Wavelet Theory and Applications

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1 Introduction

The history and theory of wavelet analysis requires some motivation. Experiments that produce sequences of measurements, or *signals*, generate large amounts of data from which a few quantities are to be determined. This data reduction involves signal processing, feature detection, and numerical computation, all of which demand efficient mathematical tools. *Wavelet analysis* is one such tool. It was developed over several centuries, mainly to solve various practical problems, but with present-day computers has become a standard method for automatic data analysis.

This article will present a very brief sketch of the history and theory of wavelet analysis, and then list a few applications to physical and computational chemistry. The subject spans many disciplines, and its literature comprises thousands of articles and books, making it easy to venture beyond the current scope. The popular surveys[1,2] in the bibliography are a good source of more general information; the ambitious reader is invited to consult the more technical works[3–6] for the mathematical details. Most applications to date are described in scholarly journals, but many are collected in edited compilations.[7–12]

2 A Brief Theory of Wavelets

Wavelets are building blocks for signals, with nice mathematical properties. Finding which blocks comprise a signal is called *analysis*, while assembling blocks to form a signal is called *synthesis*. Both analysis and synthesis require computation with the signal, so by "nice" it is meant that these computations can be done fast either by human or machine. A good set of building blocks has two other properties: discovering that a signal contains a particular block should convey a lot of information about the signal, but the blocks themselves should be sufficiently generic that they can synthesize any signal. Attempts to resolve this conflict have yielded many different candidate building blocks, all of which look like packets of waves, or wavelets.

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2.1 Fourier analysis

Analysis of signals as superpositions of simple building blocks began in 1822 with Fourier,[13] who claimed that an "arbitrary function" $f = f(x)$ could be written as a sum of sines and cosines with integer frequencies:

$$f(x) = \sum_n a_n \cos(nx) + b_n \sin(nx) = a_0 + a_1 \cos(1x) + b_1 \sin(1x) + a_2 \cos(2x) + b_2 \sin(2x) + \cdots \quad (1)$$

One obtains the *Fourier coefficients* $\{a_0, a_1, a_2, \ldots, b_1, b_2, \ldots\}$ by computing integrals:

$$a_0 = c \int f(x)\, dx; \qquad a_n = 2c \int f(x) \cos(nx)\, dx, \quad b_n = 2c \int f(x) \sin(nx)\, dx, \quad \text{for } n = 1, 2, \ldots \quad (2)$$

Here c is a normalization factor $1/2\pi$ related to the period of sine and cosine.

The variety of arbitrary functions f has expanded considerably in the time since Fourier's monograph, and considerable effort has been devoted to the mathematical generalization of formulas 1 and 2. Even a quick survey of this large area of mathematics would consume the rest of this article, but its usefulness can be illustrated by pointing out four desirable properties.

First, Fourier's method could be regarded as a *data compression* or *data reduction* tool. Complicated functions, which did not have simple analytic formulas permitting their evaluation at any point, could be encoded as lists of numbers. In practice, knowing even a few Fourier coefficients of a function suffices to reconstruct a good approximation it. The theory of smooth or highly differentiable functions can be used to make this observation rigorous. For example, if a function has three continuous derivatives, then its Fourier coefficients a_n and b_n must decrease in proportion to $1/n^3$ as the index n increases to infinity. The coefficients after the first 100 are about one million times smaller than the first few, so using only 100 Fourier coefficients to encode such a function preserves it to about six digits of accuracy for all further calculations.

Second, sines and cosines are derivatives of each other, so the term-by-term derivative of one Fourier series is another Fourier series. Thus *physically meaningful* quantities such as energy and momentum, which are computed by differentiation, could be had easily from Fourier coefficients.

Third, Fourier series are easy to interpret because the index of a Fourier coefficient is a *feature flag*. Information about a function can be found simply by looking for a large Fourier coefficient and noting its index. If a_n or b_n is large for some integer n, it means that "the function f contains significant energy at frequency n." In this case the feature is an amplitude peak, which flags a frequency present in the function. Such a method is utilized in Fourier transform spectroscopy.

Finally, practical computation with Fourier series is easy because there are *fast algorithms* to approximate them on digital computers. One starts with the observation that the integrals in Equation 2 can be approximated by sums:

$$\tilde{a}_0 = \frac{c}{N} \sum_{k=1}^{N} f(x_k); \qquad \tilde{a}_n = \frac{2c}{N} \sum_{k=1}^{N} f(x_k) \cos(nx_k), \quad \tilde{b}_n = \frac{2c}{N} \sum_{k=1}^{N} f(x_k) \sin(nx_k), \quad \text{for } n = 1, 2, \ldots \quad (3)$$

The numbers $\tilde{a}_n$ and $\tilde{b}_n$ are called *discrete Fourier coefficients*. They are obtained by sampling f and the sine and cosine functions within one period 2π, at N equally spaced points $x_k = 2\pi k/N$, $k = 1, \ldots, N$, where N is fixed and usually large. The normalization factor $c = 1/2\pi$ is the same as the one in Equation 2.

