Computer Software Reviews

STATPAK. Version 4.12. Northwest Analytical, Inc., 520 NW Davis St., Portland, OR 97209. List price $495.00; educational discounted price $350.00; source code $75.00. Not copy protected.

Statpak is a "multi-function library of statistical analysis and support routines" for the IBM-PC, XT, AT, and compatibles. There are 67 compiled BASIC routines that are written in Microsoft BASIC and compiled with the Microsoft QuickBasic compiler. All computations are done in single precision except the routine MLINREG (multiple linear regression) which is in double precision. The source code is available to registered users from the vendor for $75.00.

To run Statpak, DOS 2.0 or higher is needed with a minimum of 512K RAM (384K user free). The software supports IBM-PC/XT/AT and PC compatibles with color graphics adapter (CGA), enhanced graphics adapter (EGA), or compatible Hercules Monochrome Graphics' cards. STATPAK supports the following printers: Hewlett-Packard Series (Laserjet+, Thinkjet, and 82905 Dot-Matrix), C-Itoh Prowriter, DEC LA50, Epson MX, IBM Graphics Printer and Proprinter, NEC 8023, and Okidata Microline 92. I had to call the vendor to request a driver for the Hewlett Packard LaserJet series II printer that was not included on the 9 disks. There is also support for 5 different plotters. There is no support for a mouse, math coprocessor, or fonts and no on-line help.

Statpak is supplied on 9 MS-DOS 5.25 in. low-density double-sided disks that are not copy protected. If loaded onto a hard disk, which is highly recommended, it will occupy 2.37 mb of space.

Installation of Statpak was extremely simple and fast taking approximately 5 min. There is no "SETUP" utility, and all you do is copy the 7 distribution disks onto your hard disk and copy three files from the remaining 2 disks that are drivers for the type of graphics, printer, and plotter device you are using. Statpak can be run from a floppy disk system, but performance and versatility will be greatly affected.

The work flow of Statpak begins with the main menu that includes utilities (some DOS routines), system initialization (color configuration, path assignments, etc.), and entry to the menu (SPMENU) for the statistical routines. Statpak is menu driven, and the routines are selected by letter or can be started by typing in the name of the routine.

Once in the statistical menu (SPMENU), there are (A) data entry and file utilities, (B) conversion utilities, (C) mathematical utilities, (D) graphics and plotting, (E) probability calculations, (F) single-variable statistics, (G) distribution functions, (H) regression and correlation, (I) means testing and χ^2 analysis, (J) nonparametric statistics, and (K) analysis of variance (ANOVA).

Starting in (A) data entry and file utilities, the user will find a spreadsheet-like screen editor for data input. Once the data have been saved, it becomes the default data set for all the routines. This meant that the user can run the various routines of Statpak with minimum typing, a nice time saving feature. Statpak can import/export .DIF, SYLK, ASCII, and Lotus 1-2-3 .PRN files.

Using the editor was simple and fast and you can only enter and delete data. To transform variables into new variables, you have to exit this routine and enter the "SPLICE" routine. This was tedious and time consuming. Trying to edit the data with the SPEED (line oriented file editor) routine was difficult because the user must use many commands. I decided that this routine was totally useless. I found it more useful to use EXCEL (Microsoft Corp.) or LOTUS 1-2-3 for data entry, editing, and transformations and then save the file in ASCII or in .PRN (LOTUS output format) and import it using Statpak's file conversion utility.

I evaluated the software on an IBM-PC XT with an 8088 processor running at 4.72 MHz and on an Advanced Logic Research (ALR) machine with an 80386 processor running at 25 MHz. The routines ran extremely fast, even on the XT. I reviewed the various routines of Statpak using my tree-ring data set that consisted of 36 variables (12 elements, 12 months of temperature and precipitation data) on trees of age 110 years. To compare the results, performance, and general usefulness of Statpak, the data set was previously analyzed with use of SAS (Statistical Analysis System) on a mainframe.

For the trace elements in tree-rings, I wanted to determine how the 12 elements (dependent variables) in the tree-rings were influenced by the 24 climate variables (independent variables). This was a multivariate problem for which I used Statpak's MLINREG (multiple linear regression) routine with forward stepwise to select the best subset of climate variables that could predict the element concentrations in the rings. Since the independent variables (temperature and precipitation) consisted of two different units of different magnitude, the variables had to be standardized to a mean of 0 and standard deviation of 1. I used Statpak's STDSCORE (standardized scores) routine. The major drawback of this routine is that only one variable can be standardized at a time. This meant that I would have had to create 24 different output files, merge them, extract the standardized variables, and do the regression analysis. This turned out to be much work and it was abandoned.

Statpak also has graphics routines that are easy to use. To create a graph and print it, the user must go thru three plotting routines that can be time consuming. The user can request that output from several statistical routines be sent to a high-resolution graphics file that can be edited. However, you cannot put labels on the x-axis and there are only two locations for the y-axis label. Graphs are only printed in portrait orientation. A high-resolution graphics file was sent to a Hewlett Packard LaserJet II printer for review, and the output was not publication quality.

