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Chemometrics

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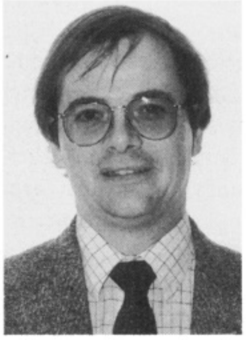
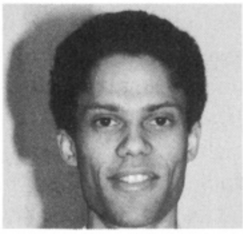
Review Contents



Steven D. Brown is Associate Professor of Chemistry at the University of Delaware. In 1977, he received his Ph.D. from the University of Washington. He has served on the faculty at the University of California, Berkeley, and Washington State University prior to joining the faculty at the University of Delaware in 1986. He is currently North American Editor of the Journal of Chemometrics and Editor of the CRC Chemometrics Series. He also serves as an officer in the International Chemometrics Society and as a member of the Chemstatistics committee of the American Statistical Association. His research interests encompass many aspects of the application of computers to chemical analysis, including signal processing methods, neural networks, digital filters, and modeling of interfacial and transport processes.

Thomas B. Blank received his B.S. in chemistry from Glassboro State College in 1990. The same year, he began Ph.D. studies in chemistry at the University of Delaware. His research interests include many aspects of design and implementation of connectionist models for the purposes of pattern recognition and nonlinear multivariate calibration of chemical systems.



Stephen T. Sum received a B.Sc. in applied chemistry (mathematics option) from the University of Waterloo in 1990. He then pursued his studies in the computer science department at Carleton University where he earned an M.Sc. in information and systems science in 1993. He is currently studying for the Ph.D. at the University of Delaware.

Lois G. Weyer earned a B.A. in chemistry from Douglass College, Rutgers University, in 1968 and an M.S. in physical chemistry from the University of Delaware in 1971. After two years at Central Chemical Corp., she joined Hercules Inc. in 1973. She is an editor of the *Journal of Near-Infrared Spectroscopy*, a member of the ASTM committee on near-infrared spectroscopy, a past chairman and past editor of the newsletter of the Council for near-IR Spectroscopy, and a member of the ACS, SAS, and ISA. Currently a Senior Research Chemist at Hercules, her work has become focused on spectroscopic methods for process monitoring. She entered the Ph.D. program at the University of Delaware in 1993.

INTRODUCTION

Chemometrics is the discipline concerned with the application of statistical and mathematical methods, as well as those methods based on mathematical logic, to chemistry. This review, the tenth of the series, and the eighth with the title Chemometrics, covers the more significant developments in the field from December 1991 to December 1993. The format follows that used in the previous review (*A1*), with some exceptions. We no longer include a separate section called Factor Analysis to account for changes in the literature and to better reflect the way in which methods based on principal component analysis are used in chemometric work. The reader will note an increase in the modeling, calibration, and pattern recognition sections, the areas where most of the work previously assigned to the section on factor analysis now appear. We have also tended to group reviews and tutorials concerned with specific chemometric methods under the appropriate heading.

As we have noted in the introduction to previous fundamental reviews, the field of chemometrics continues to enjoy steady growth. For this review, almost 20 000 computer-generated citations were examined, a significant increase over the last two-year period. As noted before, hand searches were necessary to find papers missed by the computer search; amazingly, some 10% of the references listed were not detected by the computer search. From an examination of the papers found in the computer and hand searches, it was apparent that much of the growth in the number of references was due to publications produced by authors from outside of the "usual" location of chemometrics research. The largest amount of work by far originated in the Far East. Papers dealing with subjects relevant to chemometrics and published in English from addresses in Japan, China, and Korea have gone from a handful in 1988–1990 to about 2000 during 1992–1994. Similar, but smaller, increases were seen in works originating in the former Soviet Union, Eastern Europe, Central Asia, and South America. A large number of chemometric papers were published in languages other than English. It should therefore come as no surprise that, during the past two years,

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most of the reviews of chemometrics were published in languages other than English.

An ever-widening array of applications of chemometric methods also seems responsible for this increase in the rate of growth of the literature of chemometrics. A very large number of authors not formally trained in chemometrics have published applications of chemometric methods in chemical journals during the past two years. These authors include those pursuing fundamental research in analytical chemistry, a field closely related to chemometrics for historical and other reasons. This group has always been a source of papers concerning applications of chemometric methods. Over the past two years, their interest in chemometrics has increased—a statistic which is strongly correlated with the increased power of small, desktop computers and the ready availability of commercial and other chemometrics software. However, analytical chemists are not the only group seeing possibilities in using chemometrics to explore data. Even synthetic chemists and theoretical chemists have begun to realize that chemometrics offers a route to get more from their data. Research work has begun to appear from groups who would seldom attend a chemometrics seminar, let alone publish work in the field. Chemical engineers have also discovered the advantages of chemometrics. Over the past two years, the number of chemical engineers using routine and not-so-routine chemometric techniques has shown a steep increase. This review does not include papers from the mainstream chemical engineering literature, because the scope of this review is limited to chemical applications. However, a brief examination of papers in chemical engineering journals suggests that their inclusion in the next fundamental review may be appropriate. The third group with a strong interest in chemometrics are the statisticians. Many of the papers appearing chemical journals and cited in this review come from authors with formal training not in chemistry, but in mathematics and statistics. It is therefore not surprising that papers on chemometric methods have begun to appear more regularly in the more applied statistical journals. At present, statistics journals also fall outside of the scope of journals abstracted for this review, but a very few papers from the statistics literature which are likely to be of special interest to chemometricians are cited below.

The danger inherent in the expansion of chemometrics to areas as diverse as chemical engineering and statistics on the one hand and traditional chemistry on the other lies in that the "core" of chemometrics has become harder to discern. Unlike other, more traditional areas of analytical chemistry, for example, chemometrics is not inextricably associated with a particular instrumental method for measuring chemical data. Multivariate mathematical methods are as suited for analysis of economic trends, for example, as chromatographic traces. The computer, when used with general software for mathematical data analysis, is equally adept at examining data from a chemical process or a mass spectrum or relating boiling points to chemical structure. This generality has worked to the advantage of chemometrics research in the past, when methods developed in other fields such as econometrics, psychometrics, or electrical engineering could be brought to the attention of chemists by publishing the "new" method and a small chemical application in the chemical literature. Now, however, the increased mathematical sophistication of chemists, when coupled with easy access to data analysis, has placed the field at a crossroads. Research at the "core" of chemometrics can emphasize chemical relevance by focusing on the creation of new methods especially suited to the unique aspects of chemical data and chemical problems, or it can instead focus on more general, sophisticated mathematical methods for data analysis and assign less importance to the relevance to chemical applications. Both of these directions are apparent in the citations extracted during the last two years.

The breadth of the field makes a comprehensive review of chemometrics increasingly difficult. Possibly for that reason, the fundamental review published in this journal continues to be the most comprehensive collection of chemometrics research (*A1*). With the 1993 edition, the applications reviews published in *Analytical Chemistry* now include a section called Process Analytical Chemistry, in which some applications of chemometrics receive fairly extensive coverage (*A2*). Wold has considered the motivation for, and the likely trends in, chemometrics as applied to biomedical and pharmaceutical analysis (*A3*). Other reviews included a summary of recent chemometrics research in China (*A4*) in English by Yu, and a more complete review of the current state of Chinese chemometrics (but in Chinese) by Deng (*A5*).

Many other reviews have focused on applications of chemometric methods in a particular subfield of chemistry. Over the past two years, several subfields of chemometrics have been defined as a consequence of these applications, usually as new "metrics". Carlson reviewed the use of chemometrics in organic synthesis, an area he calls "synthometrics" (*A6*). The use of chemometrics in analysis of environmental applications was the subject of several reviews. Cerda et al. discussed chemometric methods for multicomponent analysis of complex matrices (*A7*), while Vogt considered the use of chemometrics on environmental data. He has coined the term "envirometrics" to describe this research area (*A8*). Qualimetrics—a subfield of chemometrics defined earlier by Martens as one that is concerned with the use of chemometric methods to improve quality control and quality assurance—was the subject of reviews by Vogt (*A9*) and Tranter (*A10*). The use of chemometric methods in the synthesis, analysis, and formulation of pharmaceuticals was reviewed by Aanstad et al (*A11*), who call this subfield "pharmacometrics", by Berridge (*A12*), who provided an extensive review, but under a more traditional title, and by De Boer (*A13*), who offered a brief overview of the field. Kauffman reviewed chemometric methods applied to analysis of lipids (*A14*) and modeling of lipid properties (*A14*, *A15*). NMR spectroscopy is an area where increasing use is made of sophisticated chemometric methods. Hoffman and levy reviewed modern methods for data analysis in NMR (*A16*), while Hoch et al. focused on the use of chemometrics for analysis of protein NMR spectra (*A17*). Analysis of spectral data generated by other spectroscopic techniques was the subject of a number of reviews. The use of chemometric methods on ultraviolet, visible, and infrared spectra of pigments was the subject of a short review by Oka and co-workers (*A18*). Barton and Himmelsbach discussed chemometric methods in the near-infrared analysis of feed materials, with an emphasis on future directions in this research area (*A19*). A review of photothermal spectroscopy included a summary of various chemometric methods found to be helpful in data reduction (*A20*). Patonay and Warner discussed the use of chemometric methods in their review of the field of multidimensional luminescence (*A21*). Boumans considered the impact of chemometric methods on the field of plasma spectrometry in another review (*A22*). The need for chemometric methods for enhancing the selectivity of new optical sensors was the subject of a review by Gauglitz (*A23*). Even the most sophisticated optical sensors lack adequate selectivity for practical analysis, and computer-based data reduction is a necessity. Carey discussed the use of sensor arrays with multivariate data analysis methods (*A24*). Examples of the use of this chemometrically enhanced sensor array to process control and pollution prevention were provided. Mass spectrometry has long been associated with chemometrics. Varmuza reviewed new applications of chemometric methods to mass spectral analysis (*A25*). He focused on computer-assisted methods for interpretation of mass spectra and on analytical applications. Chromatography, normally an area where many workers apply chemometrics with good success, was the subject of only one review: Munk evaluated the use of chemometrics and inverse gas chromatography for the characterization of polymers (*A26*). Finally, Bear and Brown reviewed the use of chemometric methods in electroanalytical chemistry (*A27*).

Many reviews of chemometric methods also appeared. However, most of these focused on a particular method, and these papers are referenced below, under the appropriate heading. Some reviews are actually more tutorial in nature, and these are listed in the Tutorial section below. The use of chaotic systems in chemistry, and chemometric methods for dealing with them, was the subject of a review by Bishop (*A28*). Kalivas reviewed his work with undergraduates in chemometric research (*A29*).

Chemometrics continues to be stressed as an essential part of the teaching of analytical chemistry, especially by European authors and groups. The subdiscipline concerned with analytical chemistry of the Gesselschaft der Deutscher Chemiker published a position paper on the nature and importance of chemometrics to analytical chemists (*A30*). They see the field of chemometrics as no less than the theoretical basis of analytical chemistry. The relationship between chemometrics and analytical chemistry was on many minds as the result of a competition to define the scope and direction of analytical chemistry, proposed by Grasserbauer in *Fresenius' Journal of Analytical Chemistry* (*A31*). Many of the responses to this challenge were published in a subsequent issue of that journal (*A32*). Interestingly, most of the responses were from Europe or Asia, and most of them mention chemometrics very prominently. Many stressed information as a result from analytical chemistry, rather than just data. Grasserbauer reflected on the scope and direction of research in analytical chemistry in reporting the decision of the committee concerning the award (*A33*). In his opinion, the needs for a curriculum in analytics/analytical science/analytical chemistry include a significant background in advanced data analysis. The relationship of chemometrics to metrology, informatics, and analytical chemistry was also examined by Shaevich (*A34*). Postma and Kateman applied some of the methods of chemometrics to representing analytical procedures. They described a formalism for analytical methods, based on information theory (*A35*).

Despite the strong interest in chemometrics by analytical and other chemists, courses in chemometrics remain fairly uncommon. Teaching of chemometrics—to analytical chemists, synthetic chemists, chemical engineers, or whomever—probably remains the rate-limiting step in the advancement of the field. As the newer work in chemometrics becomes more mathematically sophisticated, it becomes more difficult for those with inadequate preparation in mathematics to enter the field or even to read the recent literature of chemometrics. The need to offer more introductory and intermediate instruction in chemometrics remains, both to train those using the software packages and to find ways of bringing a constant flow of new workers into the field. For the present, short courses, tutorials, and recent texts continue to be the main routes for students as well as practicing chemists to learn about chemometrics.

Short courses on chemometrics are increasingly available, and they offer the easiest way for a novice to gain some exposure to chemometrics. These range from the brief, two-day courses now offered by the American Chemical Society at national ACS conferences to the five-day schools in chemometrics offered in Britain each fall by the University of Bristol. Some commercial companies are now offering regular short courses on specialized areas of chemometrics, too. These include vendors of chemometrics software and also consultants. The video revolution has made few inroads into the teaching of mathematically oriented subjects such as chemometrics, but for those who cannot attend a short course, one company now offers taped training series on introductory statistics, experimental design, and quality assurance. Instructors for these courses are well-known statisticians, including George Box, Søren Bisgaard, Conrad Fung, and J. Stuart Hunter.

Cross-fertilization in chemometrics can also come from conferences. Major research conferences in chemometrics help during the past two years included the fifth Chemometrics in Analytical Chemistry Conference (CAC-V) held in Montreal, Canada, in July 1992, Computer Applications in Analytical Chemistry (COMPANA-92) held in Jena, Germany, in August 1992, the Third Chemometrics Conference, held in Brno, Czech Republic, and the Chemometrics and Environmetrics meeting (CHESM-93) held in Bologna, Italy in August 1993. The Gordon Research Conference (GRC) on Statistics in Chemistry and Chemical Engineering continued to have a strong chemometric component, reflecting an increased interest by many statisticians in chemometric methods. Other conferences with a significant chemometrics component included ICCCRE 10 in Jerusalem, Israel, and the 28th Colloquium Spectroscopicum Internationale, in York, England. Yearly conferences in the United States, including the EAS Conference, the FACSS Conference, and the Pittsburgh Conference also had significant chemometric components. Vandeginste reported on the 1993 Pittsburgh Conference (*A36*). His report noted the changed emphasis at PittCon: there is a strong focus by vendors on qualimetrics and chemometrics, for it is here that many instrument vendors see a chance to add value to their product.

Publishing the proceedings of conferences with a heavy emphasis on chemometrics is the rule, not the exception. Conferences held during the past two years whose proceedings were published in *Analytica Chimica Acta* included CAC V and the 6th CIC Workshop on Software Development in Chemistry. The proceedings from COMPANA 92 and The 2nd Scandinavian Symposium on Chemometrics (SSC2) appeared in *Chemometrics and Intelligent Laboratory Systems*. The proceedings from the COMPANA conference are especially noteworthy because one paper published from this conference asked the question "Does COMPANA accomplish what it should?" (*A37*). With the number of conferences increasing, and the number of workers doing research in fundamental chemometrics remaining level, questions of this sort seem to be on the minds of many conference organizers. For example, several Gordon Research Conferences have been scaled back to reflect declines in attendance: the GRC in Analytical Chemistry has been suspended for now, while the GRC on Statistics in Chemistry and Chemical Engineering has been slated to be held every two years, starting in 1994.

Conferences upcoming in 1994 with significant chemometrics content include the International Chemometrics Research Meeting, to be held in Veldhoven, Holland, in June 1994, the fifth Snowbird Conference on Chemometrics in Analytical Spectroscopy, to be held outside of Salt Lake City, UT, also in June 1994, and the 1994 GRC, in July. Many journals now offer some sort of calendar section listing conferences for those looking for one at just the right time and location.

One unusual chemometrics conference to be held in 1994 has no physical location. The North American Chapter of the International Chemometrics Society (NAmICS) will hold the First International Chemometrics Internet Conference (INCINC) during September–November 1994. Papers will be "presented" by posting the manuscripts over the Internet through session chairs to the interested (and registered!) community, and discussion of those papers will take place over a specified time period though the NAmICS Internet listserver. Proceedings from this conference will appear in *Chemometrics and Intelligent Laboratory Systems*, though those registered for the conference will have access to the manuscripts a good while before any hard copy appears in print.

The increasing use of the Internet by chemometricians—as indicated by the upcoming Internet Conference—is worthy of further comment here. It is now simple to use Internet resources to get reports, transfer data sets, exchange software, and even submit manuscripts anywhere in the world. Yet, chemists—including those in chemometrics—remain well behind the curve established for efficient use of networks by information scientists, statisticians, and many others. For example, neuroprose, a neural networks manuscript repository, has been in existence for some time at Ohio State University. Many authors in this field routinely make their work available to neuroprose (archive.cis.ohio-state.edu) by anonymous ftp. In this field, it is not uncommon to learn of a new paper in the morning, ftp the paper to a local computer, print the paper, and test the results by the next day! Statisticians also have been taking advantage of Internet capabilities for some time. The statlib (temper.stat.cmu.edu) software and data repository for statistics, located at Carnegie Mellon University, has all sorts of public-domain statistical software available by anonymous ftp. Several well-known statisticians make their "reprints" available by anonymous ftp from their computers. With the high cost of reprints and decreasing funds, this is an attractive idea. Using the Internet to make work available to any interested person with knowledge of the Internet and access to it raises several questions concerning the meaning of publication and of peer review, however. The way in which journals—especially the two commercial journals publishing much of chemometrics research—will deal with issues raised by electronic release of research work has yet to be made clear.

Awards announced during the last two years included two for Statistics in Chemistry. The 1992 award, given to the best industrial application of statistics in chemistry went to DuPont for research on mixture designs and neural networks. The 1993 award was given to Cheng Yu Ma and Chuck Bayne of Oak Ridge National Laboratory for their work on differentiation of environmental samples by linear discriminants applied to the chemical ionization mass spectra of arochlor contaminants. The first Elsevier Award in Chemometrics, given to a chemometrician under 40, was presented to Lutgard Buydens, of The Catholic University of Nijmegen.

During the past two years, two noted supporters of chemometrics passed on. Herman Wold, a noted econometrician responsible for the NIPALS algorithm and many other ideas now routine in chemometrics (and partially responsible for Svante Wold, a noted researcher in the field) died in 1992 (*A38*). L. B. (Buck) Rodgers, a well-known analytical chemist who recognized the utility of modern data analysis and was an early, powerful supporter of chemometrics in the United States, also died in 1992. Rodgers' work spanned most areas of analytical chemistry, but his last efforts were directed toward data analysis. The goodwill and enthusiasm of both will be missed.

Having data sets to test new methods for data analysis has long been a concern for those in chemometrics. This issue has also been a concern to those in information sciences and statistics. These groups have set up a number of Internet data set repositories. One site at UC Irvine (ics.uci.edu) intended for testing out neural networks contains many classification sets and may be of interest to those in chemometrics. The statlib statistics repository has some well-characterized data sets for testing certain statistical software. Chemometricians will be interested in the first attempt to offer well-studied data sets in this field (*A39*). For $10, a floppy disk containing four well-studied data sets can be obtained from the authors. Another way of testing a chemometric method—and one favored by this group—is with simulated data. Voightman has reviewed his approach for simulating an analytical instrument with Mueller calculus (*A40*). His simulated instruments produce very good, simulated data. Visual BASIC has also been used to simulate analytical processes (*A41*). Even Fourier transform NMR can be simulated, as Ratzlaff and VanderVelde demonstrate (*A42*). Pool and co-workers reported an algorithm for simulating gas chromatographic/mass spectrometric (GC/MS) data (*A43*). The simulated data was validated with real GC/MS data. Yang et al. used simulation methods for multiplex chromatography to test several different methods for quantitation (*A44*). Lewis et al. used the DryLab I/mp package to simulate chromatographic separations as a function of changes in the mobile-phase pH (*A45*).

Two new journals will be of considerable interest to chemometricians. One, *Spectrochimica Acta Electronica*, the electronic supplement to *Spectrochimica Acta, Part B,* publishes computer applications in spectrochemical analysis. This journal provides a hard copy text and a floppy disk containing the software associated with each article. The approach employed here is not novel; *The Mathematica Journal* has done the same thing for some time, but *Spectrochimica Acta Electronica*, represents the first chemical journal to offer this feature. Judging from the number of books being published with accompanying software and disks (see the section below for more on this), providing an executable version of software with a publication reporting that software is a feature that is likely to become more common in the near future. The second new journal of interest to those in chemometrics publishes no papers. Instead, new papers on chemometrics are summarized in *Window on Chemometrics*, a service begun by the Royal Society of Chemistry in July 1993. *Window on Chemometrics* offers brief abstracts of articles of interest to those developing chemometric methods or applying chemometric techniques. The scope for the abstract list includes general techniques and statistics, calibration and validation, computer programs, and expert systems, as well as chemometric application to standard analytical methods in spectrometry, chromatography, and other methods. Some 250 journals are scanned for articles relevant to chemometrics, and abstracts are provided monthly. The existence of this abstracting service is another indication of the increasing use of chemometric methods throughout chemistry, and it is a welcome aid for those wishing to keep abreast of the latest work in chemometrics without scanning more general abstracts.

Books. During the last two years, a surprisingly large number of texts on chemometric methods were published. Many were intended for an audience new to chemometrics. Haswell edited a multiauthor book offering introductory treatments of several areas important to modern chemometrics (*A46*). A second in the series of books made from the tutorials published in *Chemometrics and Intelligent Laboratory Systems* appeared (*A47*). This book included tutorial articles from mid-1989 to late 1991. Brereton edited an introductory, multiauthor volume on the use of pattern recognition methods in chemistry (*A48*). Case studies served to illustrate the principles, and an optional, tutorial software supplement distinguishes their approach, the one used at the Bristol short course. Kateman and Buydens teach introductory chemometrics from the perspective of considering the influence of the analytical process on the quality of an analytical result in a revision of an early text on chemometrics (*A49*). Meloun and co-workers published the first in their series of texts on chemometrics in analytical chemistry (*A50*). The book, which focuses on introductory statistical methods and exploratory data analysis, is intended for use with their commercial CHEMSTAT package. Buydens and Schoenmakers edited a multiauthor text on software approaches for implementing expert systems, neural networks, and genetic algorithms (*A51*). Analysis of spectral data with the help of chemometrics continues to receive a lot of attention. Kalivas and Lang discuss the mathematical aspects of multivariate calibration of spectra in their new book (*A52*). Pelikán and co-workers offered a fairly complete text on the applications of chemometrics and other numerical methods applied to several different spectroscopies (*A53*). A more introductory treatment of the analysis of data from electronic and vibrational spectroscopy also appeared (*A54*). Several multiauthor books appeared on near-infrared spectroscopy. The use of chemometrics in qualitative and quantitative analysis of samples by near-infrared (near-IR) spectrometry is emphasized in all three books. The book edited by Hildrum et al. emphasizes applications, but includes a section on developments in multivariate calibration (*A55*). The book edited by Burns and Ciurczak focuses more on introductory theory of near-infrared spectroscopy and on the basics of multivariate calibration (*A56*). There is a sizable section on applications in this book, too. The third book, edited by Murray and Cowe, contains proceedings from the 4th International Conference on Near-Infrared Spectroscopy (*A57*). Many of the papers included here concern details of the chemometrics used in the data analysis. This book is more suited to the expert at near-IR and chemometrics. Other books on chemometrics applications that resulted from conferences included the third volume in the series covering the Snowbird Conference (*A58*). This book has a nice chapter on multivariate calibration by Haaland.

