Computer Software Reviews

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MINPACK1-LIB. PC Scientific, M. G. Tuttle/PC Software. McGraw-Hill Book Company: 11 West 19th Street, New York, New York 10011. List price $465.00.

MINPACK1 is a FORTRAN library package for solving systems of nonlinear equations and nonlinear least-squares problems. It runs on IBM PC, XT, AT, or PS/2 computers and compatibles that can use any of the following FORTRAN compilers: IBM 2.0, IBM Professional 1.30, Lahey F77L2.22, Microsoft 3.31 or 4.01, and Ryan-McFarland 2.42. The package is available in compiler specific versions on both $5^1/_4$ in. and $3^1/_2$ in. diskettes. Routines providing support for 80X87 coprocessors as well as emulation are provided. There is no copy protection on the package and users can backup as they wish.

The package provides implementations of the Powell hybrid method for solving nonlinear equations and of the modified Levenberg-Marquardt algorithm for fitting nonlinear functions by minimizing the sum of the squares of their deviations. Both academic and industrial chemists will benefit from this package when they need to utilize these methods.

There are eleven machine language subroutines supplied in the package. Subroutines with names ending in "1" utilize default parameters and offer little flexibility with regard to convergence criteria, whereas those without the "1" are more general (and harder to use). Subroutines whose names contain "J", "DER", or "STR" require the user to supply the Jacobian matrix for the functions, otherwise a finite difference approximation to the Jacobian is provided by the package. HYBRD, HYBRD1, HYBRJ, and HYBRJ1 are used to solve systems of nonlinear equations. LMDIF1, LMDIF, LMDER1, LMDER, LMSTR1, and LMSTR are used for solving nonlinear least-squares problems, with the last two for use when limited memory is available. Finally, the subroutine CHKDER is provided to check the consistency of the Jacobian matrix with its corresponding functions.

The demonstration and test programs provided in the package are straightforward and clear. There is no problem for the user to implement them in a short period of time. The use of individual subroutines for specific chemical applications will, however, depend on the users' familiarity with FORTRAN. The whole package does what it is sold to do, but how effectively it can be used could be very different for different users. For those who are using the mainframe MINPACK-1 product, it would be a simple matter to move their programs to micro. Others must spend some time to familiarize themselves with the skeleton files provided in the package so as to have a good understanding of the calling sequences and the variables used, before they can adapt or modify them for their specific applications.

We tested the LM subroutines in both the Jacobian and finite different approximation by fitting experimental kinetic data to single and double exponential functions. The subroutines yielded identical results that were in agreement with independently derived values. The nonlinear equation solving algorithms were also tested with a real world system of nonlinear equations: a multivalued pair of equations describing steady state behavior of a bistable photochemical reaction. Although results in agreement with other methods were obtained, the internal scaling of the algorithm was inadequate to solve the problem and rescaling of the functions as well as initial estimates very close to the solutions were needed. The algorithm and documentation provided no help in resolving the problems encountered.

Borland's Numerical Methods Toolbox and Precision Plus' MATH-PAK 87 provide similar algorithms. The Borland product is, however, available only for Pascal. The Precision Plus product is available in versions for several languages including FORTRAN and Pascal. Finally, the book *Numerical Recipes* by Press et al. provides excellent and well-written discussion of the algorithms as well as source code (optionally available in machine-readable form) in several high-level languages.

Although the documentation provided is more than adequate to get the package working we found it rather dry (too much word processing, not enough style!) and incomplete as regards both the functioning of the algorithms and the use of the screen interface provided in the package.

We have successfully run the package on AT type microcomputers with and without coprocessors as well as on a PC clone without a hard drive. It is extremely inconvenient to use the package (or for that matter, the Microsoft FORTRAN Compiler, itself) in a computer having only floppy disk drives; a minimal system for compiling and running these routines would have 2 floppies with a hard disk or a large (>1Mbyte) expanded memory to use in place of the hard drive.

These routines are very fast; a few seconds suffice to determine four parameters in the least-squares fit of ca. 30 data pairs. We made no attempt to quantitate speed; means of estimating speed and memory requirements are given in the documentation which should be useful to those who must deal with large data sets or real time computation.

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Current Contents on Diskette. Institute for Scientific Information: 3501 Market Street, Philadelphia, PA 19104. List Price $600.00; publication series for IBM and Macintosh $380.00 (or $550.00 with subscription to printed version); 1200 publication series for IBM $725.00 ($895.00 with printed version).

The impact of the microcomputer on this profession has steadily grown and it is now actually uncommon to find a chemist's office lacking a personal computer. Until recently, the PC has been used mainly as a means of facilitating written communication (word processing and drawing programs) and as a means of conveniently interfacing with mainframe computers through terminal emulation programs. However, recent advances in the speed of microcomputers and in the reduction of hard disk storage costs have opened the microcomputer as a convenient means for data storage and retrieval. Current Contents on Diskette represents a critically important addition to the library of PC applications. The current review deals only with the Macintosh version. A review of the IBM version is underway.

