

Let the buyer be aware . . . ,

Methods in Enzymology, Vol. 210. Numerical computer methods. Ludwig Brand and Michael L. Johnson, editors. Academic Press, San Diego. 1992. 718 pp. \$95.00.

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A current magazine aimed at buyers of scientific biomedical instruments shows that nearly every device made now is linked to computer technology. The main aim of this volume is to make the buyers aware of the numerical computer methods that have developed in parallel to the hardware.

A section of the book discusses transformed data, e.g., a Scatchard plot, or a double reciprocal plot of Lineweaver and Burk. This methodology was used to transform a set of data to a straight line, and then to fit the transformed data to extract some set of parameters. A recent article by Dean Burk about the origin of his paper with H. Lineweaver's, some 50 years later (Burk, D., 1985. *TIBS*. 11:202-204), reports that the double reciprocal plot, "has continued to reign essentially unchallenged." However, fitting to a linear least-squares straight line assumes that the experimental uncertainties follow a random distribution (they don't), and are parallel to the Y-axis (they might not be). Now, with high-speed computers capable of nonlinear least-squares analysis, there's no need to first transform the data before analysis.

And that's just from the three page preface!

The thirty chapters of the book are separated into three sections. In the first section, basic methods such as nonlinear least squares analysis, global analysis, weighting functions, analysis of residuals, singular value decomposition, and interpolation methods, are described. Many of these were written by Michael Johnson and his colleagues, and they are excellent.

The second section presents specific examples of biomedical research, part of it coming from Lennie Brand's own investigations on time-resolved fluorescence spectroscopy. Included are ligand-binding data, enzyme-cata-

lyzed reactions, protein-DNA complexes, circular dichroism spectra, photoacoustics, binary mixtures of phospholipids, deconvolution analysis of hormone data, and time-resolved fluorescence spectroscopy. I almost missed a section on phase fluorometry ("Alternatives to Consider in Fluorescence Decay Analysis," by J. R. Knutson), which gives a brief history of the technique, then contrasts it with pulse fluorometry. Knutson refers to "pulse partisans" and "phase partisans" when talking about the members of the two groups, but his preliminary analysis shows that neither method can claim a clear advantage in general purpose fluorometry.

The third section introduces new methods that are currently being developed, such as biological sequence comparison, symbolic mathematics, fractal applications, and artificial neural networks. These are fascinating, and I have already purchased a symbolic mathematics software package.

In a recent special section in *Science* (Pool, R., 1992. *Computing in Science. Science (Wash. DC)*. 256:44-62), the issue of software packages was previously brought up. The article said that: "Just a few years ago, (a scientist) faced an unpleasant choice: either write his own software, a tedious and difficult job, or else use programs written by another researcher, which would most likely be idiosyncratic and difficult to learn." The article was speaking about molecular modelling, although it could have been addressing the topics in this volume. Today, for some tasks, the job is being done by commercial software packages. For the most part, however, it is not being done for the computer methods at hand, because (aside from symbolic mathematics and one or two others) the demand is seen as far too small. However, this book makes a good case for spreading the word about numerical computer methods.

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