Several other books appeared which are of interest to data analysts. Gans examined the statistical theory and practice of fitting chemical data to models (*A59*). Noggle published an introductory text on curve fitting with the MS-DOS-based EZ-FIT software, a copy of which is provided with the text (*A60*). Miller and Miller updated their well-known text on statistics for analytical chemistry (*A61*). Their new version places more emphasis on computer methods and chemometrics. Meier and Zünd consider the use of statistical methods in analytical chemistry too, but from the perspective of case studies (*A62*). This new text also includes a disk with software in BASIC. Experimental design is an area that now attracts a great deal of interest from chemists and others. That interest spurred the publication of new books on experimental design and the revision or rerelease of older classics. Goupy offered an experimenter's approach to experimental design, but with an emphasis on designs requiring computer-based calculations (*A63*). Davies published a nice introduction to experimental design for chemists (*A64*). This text covers designs up to those requiring the use of computer methods. Deming and Morgan updated their introductory text on experimental designs in chemistry (*A65*). Finally, the classic text on experimental design by Cochran and Cox was rereleased, in paperback form (*A66*).

Several other statistics books appeared whose topics are of special interest to workers in chemometrics. McLachlan published a new book on statistical methods for pattern recognition (*A67*). This well-written book includes discussion of chemometric methods as well as the usual statistical theory. It will be of interest to anyone doing classification work. Several books appeared on the bootstrap, a validation method gaining attention in chemometrics. Efron and Tibshirani published a book introducing the bootstrap and examining its applications (*A68*). Hall offered a text on the theory of the bootstrap (*A69*), while Mammen published work on the utility of bootstrapping in book form (*A70*). Brown considered the statistical theory behind calibration and related regression problems in a new book (*A71*). Van de Geer examined the theory behind nonlinear analysis of categorical variables in a monograph (*A72*). In a second monograph, he reported on the use of standard statistical packages, such as SPSS, to implement the GIFI system for nonlinear analysis of several experimental data sets (*A73*). Jobson surveyed the theory and applications of multivariate data analysis in a two-volume set (*A74*, *A75*). A diskette with the example data sets accompanies volume 1. Afifi and Clark used geometrical and graphical explanations to teach multivariate analysis in their new book (*A76*). They also offer introductions to several statistical packages. Kirby focuses on a single package, the SYSTAT statistical software package, to illustrate some advanced statistical methods (*A77*). Cressle offered a compendium of knowledge on spatial statistics in a new book (*A78*). Bandemer and Näther published an extensive monograph on the theory of fuzzy modeling methods (*A79*).

Neural nets are attracting attention from several groups. Among the many new books published in this area, a few stand out as especially interesting. Kosko summarized the literature on fuzzy methods and neural networks in a new book, which also includes C language software for fuzzy analysis and fuzzy nets (*A80*). Chemists, especially those new to the area of neural nets, will find the new book by Zupan and Gasteiger very helpful (*A81*). This book is filled with clear discussions of many types of networks, and many example applications relevant to chemistry are presented. Other new books on neural networks included those on statistical modeling with nets by Smith (*A82*), a new book by Freeman on generating nets with the Mathematica symbolic computing package (*A83*), and a book on advanced methods by Wasserman which supplements his earlier, more introductory text (*A84*). Another book suited for those with expertise in neural nets is concerned with the combination of nets and genetic algorithms (*A85*). Applications of neural nets to pattern recognition are covered in a new book by Nigrin (*A86*) and a book comparing traditional and net-based approaches by Schalkoff (*A87*). Those chemometricians interested in keeping up with the latest developments in computational chemistry will want to examine the multiauthor text edited by Lipkowitz and Boyd (*A88*). A very useful chapter on computational software is included.

And, finally, although it is not particularly recently published, mention should be made here of an unusual book containing only data. Andrews and Herzberg have collected several data sets from different disciplines in a single source (*A89*). They intended it for statisticians, but those seeking data sets for testing chemometric methods may find this a useful source book.

Software. Chemometrics is an algorithm-based field, and the development of software continues to be an important part of research in this field. Not surprisingly, many papers concerned with chemometrics included discussion of in-house chemometrics software of some type. These in-house packages continue to grow in both size and sophistication. The area of optimization is especially active. Tchapla reviewed optimization software available for chromatography and gave suggestions on the selection of a suitable optimization package (*A90*). One of the most frustrating aspects of a chemometric analysis can be getting the data from the instrument to the computer where the analysis is to take place. Fennema and co-workers discuss their solution to this problem in a two-part series (*A91*, *A92*). Progress toward the eventual standardization of data formats and simplification of interchange of analytical data was evaluated (*A93*). A noncommercial standard for storage and transfer of Auger and X-ray photoelectron spectra between machines and computers of all types has been developed by a consortium of Japanese researchers in this area (*A94*). They propose it as a standard. The use of laboratory information management systems (LIMS) has become much more common. McDowall and co-workers considered applications where LIMS and chemometrics are complimentary (*A95*). Levey and Leonard discussed the important issues to be considered in attempting to validate LIMS (*A96*). Miller and Mason offer a computer performance analysis of a LIMS for use in the pharmaceutical industry (*A97*). The issue of software and method validation was a popular subject during the past two years. Several reports concerned software for validation of analytical methods. The AMIQAS package was developed and used for quality control, proficiency testing, and method evaluation on lead analyses in blood (*A98*). A program based on maximum likelihood fitting of a functional relationship was also proposed as a means of method validation (*A99*). Biochemical and bioanalytical data were validated by an expert system-based approach implemented in the VALAB package (*A100*). Automated analysis of quality control data was accomplished by a new software package based on Westgard's multirule (*A101*). Database search and interpretation software continues to be refined. The SpecInfo system, a spectroscopic search package used with NMR, IR, and MS databases, was reviewed (*A102*) and evaluated for estimation of the ^{13}C NMR of organic molecules (*A103*). The SCANNET database, a system suited for NMR, IR, MS, Raman, and UV spectra searches and structural elucidation, was described in two reports (*A104*, *A105*). Berrueta and co-workers describe the FLUORIM package for collection, evaluation, and storage of fluorescence data (*A106*). The Beilstein database and search system for current facts in chemistry was also described (*A107*).

Many authors considered the improvement of analytical methods with a chemometrics software package. The use of chemometric "detectors" for chromatographic separations was the subject of three reports. Cardot et al. described a program for automatic detection and description of chromatographic peaks (*A108*). Jurasek and co-workers reported a chemometric detector based on the ISODET software package that recognizes Cl-, Br-, and S-containing compounds from the isotope cluster patterns in their mass spectra (*A109*). Werther, Lohninger, and Varmuza discussed the use of the SpecInfo and MASS-LIB information systems with the EDAS software package as a classifier for GC/MS data (*A110*). Two disjoint classes are nicely separated. Another application in chromatography was concerned with the use of symbolic programming for automated estimation of retention data from chromatograms (*A111*). Atomic spectroscopy, an area not usually of interest to those in chemometrics, also received some attention during the past two years. Webb and Salin report an electronic aid based on a small expert system for line selection in inductively coupled plasma spectrometry (*A112*). Hypertext tools have been published for selection of dissolution methods prior to atomic absorption analysis (*A113*). Burton and Horlick reported on the MS Interview database for plasma mass spectrometry and related techniques (*A114*). Their program is suited for use with MS sources other than the plasma torch or glow discharge. Analysis of mass spectra is always challenging, something that attracts the interest of chemometricians. The last two years saw the publication of many packages for mass spectral analysis. A set of simple software tools for elucidation of mass spectra was offered in one paper (*A115*), and the SpecTool hypermedia tool kit for interpretation of mass spectra was described in two others (*A116, A117*). Rules for identification of substructure from tandem mass spectra by the MAPS software package were the subject of a paper by Hart and co-workers (*A118*). Software for the analysis of data from plasma desorption mass spectrometry was also discussed (*A119*). King and Horlick offered SpectroPlot, a general user interface for processing spectral and interferometric data on Macintosh computers (*A120*). Programs with more specific uses included the STAR package for evaluation of stability constants from multiwavelength absorbance data (*A121*) and the RAMPAC package for background correction, peak fitting, and deconvolution of Raman spectra (*A122*). A subroutine for the MINUIT package that performs deconvolution of spectra containing up to 13 peaks was the subject of one report (*A123*). NMR, especially multidimensional NMR and NMR imaging, is another area where chemometrics software continues to evolve. The PROSA package performs many common preprocessing operations on large multidimensional NMR spectra (*A124*). Another paper reported on what the authors called a "seraglio of programs" for human-aided assignment of 2-D ^{1}H NMR (*A125*). NMR microscopic imaging using projection reconstruction and the interpretation of multivoxel spectra with the MIMSTATS software package were the subject of two papers (*A126, A127*). A novel, extensible NMR signal processing package made by embedding Matlab into a UNIX-based expert system was the subject of another report (*A128*). Fitting of high-resolution electron spin resonance spectra was discussed by Kirste (*A129*). Surface spectra are also amenable to chemometric assistance, and new software for that continues to appear. Software for automated analysis of ion scattering spectrometry data was reported (*A130*). Time-resolved acoustic emission produces a kind of spectrum which has been the subject of several papers by Wade's group. They reported on an extensible toolbox of signal processing methods for examining these acoustic emission "spectra" (*A131*).

Development of general-purpose chemometric software continues to attract interest, but less than in previous review periods. Militky and Meloun added to their series of papers on the CHEMSTAT package with two papers on the nonlinear least squares package MINOPT (*A132, A133*). The second paper in a series describing a computer tool kit for chemists, one dealing with maximum tolerance procedures for fitting data to models, also appeared (*A134*). Several rather novel software packages conclude our examination of this subject. The CFIT package, a genetic algorithm-based method for spectral curve fitting, was discussed by Lucasius et al. (*A135*). Software for image segmentation was the subject of a report by Mitev and Ivanova (*A136*). This is very useful for automating biological assays and classifying image parts. Software for fully automated, adaptive analysis has long been a goal of some groups in chemometrics. Plouvier et al. reported on their experiment planner software package (*A137*). This software is capable of making strategic decisions concerning experiments and can alter ongoing experiments—or decide to terminate them—based on new experimental data. Finally, two reports on new software for teaching chemometrics appeared. One based the chemometric analysis on commercial spreadsheet packages (*A138*). The second announced a new module for the commercial CLEOPATRA chemometrics teaching package (*A139*).

Commercial chemometrics software has changed a good deal during the last two years, as vendors began to take advantage of improvements in computer hardware and system software. Commercial statistical software—much of which can be used to do considerable "chemometric analysis"—has matured significantly during this period. Very sophisticated user interfaces coupled to high-performance software for data analysis are now common on general-purpose statistical packages. Commercial chemometrics software, with a smaller audience and smaller budgets for development, cannot at present match the quality of these packages. However, the past two years has seen a gradual improvement in the quality of most of the established commercial packages for chemometrics. Pirouette and Unscrambler both were upgraded recently, and both have focused on the new issue of software validation. Unscrambler now offers capabilities for experimental design and the examination of response surfaces. Many other incremental improvements were also made. An upgrade to the Pirouette package focused on better file translation capabilities, improved display, and improved regression diagnostics for the soft modeling. InStep, a companion product to Pirouette which permits automated use of Pirouette-generated models under Microsoft Windows, also appeared. A new version of GOLPE, a package for variable selection released by Multivariate Infometric Analysis, is also available for purchase. This software is especially suited for work concerned with drug design and multivariate calibration. A few new packages suited to chemometrics also appeared. The SCAN software package, a general package produced by Jerll for exploratory data analysis, calibration, and classification, made its debut in late 1992. This package offers several unusual chemometric methods not found in other chemometric packages. The MODDE package was announced by Umetrics in 1993. This software package combines partial least squares (PLS) modeling and experimental design with a Windows-based graphical user interface that is more mature than many other packages. The last two years saw the release of a new version of the PLS Toolbox by Barry Wise. This shareware toolbox, which runs under the Matlab numerical computation and visualization package available from the Mathworks, offers m-files in source form for multivariate calibration methods of all sorts, including some newer methods not provided in commercial packages. The Matlab software package itself also underwent a major revision in 1992; the new version offers much improved graphical user interfaces and visualization capabilities, along with some changes in the Matlab language. Toolboxes with m-files for neural networks, statistics, and image processing appeared during the last two years. Matlab continues to gain supporters among chemometricians, and many papers published during the last two years included Matlab code. The Mathworks now provides an anonymous ftp site (ftp.mathworks.com) with public-domain Matlab code, some of which is of interest to those in chemometrics. A new Windows version of S-plus also was released during the past two years. This language also offers many attractive features, and it has become the favorite of many statisticians. The statlib repository has a fairly large amount of S-plus code useful in chemometrics applications.

Tutorials. With the gradual entry of chemometric methods and concepts into most analytical instrumentation, the need for tutorial articles in chemometrics has grown. Here, at least, the supply has kept up with demand. Now, there are many tutorials published on all areas of chemometrics. Regular columns on introductory statistical and chemometric methods appear in *Spectroscopy* and *LC-GC*, for example. Some of the tutorial articles being published now, of course, are more tutorial than others, which seem more like reviews. Only general tutorials are listed here; ones with a specific topic are referenced in an appropriate section below. Gardner et al. offer two brief tutorials on the need for chemometric and statistical methods in monitoring data from processes and routine analytical runs (*A140*, *A141*). As usual, many tutorial articles addressed issues concerning regression in one form or another. Johnson considered why, when, and how biochemists should use least squares analysis in dealing with their data (*A142*). The application of multivariate methods to multidimensional NMR was the subject of a tutorial that focuses on the relation between the mathematics and the physics of the measurement process (*A143*). Wythoff introduced the back-propagation method for training feed-forward neural networks (*A144*). The mathematical modeling required for analysis of immunoassay data was the subject of a tutorial by Baud (*A145*). Statistical methods receiving examination included empirical Bayes methods for parameter estimation (*A146*) and validation procedures for regression and classification (*A147*).

STATISTICS

A substantial increase in the number of literature references describing the use of statistics in chemical data analysis occurred during this review period. As in previous years, a number of papers merely incorporated basic statistical methods into the chemical analysis. These works are omitted here; instead, only those studies whose focus was on the development or evaluation of statistical procedures for analytical chemistry are cited. During the past two years, procedures were reported for diverse purposes such as method comparison and validation, quality assurance and control, estimation of detection limits, sampling, outlier detection, error estimation, and derivation of confidence intervals. Many of the articles published in these areas are beyond the scope of this review and are not referenced here. The interested reader is referred to statistics journals such as *Technometrics* and the *Journal of the American Statistical Association*.

Several reviews of statistical techniques for chemical data analysis appeared in the literature. In particular, the use of statistics for method validation was often discussed. Castledine and Fell reviewed schemes for assessing the purity of liquid chromatography (LC) peaks as part of the validation procedure for pharmaceutical analyses (*B1*). In addition, method validation was the topic of two other reviews regarding biopharmaceutical assays (*B2*) and food analysis (*B3*). The interlaboratory validation of analytical measurements was also of concern. The importance of assessing and comparing the accuracy of analyses performed by different laboratories was discussed in the context of pesticide residue analyses (*B4*), wastewater monitoring (*B5*), and chemical analyses in general (*B6*). Currie addressed the issue of accuracy in analytical science in a review which included an illustration of exploratory statistical graphics for appraising data quality and uncovering relationships (*B7*). In an introductory review of chemical analysis in complex matrices, Smyth described statistical data evaluation (*B8*). The subject of statistical sampling was discussed by two reviewers. The first provided an overview of groundwater monitoring at waste disposal sites (*B9*), while the second reviewed coal process and quality control in power plants (*B10*). Duca considered several statistical aspects of the estimation of reference limits in biological monitoring (*B11*). The detection and handling of outliers in analytical data was also considered. In this regard, Miller reviewed parametric, nonparametric, and robust statistical methods for treating outliers (*B12*). In still another review, Piegorsch and Haseman discussed various parametric and nonparametric procedures for the analysis of toxicity data (*B13*). The use of flow statistics in nuclear magnetic resonance (NMR) spectrometry was also discussed (*B14*). A new area named informational statistics was described as comparable to robust statistics in terms of resistance to uncertainty. Sarbu explained the basics of this field as applied to analytical chemistry (*B15*).

Statistical procedures were utilized to either combine or compare chemical data for a given determination obtained from different analytical methods. These procedures account for differences in the accuracy and precision of the various analytical methods. For example, Schiller and Eberhard described a technique for presenting the combined results from several different chemical methods as a weighted mean and a corresponding uncertainty (*B16*). Moreover, Rasemann and Peter defined the degree of efficiency, the degree of (mutual) reproducibility, and the equivalence probability as measures for comparing the results of tin analyses from various chemical procedures (*B17*). Another method comparison technique based on statistical power calculations was also reported by Mazzo and Connolly (*B18*). Statistical procedures for evaluating results from different laboratories were discussed by several researchers. Henrion et al. again reported on applying three-way principal components analysis (PCA) to multivariate data for the detection of error in round robin tests (*B19*). In a large interlaboratory and method comparison study, the World Health Organization determined that the laboratory constituted the single most significant factor affecting the accuracy and precision of toxicological assays (*B20*). Thompson and co-workers compared the robust analysis of variance (ANOVA) method outlined by the Analytical Methods Committee (AMC) with the Harmonized Protocol. They found that the former was markedly more reliable for interpreting data from collaborative trials (*B21*). De Beer et al. evaluated three volumetric procedures for pharmaceuticals, using ANOVA and box plots to show that interlaboratory variations were significant (*B22*).

A number of papers published over the last two years described the use of statistical procedures for analytical method validation as well as for quality assurance and control. In a two-part report, Lang and Bolton presented a scheme for validating bioanalytical methods for pharmaceuticals (*B23*, *B24*). Another report discussed the design and interpretation of a method evaluation in atomic absorption spectrometry. The design used here permits estimation of the systematic error, the limit of detection, and the limit of quantification (*B25*). Method evaluation functions (MEF), defined as the expected value of the analysis as a function of the true analyte content, were also described for inductively coupled plasma atomic emission spectrometry (ICP-AES) (*B26*). Critchfield and co-workers explained a new bootstrapping technique which provides a probabilistic assessment of confidence on the linearity of a calibration curve (*B27*). In the area of quality assurance and control, an analysis of precision based on the χ^2 distribution was described in the general case (*B28*) and in the specific case of activation analysis (*B29*). Quality control and standardization in analytical systems were addressed by examining the statistical properties of immunoanalytic systems (*B30*). For the purpose of quality assurance and control in spectrochemical methods, Pasky described statistical evaluations for normality, trends, and outliers (*B31*). Caudill et al. reported the results of testing a composite multivariate quality control (CMQC) system which detects systematic errors, random errors, and correlation changes under various typical measurement conditions (*B32*).

The estimation of detection limits by statistical means continues to be of significant interest. Work in this area was undertaken by several research groups. Yang and co-workers investigated determination errors arising when multicomponent analysis (MCA) methods are employed for correcting line interferences in ICP-AES. The development of a relationship between the relative error in analyte concentration and the extent of line overlap, bandwidth, and magnitude of wavelength positioning error allowed the derivation of an expression for the true detection limit (*B33*). In another study, a statistical model was designed to ascertain the analytical sensitivity, the limit of detection, the limit of determination, and the precision of spectrometric and chromatographic methods on the basis of linear calibration data (*B34*). Singh employed PCA to estimate multivariate decision and detection limits for gas chromatography/mass spectrometry data (*B35*). The estimation of detection and decision limits is rendered more difficult when the variance of the instrument response is not constant. Torrades and Garcia Raurich suggested a model which transforms heteroscedastic data to homoscedastic data in order to enable an estimation of the detection limit from the projection of the confidence interval about the regression line (*B36*). Gibbons and co-workers also proposed a detection limit estimator which allows for a concentration-dependent variability in the analyte signal and multiple future detection decisions (*B37*). In addition, Gibbons et al. described an approach for calculating practical quantitation limits from calibration data (*B38*). A replacement method for estimating normal and log-normal distribution parameters was described which accommodates samples with concentrations that fall below the detection limit by assigning them a value between zero and the detection limit. This technique was compared with the methods of maximum likelihood and log-probability regression (*B39*). The treatment of values below the detection limit with a parametric estimation method was also discussed by Hartmann and Walter (*B40*). Wegscheider and co-workers described an error model for (locally) linear systems which could be employed for estimating detection limits in spectral measurements (*B41*). The definition of detection limit was revised in a new statistical technique applied to bilinear chromatography. The method uses regions in which no chemical components are eluting as repeated analytical blanks to formulate a multivariate detection limit for measuring the number of species in local regions of a chromatogram (*B42*).

Sampling strategies and outlier detection were also investigated by a variety of statistical means. Dale et al. recommended the use of the standard error-to-mean ratio, kurtosis, and skewness to aid in determining a suitable sample size for estimating the distribution of soil nitrogen (*B43*). Representative soil sampling for heavy metal analysis was discussed by Einax and co-workers, who employed cluster, discriminant, and principal components analysis, as well as a multivariate autocorrelation function to evaluate the sampling (*B44*). Soil contamination was the subject of another study in which different sampling strategies were statistically compared (*B45*). In a biological application, Traut and Scheid reported the dependence of the statistical power on the control sample size in mutagen screening (*B46*). The appropriate number of samples for the *Ceriodaphnia* reproduction toxicity test was also ascertained statistically (*B47*). Signal-to-noise ratio measurements in electron spectroscopy were performed by Seah and Cumpson. They determined the minimum number of counts necessary to accurately measure the noise statistics assuming Poisson behavior (*B48*). Several methods for detecting outliers in measurements were discussed. Critical Q-test (*B49*) and QP-test (*B50*) values obtained from a stochastic procedure were described for this purpose. A robust, alternating regression method was suggested as an alternative to the least squares regression technique that underlies a principal components analysis. The robust regression approach allows the elimination of outliers which could otherwise lead to an erroneous set of principal components (*B51*). Residual analysis and outlier detection were carried out using a robust bivariate regression model which accounts for error in both variables (*B52*). Moen et al. described the median method as a nonparametric linear regression technique which is resistant to outliers. In their approach, the median of all the absolute y deviations is used as a robust measure of the dispersion of the individual y deviations from the regression line (*B53*). A new technique called the gnostical method was discussed by Paukert and co-workers for identifying outliers, evaluating the homogeneity of data sets, and classifying individual data (*B54*). In a novel approach based on multivariate analysis, Stapanian et al. described a method for identifying outliers as well as their suspected causes. The procedure was illustrated with a large multivariate environmental data set (*B55*).