There are several very useful routines in Statpak. One of them is ONEVREG (one independent variable regression). In this routine, the least-squares coefficients are calculated for four function types that include (1) linear, (2) exponential, (3) logarithmic, and (4) power law. The detailed output includes standard error of estimate for the regression coefficients and R^2. The regression coefficients can then be saved to a file and recalled later with the routine FUNGEN. Another useful routine of Statpak is FUNGEN (function generator) where the user enters an equation with one or more independent variables. The user is then prompted for input and the results can be output to screen or file. However, if a syntax error is made, you have to retype the entire equation, which can be annoying for long equations. Additional useful routines of Statpak are time series analysis, ANOVA, general means testing, descriptive statistics, correlation and covariance, and t-test.

I was impressed with the detailed output from the descriptive statistics routine that included arithmetic (95% confidence interval), geometric, harmonic, and quadratic means, sum, min, max, std, %RSD, variance, standard error, and coefficients of skewness and Kurtosis. The user can request that the output be sent to screen, printer, or file (ASCII). I sent the output to a file and recalled it later using a word processor. I was shocked that the impressive output that appeared on the screen and printer was not the same output that was sent to the file. The output file consisted of the variable names and only the raw numbers with no format or titles. You need the manual to decipher what the numbers represent and it is a useless option because the file cannot be incorporated into a document with use of a word processor.

The manual, 590 pages, was well-written and organized. For each routine, there was a clear description of its purpose with a detailed example on how to use it. What I really enjoyed most about the manual was that it was very honest. It explicitly stated what the software can and cannot do. If the user tries to run the software without reading the manual, they may be disappointed in the usefulness of Statpak. There is an appendix that gives the formulas for all the statistical computations used in Statpak. For registered users of Statpak, there is technical phone support from the vendor.

In summary, Statpak is a very simple-to-use statistic package that can be very useful to both the academic and industrial chemist. The user can be proficient in using Statpak in less than 10 min. It is ideal for use in the undergraduate laboratory and no knowledge of statistics is needed to run the routines, and the results are comparable to those from SAS. It is extremely user friendly, and it is much easier to learn and use than SAS-PC, SYSTAT, and STATGRAPHICS, although not as powerful. There are no cluster analysis routines, principal components, and factor analysis. I highly recommend Statpak for routine statistical analysis despite some of its shortfalls. The routines execute quickly and no elaborate computer or high-powered CPU's are needed to run Statpak. If what you need is a statistical package that is extremely easy to learn and use, then Statpak is your statistician.

Gene S. Hall, *Rutgers, The State University of New Jersey*

Expressionist. Prescience Corporation: 814 Castro Street, San Francisco, California. List price $129.95. Academic discount available by contacting the company directly.

Expressionist is a program for equation typesetting for use in the Macintosh computer.

The program is contained on a single disk and the package includes a user's manual and a quick (and useful) keystroke reference card. It

can be used on all Macintosh computers and is extremely straightforward and uncomplicated to use. It allows easy editing of an expression in a similar manner as MacWrite. Prescience Corporation informs you that the use of Expressionist with Microsoft 4.0 can present a problem in terms of Microsoft 4.0 corrupting picture information when you paste a picture in. This results in Expressionist not recognizing the picture and it "chokes". Prescience Corporation has determined that the fault lies in a bug in Microsoft 4.0 and suggests several options to work around this problem.

It will be a useful addition to a laboratory that requires complex equations with unorthodox symbols in reports and communications. Prior to this program (and others), typesetting of these equations has been difficult and tedious, but now it has been reduced to a simple and straightforward task. It adds a professional touch to reports and will be particularly useful for publications submitted to journals that require the manuscript to be camera-ready. Numerous journals and book companies now require camera-ready manuscripts in order to improve the speed of publication and reduce cost. A professionally produced complex equation appears so much better than the hand-drawn equations one finds frequently in the literature.

Joseph Sneddon, *University of Lowell*

CLR ANOVA. Clear Lake Research: 5616 Morningside, No. 127, Houston, TX 77005. List Price Unknown.

CLR ANOVA is an analysis of a variance package written for the MacIntosh which can compute up to 10 factors with 5 between and 5 within subject variables with equal or unequal sample sizes. After computing the anova, the program can compute marginal means, pairwise comparisons, simple effects, and specific contrasts. Furthermore, interactions can be plotted graphically. The graph can then be pasted into a file which can be accessed by MacPaint, Superpaint, or MacDraw or sent directly to the printer.

CLR ANOVA does exactly with it is supposed to do. Furthermore, the package is very easy to learn and operate. One can become an expert in use and operation in under an hour, as long as one knows how to use pull down menus. Unfortunately, the data files must be constructed with the raw data only; labels and headings are not allowed. After the anova is performed, the statistical analysis does not take full advantage of the window techniques of the MacIntosh in that only one analysis window can be open at a given time. This necessitates printing or saving each window, a potentially tedious operation when many variables are present. The graphs, once produced, can only be crudely modified in CLR ANOVA. A custom designed graph can be created by transferring the graph to a graphics package such as Superpaint. While none of these objections are at all serious, it seems that such a narrowly focused statistics package would perform these tasks well.