The coefficients repeat themselves as the frequency n passes N, $2N$, $3N$, and so on, limiting the amount of frequency information that such an approximation can contain. In fact, the $2N$ "distinct" Fourier coefficients computable from formula 3 can only resolve N frequencies. (This observation is called *Nyquist's Theorem.*) The samples of f can be recovered from the $2N$ coefficients through the following formula:

$$f(x_k) = \tilde{a}_0 + \tilde{a}_1 \cos(1x_k) + \cdots + \tilde{a}_N \cos(Nx_k) + \tilde{b}_1 \sin(1x_k) + \cdots + \tilde{b}_N \sin(Nx_k), \quad \text{for } k = 1, \ldots, N. \tag{4}$$

It seems to take about N^2 arithmetic operations to find $\{\tilde{a}_n, \tilde{b}_n : n = 1, \ldots, N\}$, and another N^2 operations to reassemble $f(x_k)$ for all $k = 1, 2, \ldots, N$. However, by exploiting algebraic identities relating sine and cosine, Cooley and Tukey[14] found a method for evaluating formulas 3 and 4 in about $N \log N$ arithmetic operations, which is much faster when N is bigger than 100 or so. This method is now called the *fast Fourier transform*, or FFT.

Samples of f at intervals of $1/N$ can be used to interpolate approximate values between samples. If f is smooth, the interpolated values will be very accurate even if N is not too big and the sampling interval is thus quite large. Since the number of Fourier coefficients is $2N$, this observation shows how smooth functions are accurately and efficiently coded by Fourier series.

2.2 Gabor analysis

Variations of Fourier series were developed over time to solve certain practical problems. For example, the sine and cosine building-block functions are not concentrated near any particular x value. No position information can be gleaned from just the coefficients at a single frequency index n. On the other hand, an individual sample $f(x_k)$ of a smooth function f indicates roughly how big the function is near x_k, but confers no frequency information. What was sought was a collection of nice functions $w = w_{nk}(x)$, with two indices n, k, such that an "arbitrary function" $f = f(x)$ could be written as a superposition:

$$f(x) = \sum_{n,k} a_{nk} w_{nk}(x) \tag{5}$$

The building blocks w_{nk} should be chosen so that n is a feature flag for frequency and k is a feature flag for position. That is, if a_{nk} is large, one can conclude that f has significant energy at frequency n located near the position x_k. In other words, wavelet series should somehow encode position and frequency information simultaneously. This is to be accomplished by using waveforms w_{nk} which have identifiable frequency n and position x_k. But, any smooth waveform that is confined to a position interval can have its frequency measured only with limited precision, since the distortions imposed by confinement contaminate it with many nearby frequencies. The rigorous version of this statement, called the *Heisenberg uncertainty principle*, can be rendered as follows: if $w = w(x)$ is any function confined to an interval of width Δx, and $\Delta\xi$ is the uncertainty in its frequency, then the product $\Delta x\, \Delta\xi$ must be greater than or equal to 1. This fact, observed in the 1920s, is central to the modern description of nature via quantum mechanics.

The finest possible simultaneous encoding of position and frequency requires wavelets which minimize the product $\Delta x\, \Delta\xi$. Such functions are called *Gabor wavelets* and have the form depicted in Figure 1, that is, sine and cosine oscillations confined by a *Gaussian* envelope function e^{-x^2}.

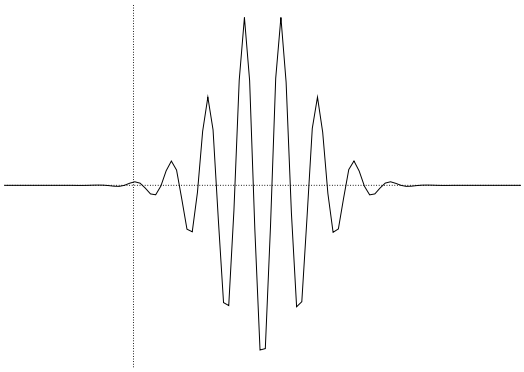

Figure 1: Gabor wavelet.

Defining $w_{nk}(x) = \cos(nx)e^{-(x-k)^2}$ for integers n, k produces a *Gabor basis* with the desired properties. Gabor wavelets need not have integer freqiuencies or be localized at integer coordinates. The frequency n, for example, can be *modulated* to any real number ξ_0. Likewise, the function can be *shifted* to any position x_0 by using $x - x_0$ instead of $x - k$, and can be *dilated* so it is concentrated within Δx of there by using the envelope $e^{-(x-x_0)^2/\Delta x^2}$. Finally, Gabor functions can be multiplied by an *amplitude* to adjust their size.