The estimation of error in analytical measurements by statistical methods was the focus of many studies. Several authors critically examined the common practice of least squares fitting to spectroscopic data. Yamada argued that the standard deviation of the fit is poorly defined, particularly when the data comprise several sets of data with varying precision. The significance of the uncertainty of the fit was evaluated for absolute and relative weighing strategies (*B56*). Martin also investigated the uncertainty of fitting a function to spectral data and compared results from the least squares method with one based on cubic splines (*B57*). Using Monte Carlo calculations, the applicability of estimating the error by the covariance matrix in a least squares fitting procedure was examined (*B58*). An approach in which the residuals of a least squares fitting to spectroscopic data are extensively studied to evaluate the quality of the linear model was also described (*B59*). Tellinghuisen reported a technique which greatly reduces the detrimental effects of background on the precision of the least squares estimate of exponential decay parameters (*B60*). Another study explained a statistical test for determining the significant number of spectral lines to be included in a least squares fitting (*B61*). In an analytical method comparison application, the performance of ordinary least squares was compared to that of another regression technique which accounts for error in both variables (*B62*). The problems associated with multicollinearity were addressed by the use of biased linear models based on the mean quadratic error of prediction (*B63*). Giorgini et al. developed a method for assessing the influence of signal noise characterized by Poisson statistics on vibrational correlation functions and relaxation times in Raman spectrometry (*B64*). The propagation of error in γ spectroscopy and neutron coincidence counting for plutonium materials was also modeled (*B65*). Several researchers investigated the uncertainties associated with measurements in Auger (AES) and X-ray photoelectron (XPS) spectroscopies using χ^2 (*B66*), Bayesian (*B67*), minimum χ^2 and unweighted least squares procedures (*B68*). In addition, Harrison and Hazel proposed XPS/AES data acquisition strategies on the basis of uncertainty determinations (*B69*). Atomic models are employed in interpreting nuclear Overhauser effect (NOE) data for macromolecular structure determinations. A cross-validation procedure was implemented to define reliable criteria for evaluating the quality of solution NMR structures (*B70*). Protein structure elucidation by NMR was also the subject of error analysis by Hoch (*B71*). Coates formulated corrections for dead time effects in the measurement of time-interval distributions, where the form of the probability distribution is arbitrary but known. The method was illustrated with a time-of-flight mass spectrometry application (*B72*). Several studies investigated the effect of measurement error on the determination of principal components. In one study, Simeon and Pavkovic evaluated two methods for calculating statistical weights based on variances and concluded that such weights improve the analysis of principal components (*B73*). A second study examined the influence of white noise in equilibrium data on abstract factor analysis. The perturbation of the data with normally distributed error prior to factor analysis was proposed as an aid in data modeling (*B74*). In another study, it was argued that the principal component and factor analysis modes (Q-mode and R-mode) typically selected assume error estimates that are not commonly encountered in chemistry. Two new scaling methods were proposed to improve the accuracy of the factors (*B75*). Error analysis of calibration curves was also performed by several workers. For instance, Cabral utilized an analysis of covariance of the regression lines to evaluate the repeatability of ion-selective electrodes (*B76*). Others characterized the error in a calibration curve from flow injection and chemiluminescence data by calculating the bias, excess variance, skewness, and excess kurtosis (*B77*). Four statistical methods which account for error in both the x and y variables in linear regression were evaluated by MacTaggart and Farwell (*B78*). The H-point standard addition method, a technique for eliminating the blank bias error, was evaluated using ANOVA and the Bartlett statistic in a spectrophotometric application (*B79*). A bootstrap method was also employed to determine the reliability of calculated imprecision profiles in immunoassays (*B80*). In an environmental application, Ramsey et al. described the merits of robust ANOVA over classical ANOVA in the presence of outliers for geochemical surveys (*B81*, *B82*).

Confidence intervals for analytical determinations were also obtained by statistical means. Krouwer and Schlain described a method for calculating a least squares estimate and a corresponding confidence interval for the extent of deviation from assay linearity (*B83*). Another method was presented by Alvord and Rossio for determining confidence intervals for dose potency estimates obtained from various nonlinear dose–response models (*B84*). An existing procedure was modified to account for the uncertainty in predictions of hazardous concentrations of toxic substances and to derive one-sided 95% and 50% confidence limits (*B85*). In a discussion on linear regression, MacTaggart and Farwell explained the influences of various assumptions on calibration and described several approaches to calculating confidence intervals (*B86*). Phatak and co-workers developed a technique for obtaining approximate confidence intervals for partial least squares estimates on the basis of a linearized PLS estimator (*B87*). Confidence intervals were also calculated using a Monte Carlo method and their uncertainties were determined by a nonparametric regression technique. The approach was considered best suited to nonlinear regression problems not easily solved by conventional means (*B88*). In another study, confidence intervals obtained from a bias-corrected bootstrap method were compared with those calculated with various parametric methods for accuracy and precision (*B89*).

Several other papers concerning statistical analysis were published in the chemistry literature. For instance, a procedure for fitting electron energy loss spectra using unweighted least squares on the log–log transformed data was described. The residual variance of the fit instead of the χ^2 test was suggested as a means of determining the optimum width of the fitting window (*B90*). Bielsa and Meira investigated the propagation of error in the correction of the combined distributions of molecular weights and chemical composition of copolymers for instrumental broadening in size exclusion chromatography (*B91*). Using microbial toxicity measurements, concentration–response curves were generated by nonlinear regression of the raw data and by weighted linear regression of the linearly transformed data (*B92*). Based on a modified normal function for modeling asymmetry in chromatographic peaks, equations were also formulated for calculating various chromatographic figures of merit (*B93*). Hotelling's T2 test, canonical correlation analysis, and PCA were used to compare estimates of Hilditch's theory and LC determinations of triacylglycerols in olive oil (*B94*, *B95*). The interaction of components in a mixture could lead to nonadditivity in spectra. Khots and co-workers investigated this phenomenon using simplex–lattice designs (*B96*). An interesting study was also reported on the influence of chance effects on the cross-validation of partial least squares regression models (*B97*). Finally, Mandel argued that all models should be validated prior to their application to data. He presented a graphical procedure for achieving such validation (*B98*).

OPTIMIZATION

The optimization of chemical systems using mathematical methods has become widespread in the chemical sciences. Hundreds of research efforts published in the most recent reporting period utilized some sort of mathematical optimization, but most of these involved only straightforward application of well-known methods. Due to space constraints, however, only relatively new methods and applications are included in this section.

A number of reviews on some of the more popular optimization methods were given. One paper discussed statistical modeling and experimental design strategies in the pharmaceutical industry (*C1*). Two general reviews pertaining to the use of information theory in analytical chemistry were published (*C2*, *C3*), while another review focused on the use of information theory in the optimization of chromatographic systems (*C4*). The simplex optimization method was by far the most popular multiparameter optimization technique cited in the chemical literature. Those looking for an introduction to the simplex method will want to examine the review by Reh (*C5*). Simulated annealing optimization, including a variable step size modification, was discussed in a tutorial (*C6*). Multicriteria optimization by genetic algorithms represents a new area in the field of chemometrics. Those interested in this rapidly growing research area are referred to two tutorials on the use of genetic programming in analytical chemistry (*C7*, *C8*).

The early, widespread use of simplex optimization in chemistry can be explained by its simplicity and its relatively modest demands on the computer as compared to many other nonlinear optimization methods. Even though modern day desktop computers offer substantially more power than earlier machines, the simplex continues to be very popular among chemists. Modifications and developments of the simplex algorithm also continue to be well represented in chemical optimization research. In one paper, the convergence properties of several different modifications of the simplex method were examined (*C9*). A modified and weighted centroid simplex method (CMWCS) was presented and employed in the optimization of the heating program parameters in graphite furnace atomic absorption spectroscopy (*C10*). A weighted, variable step size simplex method was used to optimize buffer pH, sodium dodecyl sulfate concentration, and percentage of organic solvent in micellar electrokinetic chromatography (*C11*). Brumby studied the effect of different quadratic convergence criteria on the computer time required to optimize some benchmark problems with the simplex method (*C12*). A new application of the simplex method involved the detection and following of a discontinuity (*C13*).

A number of other optimization techniques are known to have better convergence characteristics than the simplex method on complex or high-dimensional error surfaces. Several researchers have compared the simplex with some of these optimization methods during the most recent reporting period. For example, Monte Carlo optimization was compared with the simplex method in the fitting of physiological toxicokinetic models (*C14*). The application of the simplex method resulted in better fits to the toxicokinetic model, but results obtained from the Monte Carlo method contained a smaller measurement of uncertainty. Simplex and steepest ascent methods were compared in the optimization of flow injection reactor conditions used in postcolumn detection chromatography (*C15*). The quality of the solutions obtained from the two optimization methods was very similar. In another study, the simplex method was compared with the conjugate direction set method of Powell in the optimization of the flow injection analysis for nitrite in water (*C16*). In a new application, the steepest ascent method was applied to the optimization of the separation of enantiomers on a chiral stationary phase in open tubular column supercritical fluid chromatography (*C17*). Error-compensated kinetic determinations of mixed first- and second-order reaction systems were accomplished with a Levenberg–Marquardt-based nonlinear optimization scheme (*C18*). The method was demonstrated on simulated data with various amounts of additive noise. Multiple parameters in micellar liquid chromatography were optimized using an optimization strategy based on an extension of iterative regression (*C19*). Amino acid and peptide separations were achieved by optimizing pH, concentration of surfactant, and 2-propanol solvent. An optimization procedure for the simulation of proton elastic recoil spectra induced by low-energy helium ions was reported (*C20*). The optimization was conducted according to Poisson, maximum likelihood, or χ^2 statistics, according to the authors. The signal-to-noise ratio for an electrothermal atomizer was optimized using Monte Carlo simulations (*C21*). The optimization was conducted with a two-dimensional grid design in length and diameter of the electrothermal atomizer. Simulated annealing was used to optimize the gradient-coil design in a NMR spectrometer (*C22*) and in multicomponent calibration designs (*C23*). Window diagram and overlapping resolution maps were the most popular techniques utilized by researchers in the optimization of chromatographic systems. A comparison of these two methods was conducted in the optimization of planar chromatographic experiments (*C24*). The overlapping resolution map method was reported to be more robust with respect to variations between the development distance, spot diameter, and average plate height. The overlapping resolution map was also used to optimize the separation of porphyrins by micellar electrokinetic chromatography (*C25*), the HPLC separation of nitroaromatics (*C26*), and the gradient HPLC separation of selected phthalates (*C27*). The window diagram technique was also used to optimize gas chromatographic (*C28*), and capillary zone electrophoretic experiments (*C29*). A three-part optimization method called PRISMA was used to optimize HPLC mobile-phase composition that included up to four solvents (*C30*). A graphical method was used to predict the combined effect of mobile-phase variables on resolution, peak height, and retention time in ion chromatography (*C31*).

A significant number of studies involving information theory in the optimization of analytical experiments were reported during the last two years. A tutorial on the application of information theory to the optimization of neutron activation analysis of trace constituents in certified reference materials was published (*C32*). It was demonstrated that the information could be used as an evaluation criterion as well as an objective function in the optimization process. A gas chromatographic screening method for the determination of chemical warfare agents, precursors, and degradation products was optimized by considering the information power in the chromatographic distribution profiles of sequentially connected columns (*C33*). In an experiment that coupled information theory with nonlinear optimization, the function of mutual information was used as an objective function in the simplex optimization of the mobile-phase composition in liquid chromatographic analysis (*C34*). A discussion on the use of the function of mutual information as an evaluation criterion in the optimization of multielemental atomic spectroscopy was the subject of a paper by Matherny and Eckslager (*C35*). Simulations were used to evaluate the effect of different analytical performance parameters on the effectiveness of the method. In a more general discussion, it was argued that the spatial resolving power of the information theory approach should exceed that attainable by integral analysis (*C36*). The mutual information and information throughput were maximized in an optimization of micellar electrokinetic chromatography (*C37*). The variables that were optimized included micelle concentration, applied voltage, and temperature. Other applications of information theory that were reported during the last two years included optical resolution of enantiomeric amino acids (*C38*) and the analysis of natural products (*C39*).

Statistical experimental design has become one of the most widely used optimization tools in the chemical literature during the past two years. More than 60 applications of experimental designs were cited. The references listed here involve only new designs or applications. A factorial design was used to establish optimal sequences for data pretreatment in near-infrared spectroscopy calibrations (*C40*). The pointwise resolutive significance of each design point with regard to a number of parameters was discussed (*C41*). The sum of all the pointwise resolutive significance was proposed as a measure of the overall resolution of the data set, and simulations were used to validate the conclusions. A factorial design was also used to study the effects of flow rate, injection volume, and coil length on the experimental fluctuations of flow injection signals (*C42*). An analysis of the fluctuations revealed that interaction between the parameters studied was always significant. Several efforts addressed the use of experimental designs that used process and mixture variables in combination. A two-part study was conducted that gave first a theoretical evaluation of the process and mixed-variable model (*C43*), followed by an application using pharmaceutical data (*C44*). Designs for mixture and process variables were also applied to the problem of pharmaceutical tablet formulations (*C45*). The optimization of TLC separations of alkaloids was approached with a mixture design and response surface modeling (*C46*). The number of mobile-phase solvents used for the separation was reduced from eight, recommended by the European Pharmacopoeia, to four without a loss in resolution. It is often desirable to conduct experimental designs with a minimum number of examples. Wegsheider and Walner used a partial least squares model to study the sparse effects of sparse mixed-variable mixture models (*C47*). The effectiveness of Doehlert designs was explored in the chromatographic separation of chlorophenols (*C48*), the use of microemulsions as drug carriers (*C49*), and the interpretation of atomization interferences in electrothermal atomic absorption spectroscopy (*C50*, *C51*). Several Plackett–Burman designs were examined for the optimization or ruggedness testing of analytical procedures (*C52*). The authors demonstrated that erroneous conclusions may result in the case of an improperly balanced three-level design. Taguchi experimental designs were used in the optimization of the chromatographic separation of 25 solvents commonly found in bulk pharmaceuticals (*C53*).

Optimization methods are sometimes used in conjunction with an experimental design strategy. The initial experimental design step can often improve the chances for a good solution by providing more information about the response surface. A coupled strategy based on experimental design and simplex optimization was used to optimize the supercritical fluid extraction of PAHs and organochlorine pesticide compounds from the environmental samples using a liquid–solid extraction cartridge (*C54*). Pijnappel compared variable projection and Gauss–Newton optimizations in an experimental design–optimization strategy that was designed to quantify model parameters from one- and two-dimensional NMR (*C55*) while Cladera et al. used an experimentally designed data set to compare Gauss–Newton and simplex optimization methods in a study of the simultaneous kinetic analysis of catalysts and activators (*C56*). The reversed-phase ion interaction liquid chromatographic separation of nitrite, nitrate, and phenylenediamine isomers was optimized with an experimental design followed by partial least squares regression (*C57*).

The use of genetic algorithms in chemical research represents the fastest growing research area concerned with the optimization of chemical systems during the reporting period. Genetic algorithms are used to perform an evolutionary search of the optimization space defined by the chemical system of interest. The property most promoted of the genetic class of optimization techniques in the literature is their ability to avoid trapping in local minima on the optimization error surface. Optimization surfaces that contain multiple local minima can trap gradient-based optimization methods in undesirable solutions. The genetic algorithm avoids this difficulty by the development of multiple evolutionary searches in parallel. The optimized parameters are chosen from the search with the minimum error solution. The cost of parallel evolutionary searches can be substantial in terms of execution time and computer memory requirements, particularly when many variables are to be optimized, however. Wienke et al. have compared the performance of simplex, steepest ascent, overlapping resolution map, pattern search, and simulated annealing with a genetic algorithm in the optimization of spectroscopic excitation conditions for the simultaneous analysis of six trace elements in atomic emission spectroscopy (*C58*). A second comparison of the same methods involved the optimization of six properties of a biochemical test strip for human blood glucose determination as a function of 12 chemical and technological parameters (*C59*). In this study, a substantial advantage of the genetic algorithm method as compared to other optimization approaches was reported. Optimal selection of wavelengths in multicomponent analysis was performed by genetic algorithm (*C60*), and the selection of an optimal calibration set was reported using a dynamic version of a genetic algorithm (*C61*). Genetic algorithms have also been applied to other optimizations involving spectral curve fitting (*C62*) and the assignment of 2-D NMR spectra of proteins (*C63*). The optimization of biological media by a genetic algorithm was also reported (*C64*). In this study of benzoate degradation by *Pseudomonas pudita*, optimization with the genetic algorithm allowed for an 80-fold increase in the biomass concentration and a 3-fold increase in the biomass yield coefficient. Genetic algorithms have also been applied to the determination of chemical structures. An atom-to-atom mapping was conducted by optimizing the minimum chemical distance parameter (*C65*), and feasible isomeric structures were determined from the molecular formula (*C66*). In another study, a genetic algorithm was used to infer hypothetical physical structures that corresponded to physical properties exhibited by poly(ethylene terephthalate) yarns (*C67*). The genetic algorithm used a validated neural network model that was developed from a structure–property mapping of yarn exemplars. A novel hybrid scheme that utilized a genetic algorithm in the determination of kinetic rate coefficients in the hydrolysis of adenosine 5′-triphosphate was also reported (*C68*). Of several approaches examined, including hybrid and pure genetic methods, the most rapid convergence resulted when the genetic algorithm was used to select initial starting point for a quasi-Newton optimizer.

SIGNAL PROCESSING

Signal processing techniques are defined here as data transformations that improve the accessibility of physically significant information in analytical signals. A large number of papers that include digital filtering, smoothing, deconvolution, and transformation of data into alternate domains were in evidence during this reporting period, partly due to the wide availability of software packages that contain these signal processing routines. In order to meet practical space limitations, references in this section were restricted to research efforts that featured signal processing techniques in a major role. A number of articles that reviewed signal processing techniques were published over the past two years. A review of Fourier methods was given (*D1*), as well as a more specific review of Fourier smoothing and filtering of α-particle spectra (*D2*). Two reviews on Hadamard transform IR spectrometry were given during the reporting period. The scope of the discussions included basic concepts and more recent advances in stationary encoding masks and appropriate spectrum recovery techniques that make Hadamard transform spectrometry more attractive (*D3*, *D4*). Applications of matched filtering and correlation techniques in (Multiplex) chromatography were reviewed with a focus on applications in environmental chemistry (*D5*). Two reviews appeared on the use of signal processing techniques in Raman spectroscopy. In the first review, autocorrelation functions, Fourier power spectra, signal intensity distributions, and correlation between Raman and elastic scattering were covered (*D6*). The second review addressed the determination of line frequency shifts in Raman difference spectroscopy, the study of line width changes by Raman difference spectroscopy (RDS), and described experimental techniques and applications (*D7*).

The smoothing of analytical data has become common practice in many chemical laboratories. Many instrumental software packages provide smoothing options for the analytical chemist. A limited number of research efforts that focused on the details of smoothing are covered in this review. Least squares polynomial smoothing of inductively coupled plasma atomic emission spectra was discussed with respect to point insertion into spectral scanning intervals and the minimization of spectral distortions (*D8*). A new, computationally efficient method for estimating the background in electron energy loss spectra was given (*D9*). The new least squares method was reported to be more robust and efficient than the traditional method of calculating a least squares fit of a power law model. A novel method for enhancing detection limits in flow injection analysis was reported by Bos and Hoogendam (*D10*). The authors reported that under conditions of white noise and favorable peak shapes, a wavelet transform of the spectral data allowed the detection of analytes below the conventional statistical detection limit. In another smoothing paper, a general framework for the representation of spectra by continuous functions was given by Alsberg (*D11*). Two ways of dealing with objects in function space were investigated: operation on functions only and operation on functional coefficients only.

A substantial number of authors reported the use of digital filtering methods in the analysis of analytical data. Hyde et al. presented a novel filtering technique for the resolution enhancement of magnetic resonance spectra that uses computer-simulated sinusoidal field modulation with phase-sensitive detection at selected fundamental or harmonic frequencies. The pseudomodulation method was applied to simulated data (*D12*), and strategies were given for use with EPR spectra (*D13*). Moore and Jorgenson reported a simple method of removing baseline drift in chromatographic data by use of a moving median digital filter (*D14*). The moving median filter removes impulse characteristics but preserves sudden changes such as baseline shifts and drifting. Two research efforts reported the use of matched filters in data treatment. The first paper reported on the robustness of the matched filter toward noise model errors in the quantification of chromatographic data (*D15*). In the second study involving matched filtering, signal model errors were minimized using a simplex optimization (*D16*). Infinite impulse response (IIR) and finite impulse response (FIR) filters were compared in flow injection simulations (*D17*) and in experimental applications (*D18*). It was reported that the low-pass Chebyshev type II filter was the most effective. A variable digital filter was used to obtain well-resolved solid-state electronic spectra of Cr(III) complexes (*D19*). The resolved spectra allowed for interpretations in terms of tetragonal distortions in the coordination sphere of the Cr(III) ion. Tunable parameters of the SR250 boxcar integrator–averager system were optimized for the analysis of excited-state lifetime decay waveforms produced from a pulsed-laser luminescence spectrometer (*D20*). Harada and Tanuma compared top-hat, first-derivative and second-derivative digital filters in subtracting the background of overlapped low-energy Auger spectra (*D21*). The authors reported that the top-hat filtered spectra gave the best separation of the Cu and Au analytes. In another study involving the filtering of Auger spectra, the suppression of noise in scanning Auger images was addressed with several different digital filters (*D22*). Strategies for coupling Gaussian-shaped bandpass digital filtering with partial least squares regression were reported and applied to the determination of glucose in plasma by Fourier transform near-infrared spectroscopy (*D23*). Piyakis and Sacher used Savitsky–Golay filtering and an automated optimal Wiener filter in the removal of noise from the spectra of different surface analysis instruments (*D24*). An exchange of comments pertaining to the conclusions reported in this paper concerned a disagreement about the relative merits of the two filtering methods. Seah and Cumpson maintained that the optimal Wiener filter was the faster algorithm but that the application of the Savitsky–Golay method was more transparent (*D25*). The authors of the original paper responded that the application of the automated version of the Wiener filter was actually more straightforward (*D26*). Janssens and Francois proposed the use of two consecutive applications of zero-area Gaussian filters for the resolution enhancement of complex spectra (*D27*). The use of consecutive filters of this type was demonstrated to produce significant improvements in the resolution of atomic emission, NMR, IR, and UV–visible spectra.