Current Contents on Diskette is implemented through the Apple Macintosh Hypercard environment. It makes available to the user the information in the printed issues of *Current Contents* but implements as well the extremely valuable bonus of permitting the user to find searches that go far beyond the keyword index found in the printed version. Further, the retrieved information can be exported from the Hypercard environment in a number of very useful ways.

The program is supplied on a double sided, 800K floppy disk and requires that the user already have Hypercard. It is not, however, necessary that the user have previous experience with Hypercard and indeed this evaluation of Current Contents on Diskette was the reviewers first experience with Hypercard. The actual information is supplied in a compressed form so that each issue's data can fit on a single floppy. A proprietary compacting scheme (StuffIt and UnStuffIt) is called upon to decompress the information simply by double clicking on the file. This process is very space intensive, as, at least temporarily, both the original and decompressed versions of the data must co-exist on the hard disk. After decompression the original file can be deleted. Nonetheless, maintaining several weekly issues will require extensive hard disk space as, for example, the June 20 issue of *Life Sciences* occupies 1.2 megabytes once decompressed. Double clicking on the decompressed version of the file then implements the Hypercard routines that make the data available. The information can be scanned in very much the same fashion that one would use the printed version and indeed the layout is quite similar and very readable. Conversely, individual searches can be implemented with either AND or OR logic searching either for strings (where, for example, a search for "gene" would be found in a title containing the word "general") or word searches where the previous example match would be excluded. It is in these search routines that the version on diskette has greatly enhanced value over the printed issues. For example, the reviewers own attempted use of the printed physical sciences version for searches of "non-linear optical materials" was greatly frustrated by the very much more prevalent reference to the term "non-linear" by mathematicians.

Once a search has been executed, the information is displayed with the standard Macintosh scroll bar permitting movement from one reference to another. This is, however, rather inconvenient and scanning a large number of search hits would be greatly facilitated if a method were available to jump from one to another with the information for each starting at the top of the screen. Further, there is no indication of the number of hits that have been obtained and to determine if one's search has been too broad, the rather slow process of scrolling through the hits must be executed. Once a subset of the file has been obtained it can be printed, or exported to a text file on disk. Further, routines are provided that permit ready printing of "Request-A-Print" forms for requesting reprints from the author or for printing requests to be sent to ISI for copies of the "Genuine Article" (for a fee).

2748 *J. Am. Chem. Soc., Vol. 111, No. 7, 1989*

Book Reviews

Overall, this is a very nice implementation of Hypercard that represents a real advance in current awareness. Deficiencies are minor and include, in addition to the aforementioned difficulty of scrolling through

hits, relatively slow searches. While the current release covers only the life sciences issues of Current Contents, future release of the Physical Sciences issues on diskette is planned.

Book Reviews[*]

Methods in Enzymology. Volume 158, Part A, and Volume 159. Volume 158: Edited by James F. Riordan (Harvard Medical School) and Bert L. Vallee (Harvard Medical School). Academic: New York and Orlando. 1988. xxv + 464 pp. $59.00. ISBN 0-12-182059-9. Volume 159: Edited by Jackie D. Corbin (Vanderbilt University) and Roger A. Johnson (State University of New York at Stony Brook). Academic: New York and Orlando. 1988. xxxvii + 849 pp. $89.00. ISBN 0-12-182060-2.

Volume 158, Part A, is subtitled "Metallobiochemistry". It consists of 33 contributions under three headings: "Sample Preparation", "Analytical Techniques", and "Analysis of Metals".

Volume 159 is subtitled "Initiation and Termination of Cyclic Nucleotide Action". It consists of 74 contributions, under six section headings: "Cyclic Nucleotide Cascades", "Assays of Cyclic Nucleotide Levels, Turnover, and Transport", "Cyclic Nucleotide Action", "Protein Phosphates", "General Methods for Studies of Phosphodiesterases", and "Methods for Isolation and Studies of Various Phosphodiesterase Isoenzymes". Each book has a true author index and a substantial subject index.

Marvels of the Molecule. By L. Salem (Universite de Paris-Sud). VCH: New York and Weinheim. 1987. xii + 88 pp. $16.95. ISBN 0-89573-345-5.

This little book is essentially an essay, written to "demystify modern chemistry". To do so, it avoids arcane scientific terminology (there is a glossary, however) and relates the phenomena of chemistry to things encountered in everyday life. In a foreword, Roald Hoffmann describes this book as "a modern Baedeker, a guide to the seemingly strange country of the chemists." Indeed, it succeeds in making such concepts as molecular bonding, reaction kinetics, catalysis, etc., reasonably comprehensible at a nearly intuitive level. It is written for the lay reader, but could be very helpful to the beginning student as well (and to instructors looking for ways to explain basic concepts).

Grosse Molekuele. By Hans-Georg Elias. In German. Springer Verlag: Heidelberg and New York. 1985. 204 pp. ISBN 3-540-15599-6 and 0-387-15599-6.