There are other variants of Gabor functions; some use different envelope functions, or vary the envelope width at different positions. They also have various other names, like short-time or windowed Fourier transforms. Most technical details concerning these functions have been omitted here, but can be found in a basic text.[15]

Each Gabor component of a function can be visualized as a density plot in the position-frequency plane, indicating at each (x, ξ) the amount of energy in frequency ξ present in the Gabor function at that position x. The *Wigner distribution* of a Gabor function is just such a density; it has elliptical level sets and has most of its mass concentrated near the central position and frequency (x_0, ξ_0) of the waveform. Figure 2 shows the idealized Wigner distribution of a Gabor function as a density plot, with darker shading indicating larger values. The x and ξ dimensions of the medium-dark ellipse give the position and frequency uncertainties Δx and $\Delta\xi$, respectively, of the Gabor function. Thus $\Delta x\,\Delta\xi = 1$. The *aspect ratio* of the ellipses, $\Delta\xi/\Delta x$, is arbitrary.

Unfortunately, the actual Wigner transform of several Gabor wavelets will contain spurious shaded regions caused by interference or "cross terms," especially near 0. Thus it is useful to further idealize by replacing the contour plots with rectangular tiles, one centered at the appropriate (x_0, ξ_0) for each wavelet, with sides Δx and $\Delta\xi$, as shown in Figure 3. A signal can be analyzed by such a tiling; the pattern of lighter and darker tiles indicates where the signal is most energetic, and which frequencies contain the most energy.

The final idealization is to reduce the signal to musical notation, where instead of rectangular tiles there are stylized notes. The shape of a note indicates its duration Δx, and other other clues besides shading indicate the amplitude. By analogy, Gabor analysis is the task of finding the musical score by listening to the music. This can surely be done by musicians within some acceptable error margin. The issue is to devise efficient automatic methods to do it in other contexts, where the

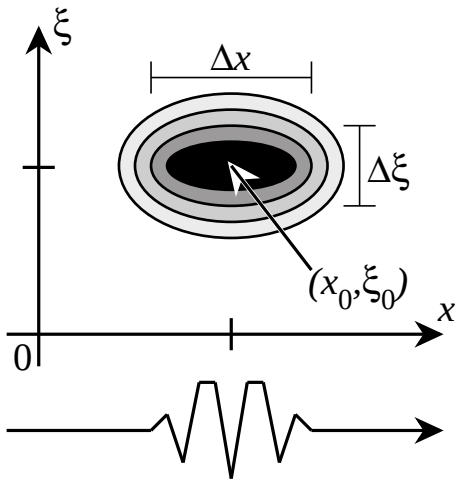

Figure 2: Contour-density plot of the idealized Wigner distribution of a Gabor wavelet.

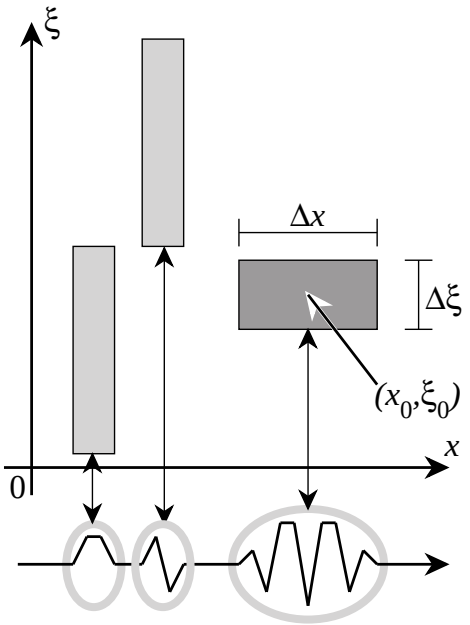

Figure 3: Idealized Wigner transforms of three Gabor wavelets.

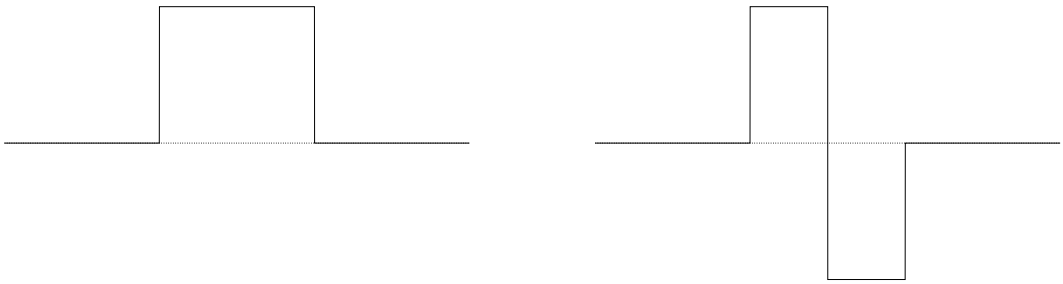

Figure 4: Indicator function of the interval $[0, 1]$, and its associated mother wavelet

signal is not music.

