (14)$$

and so $L^2(\mathbb{R}) = \bigoplus_{m=-\infty}^{\infty} W_m$. By this kind of decomposition, components in each space W_j, contain different details of the function, or from the view of signal processing, the original signal is decomposed by a group of orthogonal filters. From Mra, Mallat developed a fast algorithm to compute DWT of a given signal. Associated with the wavelet function $\psi(t)$ is a scaling function, $\varphi(t)$, and scaling coefficients, a_n^m. The scaling and wavelet coefficients at scale m can be computed from the scaling coefficients at the next finer scale $m+1$ using

$$a_n^m = \sum_l h[l-2n]a_l^{m+1}, \quad (15)$$

$$d_n^m = \sum_l g[l-2n]a_l^{m+1}, \quad (16)$$

where $h[n]$ and $g[n]$ are tipically called lowpass and highpass filters in the associated filter banks. Eqns. (15) and (16) represent the fast wavelet transform (FWT) for computing (5).

In fact, the signal a_n^m and d_n^m are the convolution of a_n^{m+1} with the filters $h[n]$ and $g[n]$ followed by a downsampling of factor 2. Conversely, a reconstruction of the original scaling coefficients a_n^{m+1} can be made from

$$a_n^{m+1} = \sum_l (h[2l-n]\, a_l^m + \sum_l g[2l-n]\, d_l^m), \tag{17}$$

A combination of the scaling and wavelet coefficient at a coarse scale. This equation represents the inverse of FWT for computing:

$$y(t) = \sum_m \sum_n d_n^m \psi_n^m(t)\,, \tag{18}$$

And it corresponds to the synthesis filter bank. This part can be viewed as the discrete convolution between the upsampled signal a_l^m and the filters $h[n]$ and $g[n]$, that is, following an "upsampling" of factor 2 one calculates the convolutions between the upsampled signal and the filters $h[n]$ and $g[n]$. The number of levels in the multiresolution algorithm depends on the length of the signal. A signal with 2^k values can be composed into $k+1$ levels.

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