The book *Grosse Molekuele* (Giant Molecules) with its subtitle, Popular Talks about Synthetic and Natural Polymers, is a most delightful book and is recommended for scientists and nonscientists alike. It is one of the few books on scientific subjects that can be understood and appreciated by almost everybody. The author introduces the subjects by saying: "if macromolecules did not exist there would be no life; people, animals and plants would be without structural, storage and transport materials; without macromolecules, life would not propagate."

The author provides an amazing amount of information on how much can be produced on an acre of land in wool, natural rubber, cotton, meat, rice and on synthetic fibers. We find in the book information on fibers, adhesives, motor oils, foams, rubbers, glasses, and many other materials; how they are made and how they are used. The book describes the structures of chemical molecules, monomeric building elements that ultimately result in high molecular weight substances; he describes the enzymatic degradation of polysaccharides and the similar enzymatic tenderizing of meat. He points out the relation between sweet potatoes and tough meat, what happens when spaghetti foams, what happens when bread becomes old, what processes occur when we iron clothes or when we shave, and how the Xerox machine works.

The author educates the reader with the structures of stereoregular macromolecules, helical macromolecules, synthetic and natural fibers. The composition of paper and leather, their fabrication, and the optimization of their properties, including their texture, are mentioned. He emphasizes that some of the polymers are not only cheaper but also

stronger than steel; the author takes advantage of his extensive knowledge of history and refers to the use of polymeric materials (not then recognized as such) from the Roman and even Egyptian times.

Elias' book on Giant Molecules is delightful to read; I have read it several times and still occasionally read one or the other chapter. I consequently recommend it for people that enjoy scientific reading that is close to everyday life.

Otto Vogl, *Polytechnic University, Brooklyn*

Teratogens: Chemicals Which Cause Birth Defects. Edited by Vera Kolb Meyers (University of Wisconsin—Parkside). Elsevier: New York, NY. 1988. xii + 472 pp. $171.00. ISBN 0-444-42914-X.

This book is Volume 31 in the series *Studies in Environmental Science.* The stated aim of the monograph is to address the practical aspects of teratogens, particularly the need to obtain information about the potential of chemicals as reproductive hazards. The book consists of eight chapters: (1) How to Obtain Information About the Teratogenic Potential of Chemicals by H. B. Morgan, G. S. Danford, F. M. Holland, K. C. Miller, E. T. Owens, B. E. Ricci, S. Y. Uppuluri, and J. K. Wassom, (2) Registry of Toxic Effects of Chemical Substances as a Source for Compiling a List of Teratogens by V. K. Meyers, (3) Reproductive Hazards in Industry: Identification and Prevention by K. Hemminki and M. Lindbohm, (4) Teratogenic Chemicals in Undergraduate General Chemistry Laboratories by D. K. Kolb, (5) Safe Handling of Teratogenic Chemicals by B. C. McKusick, (6) Use of Registered Data in Studies of Occupational Exposure and Pregnancy Outcome by M. Lindbohm and K. Hemminki, (7) Long-term Effects of Chemicals on Developing Brain and Behavior by M. Mirmiran and S. De Boer, and (8) Teratogenicity of Pesticides and other Environmental Pollutants by M. J. Kland.

The first two chapters provide an introduction to numerous databases of information on teratogenic chemicals. Chapter 2 is followed by two appendices which list over 5000 compounds and mixtures for which reproductive effects have been reported. Substances are tabulated alphabetically by parent compound names, along with CAS registry numbers, as they appear in the Registry of Toxic Effects of Chemical Substances (RTECS). The authors have made an extra effort to provide a comprehensive listing of teratogens. However, the appendices include many laboratory reagents not normally associated with serious toxic hazard (e.g., sodium chloride, magnesium sulfate, most amino acids, carbon dioxide, sucrose, carbon), and no comparative data from animal tests are included with the compounds. Therefore, chemists using the tables must seek more detailed data on the teratogenicity of specific compounds from the original RTECS files or other sources.

The two chapters by Hemmicki and Lindbohm address the occupational risks associated with teratogens. The essays are very general in scope and focus on Scandinavian studies of industrial exposure.

Kolb's discussion of teratogenic compounds in undergraduate laboratories will be of interest to educators. Several compounds with teratogenic potential are widely used in undergraduate laboratories; the potential hazards associated with such substances are described and handling procedures to minimize exposure are suggested. The safe handling of teratogens is given additional coverage in the chapter by McKusick.

The effects of chemicals on neurobehavioral development are reviewed in the chapter by Mirmiran and De Boer. Numerous compounds and their specific developmental effects are discussed. A large number of references to experimental studies are provided.

The chapter by Kland reviews studies on the teratogenic potential of pesticides and other environmental agents. Some particularly notorious compounds, such as dioxins, PCB's, and PBB's, are given special attention; both epidemiological studies and anecdotal accounts of the teratogenicity of these compounds are summarized. One error in this chapter may mislead some readers. It is stated that pentachlorophenol, often called PCP, is the same compound as the street drug, "angel dust"; the latter substance is actually phencyclidine (1-(1-phenylcyclohexyl)-

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[*] Unsigned book reviews are by the Book Review Editor.