2.3 Multiresolution Analysis

To be useful, wavelet series must come with fast algorithms for machine computation, that is, a method like FFT both for finding the expansion amplitudes a_{nk} and for reconstructing the function they represent. Since Gabor functions are so closely related to sines and cosines, the FFT can be applied to them as well. However, there is an even faster family of algorithms based on a completely different idea, namely that of *multiresolution analysis*, or MRA. To perform such an analysis, one needs a building block function $v = v(x)$ with a definite position and size. One could use $v = \mathbf{1}_{[0,1)}$, the indicator function of the interval $[0, 1)$ depicted on the left side of Figure 4 and defined by the following formula:

$$\mathbf{1}_{[0,1)}(x) \stackrel{\text{def}}{=} \begin{cases} 1, & \text{if } 0 \le x < 1; \\ 0, & \text{if } x < 0 \text{ or } x \ge 1. \end{cases} \tag{6}$$

This v is evidently located at $x = 0$ and has unit scale, since it is nonzero on an interval of length 1. It can be *translated* to a new position, the interval $[k, k + 1)$, using the following formula:

$$v_k(x) \stackrel{\text{def}}{=} v(x - k) = \begin{cases} 1, & \text{if } k \le x < k + 1; \\ 0, & \text{if } x < k \text{ or } x \ge k + 1. \end{cases} \qquad k = \pm 1, \pm 2, \ldots \tag{7}$$

An arbitrary function f can be described *at unit resolution* with a series of the form

$$f_0(x) = \sum_k a_k w_k(x) \tag{8}$$

The "step" function f_0 is constant on the interval $[k, k + 1)$ at integer k, where it takes the value $a_k = \int f(x)v_k(x)\,dx$, the average value of f there. If f does not change too much over such intervals, then f_0 will approximate f reasonably well at all x. An example of this is shown in Figure 5.

To obtain a better approximation of f, one increases the resolution in Equation 8 by using skinnier versions of the functions v_k. The formula for these is given by *dilating* the variable x by a power of 2:

$$v_{jk}(x) \stackrel{\text{def}}{=} v(2^j x - k); \qquad j = 0, 1, 2, \ldots; \quad k = \pm 1, \pm 2, \ldots \tag{9}$$

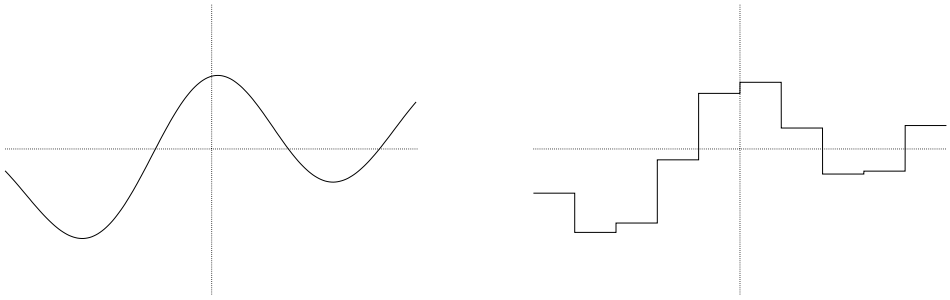

Figure 5: The original function f and its unit-resolution approximation f_0.

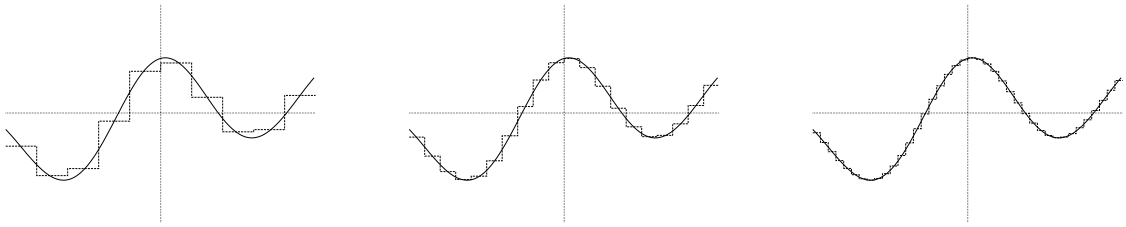

Figure 6: Three approximations to f: unit resolution f_0, double resolution f_1, and quadruple resolution f_2.

The original v is v_{00}, and the earlier v_k are v_{0k}, in this two-index notation. The unit-resolution approximation corresponds to $j = 0$, and the resolution doubles with each unit increase in j. Approximations of f corresponding to $j = 0, 1, 2$ are shown in Figure 6.