Time series analysis is often performed using digital filtering methods. Simulations were used to show that a two-phase approach using nonlinear state-space models performs more effectively than the previously favored linear approach in the adaptive on-line control of bioreactor processes (*D28*). Doerffel et al. proposed the cumulative sum, CUMSUM, as an indicator of tendencies in time series analysis (*D29*). The theoretical background on the interpretation of the CUMSUM shape was given and several applications of the method were demonstrated. Other studies involving time series methods included the analysis of scanned data (*D30*) and the evaluation of noisy data in distribution analysis (*D31*).

Researchers continue to find Kalman filtering a useful technique in the signal processing of analytical data. Xie et al. presented a robust version of the Kalman filter that was designed to be insensitive to outliers (*D32*). A limiting transformation on the innovation term was used to make the filter more robust. Information theory was used to predict the precision and evaluate the accuracy of an adaptive version of the Kalman filter in the mathematical separation of overlapped target and interferent peaks (*D33*). In this study using simulated data, the precision and accuracy of the filter were predicted with the function of mutual information and a single spectrum. The reliability of Kalman filtering in the correction of wavelength positioning errors in inductively coupled plasma atomic emission spectroscopy was examined with two different evaluation criteria: (1) the NAC criteria that is based on the autocorrelation analysis of the innovation sequence; (2) the innovations number, which is the autocorrelation coefficient of the innovation sequence, at the initial wavelength. It was determined that the application of both criteria was necessary for the modeling of continuous backgrounds and for obtaining estimates of the reliability of the analytical result (*D34*). The Kalman filter was used for background correction by three researchers. In the first study, the filter was used in conjunction with a lock-in amplifier for background suppression of argon spectral lines in glow discharge atomic emission experiments (*D35*). It was reported that the background suppression of argon lines by Kalman filtering improved the detection limit by 1 order of magnitude. In a third study, the determination of trace elements in uranium was enhanced by the Kalman filter correction of substantial background interferences (*D36*). A two-part study employed the Kalman filter as a noise reduction tool. In the first part, the improvement in calibration accuracy using simulated transient signals was addressed (*D37*), while the second part of the study examined the application to atomic absorption spectrometry with hydride generation (*D38*).

Several researchers reported on the use of Fourier transform methods in the signal processing of analytical data. A new recursive method for computing fast Fourier transforms was presented by Wu and Chin (*D39*). The algorithm uses a three-stage, correlation-based approach. Fourier convolution was used to calculate the Hilbert transform, which relates components of immittance (*D40*). A nonlinear transformation of the immittance data was used to convert the data into a usable form. Fourier convolution of the raw immittance data is not possible because immittance data are not equispaced on a linear scale. Three studies involved investigations of apodization functions used in Fourier smoothing or filtering. Larivee and Brown used a maximum entropy criterion for finding near-optimal apodization functions that enhance signal-to-noise ratios in noisy data environments (*D41*). The method, which required no *a* priori knowledge of the signal shape, performed as well as an optimal filter that used the true signal shape. Appropriate apodization functions for NMR data were determined interactively using a constrained least squares technique with free induction decay measurements and the signal-to-noise ratio (*D42*). Peak broadening and baseline instabilities in ion mobility spectra were corrected with Fourier filtering (*D43*). Hanning, Hamming, super-Gaussian, and rectangular apodization functions were applied to the ion mobility spectra. Fourier filtering techniques have also been used to enhance signal-to-noise ratios in Rutherford backscattering spectra (*D44*) and Fourier transform hydrodynamic modulation voltammetry (*D45*). Filtering was used to improve the resolution of electronic spectra (*D46*). A time domain filtering technique that used a narrow stop band in the frequency domain was used to suppress the solvent signal in NMR experiments (*D47*). In another filtering study, time domain and frequency domain filters were compared in the determination of glucose in aqueous samples by FT-IR detection flow injection analysis (*D48*). It was reported that superior results could be obtained with frequency domain filtering by using the enzymatic degradation of glucose for its measurement. Subtraction of background fluorescence in twin-beam, time-resolved microfluorometry studies of biological samples was accomplished by subtracting the background reference in the time domain before transforming the signal into the frequency domain for analysis of lifetime and decay measurements (*D49*). Two research efforts used Fourier transform methods in investigations of the failure analysis of materials. In the first study, a numerical Laplace transform and inversion using the fast Fourier transform was used in the stress analysis of samples subjected to impact testing (*D50*). In a second study, Fourier transform methods were used to investigate the relation of geometrical features on fatigue fracture surfaces to microstructure (*D51*). Two studies involved the examination of chromatographic experiments with Fourier analysis. The recognition of chromatographic retention patterns was accomplished by fitting the experimental autocovariance function to theoretical models (*D52*). In a second study, Fourier analysis was used to quantitatively estimate both the separation performance and the retention pattern under programmed elution conditions (*D53*).

A limited number of studies on Hadamard transform methods appeared over the last two years. Fateley et al. reported the use of a two-dimensional encoding mask for the imaging of thin-layer chromatography plates by laser-induced fluorescence or surface-enhanced Raman scattering (*D54*). The authors also examined three-dimensional imaging using the two-dimensional encoding mask with the depth profiling capabilities of photoacoustic detection. A novel imaging technique was described that combines tomography, Hadamard signal encoding, and a patented FT-IR emission–transmission method for spatially resolving chemical species in a sooting flame from their infrared spectra (*D55*). Harms et al. reported a new, more efficient method for spectrum recovery by fast Hadamard transform (*D56*). The new method allows a permutation scheme to be applied to any Hadamard or simplex matrix in the appropriate equivalent class. A computer code was developed that facilitates exhaustive generation of Skew–Hadamard matrices by using elegant bit-manipulation techniques for matrix multiplication (*D57*). The bit-manipulation-based codes required 124 h of CPU time on an IBM RS6000/560 to generate all combinatorial possibilities of Skew–Hadamard matrices of order 100 × 100.

As has been true for previous reviews, the deconvolution of analytical signals represented a significant portion of signal processing research during the latest reporting period. An improved method for deconvolving atmospheric absorption spectra using Newton's iterative method and line shape theory was reported by Xu and Wang (*D58*). Several researchers reported on the use of deconvolution methods in chemical imaging. Spatial resolution in photoresist materials was reported by deconvolution of ESR spectra (*D59*). ESR imaging reportedly revealed that UV light was absorbed at the surface. Deconvolution techniques were also applied to secondary ion mass spectrometric (SIMS) image analysis data with a goal of improving detection limits (*D60*). In two other SIMS studies, the deconvolution of depth profiles using a model depth resolution function (*D61*) and a comparison of inversion techniques using measured response functions and indirect techniques were investigated (*D62*). The enhancement of resolution by deconvolution methods was reported by several researchers. The degree of crystallinity in cellulose was determined by deconvolution of unresolved infrared OH bands (*D63*), while in another study the simplification of one- and two-dimensional NMR multiplets using several successive deconvolutions was reported (*D64*). A modified Wiener filter algorithm was used to improve the resolution of electron energy loss spectra to 0.1 eV (*D65*). Fourier self-deconvolution was used to study the structure of arrestin from bovine photoreceptors (*D66*). The resolution of secondary structure–sensitive overlapped amide I bands allowed for a quantitative determination of the number of α-helices, extended strands, turns, and bends in the arrestin structure. The resolution of line-overlapping broadened Moessbauer, EPR, and thermoluminescence spectra was examined with deconvolution (*D67*). The deconvolved spectra reportedly improved the quality of information available for characterization. Two papers reported the application of deconvolution methods to the resolution of overlapped voltammograms (*D68, D69*). A time-dependent, Fourier transform deconvolution of Raman spectra between 950 and 1500 cm^{-1} was used to obtain estimates of crystallinity in polyethylene samples (*D70*). Circular dichroism spectra of β-turn conformers of pseudocyclic hexapeptides were resolved by deconvolution (*D71*). Circular dichroism, NOE, and X-ray crystallographic data were used in the resolution of the conformational spectra. The effect of an electrochemical concentration modulator injection device on the chromatographic signal was removed using time domain deconvolution (*D72*). An overview of different time domain deconvolution methods was given with emphasis on the shape of the virtual injection.

The use of maximum entropy methods in the analysis of analytical signals continued to increase during the latest reporting period. The suppression of artifacts in the phase-modulated, rotating frame NMR imaging experiment was reported using the maximum entropy method (*D73*). Artifacts in the Fourier transform spectra arising from off-resonance effects, imperfect pulse angles, and truncation were suppressed. Two studies involved comparison of maximum entropy and Fourier methods in the processing of analytical data. In the first study, the two methods were compared for phase refinement in crystal structure determinations (*D74*), while the second comparison study involved the deconvolution of two-dimensional NMR spectra of proteins (*D75*). The deconvolution of the instrumental response function in electron energy loss spectra using maximum entropy methods was the subject of two papers (*D76, D77*), while a factor of 3 improvement in resolution was realized in the maximum entropy deconvolution of neutron tunneling spectroscopic data (*D78*). Maximum entropy methods were also used to deconvolute two-dimensional (*D79*) and COSY (*D80*) NMR data. A software package that includes maximum entropy methods was designed for the recovery of signal from noisy data (*D81*). The routines are designed to recover signal in the presence of Gaussian, binomial, or Poisson noise. A direct method for the inversion of resonant Raman excitation profiles to the time domain by maximum entropy was proposed (*D82*). The method was considered along with another direct method that used a Fourier series expansion of the Raman dispersion relation. Several intrinsic characteristics of the line shape optimized maximum entropy linear prediction (LOMEP) procedure as a line-narrowing method was discussed (*D83*). The method was demonstrated on gas-phase IR and NMR spectra. A maximum entropy fit of fluorescence intensity vs correlation time and fluorescence lifetime measurements was used to determine the physical homogeneity and state of aggregation of recombinant proteins (*D84*). Finally, Kauppinen and Saario presented their arguments against the use of maximum entropy methods in spectral recovery (*D85*).

A number of other signal processing studies were reported during the last two years. B-Splines were proposed for the compression of very large data arrays (*D86*). The mathematical relationship between the maximum entropy method for the compression of data tables and the B-spline of zeroth degree was described together with the generalization of B-spline compression of data tables and *n*th-order data array tables in matrix and tensor algebra. A conditional-access algorithm was used to determine elemental specificity in the dual-channel flame photometric detection of gas chromatographic peaks (*D87*). The method reportedly yields infinitely selective chromatograms for any chosen flame photometric detection element. The multiple signal classification method or MUSIC was compared with the Fourier transform method for spectral estimation of three simple model systems (*D88*). The method was very accurate in determining line position, but the estimates of the line amplitudes were rough. A novel, multiplex method for sampling and frequency analyzing a signal consisting of a sum of exponentially damped sinusoids of different frequency was presented (*D89*). The bipolar method of sampling used here achieves the multiplex advantage of Fourier transform analysis for time-of-flight mass spectrometers. Geladi offered a tutorial on multivariate imaging that addressed grey level operations and the general properties of images (*D90*). A new method for approximating the Kramers–Kronig transform with the finite Hilbert transform was reported (*D91*). The accuracy of transformed spectra using the BZ algorithm was the same as that obtained with the Kramers–Kronig transform. The advantages of spectral interference subtraction and extended multiplicative scatter correction in the pretreatment of near-infrared data were examined by Schonkopf et al. (*D92*). The application of these pretreatments led to a simplification of partial least squares regression models. Three principal component-based methods were used to process analytical data. In the first method, gain and offset stabilization of γ ray pulse height spectra was performed with a principal component-based target test (*D93*). In a second study, eigenstructure tracking analysis was used to identify the noise distribution and local rank in instrumental profiles (*D94*). In a demonstration of the method, the heteroscedasticity in the infrared absorbance spectra of a three-component mixture design was revealed. A two-way procedure for the background correction of chromatographic–spectroscopic data was reported by Liang et al. (*D95*). The method, a combination of a congruence analysis and a least squares fit of the zero-component regions, compared favorably with double centering without increasing the rank of the data. Haaland et al. introduced the use of classical least squares to improve the signal-to-noise ratios of the composite analyte spectra obtained from FT-IR detection chromatography (*D96*). The signal-to-noise ratios that resulted with the application of the classical least squares method were as good or better than those obtained with the more usual coaddition of spectra. A number of research efforts used some form of correlation analysis in signal processing. Cross-correlation of flow injection signals was performed by using two parallel flow lines (*D97*). The cross-correlation of the data followed by low-pass filtering resulted in 2 orders of magnitude improvement in the signal-to-noise ratio. A new method, single-sequence correlation chromatography, reportedly reduces the chromatographic detection limit (*D98*). Larger sample volumes are made possible without a loss in resolution by using a deconvolution procedure. Autocorrelation and cross-correlation techniques were used in laser microanalysis atomic emission spectrometry to detect periodicities in a line scan in the presence of noise (*D99*). Detection limits were improved in flow injection atomic absorption spectrometry by applying an ensemble summation procedure to repetitive flow injection signals (*D100*). A multiresolution algorithm that combined derivative methods with cross-correlation methods was presented as a means for signal-to-noise improvement in ion mobility spectrometry (*D101*).

RESOLUTION

Curve resolution can be achieved by a variety of techniques, from matrix manipulation methods to graphical means. One of the more interesting approaches involves the special situation in which two analytical methods are combined in hyphenated analytical techniques such as LC–UV. Here, the chromatographic peaks may be resolvable through analysis of the combined spectroscopic–chromatographic data matrix. Evolving factor analysis (EFA) has been proposed as one way to extract information on components measured by these techniques. New EFA applications and a few modifications have been reported by several research groups during the past two years. New applications of EFA have gone beyond LC–UV and included such widely diverse combinations as GC/MS (*E1*), fluorescence lifetime-resolved spectra (*E2*), pH gradients in FIA systems (*E3*), and spectra of components in an industrial process (*E4*). To balance these successes, it also should be noted that EFA was applied for the first time to an LC–UV data set in which the separation of two compounds was not achieved (*E5*). The EFA technique was reviewed by Keller and Massart (*E6*). Several research groups have reported modifications of the EFA technique to improve its performance. A fixed-size, moving window (FSMW) modification to EFA was introduced by Keller and Massart to take instrumental and experimental artifacts into account (*E7*), to correct for heteroscedastic noise (*E8*), and to correct for the nonlinear response of photodiode array UV detectors (*E9*). An algorithm for another modification of EFA was suggested by a Belgian group concerned with the efficiency of an automatic peak purity control procedure (*E10*). Window factor analysis (WFA) is a third modification, introduced by Malinowski (*E11*) and applied to FIA data. This approach was further applied to EDTA complexation (*E12*) and HPLC data (*E13*). Heuristic evolving latent projections (HELP) was proposed by Kvalheim and Liang as a new method to resolve 2-D data (*E14*). HELP was compared to EFA (*E15*), and both were found to perform equally well on the data sets studied. The HELP algorithm was also used in an LC–UV study involving drug isomers (*E16*) and chlorophyll degradation experiments (*E17*). Limitations of evolving principal component innovation analysis, another resolution technique similar to EFA and HELP, were discussed in a paper by Vanslyke and Wentzell (*E18*). Other principal component-based methods have also been reported to be useful in analysis of 2-D and 3-D data. Generalized rank annihilation factor analysis (GRAFA), iterative target transformation factor analysis (ITTFA), and residual bilinearization were all used on real LC–UV data in a comparative study (*E19*). ITTFA was compared to curve fitting and local curve fitting in an examination of methods for background correction (*E20*). The curve fitting methods gave the best results in these studies. The generalized rank annihilation method was modified with similarity transforms to avoid problems that arise with complex eigenvectors (*E21*). This approach was further advanced with a decomposition algorithm called the direct trilinear decomposition method (DTDM) (*E22*). One-dimensional chromatograms were resolved by combining several runs using simplex optimization of cross-correlation matrices and then applying HELP to the 2-D data (*E23*). Three-way arrays were resolved by a generalized eigenvalue approach, which was reported to be more effective than parallel factor analysis (PARAFAC) (*E24*). Overlapping resolution mapping (ORM), which had originally been developed for chromatography, was modified and applied to atomic emission spectroscopy (*E25*). ITTFA was applied to time-dependent direct-inlet mass spectrometry (*E26*). A comparison of the performance of several noniterative factor analysis algorithms on noisy and overlapped data was reported by Neal (*E27*). The results indicated that the conventions used to exclude some of the noise have a significant effect on the algorithm performance. A theory of overlap for 2-D separations was tested by computer simulation of 3-D concentration profiles (*E28*). Principal component analysis and self-modeling, along with nonlinear least squares fitting, was applied to 2-D fluorescence data (*E29*). Lastly, alternating regression (AR) was recommended as a non-factor-based analysis approach to the resolution of 2-D data sets (*E30*).

Progress has also been made in the application of PCA methods to one-dimensional curve resolution problems. A program called OBLIQUE was offered to assist in performing nonorthogonal rotations (*E31*). It was applied to gas chromatographic data. Principal components analysis of infrared microscopic data provided information on the number of spectrally different layers, which were subsequently resolved by a nonlinear optimization (*E32*). The effect of white noise on abstract factor analysis was studied using varimax rotated factor loadings to observe the effects on loading interpretations (*E33*). Self-modeling curve resolution techniques also continue to receive attention, mostly through new applications. PCA self-modeling was applied to fluorescence spectra, with an improved procedure to address more complex systems (*E34*). PCA, followed by self-modeling spectral resolution, was used for quantitative analysis of tetraphenylethylene photochemical reactions (*E35*). A photophysical constraint was introduced to justify the results of the self-modeling. The correction of overlapped spectral interferences in ICP-AES was accomplished by self-modeling curve resolution, and the effect of measurement errors on the results was investigated (*E36*). A tutorial on self-modeling techniques was offered by Windig (*E37*). A review of the SIMPLISMA method for interactive self-modeling mixture analysis, which uses a relatively simple algorithm rather than PCA and displays intermediate steps as spectra, was also published (*E38*). The SIMPLISMA method was also applied to second-derivative near-IR spectra (*E39*), IR microscopy (*E40*), and mass spectral data (*E41*).

Kalman filtering offers another approach to resolving peak overlap in analytical data. Several studies and applications of recursive filtering have appeared during this review period. Two new methods, fading Kalman filtering (FKF) and networked Kalman filtering (NKF), were introduced (*E42*). Kalman filtering was applied after an optimized alignment by simulated annealing to the quantitative analysis of ESCA spectra (*E43*). A combination of steepest descent minimization and Kalman filtering was applied to HPLC peaks (*E44*). The precision and accuracy of results from an adaptive Kalman filter used with Gaussian peaks were modeled (*E45*). A comparative study was done with Kalman filtering, synchronous excitation, and numerical derivative techniques in fluorometry (*E46*). Synchronous excitation can be combined with Kalman filtering to improve results. Kalman filtering applications have included simultaneous kinetic determination of phenols by visible spectroscopy (*E47*), the quantification of pyrazines by polarography (*E48*), and the separation of the signals which results from multiinjection chromatography (*E49*).

Fourier self-deconvolution techniques and curve fitting in Fourier space are still receiving some attention. Several advantages for curve fitting in Fourier space, for example, were reported in a review relating to Moessbauer spectroscopy (*E50*). A method which was based on Fourier deconvolution was presented for EPR peaks (*E51*). A program called Asymgrad was written to perform deconvolution of multiple peaks in a narrow spectral range (*E52*). Applications of Fourier self-deconvolution included the resolution enhancement of polarographic adsorption peaks (*E53*), cyclic voltammetry (*E54*), and infrared spectra of rhodopsin in disk membranes (*E55*).

Maximum likelihood and/or maximum entropy methods have also been applied to resolution problems, often in conjunction with other techniques. Maximum likelihood factor analysis (MLCFA) was used to resolve EPR powder spectra (*E56*) and Auger depth profiles (*E57*). In the latter study, the combined technique was found to be superior to ordinary PCA. A maximum likelihood method involving symmetrized spectral resolution yielded improved noise suppression and marked resolution enhancement for 2-D NMR spectra (*E58*). Maximum likelihood and maximum entropy estimation were jointly applied in a neutron spectroscopy experiment (*E59*). The study also involved spectral unfolding, using information theory as a base. Software using maximum entropy was developed and applied to electrospray mass spectra of protein mixtures (*E60*). The program automatically produces zero-charge mass spectra, along with a probabilistic quantification. Another novel, entropy-based algorithm for extracting parent masses was presented for electrospray spectra (*E61*). The nonlinearity of the maximum entropy method was investigated (*E62*). Additional maximum entropy-based resolution applications were reported for the study of depth profiles from XPS (*E63*) and SIMS (*E64*). A method called expectation maximization was also employed in conjunction with regularized least squares to resolve single-exponential kernels from kinetic data (*E65*). The regularized least squares analysis was performed by ridge regression using generalized cross-validation to optimize the regularization parameter.

Several recent papers described methods based on statistical or neural network-based approaches to curve resolution. A comparison between Bayesian and maximum likelihood peak fitting techniques showed that the former was very effective in reducing peak intensity uncertainties (*E66*). Bayesian probability was also applied to the estimation of true line shapes, even from strongly overlapped or broadened peaks (*E67*). A method employing apparent content curves was proposed to resolve analytes' spectral peaks from those of unknown interferents (*E68*). A cerebellar model arithmetic computer neural network was reported for the resolution of chromatographic peaks (*E69*). An artificial neural network was also applied to pyrolysis mass spectra (*E70*). Fuzzy linear programming formed the basis of a new method for resolving spectral peaks (*E71*).

Convergence issues for several iterative resolution algorithms were discussed in a general paper (*E72*). Also, a statistical theory for spot overlap for two-dimensional separations was expanded and applied (*E73*, *E74*).

CALIBRATION

Calibration refers to the process of relating a measured response to the amount of a chemical entity or property. Calibration techniques are of critical importance to most analytical work, and analytical chemists have explored statistical and mathematical methods to improve their results for many years. This review will focus on only the most recent approaches, including new types of regression, principal component-based methods, Kalman filtering, and artificial neural networks.

In addition to the many technique-related and application studies, reviews, comparative studies, and general papers have appeared recently. A global perspective on multivariate methods including **K**-matrix and **P**-matrix calibration, principal components regression, and partial least squares was offered by Lang and Kalivas (*F1*). Geometric theory and an understanding of projections were invoked. A comparison of linear prediction singular value decomposition (LPSVD) and total least squares (TLS) as applied to NMR data was made (*F2*). Gemperline wrote a tutorial on methods for detecting, studying, and modeling nonlinear spectral responses in multicomponent assays (*F3*). Included in the paper were tests for detecting nonlinear regions and suggestions for future study. Another review on nonlinear methods was contributed by University of Washington researchers (*F4*). PCR, PLS, locally weighted regression (LWR), projection pursuit regression (PPR), alternating conditional expectations (ACE), multivariate adaptive regression splines (MARS), and artificial neural networks (ANN) were applied to six data sets and results were compared. Weighted nonlinear PCR, PLS, and canonical correlation (CCA) in latent variables were compared with classical calibration by Wienke and Kateman (*F5*). Sekulic and Kowalski contributed a tutorial paper on MARS, complete with examples which explain the mechanics of the algorithm (*F6*). Multivariate calibration methods were examined with respect to a proposed classification of analytical mixture types (*F7*). Mark reviewed MLR and principal component-based methods and discussed the effects of errors (*F8*). The relationship between digital filtering and multivariate regression as applied to quantitative analysis was discussed by Erickson, Lysaght, and Callis (*F9*). Plotting aids to assist in characterizing multivariate calibration data were offered by Spiegelman (*F10*).

