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Book Review

Wavelets in Chemistry
B. Walczak, 2000, Elsevier, Amsterdam, ISBN: 0444501118, Price: GBP £184.00, USD $276.95, € EUR 276

The book is available in Europe, Middle East and Africa from Elsevier, Customer Service Department, Linacre House, Jordan Hill, Oxford OX2 8DP, UK, and in the USA/Canada from Elsevier, Customer Service Department, 11830 Westline Industrial Drive, St. Louis, MO 63146, USA.

Wavelets in Chemistry is the 22nd volume of the series of Data Handling in Science and Technology. The book, which was written by authors in chemistry and chemical engineering, attempts to provide a tutorial and reference work for people working in the same disciplines.

The book is divided into two parts. The first part addresses the relationship of wavelet transforms to the Fourier transform, the detailed background and the theory of its application. The second part consists of applications of the wavelet transform to chromatographic data, electrochemistry, spectroscopy, physical chemistry, library compression, searching and reconstruction, online detection of transitions in time series, calibration, parsimonious functional data analysis models, multi-scale statistical process control, classification and regression, image compression, analysis of 2-D and 3-D analytical images, etc. Even though it was published in 2000 the coverage of the topics is still very complete and not out-of-date.

The first two chapters cover all the basic properties and calculation techniques needed to know about the wavelet transform. The Fourier transform has a direct link to the wavelet transform and therefore an understanding of it will benefit the understanding of the wavelet transform. Chapter 1 uses proper formulae and well prepared figures to help the reader understand the basic ideas and usages of the Fourier transform in signal processing. Although the major topic of this chapter is about the Fourier transform, using the comparisons of some essential characteristics between Fourier and wavelet transforms is a good idea to introduce wavelets. Chapter 2 starts from the introduction of the short-time Fourier transform then introduces the wavelet transform and the wavelet packet transform. The first two chapters as an overall introduction are really readable and should be comprehensively studied by a reader who does not know, or is not an expert of, the Fourier or the wavelet transforms.

Details of the fundamentals of wavelet transforms are presented in Chapters 3 and 4. The continuous wavelet transform and its inverse transform are introduced at the beginning of Chapter 3. Then the practical form of the wavelet transform—discrete wavelet transform and multiresolution analysis, fast wavelet transform and the wavelet families are described accompanied by examples of continuous functions. The major problem that arises when a finite-length signal is analysed using the discrete wavelet transform (DWT) is how to generate a treatable signal of DWT based on the real signal. A thorough discussion of the boundary handling and other practical issues of discrete wavelet transform for discrete data are presented in Chapter 4, after a brief introduction to matrix theory at the beginning.

Because de-noising and compression are major interests in signal processing and image analysis, the content of Chapter 5 (Multiscale methods for denoising and compression) is repeated and extended in a number of subsequent chapters. It is important to characterize noise, and three techniques are roughly described for this aim. De-noising and compression are not separated in this chapter even though there is a common view that they do have some different aspects, since redundant information does not equal noise (although similar techniques can be used in both cases). Compression is used to reduce storage space, although it seems that the demands for compression are not as critical as few years ago because rapidly evolving technology is providing cheaper and bigger storage capacity and wider network transform bandwidth. I would like to suggest that now, simplification is the main aim of compression in situations where stor-

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age is not an issue. For filtering data with Gaussian error simple linear methods can solve the problem but for non-Gaussian error different median methods and their combinations with wavelet filters have to be used. Not only off-line but also on-line filters are introduced here. A short discussion about some indicative rules of thumb for designing wavelet filters is given at the end of the chapter. A little regret is that I had to do some web searches for the meanings of two acronyms ARMA (autoregressive moving average) and ARIMA (autoregressive integrated moving average) which are used in more than one place. And I cannot agree with the statement on page 123, which claims that random error is normally distributed (random error might be normally distributed, but it might not).

The wavelet packet transform (WPT) is presented in Chapter 6. Since it has plentiful coefficients which could be redundant compared to DWT, a best-basis algorithm can be used to optimize a WPT with particular criteria. Similarly, but for a different purpose, this approach is described in Chapter 8. The first two sections introduce higher multiplicity wavelets, which have one low-pass filter and $m-1$ high-pass filters in an m-band wavelet. The authors argue that "in some situations it may be advantageous to rescale by some integer $m>2$." Such sophisticated wavelets can be optimized by using the adaptive wavelet algorithm which is introduced using some unpopular mathematical symbols. It would have been better to give explanation to these symbols where they are used. The correct citation to the paper of Coifman et al. used in Chapters 6 and 7 can be found in Chapter 8 on page 201.

In practice, we not only analyze a single spectrum but very often we have to treat a set of data (e.g. a group of spectra) as a whole to generate a model or do pattern recognition, etc. Chapter 7 provides some simple methods to summarize the wavelet coefficients of individual observation of the discrete wavelet transform or the wavelet packet transform to create a joint basis or a joint best-basis. The equation of entropy used here is different to the one used in the previous chapter and I suspect that a correction should be applied before it can be used.

Part II of the book consists of reviews of broad wavelet applications in different fields of chemistry and chemical engineering. Chromatographic, electrochemical and spectroscopic data are similar but also have different characteristics, therefore applications of the wavelet transform for them are divided into three chapters. Chapter 12 gives some very interesting examples of the wavelet transform in physical chemistry, which could have been overlooked by some readers. For example, we know that an electronic movement or atomic orbital can be expressed in conjugate position and momentum co-ordinates. These two spaces are complementary, therefore using the wavelet transform can give simultaneous information on position and momentum distributions. It is a natural necessity of a changeable window—wavelet for calculating/localizing (within the bounds of the Heisenberg Uncertainty Principle). Functional data analysis is good for describing spectra because a function is more meaningful than a discrete vector and consumes less storage space. Wavelets express spectra in a natural way and can "compress" spectra in an efficient way. When the wavelet transform is combined with variable selection methods, parsimonious functional data analysis models can be created. The content of parsimonious functional data analysis can be found in Chapter 16. Chapter 17 may be interesting to the engineers working in industry because it presents how to use wavelet transforms for multi-scale statistical process control. The advantages of using wavelets with control charts are shown in this chapter. In another section a methodology is developed to apply Bayesian data rectification, which is flexible and accurate in multi-scale way. In the book the reader can also find the examples of the wavelet transform used for spectral library (Chapter 13), online detection of transitions in time series (Chapter 14), calibration (Chapter 15), regression and classification (Chapter 18) and image processing and analysis (Chapters 19 and 20).

As the book is a collection of the contributions of different authors, some contents are repeated in different places in similar or different words which might help the reader to remember or rethink an idea in a different way. It might also be a source of confusion. For example, compression of data is discussed in a few chapters. In Chapter 5 the cutting-off of smaller coefficients is emphasized, while in Chapter 19 the treatment of correlated redundant information is presented. Also Chapter 19 can be compared with Chapter 20 which also describes image compression and sections of other chapters in the book. It is also possible that the reader can jump directly into the chapter which is interesting to him/her without losing much information, since every chapter can be read separately.

In general, despite these minor criticisms, the editor of this book has brought together a number of good introductions for obtaining comprehensive and essential information in the area of wavelet transforms and the related areas for a chemist/chemical engineer. This book should be of interest and some value to anyone working in these fields.

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