A successful multiresolution analysis of f must have the property that the error $|f - f_j|$ tends to 0 as j tends to ∞. This obviously depends on the choice of v and nothing else, since v completely determines f_j for all $j = 0, 1, 2, \ldots$. The indicator function $\mathbf{1}_{[0,1)}$ has this property, but there are other choices for v which work and give faster rates of approximation. One way to generate them is to look for solutions to the *two-scale equation*:

$$v(x) = \sum_k h_k v(2x - k); \qquad \int v(x)\,dx = 1. \tag{10}$$

A solution v to this pair of equations is called a *scaling function*. It in turn is determined by the numbers $\{h_k\}$, indexed by integers k, which are called *(low-pass) filter coefficients*. There will be a unique solution v if the following conditions are met:

$$\{h_k\} \text{ has only finitely many nonzero coefficients, and } \textstyle\sum_k h_k = 2; \tag{11}$$

$$\sum_k h_k h_{k+2n} = 0, \quad \text{for } n \neq 0; \qquad \sum_k h_k^2 = 2. \tag{12}$$

(Some of these conditions can be weakened.[16]) The indicator function $\mathbf{1}_{[0,1)}$ solves Equation 10 with $h_0 = h_1 = 1$ and $h_k = 0$ for all $k \neq 0, 1$. This is the simplest possible filter sequence. A fancier example is listed in Table 1, with its corresponding solution v to Equation 10 plotted in Figure 7.

k	Exact value of h_k	Numerical value of h_k
< 0	0	0.0000000000000000
0	$(\sqrt{15}-3)/16$	0.0545614591379636
1	$(1-\sqrt{15})/16$	-0.1795614591379636
2	$(3-\sqrt{15})/8$	-0.1091229182759271
3	$(3+\sqrt{15})/8$	0.8591229182759271
4	$(13+\sqrt{15})/16$	1.0545614591379636
5	$(9-\sqrt{15})/16$	0.3204385408620364
> 5	0	0.0000000000000000

Table 1: "Coiflet 6" low-pass filter coefficients for the two-scale equation.

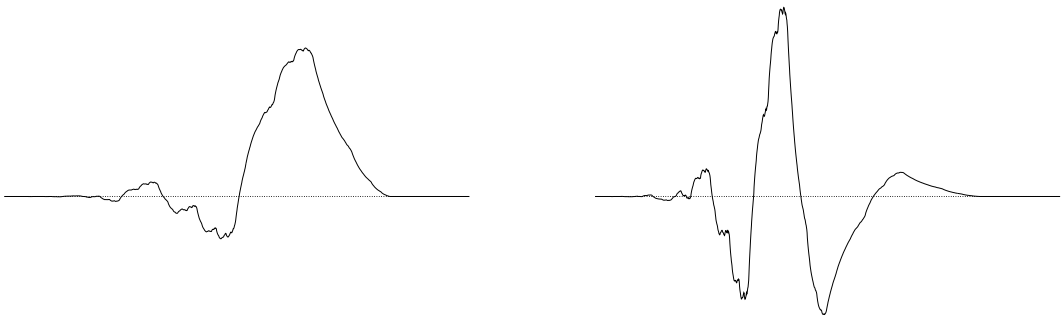

Figure 7: Solution to the two-scale equation with Coiflet 6 filter coefficients, and its associated mother wavelet.

Any sequence $\{h_k\}$ that satisfies Equations 11 and 12 produces a function v that is *orthogonal to its integer translates:*

$$\int v(x)v(x-k)\,dx = 0, \quad \text{if } k \text{ is a nonzero integer;} \qquad \int v(x)^2\,dx = 1. \tag{13}$$

In such cases, the formula for a resolution-j expansion of a function f looks just like the Fourier series formula:

$$f_j(x) = \sum_k a_k v_{jk}(x); \qquad a_k = 2^j \int f(x)v_{jk}(x)\,dx. \tag{14}$$

The extra factor 2^j is needed to compensate for the slimming of v at resolution j. However, such an expansion differs little from a list of samples of f at points separated by 2^{-j}, and thus provides little compression or feature tagging. But, it is possible to encode only the differences between successive approximations to f:

$$f = f_0 + (f_1 - f_0) + (f_2 - f_1) + (f_3 - f_2) + \cdots \tag{15}$$

This works because $|fj - f_{j-1}|$ tends to zero as j tends to infinity, so the coefficients needed to encode $f_j - f_{j-1}$ must become small for large j. This difference decreases faster for smoother f. Also, the number of coefficients needed to encode $f_j - f_{j-1}$ is proportional to 2^j, so that for smooth f only a few nonnegligible difference coefficients suffice for a close approximation. The trick is to expand the differences as superpositions of another function:

$$f(x) = \sum_k a_{0k}v_{0k}(x) + \sum_k b_{0k}w_{0k}(x) + \sum_k b_{1k}w_{1k}(x) + \sum_k b_{2k}w_{2k}(x) + \cdots, \tag{16}$$

where a_{0k} and b_{jk}, $j = 0, 1, 2, \ldots$ are amplitudes to be determined for each function f. Such a formula holds because the scaling function v satisfies the two-scale equation. As a result, there is a function, called the *mother wavelet* w, which generates the components in Equation 16 by dilation and translation:

$$w_{jk}(x) \stackrel{\text{def}}{=} w(2^j x - k); \qquad j = 0, 1, 2, \ldots; \quad k = \pm 1, \pm 2, \ldots \tag{17}$$

Note the similarity with Equation 9. Roughly speaking, the mother wavelet w is the difference between $v(x)$ and $v(2x)$. The actual formula is somewhat more complicated:

$$w(x) = \sum_k g_k v(2x - k); \qquad g_k = (-1)^k h_{1-k}(x), \quad k = 0, \pm 1, \pm 2, \ldots \tag{18}$$

Notice that the low pass filter $\{h_k\}$ determines the differencing or *high-pass filter* $\{g_k\}$ that generates w. Figures 4 and 7 show two example pairs of scaling functions and mother wavelets.

The two sequences $\{h_k\}$, $\{g_k\}$ are called *conjugate quadrature filters*, and with them it is possible to find the coefficients a_{0k} and b_{jk} of Equation 16 efficiently. There are fast algorithms that do this,[6] and also many methods to find conjugate quadrature filters.[5,17] If the filters are designed well, then the mother wavelet w will be well-localized in position and frequency, namely its uncertainty product $\Delta x\,\Delta\xi$ will be not much bigger than 1. In that case, w may be depicted as a rectangular 1×1 tile centered above the origin in the $x\xi$ plane, and w_{jk} may be depicted as a tile with $\Delta x = 2^{-j}$ and $\Delta\xi = 2^j$, centered at $x_0 = 2^{-j}k$ and $\xi_0 = \frac{1}{2}2^j$. Notice that $\xi_0 = \frac{1}{2}\Delta\xi_0$ for all of these wavelets.

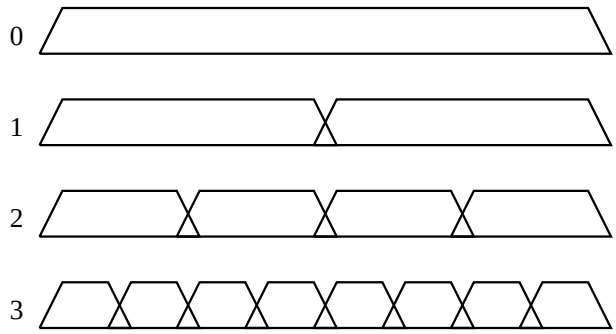

Figure 8: Adapted Gabor analysis with four different window widths.

2.4 Adapted waveform analysis

There are various kinds of wavelets, including continuous wavelets,[18] discrete orthogonal wavelets,[5] spline wavelets,[4] local cosines,[19] and wavelet packets.[6] Different applications benefit differently from these varieties, and the procedure of selecting the appropriate one is called *adapted waveform analysis*.

One way of adapting the analysis to the problem is to perform a Gabor analysis with window widths $\Delta\xi$ determined by the signal. Figure 8 shows how four different window sizes, each half the width of the previous, may be used to partition a signal. Within each window one does a Fourier transform, so that the four lines constitute four different Gabor analyses. Each analysis yields an equally long list of coefficients: the one to use is the list with the *smallest number of large coefficients*. There are many ways to judge coefficients and decide which are large enough to be nonnegligible.[20] The count of nonnegligible coefficients may be called the *information cost* of representing the signal. Adapting the analysis seeks to minimize this cost to the *theoretical dimension*, which is the lowest cost achievable with the available set of waveforms.

To illustrate this procedure, consider a musical signal that changes in the middle of the interval from one pure tone to a second. In this ideal case, all the analyses will contain at least two large coefficients, one for each of the two frequencies. Analysis "0" will have those, plus extra coefficients for the "cross terms" needed to cancel the first tone in the second half and to cancel the second tone in the first half. Analyses "1," "2" and "3" will contain just one large coefficient per window, determining the frequency present in the window. Of these, analysis "1" will have the fewest total coefficients, since it has the fewest windows. There are three pieces of information conveyed by the adapted analysis: the two frequencies and the place where the change occurs.

More sophisticated adaption is possible, since the decision to use a large window or a small one can be made locally. A window should be split whenever doing so reduces the total cost of representing the signal.[21] Alternatively, a window may be grown as long as its information cost decreases, after which a new window should be started.[22] Where the algorithm places windows conveys information about frequency changes in the signal. This is another kind of feature flagging.