While the program has no serious problems, I question how generally useful the package is for the average chemist. This program does not perform other more common statistical tests which the program Statview does. Statview also computes anovas, but it does not allow any further analysis once the anova is computed. Essentially CLR ANOVA performs tasks that the vast majority of chemists may never need, while neglecting to perform the less sophisticated routine statistical operations needed. This reviewer would recommend a broader based statistics package such as Statview, rather than CLR ANOVA.

Robert E. Rosenberg, *Columbia University*

*Book Reviews**

Advances in Polymer Science. Volume 94, New Polymer Materials. With contributions by Tohru Takekoshi (General Electric Corp.), Masahiro Irie (Kyushu University, Japan), B. Boutevin (Ecole Nationale Superieure de Chimie, France), and Yasuhiko Tobato and Yoshito Ikada (Kyoto University, Japan). Springer-Verlag: New York and Berlin. 1990. xii + 160 pp. $74.50. ISBN 0-387-51547-X.

This is a poorly edited and poorly typeset volume containing three good reviews and one very poor review of very different areas of polymer chemistry. The review of Polyimides by Tohru Takekoshi is a well-written presentation of the advances of the past 10 years in preparation of polyimides with better processability or applications in composites. The extensive emphasis on monomer and polymer synthesis is supported by tabulations of data and illustrative examples. The synthesis compendium is arranged by desired properties (processability, crystallinity, composite use, etc.) or by products (monomers dianhydrides, diamines, etc.). The review is current, well organized, and well referenced.

The review of Photoresponsive Polymers by Masahiro Irie is clearly written, well supported by both structural equations and data compilations, comprehensive, and moderately well buttressed by references, one-half of which come from the 1980s. The topic lends itself well to review since a discussion of the seemingly infinite ways that chromophore-containing polymers adjust to and reversibly relax from exposure to light is fascinating.

The third review on Telechelic Oligomers by Radical Reactions by B. Boutevin is the nadir of the book. The English is poor with numerous sentences that are literally indecipherable. Coupling poor English with poor typesetting makes this section of the book very hard to read. Organization is wanting, illustrative examples are missing, summations of data are few and lack breadth, and the presentation of the information is choppy with subtopics, anomalies, and details of specific materials dropped into the discussion in short sentences. Only one-third of the references are from the 1980s.

The final third of the book is taken up by Yasuhiko Tabata and Yoshito Ikada's review of Phagocytosis of Polymer Microshperes by Macrophages. How the body's immune system attacks or responds to polymers is of major importance in biomedical research and controlled drug release. The review is well written, comprehensive, detailed, and well ordered and organized. The topic of how the body attacks and degrades small spheres of step-synthesized polyesters, ethers, and saccharides is extensively discussed. Properties and structures which promote or delay such degradation are defined. The review, though good, suffers from the authors' preference for giving references without the year of publication, a practice which illustrated the poor editing shown repeatedly in this volume.

The poor editing, the very poorly written review on telechelic oligomers, and the typographical errors make the information presented in this book suspect. Without obtaining the original references, I would be loathe to accept any data presented in this book. For that reason, I would not buy the book, would not request its purchase by local libraries, and would only obtain it on interlibrary loan to gain a general overview and update on the topics covered. I would not use the book as a sole reference on anything. The book does have one benefit that too many review compilations lack and that is an index. The index is cursory but still present.

John J. Meister, *University of Detroit*

Principles of Catalyst Development. By James T. Richardson (University of Houston). Plenum: New York and London. 1989. ix + 288 pp. $49.50. ISBN 0-306-43162-9.

During the early part of my graduate studies about 15 years ago, I had the opportunity to attend a short course "The Uses of Heterogeneous Catalysis". This short course was, and still is, extremely popular. At the time I attended, it was taught by Joe Hightower (Rice University), Dan Luss (University of Houston), John Sinfelt (Exxon Research and Engineering), and the author of *Principles of Catalyst Development*, James Richardson. The course was designed to teach the fundamental aspects of catalysis to students who had a background in chemistry or chemical engineering but lacked formal training in catalysis. This short course truly helped me get started in research in heterogeneous catalysis.

Principles of Catalyst Development is based upon and is similar in scope to the short course. The practice of heterogeneous catalysis relies upon utilizing scientific skills from diverse backgrounds, and coherent coverage of the material for beginners is difficult. Relying upon his many years of experience in teaching not only short courses but also as a chemical engineering faculty member, Professor Richardson has, in my opinion, presented a textbook which covers the important aspects of catalysis very clearly.

Each chapter in the book is, in essence, an introduction to a particular facet of catalysis. Major topics include a vital introduction to heterogeneous catalysis along with chapters dealing with structures, catalyst development, common catalytic materials, design, preparation, characterization, and deactivation. The topics are not covered in great detail, which is as expected for a book designed to be an overview. However, 283 references (mostly to books and review articles) are given which

*Unsigned book reviews are by the Book Review Editor.