

Chemometrics: From Basics to Wavelet Transform, Foo-Tim CHAU, Yi-Zeng LIANG, Junbin GAO, and Xue-Guang SHAO, Hoboken, NJ: Wiley-Interscience, 2004, ISBN 0-471-20242-8, xiv + 316 pp., \$99.95.

This is not your father's chemometrics book. Even though the word "basics" appears in the title, there is no discussion of PLS, SIMCA, experimental design, or any of the other topics that one might expect in a book with this title. What is here is an introduction to signal analysis, especially using the wavelet transform, for signals from analytical chemical instruments. If that sounds like what you do, this may be a good book to check out. Even though there are appendices for both matrix algebra and the MATLAB programming language, in my opinion the reader needs a background in linear algebra and statistics, at least through covariance matrices, to get the most from this book.

Chapter 1 is an introduction that includes brief descriptions of a number of websites that provide the reader with much useful information. Chapters 2 and 3 provide brief overviews of standard one- and two-dimensional signal processing techniques that are useful in analytical chemical work. Some of the one-dimensional topics of Chapter 2 are as follows:

1. An introduction to the Savitsky–Golay smoothing algorithm. Unfortunately, only the original paper is referenced. The two papers that corrected some computational errors are missed (see Sebastian, Booth, and Hu 1995 for details and the citations).
2. An introduction to the Kalman filter that is both short and very well done.
3. An introduction to cubic spline smoothing, including a MATLAB program. Again, this is well done. This topic is important, because these smoothers are differentiable over the entire measurement domain. A reference would have been helpful for those who need or want more detail.
4. An introduction to both the Hadamard and Fourier transforms is given. This is well done, but most readers will probably already be familiar with this material. The applications mentioned are both interesting and thought-provoking.
5. An introduction to numerical differentiation is too short. In particular, no discussion of the possible numerical instability of some algorithms is given.
6. A discussion of data compression is quite good.

The two-dimensional topics of Chapter 3 include the following:

1. A discussion of PCA and its use with hyphenated analytical chemical techniques is very good. The use of hyphenated techniques throughout Chapter 3 illustrates both the application and importance of both the chemical and statistical methods.
2. A discussion of baseline offset is provided. It seems to me that outliers in the data would have the potential to cause problems with the methodology that the authors discuss. They might want to add a discussion or a reference about this topic in a second edition.
3. A discussion of differentiation for two-way data is given on page 81. The authors seem to say that one can just use the one-way algorithms. I think a bit more thought and discussion might be needed here.
4. A discussion of SMCR and evolving techniques for the analysis of data from hyphenated techniques. Again, this is well done.

Chapter 4 is where the real meat of the book begins. This chapter introduces the reader to wavelets, the wavelet transforms, and their mathematical properties. There are a few terms not clearly defined in the book that may be unfamiliar to some readers; two examples are "compact support" and "Holder continuity." The discussion stresses the similarity between wavelet basis sets and wavelet transforms to the corresponding sine and cosine basis sets and Fourier transforms. Because most readers will be familiar with the Fourier case, the mathematics are not painful.

All of the foregoing set the stage for Chapter 5, which covers application of wavelet transforms to analytical chemical data. The authors again compare wavelet methods to Fourier methods so the reader can see the advantages of each approach and the reasons why it is better to have both available. The discussions in this chapter are quite good. They include, with examples, compression, denoising and smoothing, baseline/background removal, resolution enhancement, and numerical differentiation. The discussion of application of these methods to analytical chemical procedures could be expanded, but most readers will probably be able to fill this in from their own experiences.

Discussions of combined techniques (e.g., wavelets with regression, wavelets with neural networks, etc.) are extremely helpful. Each computational

technique includes a box called "Computational Details" that describes in detail the algorithms used in the examples. This leads to the secret of the book. On both the front and back covers the book promises an ftp site with MATLAB code and datasets. Like most statisticians, I collect such things, so I wanted the site's URL. I could not find it. The secret is that the URL appears in a box on page 153. This site is a definite plus for the book.

In summary, this book provides a good but terse review of the standard signal processing methods used in analytical chemistry. It extends those methods with very good descriptions of wavelet-based approaches and then explains why one would want all of these methods to be available. This book seems to be quite useful for persons who apply signal processing methods in chemistry.

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REFERENCE

Sebastian, P. R., Booth, D. E., and Hu, M. (1995), "Using Polynomial Smoothing and Data Bounding for the Detection of Nuclear Material Diversions and Losses," *Journal of Chemical Information and Computer Science*, 35, 53–58.

Design and Analysis of Accelerated Tests for Mission-Critical Reliability, Michael J. LUVALLE, Bruce G. LEFEVRE, and SriRaman KANNAN, Boca Raton, FL: Chapman & Hall/CRC, 2004, ISBN 1-58488-471-1, xii + 236 pp., \$99.95.

This book discusses the challenges of accelerated tests for mission-critical reliability and the solutions to those challenges. For mission-critical components, which usually use ultrahighly reliable devices, the classical accelerated test methods could be problematic. Reliability data extrapolation may not be sensible, given that very few failures or little substantial degradation can be observed and that any degradation or failure actually observed during the accelerated test either disqualifies the devices, if they are relevant during operating life, or represents only an artificial mode that is irrelevant during operating life.

The authors, with many years of experience in electronics reliability analysis (first at Bell Labs and now at OFS Labs), present an alternative approach that they call "physical statistics." The essence of the approach, according to my understanding, is to use the knowledge of physics (chemical kinetics in particular) to provide an underlying material failure/degradation mechanism, which can be reasonably extended for extrapolation outside the testing range. The parameters in a chemical kinetics model are estimated based on a set of accelerated test experiments. Then the questions of how to estimate the parameters, how to assess the uncertainty, and how to design an accelerated test naturally follow.

The book comprises of six chapters:

1. Background
2. Demarcation Mapping: Initial Design of Accelerated Tests
3. Interface for Building Kinetic Models
4. Evanescent Process Mapping
5. Data Analysis for Failure Time Data
6. Data Analysis for Degradation Data.

Chapters 2–4 are devoted to the development of the chemical kinetics model, whereas Chapters 5 and 6 discuss data analysis methods. The test design issue is barely discussed, except for the initial design based on the chemical kinetic models. My impression is that Chapters 2–4 could be challenging for *Technometrics* readers who do not have a background in chemical engineering.

In Chapter 5 the method for analyzing failure time data is to select from two competing models the appropriate one that best characterizes the underlying failure mechanism based on accelerated test data. The model parameters are estimated using the maximum likelihood method and selected through a chi-squared test. Chapter 6 analyzes the degradation data. A first-order differential equation is used for the degradation process, and the parameters are estimated through linear and nonlinear regression analysis. I noticed that although the authors mention both classical methods and Bayesian methods for statistical inferences in the book's introduction, the treatments in Chapters 5 and 6 actually have a heavily classical, non-Bayesian flavor.

I like the presentation in Chapters 5 and 6, where the basic approach, models, and general analysis procedure are presented in the first several subsections.