All of these procedures require that adjacent or overlapping windows contribute independently to the signal representation, which means that the collection of waveforms should constitute an orthogonal basis. Unfortunately, this is not possible for Gabor functions due to the *Balian–Low phenomenon*, a mathematical obstruction.[23] But it is possible for *lapped orthogonal functions*, also

known as *local sines and cosines*, which are very similar.[19,24]

Though it is harder to visualize, multiresolution analyses can also be done with adapted waveforms. The procedure hinges on the remarkable orthogonality properties of solutions to the two-scale equation 10 when the low-pass filter satisfies the orthogonality conditions 12. It is possible[6] to obtain orthonormal bases of waveforms with near-minimal uncertainty product $\Delta x\,\Delta\xi \approx 1$ and arbitrary position-frequency aspect ratio $\Delta x/\Delta\xi$.

3 Applications

Wavelet analysis is a generic signal processing tool that is already incorporated in commercial software packages. The applications listed below are a subset of those with which the author has personal experience, and are just a tiny fraction of what may be seen in the literature listed in the introduction. Additional references are given below to mark the trail better for the ambitious reader.

3.1 De-Noising

Automated and computer-controlled measurement produce huge amounts of data. An abundance of measurements for every computed parameter promises robustness due to redundancy, but threatens inaccuracy due to an accumulation of the noise which is present in all physical measurements.

In many signals, noise is mainly distinguished by *incoherence*, that is, the error at one measurement is not correlated with the error at any other. This property can be exploited to reduce the average amount of error, since a wavelet analysis of an incoherent signal consists of many small components. By neglecting all components in a wavelet series that fall below a threshold, the noise components will be preferentially suppressed.[25] The threshold must be chosen based on an estimate of the noise energy in the signal.

Adapted waveform analysis offers an even sharper means to divide signals into portions likely to be noise and portions likely to be non-noise.[26] The ultimate form of this algorithm is *matching pursuit*, which uses huge families of waveforms and gives up computational speed in exchange for denoising efficiency.[27]

3.2 Digital Spectral Analysis

Digital spectrophotometry can produce tens of thousands of data points per sample, at resolutions down to small fractions of a wavelength. Such data sets must be analyzed for the presence of peaks, or local extrema. The wavelength of a peak identifies its species, while the amplitude determines the quantity of that species present in the sample. Spectra are subject to various forms of random measurement error, which give them a rough appearance. Finding local extrema by the calculus of solving for zeroes of the first derivative fails from too many false positives, but the cure of filtering out the roughness before differentiating can eliminate or drastically change the amplitude of even moderately strong peaks. Wavelet theory provides an alternative method for finding peaks in noisy spectra,[28] and estimating their size.

The choice of sampling interval in digital spectrophotometry limits the wavelength resolution, and peaks in general will not lie at sample points. Furthermore, nearby peaks interfere and ob-

scure each others' locations and amplitudes. Wavelet peak-detection algorithms have been used to separate neighboring spectral peaks of comparable height, and also to remove a strong peak that distorts much weaker ones living on its slopes.[29]

Raw nuclear magnetic resonance (NMR) data consists of damped oscillations produced by choruses of nuclei with different resonant frequencies. Analysis consists of determining those resonances, and is traditionally done with the discrete Fourier transform. However, the time variation of the amplitudes introduces errors, and the weakness of the resonances forces many repetitions to get adequate height in the peaks. The continuous wavelet transform spectral estimation algorithm has recently been used instead,[30] to avoid both these problems. Without the need for repetitions, it is possible to analyze chemical reactions at time steps comparable to nuclear spin relaxation times.

3.3 Principal Component Analysis

The problem of determining p parameters from d measurements, where $d \gg p$, can be simplified by first performing a principal component analysis (PCA) of the measurements. Such pre-processing is a kind of data reduction or compression, which can have the side benefit of exposing nonobvious linear relationships among the measured quantities. Numerical algorithms for PCA are also applicable in chemometrics.[31] Their main drawbacks are high computational complexity and non-updatability: the calculation is time consuming, and must be completely repeated whenever any new data is added.

A principal component analysis for a collection of signals actually minimizes the information cost, but an adapted waveform analysis can get close to the minimum with far less computation.[32] Furthermore, the adapted waveform analysis can be updated very cheaply when new data is added.

