Fitting features

Bruno Orsi

Enzfitter 1.05. *Biosoft, 22 Hills Road, Cambridge CB2 1JP/PO Box 580, Milltown, New Jersey 08850. £125, $249.*

To the inexperienced, a result of more than six figures printed on computer paper often assumes the status of an absolute truth. The judicious use of *Enzfitter* should provide such people, and others, with a more balanced view of the use of computers and statistics in the evaluation of experimental results. It is to the author's credit that he asserts that neither of these devices, for that is what they are, can "turn bad data into good".

Enzfitter is designed to be used on an IBM-PC (XT or AT) or a "true compatible". It is intended for curve-fitting generally, and more specifically for statistical analysis of ligand binding and for handling enzyme kinetic data. The program is versatile in that it will handle various types of screen graphics (CGA, EGA or Hercules) and a variety of printers (Epson compatible). It is pleasant to record the absence of a certain type of rodent as the author has decided to use the rather more effective method of a key input to initiate the desired course of action, the options being presented in a series of well-designed and simple overlapping 'pop-down' windows with textual prompts, rather than barely comprehensible icons.

The method of calculation uses a non-linear regression, even for linear equations, based on the Marquart algorithm. It is rapid and does not depend on having good preliminary estimates of the constants. A notable feature of the program is the ability to show the fitted data in a screen graphics display. Optional numerical transformations are available, the most important of which are graphical displays of the residuals after the regression has been completed. Standard errors notwithstanding, this is surely the simplest and easiest way of assessing, literally at a glance, whether one has picked the right equation and whether the data are a good fit or not.

One of the most valuable features, that introduces a great deal of flexibility, is the capacity to input quite complex equations, or transformations of equations, of one's own choosing in an easy manner (a peculiarity of the version 1.05) I used, however, was its reluctance to accept $x \triangle n$ (n= 1,2. . .) for such equations, and it was necessary to use the rather cumbersome process of repeated multiplication). But my only real criticism of this software is in the treatment of weighting factors especially where both variables are subject to error, an extremely common situation with ligand-binding data. Another improvement, useful for inhibition studies, would be the facility to enable the program to deal with a second independent variable.

Some typographical errors apart, the manual supplied with the software is more than adequate. It is clearly written, especially the chapter on the theoretical background which is well worth study in its own right. I do not entirely agree with the author's black-and-white attitude to the linear transformations of the Michaelis–Menten equation; this, perhaps, is reflected in his very selective bibliography, in which he ignores a vast subculture that has been devoted to this problem for almost 60 years.

Is *Enzfitter* worth buying? The expert kineticist will almost certainly have his own software so this program is likely to be of passing interest only. But for the large number of research workers who want a good, rapid and visual analysis of their data, and who do not have the time or inclination to develop their own software, it is indeed a worthwhile purchase. □

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Into solution

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MathCAD 2.0. *MathSoft, One Kendall Square, Cambridge, Massachusetts 02139/ Freepost, Tamworth, Staffordshire B79 7BR. $349, £345+VAT.*

As a boy, embarking on what seems likely to be a lifetime of sums, I dreamed up the mathematician's equivalent of Sparky's Magic Piano. All you had to do was write down the sum to which you required an answer and the Magic Paper did all the work, setting everything out neatly. I have used *MathCAD* 2.0 for the past six weeks and it seems that my dream is pretty close to fulfilment.

MathCAD is "an editor that deals with equations" on an IBM-PC (or any compatible machine) with 512K RAM and CGA, EGA or Hercules graphics. The things it can do include all numerical calculations involving standard functions (including Bessel functions, statistical functions, real and complex fast Fourier transforms and their inverses). Integration is by Simpson's rule, differentiation by a four-point estimation process. Matrices are inverted and determinants evaluated by LU decomposition, using Crout's method with partial pivoting. Systems of equations and inequalities (called 'solve blocks') are solved by the Levenberg–Marquardt method. Full references are provided for all the algorithms used — the package is clearly designed by mathematicians for mathematicians. The algorithms work to specification and were extremely difficult to 'crash', despite my best efforts.

It took a day to come to terms with the editing facilities, using only the rather dry manual provided. It took me only another day to become hooked on the package. It loaded on a Toshiba T1000 laptop without the slightest difficulty, and the drivers provided for Epson dot-matrix and HP LaserJet printers worked perfectly. *MathCAD* occupied 360K of RAM but it recognized the LIM expanded memory. At first I found the whole philosophy of *MathCAD* difficult, comparing the package unfavourably with Lotus 1-2-3 and on occasion seeing it as little more than an untidy spreadsheet. But this feeling evaporated as I began to make use of its potential.

Graphs can be plotted almost instantly. The quality is adequate for most purposes, but post-processing using a graphics package would normally be required for publication. The display and the printed output (which is just a copy of the screen) are not beautiful; they rely on the use of ASCII characters in full size throughout, including super- and subscripts, integral signs and square-root signs. IBM extended characters are available if the printer can produce them.

The algorithms are versatile and robust but occasionally rather slow. For example, to invert a 7×7 matrix took 25 seconds, while Lotus 1-2-3 took less than one second. With a maths co-processor this problem would not be so serious. *MathCAD* baulked at matrices larger than 7×7 though the manual promised up to 10×10. There is some room for improvement here.

The package is almost ideal for generating work-sheets at all levels from primary-school to final-year undergraduate mathematics. It proved easy to design sheets of worked examples on Fourier series and Laplace transforms, vector and matrix operations. The possibilities for using it as a teaching and learning aid are mind-boggling. *MathCAD* does not provide facilities for drawing diagrams, nor are there 3D plotting routines — backs of envelopes will still be required. But these are minor shortcomings measured against the power of the package.

The price is currently rather high for individuals, but then the real price of a scientific calculator has fallen by 98 per cent in 15 years. If the same happens to *MathCAD* it, or something similar, will be an indispensable aid for every scientist — and every schoolchild — by 1995. □

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