Standard additions, nonlinear regression, and multiple linear regression continue to have wide application, and some unusual approaches and analyses have been reported. Standard additions combined with MLR was used for the direct analysis of solid samples by electrothermal vaporization, inductively coupled, plasma atomic emission spectrometry (*F11*). In another hybrid approach, standard additions to correct for matrix affects and constrained background bilinearization were combined along with generalized simulated annealing to measure analytes in bilinear fluorescence data (*F12*). A nonlinear addition technique and linear stepwise discriminant analysis were used to determine strontium by atomic absorption spectrometry (*F13*). Nonlinear methods are also receiving more attention. Simplex optimization and nonlinear modeling of array characteristics were applied to the measurement of salts in blood plasma using array FIA data (*F14*). Ten biopharmaceutical chromatographic methods were used to compare univariate linear regression, weighted regression, and polynomial functions (*F15*). It was found that weighted linear regression provided the most appropriate calibration function for most of the methods. Iterative weighted regression was applied to toxicity tests (*F16*). A modified stepwise regression method, which used an information criterion instead of an *F* test for variable selection, was applied to multicomponent spectrophotometric analyses in which a known range of possible interferents coexisted (*F17*). Graph theory was proposed as a means of depicting and modeling the interferences and possible interactions in an MLR calibration (*F18*). The relationships among analyte, interferents, and instrument response were approximated by a polynomial of order 3, including cross-terms. Also, multiple linear regression has been suggested as a means of detecting and classifying interferences in clinical analyses (*F19*). Several other interesting MLR applications have been reported, including the measurement of heavy metal takeup by plants (*F20*), boron in steels (*F21*), nitrobenzene oxidation and pyrolysis products in pyrolysis GC/MS experiments (*F22*), and simultaneous determination of different catalysts during a kinetic run (*F23*). MLR was also applied to the analysis of near-IR spectra of smectite minerals, with the reflectance spectra being correlated to Al, Mg, Fe, and Si (*F24*). Wavelengths selected by MLR were spectroscopically explained.

A number of researchers explored both MLR and principal component-based techniques (PCR and PLS) and compared results. The approach with which these techniques were applied, however, may play a role in the conclusion. MLR, as it is used in near-infrared spectroscopy, involves optimization and pretreatments such as derivatives and scatter corrections which remove much of the collinearity in the data. Multiple terms and divisor terms usually improve the fit. If these tools are not employed or are not applicable to the problem, MLR may not appear to be as good at predicting as PCR or PLS. For example, several ordinary MLR methods such as **K**-matrix and P-matrix regression were compared to PCR and PLS to measure dye components in the visible region, and PLS gave the best results (*F25*). Also, the salinity of seawater was determined in the 680–1230-nm near-IR region by simple, selected wavelength regression and PLS, and again the PLS calibration produced a better predictive model (*F26*). For an array of four piezoelectric crystals measuring *o*- and *m*-cresol in water, PLS performed better than MLR because there was some collinearity (*F27*). In another study, PLS gave somewhat better results than stepwise MLR in the determination of ascorbic acid in pharmaceutical preparations, but only in the more complex samples (*F28*). Slightly better results for PLS were also obtained in a near-IR tobacco analysis investigation (*F29*), a visible absorption measurement of myoglobin oxygen saturation (*F30*), and a mid-IR on-line analysis of sugars in a fermentation process (*F31*). PLS was said to offer a more workable approach than MLR in the analysis of mixtures, due to the mixture constraint (*F32*). It was also claimed that PCR and PLS could take nonlinear effects into account better than MLR (*F33*). Other the other hand, several studies indicated that MLR and PLS results were equivalent for their sample sets, which included the determination of cadmium by inductively coupled plasma mass spectrometry (*F34*), the determination of aromatics and saturates in aviation fuel by near-IR (*F35*), the correction for interferences in hydride generation atomic absorption (*F36*), and the estimation of crude lipid content in trout by near-IR (*F37*). Although equivalent results were obtained, MLR with derivatives was judged better for the determination of pesticides in mixtures because it is simpler (*F38*). In another paper, a wavelength selection approach was chosen over a calibration using the full spectrum and the conclusion was made that the leave-one-out cross-validation approach to evaluating PLS equations may be overly optimistic in estimating error of prediction (*F39*). Lastly, a locally weighted regression gave the same prediction as PLS with fewer factors in a study involving the heat treatment of meat and near-IR spectroscopy (*F40*).

Several reviews, tutorials, and software papers concerning PLS calibrations have appeared recently. Bjoersvik and Martens reviewed the mechanics of developing a PLS method for multivariate calibration (*F41*). Naes and Isaksson discussed PCR methodology applied to food analysis by near-IR spectrometry (*F42*). Williams, Sobering, and Norris compared different PLS software packages (*F43*), finding some significant discrepancies in results. The potential of the latent variable concept was examined by Kvalheim (*F44*). Computer simulations were used to investigate PLS and modifications of PLS to compare how well they estimated the true regression coefficients in the presence of simulated light scattering effects (*F45*). Haaland compared four multivariate methods including multiple linear regression based on a classical least squares criterion (CLS), inverse least squares (ILS), PLS, and PCR, using Monte Carlo simulations (*F46*). Buco used artificially generated data to illustrate the shapes of PLS loadings (*F47*), and Cowe et al. compared the shapes of PLS1 and PCR loadings (*F48*). Martens and Foulk offered a paper on how and why PLS calibrations work in near-IR spectroscopy (*F49*). A procedure named GOLPE (generating optimal linear PLS estimations) was suggested to identify those variables which increase the predictive ability of PLS models (*F50*). Protocols were reported for coupling digital filtering techniques with PLS regression (*F51*). Programs named CENTER and SELECT were developed to establish population boundaries and choose samples for near-IR PLS calibrations (*F52*). A new, efficient PLS algorithm for large matrices was offered, complete with MATLAB code, by Lindgren, Geladi, and Wold (*F53*). Helland, Bernstsen, Borgen, and Martens presented an algorithm using recursive updating for PLS regressions (*F54*). Oman, Naes, and Zube described a PCR method employing a model which includes squares and products of principal component scores to adjust for nonlinearities in the calibration model (*F55*). Wakeling and Macfie offered a robust PLS algorithm, and they made the suggestion that the angle between loading vectors should be used as a measure of robustness (*F56*).

There have been many applications of PCR and PLS published in the last two years, and only selected examples will be included here. Derivative spectroscopy was combined with PLS in a visible spectral region analysis of several aldehyde reaction products (*F57*), and also for the determination of mixtures of flavor enhancers by UV–visible spectroscopy (*F58*). In the latter case, the derivative treatments did not prove to be an advantage. Several different preprocessing treatments, including derivatives and scatter correction, were examined as part of a study concerning an automated IR interpretation system (*F59*). In a UV-absorbing drug dissolution test, Fourier smoothing was applied before PLS to reduce background and noise (*F60*). Second derivatives and Fourier transformations were used for calibration for sample composition, thickness, and temperature using infrared emission spectroscopy of liquids (*F61*). Second-derivative spectra were also used in a polymer composition study involving attenuated total reflectance IR spectroscopy (*F62*). Target factor analysis, combined with PCA, was applied to differential-pulse anodic stripping voltammograms for the measurement of lead and cadmium (*F63*). PLS was employed to determine sulfur in an X-ray fluorescence method and was instrumental in explaining spectral artifacts (*F64*). The possibility of using more than one optical emission line for calibration in ICP-OES was explored with the help of PLS, and an improvement in sensitivity was noted (*F65*). A matrix of near-IR spectra of esters was used as a probe to explore the capabilities of PLS, especially with relation to the grouping of subsets of raw materials (*F66*). A variety of analytical disciplines have explored calibration with PCR or PLS during this reporting period. Examples include trace analysis by polarography (*F67*), an ultrasound pulse method for polymer blends (*F68*), and an analysis for osmium and ruthenium in ancient coins by neutron activation analysis (*F69*). The measurement of glucose in blood by either near- or mid-infrared spectroscopy and PLS regressions has received much attention recently (*F70–F73*). Several papers have addressed the use of PLS calibrations in flow injection analysis, including one which employed a Hadamard transform spectrometer (*F74*).

The use of Kalman filtering as a calibration technique appears to have diminished recently. Gauglitz, Mettler, and Weiss reviewed its application in multicomponent analysis by UV–visible spectroscopy (*F75*). An algorithm for a two-dimensional, real-time filter was offered, along with a discussion of parameter choices for a fluorescence analysis of polynuclear aromatics (*F76*). Some studies comparing Kalman filtering to other techniques were reported. A comparison to forgetting factor analysis in an application to the analysis of dosage forms was offered (*F77*). Also, in the prediction of priority pollutants, Kalman filtering proved to be superior to classical least squares fitting (*F78*), and in an ICP-AES study of 14 elements, Kalman filtering was marginally better than multivariate analysis (*F79*). A new approach involving a Fourier domain data set employed Kalman filtering to estimate concentrations (*F80*, *F81*). The boundary conditions of the analysis were set by calculating the condition number of the calibration matrix. An enzymatic method was reported, combining stopped-flow fluorescence and Kalman filter-based resolution of alcohol mixtures (*F82*).

Artificial neural networks (ANN) have been considered for calibrations by an increasing number of researchers. Bos, Bos, and van der Linden reviewed the current usage of artificial neural networks, with emphasis on aspects such as training methods and validation (*F83*). Blank and Brown provided a report on layered, feed-forward networks as applied to the analysis of nonlinear, multivariate spectral data (*F84*). A novel transfer function and a modified conjugate gradient algorithm which converges rapidly were proposed to improve training procedures (*F85*). Interestingly, most of the papers which appeared on calibrations with ANNs during this review period involved comparisons to other chemometric techniques. In one such study, three types of ANN were compared to stepwise linear regression, PCR, PLS, and modified PLS (*F86*). In most of the calibrations based on near-infrared analyses of agricultural products, the neural networks appeared to outperform the other methods. In a comparison with a classical model and a singular value decomposition–linear learning machine method, quantitative X-ray fluorescence data were better modeled by ANNs when wide ranges were considered (*F87*). Feed-forward ANNs were compared with nonlinear matrix regression, and a trade-off was observed (*F88*). It was found that the networks required a greater sampling frequency in order to constrain the flexible models. Glucose in whole blood measured by mid-IR spectroscopy was modeled by PLS, PCR, and ANN combinations (*F89*). The best standard error of prediction was achieved via a PLS–ANN combination. An MLR–ANN comparison for quantitative ICP atomic emission spectroscopy indicated a close relationship between the two procedures (*F90*). A consideration of three nonlinear methods (projection pursuit regression, MARS, and ANNs) vs linear PLS and PCR was reported by Seasholtz and Kowalski (*F91*). The linear methods require that fewer parameters be estimated and therefore may be more parsimonious. PLS and PCA scores were used to train neural network models for protein in meat analyses by near-IR (*F92*). The results indicated that this combined approach produced a 30% improvement over standard PLS. Other nonlinear systems were also calibrated using neural networks. These included Taguchi gas sensors for monitoring organic solvents (*F93*, *F94*) and near-IR instruments for measuring octane number (*F95*). Also, qualitative and semiquantitative analysis of elements by ICP-AES was performed with a simple neural network, the bidirectional associative memory (BAM) (*F96*).

Several additional novel calibration methods and modifications of older methods have been introduced during the past two years. Two new methods rely on isolating spectral regions in order to optimize calibration results. Isaksson and Naes suggested a segmented approach with a local, linear calibration to address nonlinearity in the calibration data (*F97*). The second method involved windowing to maximize the correlation between spectral data and composition (*F98*). A graphical method for studying interferences was also introduced in a PLS-like approach (*F99*). Bayesian methods were used by two research groups. An empirical Bayesian method for processing linear calibration data using a single calibration standard was introduced (*F100*). Also, a Bayesian method for developing calibration equations by combining several calibration sets was suggested (*F101*). Several unusual types of regression were reported. A modified ridge regression was introduced as part of a study involving the relationship between the number of terms in an equation and the size of the coefficients (*F102*). Ridge trace analysis and ridge regression were used to estimate the collinearity of a system (*F103*). A new approach to PLS regression, SIMPLS, was proposed by de Jong (*F104*). This algorithm calculates the PLS factors directly as linear combinations of the original variables in such a way as to maximize covariance. Nonlinear, robust regression methods based on the single-median and repeated-median methods were developed and adapted to calibrations in flame atomic absorption spectrometry (*F105*). A method based on simultaneous minimization of residuals, with increased weight on the x variable, was proposed (*F106*). Several methods relating to bilinear or trilinear data were also introduced or modified. A new constrained optimization method was presented for background linearization with 2-D data (*F107*). A review of recent advances in second-order calibration, in particular nonbilinear rank annihilation, by Wang, Borgen, and Kowalski also appeared (*F108*, *F109*). Gemperline and co-workers offered an introduction to three-way principal components analysis (*F110*). Smilde reviewed the theory, history, and applications of three-way chemometric methods, including unfolding, Tucker methods, and parallel factor analysis (PARAFAC) (*F111*). Three-dimensional PLS of fluorometry data was employed for the determination of several polynuclear aromatic compounds (*F112*). Some additional new techniques were introduced. External differential representation (EDR) is a mathematical technique used to model systems by making estimations based on partial data (*F113*). It involves rewriting the equations in terms of higher-order differential equations on the input and output variables. Procrustes rotation is a second approach which works with partial data (*F114*). Using only the experimental spectra, the DATAN algorithm calculated spectral profiles and concentrations of components by a Procrustes rotation performed on the scores of the PLS regression. A branch and bound algorithm was applied to the analysis of mixtures having a known range of possible components (*F115*). Optimized scaling was also introduced for closed data sets that occasionally occur in multivariate calibrations (*F116*). Linear local models calculated via multidimensional simplex interpolation were also employed as a calibration aid (*F117*).

Occasionally a calibration may be performed against a physical property rather than a constituent. In particular, full-spectrum methods such as PLS and PCR are useful for including all of the subtle spectral features contributed by different chemical species, all of which may relate to a physical property such as toughness of a polymer. For example, band shape changes due to hydrogen bonding may be related to physical properties. A number of properties of water, such as the velocity of sound, surface tension, and refractive index, were measured at various temperatures by near-IR spectroscopy with calibration by PLS and MLR (*F118*). Octane number and other gasoline properties have been measured by PLS and near-IR spectroscopy in the past. Recently, horizontal ATR/FT-IR (*F119*) and proton NMR (*F120*) have also been combined with multivariate techniques to predict octane number. Several aspects of the crystalline structure of proteins as measured by IR were calibrated against X-ray data, using PLS and PCR (*F121*). A study of the effects of particle size on diffuse reflectance mid-IR spectra was done using PLS to show differences in absorption intensities (*F122*). PLS was also used to explore the problem of sample heating in near-IR Raman spectrometry (*F123*). The PLS analysis measured the shift in a thermotropic phase transition.

Discussions of calibration strategies, means of measuring errors, and different types of weighting were the subject of several papers. An improved means of describing the interdependence of the parameters involved in a multivariate fit was offered (*F124*). A procedure for choosing the optimal set of principal components for a given calibration was given (*F125*). The Heisenberg principle was invoked to determine a balance between fit and variance in a predictor and to optimize the mean square error of prediction with respect to bias and prediction variance (*F126*). The effects of spectral resolution, dynamic range, and noise on multivariate calibrations was explored using hydrocarbon mixture data sets (*F127*). The relationship among closure, mean centering, and baseline offsets to the interpretation of matrix rank in calibration sets was discussed (*F128*). Also, the effect of mean centering on PLS predictions was examined, with the conclusion that it can sometimes lead to higher prediction errors (*F129*). Several different methods for examining errors were reported. O'Connell, Belanger, and Haaland reviewed calibration and assay development for an immunosorbent assay, applying several measures of performance (*F130*). These included minimum detectable concentration, reliable detection limit, limit of quantitation, and precision profile. A modification of a previously reported technique for the estimation of prediction error within the calibration range was offered (*F131*). This approach involves removing the uncalibrated portion of a sample and using the calibrated model to predict the remaining signal. The bootstrap method was used to approximate confidence intervals (*F132*). Near-IR calibration methods were discussed with respect to their tolerance to random errors (*F133*). Residual maximum likelihood was used to evaluate the accuracy of two near-IR methods relative to a referee method (*F134*). Selection of variables was the subject of two papers. Cross-validation, Procrustes rotation, and statistical variable selection were used to reduce a battery of 26 kerosene specification tests to 10 (*F135*). Ten different strategies involving different number of principal component, scatter correction, and local regression methods were applied to a large data set of forage samples (*F136*). A local calibration with 50 samples was suggested as optimal in this study. Wise and Ricker evaluated continuum regression (CR) for the identification of optimal finite impulse response models (*F137*). Location of a minimum in the CR response surface permitted selection of an optimal number of latent variables and an optimal form for the regression. Generally, models with regression characteristics between PCR and PLS were optimal.

Transferring calibrations between two instruments has elicited several papers recently. The need for transferring calibrations occurs primarily when the calibration developed on a laboratory instrument, such as a near-infrared spectrometer, is to be used on a second instrument in a process area. Biased models such as PLS are particularly difficult to transfer because every subtle aspect of the instrument's behavior may be included in the calibration model. There have been several different approaches proposed to solve this problem. One is to collect a subset of standard samples to be used to individually match each instrument to an original master instrument on which a full calibration was performed. One recent paper compares the suitability of five different standard materials sets for this purpose (*F138*). A modification of this approach, using two-dimensional responses measured on several instruments or on a single instrument under different conditions, was reported (*F139*). This method employs banded diagonal transformation matrices to simultaneously correct for response channel shift and intensity variations in both dimensions. PLS was employed in two additional approaches. In one of these, PLS equations were modified to incorporate a repeatability file containing spectra from different instruments at different temperatures (*F140*). In the second, a new PLS-based algorithm involved relating the *x* blocks (predictor physical variables) of two instruments (*F141*). Lastly, Wang and Kowalski reported a calibration-transfer method called piecewise direct standardization (PDS), which structures a transformation matrix based on the measurement of a small set of samples run on both instruments (*F142*).

Finally, the statistical basis for, and the relative performance of, what Frank and Friedman call several "chemometric" regression methods was the topic of a critical evaluation of PLS, PCR, ridge regression, and weighted regression for a largely statistical audience (*F143*). A number of statisticians have long harbored doubts about PLS, and the paper helps by putting PLS into perspective for them. The results of the study, and the manner in which it was conducted, brought a comment from Wold (*F144*). Hastie and Mallows also commented on the paper (*F145*). Frank and Friedman provided a response to these comments in a followup discussion (*F146*).

PARAMETER ESTIMATION

Parameter estimation, as reviewed in this section, includes methods which fit experimental data to mathematical models of general chemical properties. A distinction has been made between modeling of composition (calibration) and modeling of properties. The latter include, for example, kinetic parameters, ionization constants, and spectral band shapes. Some of the more popular modeling methods include linear and nonlinear regression, recursive filtering, and principal components-based techniques.

Several comparisons between modeling approaches appeared during the review period. Simulation and modeling methods for optimizing quality control practices were reviewed (*G1*). Maximum likelihood and least squares estimation were examined for estimating exponential decay parameters (*G2*). It was found that the maximum likelihood estimator for lifetime, but not rate, exhibited divergence in its variance, indicating that lifetime is the statistically preferred parameter for characterizing exponential decay for finite observation times. The process of model fitting using binomial regression and log–linear regression was discussed and illustrated by application to end point determinations of toxicity test data (*G3*). Principal components analysis and Kalman filtering were used as examples in a review of ways to examine chemical behavior (*G4*). Discrete Fourier transform and Bayesian analyses were compared as means of estimating the signal frequency and amplitude of NMR resonances (*G5*). Three different methods were used to study in vivo magnetic resonance spectral parameters: nonlinear maximum likelihood estimation (NMLE), linear prediction, and Fourier transformation (*G6*). A comparison between three-way PLS and parallel factor analysis (PARAFAC) for estimating HPLC retention values was made with attention to validation tools (*G7*).

Several computer programs were offered to assist researchers interested in parameter estimation. These included graphical evaluation of pK_a values (*G8*), mathematical determination of equilibrium constants (*G9*), and prediction of retention values in temperature programming of chromatographic columns (*G10*). A general equation to derive kinetic models by facilitating application of the Taylor series was reported (*G11*). Another group of programs involved some statistical approaches. One employing Bayesian probabilistic reasoning was used for the analysis of output curves from a DTA curve of a soil sample (*G12*). BASIC programs employing maximum likelihood and χ^2 approaches to the estimation of lethal dosages in bioassay applications were also published (*G13*). A new algorithm for computing spectral reconstructions based on the maximum entropy principle was described (*G14*). Other new algorithms involved matrix-based methods. A procedure employing continuous regularization was suggested as an improvement in the linear prediction singular value decomposition (LPSVD) algorithm for determining spectral parameters from time domain ESR or NMR spectra (*G15*). Two new approximation methods for weighted PCA as applied to parameter estimation problems were discussed (*G16*).

Some unusual approaches to parameter estimation have been published in the last two years. Simulated annealing has been applied to NMR (*G17*) and fluorescence data (*G18*). Artificial neural networks were used to predict NMR chemical shifts (*G19*) and for modeling an enzymatic glucose determination by FIA (*G20*). A combination of neural networks and principal components analysis characterized the effect of process parameters on the optical emission and mass spectra of etching plasmas (*G21*). Pade–Laplace analysis was proposed as a method for identifying the number of exponential components in a relaxation decay curve, but was found to be no better than nonlinear least squares regression at resolving three decays with similar time constants (*G22*). Weibull, logit, and probit models estimated the risk of carcinogenesis (*G23*). New iterative methods for the analysis of potentiometric titration data were presented (*G24*). Nonparametric variogram modeling, followed by kriging, was used to characterize the extent of regions of contamination at superfund sites (*G25*).

The Kalman filter and other recursive methods continue to play a role in modeling. An extended Kalman filter approach (*G26–G28*) and a parallel Kalman filter network (*G29*) have been applied to the extraction of parameters from multicomponent kinetic data. The temperature and spectral emissivity coefficients of plasma-sprayed particles were determined simultaneously with the aid of a Kalman filter (*G30*). Kalman filtering has also been used for background correction in ICP-AES (*G31*) and for the extraction of heterogeneous rate constants and transfer coefficients when coupled to a generalized simulation for step voltammetry (*G32*).