3.4 Electrochemical Noise and Corrosion

Wavelet transforms can extract useful information from complicated signals. An example of such a signal is *electrochemical noise*, which is the time-varying difference in the voltage across two electrodes placed in a corrosive solution. This signal can have an amplitude of a few microvolts and superficially looks just like noise. The voltage fluctuations are caused by corrosion events such as pitting and cracking; these cause distinct, short-lived transients that in principle can be recognized. The problem has always been to characterize the transients. They do not have a particular frequency spectrum, indeed they have the noise-like property of nearly equal power at all frequencies. Thus Fourier analysis of the signal does not isolate the desired transients as spectral peaks. They do not have a standard size and size, since for example the size of a pit influences the amplitude and duration of the voltage fluctuation it induces. Thus it is not possible to detect them by cross-correlation or matched filtering, since there is no standard template that may be slid along the signal to find all the good fits. Finally, the rapid voltage change caused by a corrosion event is easily masked by measurement errors that are unavaoidable in microvoltmeters.

These difficulties may be overcome by expressing the signal in wavelet coordinates, interpreting the new sequence as a time-frequency pattern, and then matching that pattern against templates developed experimentally. Recent work by Dai[33] has shown that wavelet and wavelet packet transforms turn corrosion events into distinct time-frequency patterns that can be automatically classified. Both visual inspection of the pattern and numerical analysis of a *feature vector* that encodes

the pattern into 14 numbers can reveal the type and intensity of the corrosion event.

3.5 Modeled Predictive Control

Control of parameters during an industrial chemical process leads to better quality products, chiefly because of variations in the inputs and fluctuations in the quality of intermediates. The earliest applications of automatic control to chemical production involved simple independent feedback devices such as thermostats. But, as the number of inputs and variables to control grows, there will be interactions and possible instability.

One way to ensure stability in a plant under automatic control is to model the controlled variables mathematically in terms of the inputs. This technique came into vogue in the 1980's.[34] However, even a relatively simple chemical plant can fail to have a tractable mathematical model. The simplifying assumptions that make it possible to design a control function are often unrealistic, namely linearity (the outputs are linear functions of the inputs) and time-invariance (the effect of control inputs is independent of the plant's state before the current instant). These assumptions are used because they imply that the Fourier transform removes the interactions between the controlled variables, allowing them to be treated one at a time. It is an example of a preferred mathematical tool, the discrete Fourier transform, leaving its mark on the work.

More sophisticated models must allow for nonlinear relationships between inputs and outputs, and time-varying consequences of applying control changes.[35] These generalizations can be handled by using the wavelet transform,[36] which removes most of the interactions between the parameters.

3.6 Models of Turbulent Fluid Flow

Mathematical modeling of fluids can aid in the design of chemical reactors, as well as devices that move through or interact with fluids. Such models balance the energy due to chemical reactions, external pressure fluctuations, internal friction or viscosity, radiation, compression, and vorticity. At present, only the simplest models produce useful simulations, and then often with simplifying assumptions. For example, it is possible to obtain a useful simulation of a two-dimensional incompressible fluid, such as water in a shallow pool or air in the Earth's atmosphere, balancing only the energy lost to friction and that transported by vortices. Future improvements in computers hold out the hope of analyzing more complicated models.

A simple two-dimensional simulation of the Earth's atmosphere involves numerical integration of the Navier–Stokes equations. The computer generates a ballet of vortices that mimic the motion of cyclones and anti-cyclones, much like the circulation observed by meteorologists. Unfortunately, even with enormous simplifications and very coarse results, the simulation is too complex for all but the most powerful and expensive computers. One basic problem is that the number of data points vastly exceeds the number of vortices present in the simulation at any time. The data points may be regarded as fixed weather observation stations that record pressure, temperature, wind speed and direction as functions of time, whether there is cyclone nearby or not. To proceed, the simulation must calculate the new values at each station, at each time step, even if not much changes. Furthermore, the presence of a cyclone must be deduced from the readings at many stations.

The readings of many stations can be combined into one through a wavelet transform of the data. It has been shown in just this context[37] that the number of wavelet components needed to reconstruct a good approximation to the flow is roughly proportional to the number of cyclones and anticyclones.

4 Conclusion and Future Directions

Wavelets are mathematical objects originally developed to overcome the technical difficulties of the Fourier transform's sines and cosines. They serve the same purpose, that is, as simple building blocks for complicated functions.

Wavelets have location, pitch, and duration, so may be considered like musical notes. They and their more general counterparts, wavelet packets, can be superposed into a signal much as musical notes can be joined into melodies and harmonies. The list of wavelets comprising a signal gives a compact representation of the signal, just like a score gives a compact representation for recorded music.

The continuous wavelet analysis of a signal, also called its time-scale representation, produces much more data than the signal itself. It is useful for de-noising and modeling, especially of signals like music, nuclear magnetic resonances, and absorption spectra.

A signal's discrete wavelet transform contains the same or nearly the same amount of data, but in many cases the interesting part gets concentrated into a small number of large components. There is a fast algorithm for producing the discrete wavelet transform of a signal, namely multiresolution decomposition, based on recursive convolution and decimation.

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