Norton Utilities—Advanced Edition, Version 4.5†

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Received February 7, 1989

Next to DOS, the best thing to buy for an IBM-PC or IBM clone computer is Norton Utilities. Norton Utilities is a file management and data recovery package. The latest version, Advanced Edition, Version 4.5, continues the tradition of the previous versions, but with increased speed and a friendly front-end interface. The program comes in both low density 3-$^1/_2$- and 5-$^1/_4$-in. versions, so you cannot get an incorrect set of disks. Version 4.5 supports DOS 4.0, the DOS 3.3 extended disk partitions, and Compaq's DOS 3.31's large partitions, as well as PC-DOS/386. The documentation has been improved, and a new manual, "The Norton Trouble Shooter", has been written. There is also a 40-page booklet, "The Norton Disk Companion", that is a simple to understand guide to disks, but alas, has no pictures or figures. There is also a newly developed install program that makes the installation of this version very simple. This new version has a half-dozen new modules. These include a batch enhancer for helping to make batch files interactive. There is a file date and time function that lets one redate or back-date files. The Norton Control Center program allows one to control the hardware by setting the cursor size, screen colors, time and date, and so on. The Norton Disk Doctor is another new program, and it diagnoses a number of floppy- and hard-disk problems and fixes physical or logical errors on the disk. Lastly, there is the Safe Format program, a PC's version of safe sex.

Norton Utilities is a very useful collection of programs to help one correct the many mistakes likely to be made with a PC. Accidently erasing files is probably the most common error anyone makes using a PC. The Unerase program is probably the most often used routine module in the Norton Utilities package. Next there are the Wipedisk and Wipefile modules. The Wipefile program overwrites a file the user does not want anyone to see again, like the review of a research grant or research manuscript one has just bashed. Wipedisk does the same for an entire disk. Both modules use the latest U.S. Government DOD rules for assuring the data are really wiped out. Just a simple writing over the files once or twice has been found to be insufficient by those who like or need to really pry. The Text Search capabilities of the program have been improved with a faster algorithm, so searching a disk for a text string is often twice as fast as before. The System Information module summarizes all the hardware features of the user's computer and the system performance of the CPU and disk. In summary, this is a very handy and useful utility program that should be useful to everyone with an IBM-PC. I highly recommend it.

† Available from Peter Norton Computing, Inc., 9th Floor, 100 Wilshire Blvd, Santa Monica, CA 90401-1104 [(213) 319-2000; FAX (213) 458-2048]. $150.00.

MathCAD

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Received December 12, 1988

The first paragraph of the MathCAD manual states that "*the MathCAD program is a unique way to deal with formulas, numbers, text and plots. MathCAD is as versatile as the most powerful computational tools and programming languages, yet as easy to use as a text editor.*" MathCAD is certainly very versatile and user friendly, and it gave this reviewer great pleasure to learn to use it.

One of the main features of MathCAD is that mathematical formulas can be entered just as they are printed in a book. The mathematical symbols are very cleverly designed to enable one to type the formula without any problems. The range of mathematical symbols and operators is adequate for most purposes and includes summation, integral, differentiation, etc. Also included are vector operations like addition, dot product, and vector product, as well as selected matrix operations like multiplication, raising to powers, taking the inverse, etc.

The other feature that comes to mind is the ease of use of the graphics features which allow one to prepare graphs for publication or for lecturing purposes. A package like this will be of great help for the author of textbooks, for instance.

MathCAD requires the following hardware and software: IBM PC, PC/XT, PC/AT, or compatible, including PS/2 series equipped with MS-DOS or PC-DOS version 2.*x* or 3.*x* operating systems; graphics adapter like IBM Color/Graphics Adapter with color or composite monitor, IBM Enhanced Graphics Adapter with any monitor, Hercules Graphics Card with monochrome monitor, Toshiba T3100, AT&T 6300 series with monochrome or color. The memory required is 512K RAM, and the system also supports Lotus/Intel/Microsoft Expanded Memory specification. A hard disk is advantageous, but the system can also run quite comfortably on a 5-$^1/_4$- or 3-$^1/_2$-in. floppy disk drive. A math coprocessor is not needed, since the program runs quite fast on a 10-MHz PC, but it supports an Intel 8087, 80287, or 80387 coprocessor. The system can be adapted to a large range of printers, including LaserJet printers of 80 and 132 characters, as well as plotters like the Hewlett-Packard plotters.

The first question that must be asked about any program is the ease of installation. MathCAD is delivered as two floppy disks, and the installation and configuration instructions are very clear and easy to follow.

The next question always deals with the manual. The MathCAD manual comes in the form of a ringbinder inserted into a hard binder. The problem with this type of arrangement is that it is easy for the publisher to produce and to incorporate last-minute changes into the manual; such manuals are not easy to handle, and this reviewer wishes that they could be supplied in a bound form. The manual itself is a model of clarity, starting with an excellent preliminary overview of the system, its operations, and its limitations which enable the new user to start working without any problems. No printing or instruction errors were spotted, although the upright bar used to calculate the value of the determinant of a matrix is sometimes shown as a broken upright bar on some keyboards.