Principal components analysis and PLS have been extensively applied as aids in the understanding of chemical systems. Results from research on the techniques, as well as from a variety of their applications, have been reported over the past two years. An examination of the mathematical structures of PCR and PLS led to the development of a prognostic vector which contains information about the contribution of each feature in a sample spectrum to the quality of the sample (*G33*). New research into nonlinear PLS analysis was reported, invoking splined inner relations (*G34*) and quadratic and logistic link functions (*G35*). Many applications of principal components-based methods have also been reported during this review period. Several papers appeared that concerned estimation of chromatographic retention parameters (*G36–G39*). The effect of nonlinear response times of photodiode array detectors on principal components-based methods was studied (*G40*). An algorithm was provided to correct for this problem. Atomic emission spectra were combined with PCA-based methods to derive depth profiles of $TiN/Ti/SiO_2$ layers (*G41*). In this work, the authors tried to rotate factors to obtain physically meaningful spectra. Similar studies were reported with Auger sputtering (*G42*, *G43*). Some unusual applications appeared in the biomedical field. The degradation of pharmacologically active compounds was characterized with eigenvector projection (*G44*). An examination of metabolic control in brain aging studies employed PCA (*G45*). PCA was also used to determine the critical parameters which define the metabolic profile of normal and diseased brains (*G46*). DNA and peptide sequences were modeled by PLS and PCA, and a good discussion was given of the problems encountered in the modeling (*G47*). Several spectroscopic techniques also benefited from PCA/PLS modeling. Solvation effects on the NMR parameters of mercury compounds were reviewed and a new multiparametric solvent scale was derived using principal components (*G48*). Correlations of ^{13}C NMR substituent effects with electronegativities were examined (*G49*). Phase transitions and conformational changes of a stearate ester were studied by applying factor analysis to FT-IR spectra at different temperatures (*G50*). PLS-2 modeling and Raman spectroscopy were combined to improve understanding of near-IR spectra (*G51*). Also, PLS was used to generate mid-infrared spectra from near-IR spectra of molten polymers in an attempt to better understand the process (*G52*). Pure UV–visible spectra were extracted from abstract principal components in a new approach to estimate the structure of ions in solution (*G53*). Visible spectra and target transformation factor analysis were employed in a study of valence states of chromium and iron (*G54*). Near-infrared reflectance spectra of lake sediments and PLS were proposed as a means of inferring the past pH of lakes (*G55*). The Auger crater-edge profile of layered structures was examined using principal components analysis (*G56*). The NIPALS algorithm was employed to determine equilibrium constants from spectroscopic titrations (*G57*). The analysis, which does not require knowledge of the component spectra or a completed titration end point, is based on a decomposition of the spectra into target and projected matrices.

Some unusual studies involving PCA were also reported during the review period. Models for infinite dilution activity coefficients were developed using abstract factors from synthetic data matrices to target test different model parameters. The synthetic data matrices came from modified cohesive energy equations (*G58*). Target testing was also used in a PCA study relating ^{13}C NMR chemical shifts and Taft's constants (*G59*). The dewatering of clay slurries was studied using factor analysis; two factors with physicochemical meaning were obtained (*G60*). PCA and response surface modeling were used to study gases from municipal solid waste combustion (*G61*). A principal components model which accounts for variation of air pollution sources over samples of the source profiles was developed using a Bayesian approach (*G62*). In this innovative work, point estimators and confidence set estimators were obtained for the vectors of the source contributions.

Least squares regression techniques remain the most popular method for parameter estimation. Several new modifications and comparisons were published during the last two years. Constrained and restrained refinement of EXAFS data reduced the number of independent parameters required to fit the data as compared to conventional least squares (*G63*). A program named Expit was offered to fit a sum of exponential functions to experimental data points (*G64*). The program employs a new technique, based on statistical tests, to automatically locate the best number of parameters. Multistage, linear least squares modeling based on autoregressive moving average (ARMA) modeling was applied to noisy NMR signals (*G65*). A newly developed numerical integration and optimization program was proposed to estimate parallel reaction parameters (*G66*). Nonlinear least squares fitting has been applied to a number of problems, including slow amide proton exchange rates (*G67*) and extracting rate constants from UV spectra taken on reacting systems (*G68, G69*). Many spectroscopic studies included least squares regression techniques. A nonlinear, iterative least squares method was used for fitting EPR spectra to simulated spectra (*G70*). The Marquardt algorithm was employed as a search procedure for adjusting the parameters. Issues concerning the application of least squares methods to vapor FT-IR spectroscopy were addressed, with emphasis on spectral collinearity (*G71*). ^{13}C solid-state NMR, FT-IR, and near-IR spectroscopies were combined with PCA and PLS in a study of the physical properties of wood pulp (*G72*). Some applications of least squares fitting to chromatographic problems were also reported. Acidity constants from capacity factors (*G73*) and testing of columns (*G74*) were typical examples. Also, least squares curve fitting and moment analysis were compared in a solute transport study (*G75*).

Some general studies involving parameter estimation were also reported. A Bayesian approach was taken to estimate the number of excitation lines in neutron scattering molecular tunneling experiments (*G76*). One paper described methods of creating chromatographic/UV simulated data to test modeling approaches (*G77*). The simulation was done to take into account small model nonlinearities which can influence the performance of a principal components analysis. The IR spectra of functional groups were extracted from typical IR spectra via PCA and MLR (*G78*). Canonical correlation analysis of mid- and near-infrared spectra of oil was done to assign near-IR wavelengths (*G79*), and two-dimensional statistical correlation of mid- and near-infrared spectra was suggested as a means of qualitative spectral interpretation (*G80*).

STRUCTURE–ACTIVITY RELATIONSHIPS

In this section, the use of multivariate techniques in the building of models that relate molecular structure to some sort of physical, biological, or chemical property is reviewed. Also included here are studies that deal with relations between material composition and property. Studies that deal with regression or classification of spectra to property are included in the calibration or pattern recognition sections, respectively. Most research in this area focused on the development of a linear or nonlinear multiple regression model that related multiple electronic or topographical molecular descriptors as independent variables to a dependent property variable. Predictions of the activities or properties of objects that are not contained in the calibration data set are made by interpolating or extrapolating the calibration model. A very important step that is all too frequently overlooked in the development of structure–activity relationships (SAR) is that of a preliminary statistical experimental design. The key aspects of structure activity design were discussed in a review that included priority setting for risk assessment of hazardous chemicals and the statistical design of calibration models (*H1*). Different chemical or physical variables can also be used to classify different objects according to property or activity. A review addressing both classification and regression in SAR was followed by examples in structure–taste modeling (*H2*). The specific techniques that were addressed included clustering, SIMCA pattern classification, and partial least squares modeling. A large increase in the use of nonlinear modeling methods in the construction of structure–activity models was noted during the past two years. One of these nonlinear modeling techniques, the nonlinear map, was the focus of another review (*H3*). An application-specific review concerned the construction of models that relate the composition of fatty acid tissue in marine animals with the dietary intake (*H4*).

Research continued in the area of descriptor development and analysis during the most recent reporting period. Ten topological indexes were examined with principal components analysis in order to determine the nature of their contributions to structure–activity regression models (*H5*). A new physicochemical descriptor was developed as a measure of hydrophobicity (*H6*). The average molecular electrostatic field was calculated from the atomic monopoles at the points on the van der Waals surface or from bond increments.

One of the most active areas in structure–activity modeling over the last two years concerned the relation of chemical structure to biological activity. Several studies involving nonlinear regression methods have appeared recently. Structure–activity relationships have traditionally dealt with nonlinearities by using nonlinear transforms of molecular descriptors in a linear regression. Over the past two years an increasing number of researchers sought to determine the feasibility of more sophisticated nonlinear regression methods in the development of SARs. Artificial neural networks, a class of highly flexible nonlinear regression methods, were examined for modeling effectiveness in a number of these structure–activity studies. Because of the highly flexible nature of neural network models, the design of data sets is critical to preventing overfitting the calibration data. Ghosal et al. reported that smaller networks performed more effectively than larger networks in the construction of predictive models that related chemical structure information to mutagenic, enzyme inhibitor, and biochemical binding properties (*H7*). In another study that compared neural network models, the comparatively rigid functional-link network outperformed back-propagation networks of various sizes in the prediction of antileukemic activity of carboquone derivatives, and in the prediction of anti-pentylenterazole activity of benzodiazepine derivatives (*H8*). Interestingly, optimally sized back-propagation neural networks actually outperformed the functional-link networks in the fitting of the training set. In other work, back-propagation neural networks were reported to outperform multiple linear regression in the development of models that related structure with dihydropteridine reductase inhibition (*H9*). Another powerful nonlinear regression technique, that of alternate conditional expectations (ACE), performed less effectively than a linear regression of nonlinearly transformed variables in the determination of psychotomimetic activity of phenylalkylamines (*H10*). The ACE approach resulted in good fits of training set but poor predictions on the test set data. In a comparison of two nonlinear regression methods, maximum likelihood logistic regression was found to be more accurate than a weighted multiple regression using logit transformed variables in the assessment of herbicide efficacy (*H11*). Strategies on the use of logistic regression in the monitoring of herbicide efficacy over a time span of several years were discussed. A number of research efforts reported new applications of multiple regression in the relation of structure with biological or toxicological activity: the relation of structure with cyclic AMP phosphodiesterase inhibition properties of pyridines and pyramidines (*H12*), NK-2 receptor antagonist activity of neurokinin A analogues (*H13*), antibacterial activity of quinolones (*H14*), and dihydropteroate synthase inhibition of multisubstituted arylsulfones (*H15*). A model that predicts the carcinogenic activity of a series of polycyclic aromatic hydrocarbons was developed from 17 property and reactivity descriptors (*H16*). In a more structured approach, a statistical experimental design was used in the development of a regression model that related temperature, light intensity, and concentration of carbon dioxide to plant growth (*H17*). Research concerning the relation of structure with biological toxicity continues to be of interest to many scientists inside and outside the chemical sciences. Experimental design, followed by regression, was compared with blocked ANOVA design for assessing the impact of tetrachlorolphenol on zooplankton populations (*H18*). The experimental design–regression model was preferred because of the ability to extrapolate this model to the no-effect concentration. Pattern recognition methods were also employed to reveal qualitative information about structure–activity relationships during the last two years. Steric and electronic chemical structure parameters were used in clustering and principal components mapping of the effects of benzoic acid derivatives on rat metabolism (*H19*). The activities of thiocarbamates were classified as herbicidal or antifungal using PLS modeling (*H20*). Some researchers studied the contributions of individual structural parameters on biological activity. A principal components analysis of the conformers of eight known Ca channel blocking agents was used to determine the structural parameters of certain conformers that are the most likely to contributors to biological activity (*H21*). Molecular mechanics software was also used in the determination of the conformational structures that are most likely to contribute to the activity of a homologous series of HMG CoA reductase inhibitors (*H22*) The interaction of different monoamine oxidase inhibitory drugs with amino acids was studied with a principal components analysis of charge-transfer chromatographic data followed by a spectral mapping technique (*H23*). It was concluded that the amine group of the drugs interacted electrostatically with the second carboxylic acid group of the dicarboxylic amino acids. Structural features affecting the antibacterial activity of quinolones against *Staphylococcus areus* were rationalized using a calibration and design in latent variables (*H24*). An expert system for structure–activity that tests for adequate representation of important structural information was applied to increasing the informational content of several data bases (*H25*). In a study that focused on variable selection, the standard parameter sets normally used in the theoretical linear solvation energy relationship, TLSER, were compared with the use of topological indexes in the molecular transform method (*H26*). A study involving the screening of hazardous substances was updated from the previously reported model (*H27*). Five new group counting variables were employed in the new SAR model. Polynomial equations of the second degree were used to correlate the lipophilicity and surface area descriptors of various trityl derivatives with the antimicrobial activity (*H28*).

A large number of researchers sought to develop models that could predict some sort of instrumental response from chemical structure information. These structure–response relationships were often modeled using larger calibration data sets as compared to those used in structure–biological activity studies. The use of large calibration sets has probably reduced the likelihood of a sparse sampling of the calibration space—a condition that often leads to overfitting by more flexible methods based on nonlinear regression. In addition, comprehensive variable selection in structure–response modeling may be intuitively easier than for structure–biological activity relations. The overfitting of the calibration data by neural networks that was reported by several researchers in the studies involving structure–biological activity models was not reported in the structure–response research. Ball and Jurs compared multiple linear regression, gradient-descent-optimized back-propagation, and quasi-Newton-optimized back-propagation in the modeling of structure–^{13}C NMR chemical shift data (*H29*). The models generated by the Broyden, Fletcher, Goldfarb, and Shanno (BFGS) quasi-Newton method resulted in improved accuracy of prediction and decreased training time when compared with back-propagation optimized by gradient descent. Both neural network approaches outperformed multiple linear regression in the prediction of NMR chemical shifts by a wide margin. Back-propagation neural networks also outperformed multiple linear regression in the modeling of structure–retention relationships in thin-layer chromatography (*H30*). Counterpropagation neural networks, neural net algorithms that function as key-value lookup tables, were compared with multiple linear regression in the prediction of Kovats indexes of substituted phenols (*H31*). The counterpropagation network approach led to significant improvements over multiple linear regression in the prediction of Kovats indexes. Interestingly, the advantage of counterpropagation neural network modeling was most pronounced in cases where the structural descriptors and Kovats indexes were highly correlated. Back-propagation neural networks were also used to generate models for predicting gas chromatographic retention indexes (*H32*). Regression models relating structure with ^{13}C NMR chemical shift data were also developed with recurrent back-propagation neural networks (*H33*). Automated selection of appropriate neural network and multiple regression predictive models from a previously developed library was accomplished using selection criteria based on the similarity of chemical structure (*H34*, *H35*). In another study involving neural networks, graph theoretical descriptors were correlated with infrared spectra (*H36*). A wide range of test set compounds were predicted with about 80% accuracy using the calibrated neural model. Another type of nonlinear modeling method, that of nonlinear mapping, was used in conjunction with principal components analysis to determine the molecular properties that allowed the separation of a series of benzimidizole sulfoxide enantiomers in chiral liquid chromatography (*H37*). Nine important molecular properties were identified from an initial data array that contained 254 molecular descriptors. A new approach to the prediction of ^{13}C NMR spectra based on optimized spectra using increments made use of the spectra of molecular fragments in estimating the overall spectrum of a candidate molecule (*H38*). The majority of structure–instrumental response papers were concerned with developing specific applications with well-known methodologies, however. Structure–retention relationships of polychlorinated dibenzofurans (*H39*), polychlorinated dibenzodioxins (H40), and petroleum hydrocarbons (*H41*) were investigated on gas chromatographic stationary phases of varying polarity with multiple linear regression techniques. Other applications that used multiple linear regression in the construction of structure–gas chromatographic retention models included studies with sulfur vesicants (*H42*), chlorinated dibenzodioxins (*H43*), polychlorinated biphenyls (*H44*), barbituric acid derivatives (*H45*), *N*-isopropyl phosphoramidothioates (*H46*), polyhalogenated biphenyls (*H47*), trimethylsilyl ethers (*H48*), and a group of benzene derivatives (*H49*). Thin-layer chromatographic structure–retention relationships were investigated for the prediction of retention of benzodiazepines (*H50*) and for the influence of dielectric strength and refractive index effects on solvent strength and selectivity in the separation of ethylene oxide oligomer mixtures (*H51*). The feasibility of structure–retention and structure–odor intensity relationships was investigated for a diverse set of industrial compounds using multiple linear regression (*H52*). Several researchers probed the usefulness of linear free energy relationships (LFER) in chromatographic structure–retention models. The LFER relationships were used with the 77 phase McReynolds data set to characterize gas chromatographic stationary phases (*H53*). LFERs were also used in reversed-phase liquid chromatography to develop a simple structure–retention model (*H54*). The regression model used only two solvatochromatic parameters, one each for the solute and the mobile phase. The solubility parameter (SOLPAR) and LFER models were compared in the resolution of chlorinated aromatic isomers (*H55*). The SOLPAR model outperformed the LFER model in the prediction of the retention of various tetrachlorodibenzo-(*p*)dioxins on C_{18} columns. The LFER was also used to examine the solute stationary-phase interaction in gas–liquid chromatography (*H56*). Relative retention values and the corresponding energy partition were determined for a group of monosubstituted benzene derivatives. A methodology was presented for the development of quantitative structure–retention relationships in gas chromatography (*H57*). Two types of calibration models were used to study the interaction between the analyte and stationary phase. The retention behavior of some ring-substituted aniline derivatives on polyethylene and octadecylsilica columns was studied with stepwise linear regression (*H58*). The differences in retention behavior of the two types of columns were attributed to free silanol groups on the polyethylene column that were not covered. In another column comparison, the retention behavior of phenol derivatives on porous graphitized and octadecylsilica columns was qualitatively examined by principal components analysis, two-dimensional nonlinear mapping, and cluster analysis (*H59*). Two different solvation energy models were used to characterize the selectivity of different stationary phases used in gas–liquid chromatography (*H60*). It was reported that, contrary to popular beliefs, none of the stationary phases behave as significant hydrogen-bond acid solvents at the test temperature of 121.4 °C. Molecular structure descriptors have been related to retention characteristics of isomeric structures. A quantitative structure–enantiospecific retention model was developed that predicts the separation of 1,4-benzodiazepines on a human serum albumin-based HPLC stationary phase (*H61*). Molecular descriptors for 40 pairs of diastereomeric amides were used to construct structure–retention relationship with partial least squares regression (*H62*). A range of conformers were used in descriptor development prior to the regression step. Hsieh and Dorsey investigated different approaches for extrapolating the structure–retention model to the 100% water mobile-phase value (*H63*). The proposed model included mobile- and stationary-phase effects in the regression. High-performance liquid and supercritical fluid chromatographic systems were compared for retention characteristics (*H64*). Automatic classification and factor analysis were used to show the equivalence of the retention processes of the two methods. Partition coefficients between olive oil and nitrogen were determined with gas–liquid chromatography and a structure–retention model (*H65*). Target factor analysis (TFA) was used to reconstruct data matrices and make predictions with the best set of molecular descriptors (*H66*). Solutes were also classified with TFA according to their retention behavior. The effect of substituent groups on fluorescence behavior was determined with a linear regression of structure–activity data (*H67*).

A few researchers used graph theoretic approaches in their structure–activity studies during the latest reporting period. Graph theoretical constructs were used to describe NMR cross-relaxation networks in macromolecules and to analyze different experiments used in topological editing (*H68*). A constrained partitioning algorithm was reported that determines the initial assignment of proton NMR resonances of proteins from MFQ-COSY data (*H69*). The algorithm used graph theoretical indexes with a binary tree generation algorithm. The combination of two-dimensional COSY NMR spectra and graph theory was used to estimate carbon-to-carbon connectivity of some simple molecules (*H70*).

Structure–property modeling was popular in industrial quality control during the most recent reporting period. The activity of a number of paraffin inhibitors in a different crude oils was studied using clustering of principal components (*H71*). Crude oils and inhibitors tended to cluster into one of several groups that were used to develop predictive structure–paraffin inhibition activity models. A principal components study of the physicochemical measurements was used to determine the defining differences between four different breeds of cattle (*H72*), and virgin olive oil samples were characterized with principal components and canonical correlation according to their triacylglycerol composition (*H73*). A regression model was developed between the properties of magnetic tape and the maghemite morphology (*H74*). It was concluded that the electroacoustic properties of the tape were mainly determined by the length of the maghemite particles. In a study that involved the quality assessment of mold-ripened cheese, a regression model was developed that relates the chemical composition to the water activity (*H75*). Some research efforts attempted to construct regression models that used physical and chemical properties to predict the properties of agricultural soil. Regression models were developed for the effect of nitrogen and nitrogen placement on no-till small grains (*H76*) and for the estimation of soil microbial biomass as a function of organic composition (*H77*).

A number of new SAR applications have appeared in the recent literature. The relationship between chemical shift tensors and shielding parameters obtained from ^{31}P NMR experiments and molecular structure was studied with a principal components analysis (*H78*). A linear relationship between the S═P—S bond angle and anisotropy and asymmetry parameters was established. Fuzzy, adaptive least squares pattern recognition was used to develop a discriminant function of 37 variables that could be used to infer aquatic toxicity from chemical structure (*H79*). The model, representing a wide range of structures in the 394-compound training set, was verified by cross-validation. Principal components analysis was used to examine the effects of different substituents on the carbonyl stretching frequency and ^{13}C NMR chemical shift (*H80*). The validity of several substituent parameters were investigated by target testing. An integrated approach to the design and optimization of SAR experiments with a new chemometric system, SPECTRE, was discussed (*H81*). A new approach to SAR analysis, multiway principal components analysis, was used to examine the spatial and temporal factors of influence on the water quality in the Niger delta (*H82*). An advanced variable selection procedure called generating optimal PLS estimations or GOLPE was presented and demonstrated with an application on a 3-D SAR (*H83*). The strategy includes a preliminary variable selection by means of a D-optimal design in loading space, followed by an iterative evaluation of the importance of the individual variables used in the predictive performance of the regression model. Finally, Lohninger evaluated the performance of neural networks that use radial basis-transfer functions on nonlinear multivariate regression with simulated data, and also with experimental data that was used to generate a structure–boiling point relationship (*H84*). Topics that were addressed included the determination of network topological structure, the setting of adjustable network parameters, generalization, and extrapolation of the model.

PATTERN RECOGNITION

The aim of pattern recognition is ultimately to classify an unknown into one (or sometimes more) of a set of predetermined classes. Establishing a classification may be desired for any number of purposes, including the analysis of chemical composition, detection of food adulteration, food quality testing, source apportionment, and exploratory data analysis, to name but a few. The classification step is often accomplished through use of one or several chemometrics techniques that are now fairly well-established, including principal components analysis, soft independent modeling of class analogy (SIMCA), *k*-nearest neighbors (KNN) classifiers, and linear discriminant analysis. Few novel methods for pattern recognition were published over the past two years; instead, the chemical literature on pattern recognition focused on novel and not-so-novel applications of existing techniques. Nevertheless, classification of data clearly remains an important subject in chemometrics, as the number of citations appearing on applications of pattern recognition were rivaled only by calibration during this review period. References in this section are therefore grouped according to the type of application, namely, applications to general spectroscopy and chromatography, sensors, food, environment, biochemistry and pharmaceuticals, and diverse industrial applications.

Several reviews on pattern recognition were found in the literature for this period. A general overview (in Slovak) of many pattern recognition methods in mass spectrometry was published with an extensive list of references (*I1*). Geladi and co-workers discussed exploratory data analysis, classification, and regression of multivariate images in chemistry (*I2*). Exploratory data analysis was also the subject of another paper in which several graphical tools were described. These tools included quantile and quantile–box plots for data presentation, quantile–quantile plots for comparing empirical and theoretical probability distributions, and power transformations for simplifying distributions (*I3*). A number of reviews concerned the utility of pattern recognition techniques in sensing systems. Multicomponent analysis with sensors using pattern recognition was reviewed by Vaihinger and Goepel (*I4*), as well as by Gauglitz (*I5*). The use of various classification methods in gas sensing was discussed by Gardner and Bartlett (*I6*). Pattern recognition with surface acoustic wave sensors (SAW) (*I7*) and field effect gas sensors (*I8*) was also reviewed. A major concern of regulators of the food industry is commodity adulteration. Several analytical and pattern recognition techniques suitable for the detection of the adulteration of fruit juices were evaluated (*I9*). The classification of off-flavors by multivariate methods was reviewed by Zervos and Albert (*I10*). A number of reviews of environmental concern involving pattern recognition were also published. Eastwood et al. discussed spectral pattern recognition in environmental programs (*I11*). Classification techniques for fluorescence spectroscopy in environmental and hydrological sciences were described (*I12*). Hierarchical clustering and principal components analysis in the source identification of airborne mineral fibers measured by SEM and energy-dispersive X-ray spectroscopy were reported (*I13*). Einax discussed the use of several pattern recognition methods in the environmental analysis of heavy metals (*I14*). Electronic gas and odor detectors modeled after animal chemoreceptors were reviewed in conjunction with pattern recognition (*I15*).

Several different pattern recognition techniques were applied to spectral analysis in general. Not surprisingly, PCA and cluster analysis were fairly widely used in these studies. For instance, PCA was used to help interpret tandem mass spectra of organic compounds (*I16*). Three different studies identified the sources of materials with the help of pattern recognition. In one study, PCA was used in determining the origin of Chinese porcelain samples analyzed for trace elements by energy-dispersive X-ray fluorescence (*I17*). A second study also used X-ray fluorescence as the basis of determining the geographical origins of Gallo-Roman ceramics using PCA, clustering, and discriminant analysis (*I18*). Another study accounted for different sources of production of Roman pottery by applying hierarchical, agglomerative clustering, and PCA to inductively coupled plasma atomic emission and atomic absorption spectra. The SIMCA classifier was also employed to augment the PCA results where the assignments were uncertain (*I19*). Bernard and Van Grieken investigated seven different hierarchical clustering algorithms using electron probe X-ray microanalysis data from mineral mixtures. The methods were evaluated and compared by the use of κ statistics, and the influence of various experimental parameters on the clustering results was assessed (*I20*). Also, different phases of heterogeneous rock and alloy materials were identified by applying PCA to two-dimensional, X-ray microfluorescence spectra (*I21*). In another study, Linton and co-workers applied cluster analysis to secondary ion mass spectrometry images for molecular microanalysis (*I22*). Ehrentreich et al. compared *k*-means and fuzzy *c*-means cluster analysis on ^{29}Si NMR data. They showed that the *c*-means clustering provides useful information regarding outliers and hybrids (*I23*). A new approach was reported for the identification of products which exhibit very similar near-infrared spectra. This approach combines the residual variance and the Mahalanobis distance metrics with PCA-based library searching (*I24*).

Several other techniques were also used for spectral analysis. Linear discriminant analysis (LDA), following PCA, was used to automatically detect benzene in the presence of nitrobenzene from surface-of-section maps generated from digitally filtered Fourier transform infrared (FT-IR) interferograms (*I25*). The same authors also reported that pattern recognition performance is optimal for linear discriminants derived from faster sampled interferograms (*I26*). Small and Barber showed the influence of interfering species on results obtained from this technique (*I27*). Discriminant analysis applied to near-IR spectra distinguished gelatinized starch samples from up to seven classes. PCA detected an outlier among these samples and emphasized the importance of spectral variations due to scattering (*I28*). The so-called bootstrap error-adjusted, single-sample technique (BEST) classifier was also used for qualitative analysis with near-IR spectroscopy (*I29–I31*). In the mid-IR region, Werther and Varmuza also carried out exploratory data analysis for spectra-structure relationships. They employed discriminants based on partial least squares latent variables instead of ones obtained from LDA or PCA (*I32*). The knowledge of mid-IR spectra was utilized to interpret near-IR spectra through a canonical correlation analysis. The principal components were used in the data analysis due to collinearity (*I33*). In an extensive study, data on analyte elements and chemical modifiers utilized in electrothermal atomic absorption spectrometry were classified using various methods such as discriminant, correlation, cluster, and factor analysis (*I34*). Jerkovich et al. explored the mass spectra–structure relationships of organic radicals by using a linear discriminant (*I35*). Scott classified volatile organic compounds using SIMCA on low-resolution mass spectra according to six classes. The molecular weights of these classes were estimated by an expert system (*I36*). The classification of low-resolution mass spectra was also investigated in a comparison study of four supervised learning methods, namely, KNN, stepwise discriminant analysis, probabilistic classification, and centroid classification (*I37*). Davis discussed the characterization of molecular spectra using hierarchical trees (*I38*). Determining the optimum features for classification can be a difficult problem. Leardi et al. investigated genetic algorithms as a method for feature selection. Genetic algorithms were shown to be generally more efficient than classical feature selection methods for this problem in that fewer features were selected and better classification results were obtained (*I39*).

The most novel research in pattern recognition involved work with artificial neural networks. These networks were also—not coincidentally—the most frequently applied pattern recognition technique for spectral analysis over the past two years. In most cases, a layered, feed-forward neural network was used. These nets were usually trained by using back-propagation of error. Lohninger and Stancl compared the performance of back-propagation neural networks with LDA, as well as that of Kohonen feature maps with KNN clustering on mass spectra of eight classes of steroids (*I40*). Meyer and Weigelt investigated the use of a back-propagation neural network with one hidden layer for IR spectral analysis. In one case, the full, low-resolution spectrum served as the input to the network (*141*). In a second case, the scores obtained from PCA of the spectra were input rather than the entire spectrum in order to minimize the number of connections required in the network (*142*). Luinge and co-workers compared a three-layered net with a library searching system for the identification of pesticides from IR data (*143*). Others using feed-forward artificial neural networks trained with the back-propagation learning algorithm for the interpretation of IR spectra included Fessenden (*144*) and Weigel (*145*). Coenegracht applied a feed-forward neural network trained with back-propagation to the analysis of the UV spectra of mixtures of sulfonamides. From a set of spectra and the peak areas of the corresponding chromatogram, the neural network was able to identify the peaks in other chromatograms measured in different mobile phases (*146*). The relationship between the europium(II) emission spectrum in complex fluorides and the structures of host complex fluoride lattices was also studied with a neural network trained by back-propagation (*147*). Noisy spectra can cause pattern recognition to be difficult, particularly when the spectra of interest are very similar. Allanic et al. demonstrated a neural network that was used to successfully distinguish between similar two-dimensional fluorescence spectra where classical methods failed (*148*). Olmos reported a neural network which performed pattern recognition on the shape of the whole spectrum rather than on individual peaks for low-resolution γ spectroscopy (*149*). The effective prediction of sample composition based on near-IR and FT-Raman data was achieved using signal preprocessing and a neural network (*150*). Ricard et al. evaluated the performance of neural networks on IR spectra by considering statistical indexes and the connection weights of the network when the net was trained on functional groups from synthetic spectra (*151*). Several research groups investigated the use of hybrid and modular networks for pattern recognition. A modular network system was designed such that each constituent network was dedicated to a specific structural task (*152*, *153*). Another system of neural networks consisting of two steps was constructed by Tanabe. In the first step, the IR spectra are classified into one of a set of categories, and in the second step, each category is connected to another network which identifies the spectrum (*154*). Others tried unusual networks on unconventional tasks in pattern recognition. The poor resolution exhibited by ion mobility spectra renders them difficult to classify with traditional library searching or pattern recognition methods. Bell et al. studied the use of a connectionist hyperprism classification (CHC) neural network with such spectra and were able to identify the significant spectral features (*155*). An interesting study of the interpretation of IR spectra using a self-organizing feature map was undertaken by Melssen and co-workers. A Kohonen network, accelerated by a parallel implementation, was used to cluster molecular fragments on the map according to functionality. The presence, in some cases, of more than one level of clustering suggested the design of a tree-structured system of dedicated multilayered, feed-forward neural networks (*156*).

Pattern recognition methods were also employed to aid in the characterization and design of chromatographic systems. For example, various hydrophobic interaction chromatography media were grouped according to protein selectivity using PCA (*157*). Similarly, the flavonoid selectivities of several mobile and stationary phases for reversed-phase high-performance liquid chromatography (HPLC) were also classified by PCA (*158*). Forgacs et al. examined the retention of aniline derivatives on two different HPLC columns and established relationships between retention properties and physicochemical parameters. This was accomplished using several methods, including PCA followed by two-dimensional nonlinear mapping, clustering, and canonical correlation analysis. The former was found to be the most suitable for the task (*159*). Smilde and Doornbos compared two multivariate analysis techniques, namely, PARAFAC and three-way PLS, for their performance in predicting reversed-phase retention. The simple validatory tools used to carry out the comparison were described (*160*). In a gas chromatography application, linear solvation energy relationships with three solute parameters were utilized to categorize several stationary phases using a so-called phase classification triangle (*161*).

The combination of new sensors and pattern recognition has long been an active area of research, and the past two years proved no exception. Many research groups have directed their attention toward the development of sensor systems in which pattern recognition techniques play a vital role. For example, Amati et al. designed SAW sensors for the simultaneous detection of various organic solvents in dry air. The selectivity of the detectors was enhanced by the use of PLS regression (*162*). Reichert et al. reported a similar system for the detection of methanol in fuel vapors (*163*). In another study of a SAW sensor array, the responses were analyzed by disjoint principal components regression (*164*). Nayaq et al. described a gas sensor array for identifying component gases or odors in air by clustering transformed data (*165*). A technique was proposed for reducing the dimensionality of remote sensing data from an imaging spectrometer by selecting features which enabled accurate classification (*166*). PCA was used with conducting polymer gas sensors to discriminate between the responses of alcohols in a ternary mixture (*167*). Sugimoto et al. also employed PCA to categorize the responses of plasma polymer thin-film probes to organic vapor molecules (*168*). A number of papers were concerned with the analysis of flavors and aromas. The response patterns of a quartz resonator gas sensor to various types of coffee or wine aromas were distinguished with a neural network (*169*). Nakamoto et al. also developed an odor-sensing system based on a quartz resonator sensor array. The choice of suitable membrane coatings for classifying nut flavors was achieved by PCA (*170*). A PCA analysis was also used with a neural network to distinguish whiskey aromas (*171*). Pearce et al. combined an array of conducting polymers with a neural network for the headspace analysis of beer. The system was able to identify various brands of beer as well as detect tainted beer (*172*). Another back-propagation neural network was devised in order to categorize response patterns generated by a flow injection system. The system was equipped with an array detector comprised of several ion-selective electrodes (*173*). The specificity of a fuel cell array was ameliorated by the use of a neural network. Signal preprocessing as well as both supervised and unsupervised learning schemes for neural networks was discussed (*174*).

A significant number of the references involving pattern recognition concerned applications in food chemistry. Generally, routine analytical measurements, including GC, LC, and trace metals analysis were used to obtain the data, and linear discriminant and principal components analysis constituted the bulk of the multivariate data analysis techniques. Linear discriminant analysis was used to characterize red varieties of grapes from HPLC measurements of anthocyanin. (*I75*). Pino et al. also utilized LDA to categorize samples of cocoa powder into two classes on the basis of GC analysis of the volatile components (*I76, I77*). As mentioned earlier, one of the main problems facing the regulatory food agencies is adulteration. In particular, the FDA undertook a study of orange juice adulteration in which PCA and discriminant analysis were used to classify samples from HPLC measurements of volatile components and from inductively coupled plasma (ICP) spectrometric analyses of trace metals (*I78*). A group in the United Kingdom reported research results regarding the authentication of orange and other fruit juices by the application of discriminant analysis to their near-IR spectra (*I79*). Kaufmann identified illicit oil substitutes in a mixture using PCA and estimated their proportions by PLS (*I80*). In another study, Headley and Hardy used PCA to identify adulterants in whiskey from gas chromatograms (*I81*). Another issue preoccupying the food industry is that of monitoring food quality. Near-IR reflectance spectra of pea extrudates were classified according to extrudate cooking conditions using PCA. These cooking conditions were found to be correlated with protein quality (*I82*). PCA was also applied to several measured parameters of powdered black pepper in order to assess the impact of storage on quality (*I83*). Narasimhan and co-workers categorized the aromas of black pepper as well as ginger using canonical discriminant analysis (CDA) on GC data that had been correlated with sensory analysis. The change in the quality of the aroma of black pepper during storage was evaluated by PCA and quality predictions were formulated for both spices (*I84*). Chromatographic data of samples of paprika were related to the evaluations of a sensory panel for classification according to aroma quality by SIMCA (*I85*). Similarly, Huang and Zayas grouped sensory evaluations of the aroma of corn germ protein flours into four classes by CDA. Stepwise multiple regression correlated sensory and GC data to enable predictions of aroma quality (*I86*). Food source apportionment is another area where pattern recognition has been applied. Shimoda et al. analyzed the volatile compounds in the headspace of cabernet sauvignon wines by GC. They were able to correctly classify the wines by region of origin using discriminant analysis (*I87*). On the other hand, Italian peppermint oils also analyzed by GC were not successfully classified according to their geographic origin using PCA and SIMCA (*I88*). Other applications of PCA included the characterization of roasted coffee by static headspace GC or HPLC-UV of coffee extracts (*I89*) and the identification of fat substitutes in sausages by near-IR reflectance spectroscopy (*I90*). Near-IR spectra of hard red wheat harvested over a four-year period were also grouped by PCA with the objective of classifying the wheat samples according to winter or spring varieties using a discriminant function (*I91*). Murota analyzed the headspace of six coffee cultivars by GC and MS and classified them into three sensory categories using CDA (*I92*). Static headspace GC was employed to determine the volatile components in four species of Pacific salmon. The use of PCA in conjunction with discriminant analysis successfully classified the four species, where nonparametric, linear, and quadratic discriminant analysis performed in decreasing order of percent classification (*I93*).

Various methods of cluster analysis were also commonly applied to food classification problems. Wheat differentiation was again the subject of study. In this case, five classes of winter wheat samples from two different growing seasons were analyzed by Curie point pyrolysis gas chromatography. It was found that multivariate cluster analysis discriminated the five classes within a single season, whereas discriminant analysis classified the wheats correctly, regardless of growing season (*I94*). Cluster analysis was also employed in food quality tests. Martinez-Anaya et al. correlated biochemical and physical properties of breadmaking starter cultures with bread quality by three different means, namely, *k*-means clustering, discriminant analysis, and PCA (*I95*). Varadi and Toth investigated the feasibility of monitoring chocolate quality during processing by applying hierarchical clustering and discriminant analysis to near-IR spectra (*I96*). Both of these pattern recognition methods were also utilized to classify red wines and musts from their physical properties and GC measurements (*I97*). Three gin brands were discriminated by several pattern recognition techniques, including clustering, PCA, and discriminant analysis (*I98*). These methods were also used to discriminate sugars from cereals, tubers, leguminosae, fruits, and sugar plants on the basis of natural isotope measurements of hydrogen, carbon, and oxygen (*I99*).

A miscellany of other pattern recognition methods were also employed in food chemistry. For example, sensory data on apricot purees were correlated with analytical parameters as measured by GC using PLS regression. The size of the GC data set was reduced by PCA prior to performing the regression (*I100*). Alcohol distillates determined by chromatography were also classified with the help of PLS modeling (*I101*). De Jong described several techniques, namely, fuzzy set theory, PLS regression, and mixed integer programming, and illustrated their use in the classification of edible fats (*I102*). Vogels and co-workers applied KNN and PCA combined with discriminant analysis to differentiate wines characterized by NMR spectroscopy. The accuracy of the classification was improved using a partial linear fit preprocessing scheme (*I103*). Oligosaccharide residues analyzed by NMR were categorized by KNN, PCA, and SIMCA (*I104–I106*). Francelin et al. compared the performances of three neural network architectures, namely, the Hopfield model, the Hamming model, and a multilayer, feedforward network, for the classification of vegetable oils analyzed by GC (*I107*). The flavor profiles of natural orange aroma generated by both a sensory panel and GC were classified using a nonlinear mapping (NLM) technique and various other pattern recognition algorithms from the ARTHUR package (*I108*). In a novel approach, Devaux et al. determined the size and shape of granules composing the different types of starches by image analysis. The similarity maps of categories generated by multiple correspondence analysis (MCA) showed that the granule distributions were characteristic of the starch species (*I109*).

Pattern recognition methods have become an integral part of environmental studies over the past few years. During the course of this review period, PCA was most commonly used for classification of environmental data, frequently to attempt to apportion the contributions of various sources of pollution. One study with that objective was carried out by Wenning et al. to determine whether contaminants found in surficial sediments were mainly of industrial, residential, or municipal origin using PCA and polytopic vector analysis (*I110*). Giesy and Hoke classified freshwater sediment toxicities by PCA and cluster analysis (*I111*). In another sediment study, PCA and hierarchical clustering were utilized to categorize sediment toxicities in the Hamburg harbor. Varimax rotation and factor analysis established the relationship of toxic responses to sediment composition (*I112*). Cash and Breen also used PCA as well as geostatistics to discriminate two sources of pollutants in the Hamburg sediments (*I113*). In another study, data on Chatauqua Lake sediments were subjected to correspondence analysis (*I114*). Several soil analysis studies also included pattern recognition techniques. Chemical soil characterizations were classified using PCA and clustering (*I115, I116*). Kokot et al. used PCA and two multicriteria decision-making methods known as PROMOTHEE and GAIA to choose an appropriate microwave digestion procedure for metal determination (*I117*). In water research, PCA and varimax rotation were applied to rainwater samples to determine the sources of various ions (*I118*). Trace element concentrations in rainwater were determined by neutron activation analysis and the samples were categorized according to source using PCA. In addition, PLS was employed to compare the data to various source signatures of the same elements (*I119*). Rainwater composition was also interpreted by Zhang et al. using PCA (*I120*). Grimalt and Olive compared the performances of PCA and factor analysis (FA) in determining the sources of various chemical species in aquatic systems. They found that FA revealed a direct correspondence between factor loadings and geochemical origin, whereas PCA only provided classification according to major sample groups (*I121, I122*). In two separate studies of groundwater, data analysis by PCA, FA, and clustering helped to elucidate possible origins of the water (*I123*), and FA aided in identifying sources of water contaminants (*I124*). Lavine et al. investigated the feasibility of identifying the source of a jet fuel spill by applying disjoint PCA to GC analyses of the fuel (*I125*). Exploratory data analysis using PCA was again discussed and illustrated with a large environmental database by Meglen (*I126*). Physicochemical characterization of airborne dust from three cast iron foundries was subjected to PCA and cluster analysis. A relationship was uncovered between chemical composition and particulate size as well as foundry operating schedules (*I127*). Sarker et al. reported the results of a study comparing SIMCA and a library searching method for the identification of hazardous compounds from mass spectra (*I128*). The interpretation of data from chlorinated phenol analyses by GC/MS was achieved using the PRIMA (pattern recognition by independent multicategory analysis) method. Results from these studies were compared to library searching (*I129, I130*). Niemi et al. formulated a discriminant function for classifying acute toxicity syndromes in fish according to the physiological responses of fish to exposure to xenobiotic chemicals (*I131*). On the basis of GC retention indexes, Klappa and Long categorized the toxicities of polychlorinated biphenyls (PCBs) using PCA and discriminant analysis (*I132*). The quantitation of PCBs and the identification of their sources by Environmental Protection Agency (EPA) methods requires the identification of Aroclor mixtures. LDA was employed to classify PCB mixtures as a specific Aroclor from mass spectral data (*I133*). Hazardous gases analyzed by ion mobility spectrometry were identified by LDA from data processed by a finite impulse response filter (*I134*). Classification of particles is also receiving attention. A scanning nuclear microprobe was utilized to analyze atmospheric aerosol particles from several sources. PCA and hierarchical cluster analysis yielded similar classes reflecting the sources of the particles (*I135*). A new model called direct trilinear decomposition followed by a matrix reconstruction (DTDMR) was developed for identifying sources of airborne particles (*I136*). Another new approach was described for identifying the sources of contaminant emissions based on a conditional probability model named the potential source contribution function (PSCF) (*I137*). Kaltenbach and Small described a procedure in which ridge regression is employed to transform collinear IR spectral data prior to LDA. They claimed that the transformation stabilizes the data by reducing the degree of collinearity, thereby improving the piecewise linear discriminant (*I138*).

A considerable number of studies involved the use of pattern recognition techniques in pharmaceutical and biochemical analysis. Lincoln et al. compared the results of applying PCA to LC–UV and LC–MS data as a way of determining the number of components co-eluting under a single chromatographic peak. They found that PCA applied to LC–MS data afforded a better detection of low levels of coeluting impurities, particularly when the UV spectra were very similar (*I139*). Castledine et al. also reported the results of applying PCA to the LC–UV analysis of a model drug (*I140*). In another pharmaceutical study, drug solutes subjected to HPLC were classified by PCA according to the pharmacological properties of the drugs (*I141*). Both PCA and SIMCA were used to categorize samples of a Chinese traditional drug by geographical origin on the basis of pyrolysis GC (*I142*). Monfre and Brimmer described the use of PCA for classification of antibiotics characterized by near-IR spectroscopy (*I143*). Plant biochemistry, as analyzed by various types of chromatography, was the basis for discriminating species of trees (*I144, I145*), plants (*I146*), and medicinal herbs (*I147*) and shrubs (*I148*) by PCA. Baiocchi and co-workers investigated the application of both PCA and LDA to HPLC data in order to distinguish between fungus-resistant and -susceptible species of poplar trees based on the phenolic content of their bark (*I149*). Others identified several molds using SIMCA on the gas chromatograms of the fatty acids of the spores (*I150*). IR spectra of tobacco plants served to classify samples according to qualitative properties using PRIMA (*I151*) and to differentiate blends using PLS and PCA (*I152*). In another study, Canadian coniferous woods were distinguished by the application of PCA to the reflectance FT-IR spectra (*I153*). Gemperline et al. utilized PCA on three-mode data arrays to establish the relationship between trace elements and blue crab shell disease (*I154*). Several pattern recognition methods, namely, KNN, projection pursuit regression, and PCA, were tried in attempts at classifying fruit fly larvae on the basis of gas chromatograms (*I155*). Delgoda and Pulfer employed the linear learning machine to identify amino acid sequences from mass spectral data (*I156*). Another paper reported the results of categorizing molecular analogues on the basis of immunochemical cross-reactivity by the use of minimum estimate variability (MEV), PCA, and KNN (*I157*). Gelinas et al. performed multielement analyses of numerous animal tissues in order to establish relationships between elemental composition and tissue types using PCA (*I158*). In an interesting application, a system for providing diagnostic information based on qualitative and quantitative properties of human urine samples was designed with PCA and PLS (*I159*). The concentrations of 20 substances in urine samples were also determined by NMR at eight time points in rats injected with two toxins. The application of PCA and nonlinear mapping to the data yielded two distinct metabolic trajectory diagrams corresponding to the two toxins (*I160*, *I161*).

Various cluster analysis methods were also commonly employed in biochemical applications. White et al. used hierarchical clustering and PCA to classify species of fungi from LC determinations of their amino acids (*I162*). In another study, fungi and bacteria were distinguished according to their biotransformation activity. This was achieved by applying hierarchical cluster analysis to the R_f values and spot intensities of the products resulting from screening the strains with several substrates (*I163*). Fungi were also categorized by Frisvad using a number of pattern recognition techniques on LC data of secondary metabolites. These techniques included several clustering methods, correspondence analysis, SIMCA, and PLS (*I164*). Others determined the factors affecting the phenolic composition of sorghum by applying single linkage cluster analysis to HPLC and in vitro degradability data of crop residues (*I165*). PCA and clustering were also utilized to discriminate roses by HPLC analysis of their flavonoids (*I166*). These same methods were employed in another study of flavonoids where R_f values from several planar chromatography systems were classified to select the minimum number of systems required to achieve optimal separation (*I167*). Hobert and Meyer used PCA and hierarchical clustering to interpret IR spectra of urinary stones. Quantitative estimates of the compounds were obtained by multiple linear regression (*I168*). Latent variable analysis was also used to represent receptor protein sequences. Subsequent application of cluster analysis yielded the minimum number of classes reflecting distinct pharmacological types and subtypes of receptors (*I169*). Matson devised a system for diagnosing nerve diseases on the basis of cerebrospinal fluid samples from normal and abnormal persons. The analytical data were evaluated by linear and stepwise regression prior to clustering (*I170*). Maenhaut and coworkers measured minor and trace elements in brain tissue and inferred a relationship between the trace element profile of a brain structure and its function. Data analysis was performed using varimax rotation and several hierarchical clustering schemes (*I171*).

Other pattern recognition approaches were adopted for biochemical methods. For instance, Reibnegger et al. compared self-organizing neural networks with cluster analysis and PCA for classification in clinical chemistry (*I172*). A neural network was also used to distinguish classes of algae from flow cytometer data (*I173*) and to identify two-dimensional proton NMR cross peaks in the spectrum of an enzyme inhibitor (*I174*). Two-dimensional proton NMR peaks of proteins were also assigned using a novel combination of spin coupling graph theory, fuzzy graph pattern recognition, and tree searching (*I175*). McLachlan presented a new method called the multichannel Fourier transform for detecting weak, periodic patterns in protein sequences against a noisy background (*I176*). Sahota and Morgan described several feature selection methods for GC and GC/MS data of biochemicals. These methods isolate unique chemical markers which are characteristic of the different classes (*I177*, *I178*).

Pattern recognition techniques continued to be explored in the petroleum, polymer, and textile industries. Meuzelaar et al. described principal components and canonical correlation analysis of spectral data on multisource fossil fuels such as coal. The chemical trends and components represented by the canonical variate functions reflected the different coal compositions and structures (*I179*). In another study, Ismail classified coal and coal fly ash samples using PCA and cluster analysis (*I180*). Several petroleum crudes and their corresponding silica-adsorbed fractions were categorized by applying PCA to their ^{13}C NMR spectra (*I181*). Lai and co-workers described a technique which uses multivariate circular profiles to aid in distinguishing crude oils by geographical origin (*I182*). Mixtures of hydrocarbons typically observed in gas chromatograms of petroleum derivatives were oxidized for analysis by GC/MS. The resulting profiles were then subjected to cluster analysis and related to the source oils (*I183*). Using PCA, Kosman and Lukco were able to differentiate petroleum products on the basis of GC-AES multielement simulated distillation data (*I184*). Petroleum products were also categorized by applying PCA to IR spectral data (*I185*). In a polymer application, PCA successfully distinguished high- and low-temperature-cured polyimide thin films analyzed by pyrolysis MS (*I186*). PCA was also utilized to elucidate the curing reaction of an epoxy resin from time-resolved FT-IR spatial maps (*I187*). Mansueto and Wight applied the SIMPLISMA self-modeling method to IR spectra to identify two types of oligomers found during the polymerization of formaldehyde (*I188*). Others used PRIMA to interpret the IR spectra of various materials of high molecular weight or complex composition (*I189*). Applications of interest to the textile industry were also reported. Gilbert et al. described the use of PCA and SIMCA in discriminating cotton fabrics characterized by diffuse reflectance Fourier transform infrared (DRIFT) spectroscopy (*I190*). In addition, PCA, SIMCA, and fuzzy clustering were applied to DRIFT spectra of textile dye mixtures. Samples were grouped according to where they were extracted on the material (*I191*). Another paper described the analysis of polyester fibers by two-dimensional HPLC and their separation by cluster analysis into classes representing the different manufacturers (*I192*). White and Catterick compared a method called group centroid Euclidean distance measurement (GCEDM) with PCA and clustering in the classification of azo dyes (*I193*). Six other pattern recognition techniques were compared with respect to their ability to formulate decision rules for qualitative assessments of dyes. They found that the best decision rules were afforded by a nonstatistical method (*I194*). In another study, FT-IR reflectance spectra of paint binders on ground chalk were interpreted by hierarchical cluster analysis and PCA (*I195*). The phase composition of superconductors was also observed by clustering and PCA (*I196*). Glick and Hieftje reported a comparison of a neural network with other pattern recognition methods in the identification of alloys from their glow-discharge atomic emission spectra. Calibration of the spectra was achieved using stepwise multiple linear regression (*I197*). A neural network was also employed to classify laser desorption–ion mobility spectra in order to distinguish polymeric materials (*I198*).

Several researchers reported studies on the development of new pattern recognition methods or the refinement of established ones. For instance, Glick and Hieftje presented an unusual alternative to conventional multivariate data analysis methods in which stereoscopic visualization is utilized for examining three-dimensional data (*I199*). A linear discriminant hierarchical clustering technique was also devised which permits the validation of clusters by a cross-validation method (*I200*). Aeberhard and co-workers demonstrated the shortcomings of the model selection procedure of regularized discriminant analysis. They suggested modifications of the selection procedure and one of the control parameters for better classification performance (*I201*). Two new orthogonal expansion techniques, modified optimal discriminant plane (MODP) for mapping and order Gram–Schmidt orthogonalization (OGSO) for modeling, were also introduced (*I202*). Alsberg and Remseth defined noncongruent two-dimensional surfaces/images as sequences of comparable but structurally different surfaces/images. They described the use of latent variable projection for the analysis of such structures (*I203*). Krzanowski explained the problem of matrix singularity associated with the use of canonical variate analysis when more variables exist than within-group degrees of freedom. He proposed using PCA under these circumstances by ranking principal components according to the ratio of between- to within-group variances instead of the usual total variance criterion (*I204*). The utility of projection pursuit in exploratory data analysis was also described (*I205*).

LIBRARY SEARCHING

During this review period, the number of publications that appeared concerning research in library searching systems was notably few. For the most part, the literature in this area of chemometrics focused on applications of existing methods. For the purpose of this review, however, the ensuing discussion will center on new library searching procedures, the enhancement of established ones, or unusual applications.

A number of previously developed library searching methods were reexamined for the purpose of refinement or for adaptation to new applications. Scsibrany and Varmuza described a searching procedure for identifying common structural characteristics of compounds grouped by principal components analysis of their mass spectra (*J1*). Another PCA-based technique, originally devised for mid-IR spectra, was implemented for the identification of near-IR spectra. The performance of this technique was compared to that of the dot product metric, and approaches for handling spectra of poor quality were proposed (*J2*). Kauvar and Ambler cross-reacted a series of triazine analogues with monoclonal antibodies for different analyte concentrations. A number of parameter values defining the so-called survey of characteristics profiles were then measured and stored in a database for matching with those of unknown samples (*J3*). A library was also constructed for protein secondary structure elucidation on the basis of Fourier transform infrared spectra–structure correlations (*J4*, *J5*). Jarvis and Kalivas described a library searching method which employs condition index evolving profiles derived from singular value decomposition of library and time-evolving sample spectra. The procedure was demonstrated with liquid chromatography UV–visible spectrophotometry (*J6*) and gas chromatography–FT-IR spectrometry (*J7*). In an effort to characterize different library searching systems, a procedure for evaluating and optimizing spectroscopic libraries was presented (*J8*). In addition, Owens reviewed the method of correlation analysis for the interpretation of mass spectra (*J9*).

Several new techniques were devised for library searching systems. For instance, a new procedure employing the correlation coefficient and the Euclidean distance was developed for interpolating spectra at every composition of eluent in the model range of high performance liquid chromatography (*J10*). A new library searching system based on peak weighting factors was also designed for X-ray powder diffraction data (*J11*). Chen and Robien reported novel algorithms for automated extraction and analysis of substituent-induced chemical shift differences of ^{13}C NMR spectra from the CSEARCH-NMR database (*J12*). Regression techniques also formed the basis of several library systems. Data reduction of spectral databases was performed using characteristic regression analysis, an approach based on characteristic vector analysis and multiple linear regression analysis (*J13*). Methods based on the use of principal components and regression attracted several authors' attention. Lo and Brown designed procedures for searching IR spectral libraries of mixtures using principal components regression. PCR analysis in conjunction with an adaptive filter was applied to medium-size libraries (*J14*). A dot product metric in addition to PCR and an adaptive filter was used for large-size libraries (*J15*). Meyer et al. discussed the identification and quantitation of components in a mixture using a library searching method based on IR peak tables and linear regression (*J16*). In a novel approach, a Hamming neural network was utilized to devise an IR spectral library searching system (*J17*).

Molecular structure database systems were also the subject of several research papers. Chemical structure databases typically allow molecular substructure searching and full-structure similarity searching, but few permit a search based on substructure similarity. In view of this, an interactive system was devised that retrieves two-dimensional molecular structures whose substructure is similar to the query structure (*J18*). Databases of three-dimensional molecules were also investigated. Artymiuk et al. compared four techniques based on interatomic distances for measuring the extent of similarity between pairs of molecules. In addition, a new method which also incorporates angular information was demonstrated with protein structures (*J19*). Another method was designed in which the similarity between two molecules relative to their mutual orientation in three-dimensional rotational space is determined. The similarity function is based on projections of molecular property values (*J20*).

ARTIFICIAL INTELLIGENCE

Artificial intelligence (AI) continues to be of considerable interest to analytical chemists, as evidenced by the significant increase in the number of references related to this field compared to previous review periods. The areas of AI discussed in this section include neural networks, genetic algorithms, and expert systems, the latter being by far the area the most widely applied to problems in chemistry. Concepts first developed in AI have taken root in other fields of data analysis. Neural networks in particular continue to grow in popularity, and their application now extends far beyond traditionally defined areas of AI. Their use is especially common now in applications concerning multivariate calibration and pattern recognition. Authors whose work involved neural networks in either of these two chemometric fields are referenced in those sections of this review. Applications of genetic algorithms, another research area whose influence has spread beyond the confines of traditional AI, are discussed in the optimization section.

A rapidly growing area of AI that is also emerging in chemometrics is that of fuzzy set theory. Fuzzy sets were conceived as mathematical constructs some time ago as a consequence of the oft-encountered need to describe objects with inherently vague attributes. The recent genesis of a new journal, *IEEE Transactions on Fuzzy Systems*, attests to the growing importance of this field in general. Other (nonchemical) journals in this field that may be of interest to chemometricians include *AI Expert, IEEE Transactions on Neural Networks*, and *Neural Networks*. For reasons of scope, however, only those papers found in journals relevant to chemistry are referenced in this review.

A number of reviews on various facets of AI appeared in the literature in the course of the last two years. Dickinson discussed some of the problems associated with conventional rule-based expert systems and suggested a new model-based approach (*K1*). In the second part of a two-part series, Warr reviewed systems for computer-assisted molecular structure elucidation, including expert systems, neural networks, and pattern recognition techniques (*K2*). Molecular structural information was also the subject of another review focusing on the use of expert systems in the analysis of infrared and nuclear magnetic resonance spectra (*K3*). Other systems designed for spectral interpretation included the improved PAIRS (program for analysis of IR spectra) and other related knowledge-based systems (*K4*), as well as one developed for biomedical applications utilizing fluorescence spectroscopy (*K5*). Expert systems were also discussed as analytical tools for various types of chromatography. In this vein, the ESCA (expert systems applied to chemical analysis) project for high-performance liquid chromatography was summarized (*K6*), and an expert system for the selection of ion chromatographic conditions was described (*K7*). The utility of fuzzy models for chemical data analysis was also the subject of two reviews. Ebel et al. reviewed pattern recognition and the representation of near-IR spectra as fuzzy sets (*K8*), while Otto et al. discussed fuzzy logic and neural networks (*K9*).

Several new approaches to the design of neural networks for chemical analysis were found in the recent literature. One such approach was the method of optimal minimal neural-network interpretation of spectra (OMNIS), an approach which combines the principles of neural networks and principal components analysis. OMNIS was shown to outperform principal components regression and partial least squares on near-IR calibration data sets by 50–75%, as measured by the standard error of prediction (*K10*). Harrington devised minimal neural networks which, unlike other neural networks, use localized processing. Fuzzy rules are employed in the construction of classification trees whose branches consist of multiple processing units (*K11, K12*). A back-propagation neural network method was reported, which comprises a linear, orthogonal feature extraction part and a nonlinear mapping part with one or more layers (*K13*). A comparison was made of the performance of back-propagation neural networks for calibration in near-IR spectroscopy with that of principal components regression (*K14*). A smart sensing system for the detection of water pollutants based on light scattering measurements was constructed using a multilayer, back-propagation neural network (*K15*). Harrington argued that the increase in the training rate of neural networks observed by others using bipolar sigmoid functions rather than the conventional sigmoid function is artificial (*K16*). In a discussion regarding the merits of neural networks as tools in analytical chemistry, Kateman advocated rigorous testing to promote the acceptance of the technique (*K17*). The back-propagation network was not the only neural network receiving attention, however. A new neural network named the dynamically capacity allocating (DCA) network manifests the ability to learn in an incremental fashion, allowing for additional training data to be used later, as it becomes available. The DCA network was shown to perform as well or better than other existing linear and nonlinear methods on classification problems and on multivariate calibration of spectroscopic data (*K18*).

Fuzzy sets consist of a convenient mathematical way of representing imprecise data which are intuitively described by linguistic terms such as "many", "few", "somewhat", etc. Fuzzy set theory allows one to determine, say, the degree to which a pattern belongs to a given class. This contrasts with traditional (crisp) set theory which uses probability to describe the likelihood of a pattern belonging to a given class. In chemical analysis, the range of applications of fuzzy set theory is increasing rapidly. In one recent example, fuzzy models have been used in conjunction with gas sensors. Fuzzy logic enabled the representation of a human expert's interpretation of inherently imprecise data in the detection of atmospheric gases using a gas sensor array (*K19*). Similarly, fuzzy set representations of sensor signals were utilized in a fire and gas leak prevention system (*K20*). Spectral data analysis has also been performed on the basis of fuzzy models. Hoerchner and Otto used fuzzy functions to assess the degree of similarity between an unknown UV–visible spectrum and the spectra in a fuzzy database (*K21*). In another study, Neuboeck and co-workers applied fuzzy logic to aid their interpretation of atomic emission spectra (*K22*). Adler et al. implemented an expert system containing fuzzy rules for the analysis of X-ray diffraction spectra (*K23*), while another group did so for neutron activation analysis (*K24*). An unusual approach reported during the last two years involved the application of a fuzzy linear regression method to colorimetric data as an alternative to the typical calibration curve (*K25*). The applications of fuzzy logic extend beyond quantitative relationships, however. Chen described the fundamentals of fuzzy cluster analysis and its use in environmental water quality assessment (*K26*). In a comparative study, three methods of propagating uncertainty in a knowledge base were examined, namely, Bayesian logic, certainty factors, and fuzzy logic (*K27*). An interesting application of fuzzy logic was conceived in which the concentration of penicillin in a fed-batch bioreactor was controlled by fuzzy rules (*K28*). A number of mass spectrometric studies were carried out in which fuzzy models were employed for data analysis. Harrington's fuzzy rule-building expert system (FuRES) was designed to classify polymer thin films characterized by laser ionization mass spectrometry (*K29*). The interpretation of the mass spectra of chromatographically unresolved binary mixtures of alcohols were aided by a fuzzy classification of the spectral patterns (*K30*). Otto et al. devised an interesting fuzzy method for determining the influence of arsenic concentration and annealing conditions on the antimony and boron implantation (depth) profiles in silicon wafers. The profiles were measured by secondary ion mass spectrometry, and the variations in concentrations were represented by a fuzzy set (*K31*).

An expert system essentially encapsulates the knowledge or expertise of human experts in a particular domain. Such knowledge is typically represented as a set of rules from which inferences can be made about a given problem in order to arrive at a decision. As a chemometric technique, expert systems have been employed in numerous applications encompassing the design or selection of analytical systems or methods, spectral analysis, and data and test validation, to name but a few. Until recently, researchers have not tried to adapt expert systems to electrochemistry, however. Esteban and co-workers developed an expert system to direct the analyst through the simultaneous determination of trace metals by voltammetric techniques. Their knowledge base provides guidance for sample pretreatment, choice of analytical procedure, and identification of the analyte metals (*K32*–*K34*). Barthel and Popp discussed the simulation of electrolyte solutions by the expert system ELDAR (Electrolyte Data Regensburg) (*K35*).

Unlike electrochemistry, however, chromatography has been an area where the advantages of expert systems have long been recognized. A number of papers appeared in the literature concerning the use of expert systems for the development of methods or the selection of optimum conditions for chromatography. A knowledge-based system was designed to suggest the best choice of a solvent-phase extraction column for high-performance liquid chromatography in the analysis of drugs (*K36*). HPLC was also combined with several individual expert systems in order to aid the analyst in ascertaining the optimum chromatographic conditions (*K37*). Some of the common difficulties associated with the design, maintenance, and use of expert systems were addressed by Bourguignon et al. by implementing a hypermedia version of CRISE, an expert system for HPLC (*K38*). In the closing of a major undertaking, final results were reported for the ESCA (expert system for chemical analysis) project in liquid chromatography (*K39*). In ion chromatography, Mulholland and co-workers discussed the design and application of an expert system for determining suitable chromatographic conditions with respect to the column, detector, and mobile phase (*K40*). Knowledge-based systems were also employed in connection with gas chromatography. For example, Scheuer described WANDA, an expert system which assists in the interpretation of gas chromatograms of trace organic substances (*K41*). In another application, an expert system was used to detect gas chromatographic system instability during the analysis of atmospheric methane (*K42*). The combination of an expert system with various methods for multivariate data analysis was discussed and illustrated in the context of HPLC-UV data (*K43*).

Although the applications above concern quantitative analysis, most of the use of expert systems in chemistry have been directed toward qualitative analysis of spectra. The knowledge-based system ESSESA was devised for structure elucidation on the basis of spectra. The determination of chemical structure involves a novel algorithm that perceives the smallest, linear independent set of rings (SSSR) (*K44*). Infrared spectra of copolymers were interpreted by an expert system on the basis of spectrum–structure correlations derived from the spectra of homopolymers (*K45*). Perkins et al. implemented an expert system in which principal components analysis is used for infrared spectral analysis. The classification rule is generated from a training set of spectra of chemical species containing the functional group(s) of interest (*K46*). This system was applied to infrared spectra taken in both the vapor phase (*K47*, *K48*) and the condensed phase (*K49*). Other applications involving the use of expert systems in the interpretation of infrared spectra included the monitoring of oil degradation (*K50*), the detection of silicon impurities in electronic materials (*K51*), and the identification of functional substructures in various gaseous (*K52*) and condensed-phase (*K53*) mixtures. Koutny and Yeung developed an expert system to flag data points in real time for which a sufficient signal-to-noise ratio had been attained during data acquisition or processing. The omission of system-detected "inadequate data" in subsequent acquisition or processing greatly improved the efficiency of the imaging of DNA sequencing gels (*K54*). A diagnostic, knowledge-based system was reported for atomic absorption spectrometry (*K55*). Expert systems were also used for classification of fluorescence spectra of petroleum oils (*K56*), and for identification of radionuclides from γ-ray spectra (*K57*). In an arson analysis application, a knowledge-based system was designed to detect petroleum-based compounds from their GC/MS signatures (*K58*). Scott and co-workers constructed an expert system for predicting the molecular weights of organic species from low-resolution mass spectra (*K59*, *K60*). The pyrolysis mass spectra of three different classes of polymers were interpreted by another expert system (*K61*). An interesting, adaptive, hybrid expert system was reported for the interpretation of two-dimensional NMR spectra of proteins. The first two modules of this expert system are rule-based and can be trained with known spectra. The third module employs a genetic algorithm to assign the NMR spectral patterns to the amino acids in the protein sequence (*K62*).

Expert systems are potentially well-suited for assisting the analyst in planning the best approach to accomplish a particular determination with respect to analytical technique and procedure. One such system was designed for elemental analysis (*K63*) and applied to X-ray fluorescence spectrometry (*K64*). Another system was developed to help map out a strategy for analyses of soil and water pollutants (*K65*). Lee and co-workers integrated a relational database with an expert system to provide both data management and domain expertise (*K66*). In a biochemical application, decisions as to the timeliness and type of measurements to be made in a fermentation process were carried out by an expert system (*K67*). Knowledge-based systems can also serve as powerful diagnostic tools. For example, CLICHE (clinical chemist expert system) was designed using abductive reasoning for the diagnosis of inborn errors of metabolism (*K68*).

Knowledge-based systems have also served to validate data and interlaboratory comparisons. VALAB was developed to validate data in a biochemical laboratory (*K69*). Another expert system was designed to permit the transfer of standard methods between laboratories and the automatic conversion of these methods into reproducible procedures (*K70*). An expert system composed of several statistical procedures was constructed to select and evaluate the results of interlaboratory tests (*K71*).

Several other chemometric techniques also incorporated artificial intelligence. For instance, three structure–activity methods, CASE, MULTICASE, and CASE/GI, were compared for accuracy in the determination of mutagenicity (*K72*). Further, two learning schemes based on inductive logic were reported. The first consisted of a machine learning algorithm, INDUCT, which was trained on ion chromatographic methods (*K73*). The second comprised an adaptive learning network based on the abductory induction mechanism (AIM) for determining the components of a gas mixture analyzed by a sensor array (*K74*). By combining *n*-branched trees to represent coherence-transfer pathways in NMR spectroscopy, it was demonstrated that a structural matching algorithm can be used to predict NMR spectra (*K75*). Applications concerning process control continue to receive attention, too. In a novel approach, a variable structure learning automaton which can adapt to environmental changes was used to maintain optimum control of a continuous stirred tank fermenter (*K76*). Robotics and expert systems also received attention over the past two years. Isenhour et al. further refined their approach to coupled AI and robotics called the Analytical Director project, an AI system including robotics for the design, testing, modification, and implementation of its own analytical procedures (*K77*, *K78*). A robot controlled by an expert system to operate a standard additions procedure was also implemented (*K79*).

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