Another main feature of MathCAD is the mixing of text, equations, tables, and graphs on one page; this is described in five chapters and a great number of examples are given to help with the familiarization of the procedures. There are nine chapters on computational features, like equations and computation, names, numbers and imaginaries, units and dimensions (very useful), vectors and matrices, range variables, iteration, operators, and a discussion on the built-in features like statistical operations, interpolation, fast Fourier operations, Bessel functions, and random numbers. There are also sections on solving equations and how to handle data files, as well as a section on examples.

There is a brief description of the numerical methods employed by MathCAD in Appendix E, with the emphasis on brief. For instance, it is stated that the LU decomposition is used in the computation of the inverse of a square (positive definite) matrix, together with some references, and the method is very briefly discussed. This appendix may, in the opinion of the reviewer, be expanded somewhat for the person who needs more details.

The operations concerning matrices and vectors are new, and some stringent tests were conducted. One of the most sensitive tests for the efficiency of matrix operations is the inverse of matrices with small elements, or matrices for which $\det(A)$ is very small. The collection of test matrices given by R. T. Gregory and D. L. Karney in *A Collection of Test Matrices for Testing Computational Algorithms*[1] is very handy for these tests, and the following matrices were tested:

(1) The Pascal matrix A of order four, with $a = {}^1/_7$, $b = 2a$, $c = 3a$, $d = 4a$, $e = 6a$, $f = 10a$, $g = 20a$ (TOL = 1E-15)

$$\mathbf{A} = \begin{pmatrix} a & a & a & a \\ a & b & c & d \\ a & c & e & f \\ a & d & f & g \end{pmatrix}$$

with det(**A**) = 4.164 931 278 6E-4. The inverse is correctly given up to 1E-12 as

$$\mathbf{A}^{-1} = \begin{pmatrix} 28 & -42 & 28 & -7 \\ -42 & 98 & -77 & 21 \\ 28 & -77 & 70 & -21 \\ -7 & 21 & -21 & 7 \end{pmatrix}$$

with det(**A**) = 2.401E3. The product of **A** and its inverse is equal to the identity matrix within 1E-15.

(2) The Hilbert Matrix H. The following abbreviations are used for the 4×4 submatrix of the infinite Hilbert matrix: $a = {}^1/_2$, $b = {}^1/_3$, $c = {}^1/_4$, $d = {}^1/_5$, $e = {}^1/_6$, $f = {}^1/_7$, which must be input as fractions; otherwise, quite large rounding-off errors may occur that invalidate the inverse. The matrix is

$$\mathbf{H} = \begin{pmatrix} 1 & a & b & c \\ a & b & c & d \\ b & c & d & e \\ c & d & e & f \end{pmatrix}$$

with det(**H**) = 1.653E-7. The inverse is satisfactorily given up to 1E-12 as

$$\mathbf{H}^{-1} = \begin{pmatrix} 16 & -120 & 240 & -140 \\ -120 & 1200 & -2700 & 1680 \\ 240 & -2700 & 6480 & -4200 \\ -140 & 1680 & -4200 & 2800 \end{pmatrix}$$

The manual states that it is possible to input matrices with 100 elements through the matrix format Alt M operator, but this reviewer could not input matrices bigger than 7×7.

The 7×7 Hilbert matrix constitutes a reasonable good test for the arithmetical and rounding-off errors of any matrix operation. The value of this determinant is given correctly up to the seventh digit after the decimal point (the correct number is 4.835 802 623 926 116E-25), while the number of the element of the inverse matrix that should be 1 128 960.000 000 is given correctly up to 0.000 1 when the format specification has the highest precision of 1E15 and TOL = 1E-15.

The vector and matrix operations are adequate for many purposes, but the absence of all eigenvalue and eigenvector routines places a serious restraint upon the general usefulness of MathCAD for the chemist. Routines such as the Jacobi method, which diagonalizes matrices, are quite fast for matrices of order seven, especially if the matrices are symmetrical positive definite (which can also be treated by the fast Choleski decomposition and the Householder and QR algorithms). Most symmetrical matrices of molecular eigenvalue problems can be blocked by symmetry into smaller matrices that can then easily be diagonalized by such programs. It is suggested that such routines be incorporated in subsequent releases of MathCAD.

The graphics part of MathCAD, coupled to the calculation of equations and tables, was tested extensively by calculating the wave functions of metal atoms low in the periodic table, as well as the electron density in overlapping hybrid orbitals in such metal–metal bonds. The performance was adequate, fast (even without the mathematical coprocessor, but very much faster with a 80287 coprocessor), and easy to use. The numerical integrations were performed well and quickly. MathCAD was a pleasure to use in this way, and a complete scientific paper or report can be written with MathCAD.

As an elementary example of the combined use of equations, tables, graphics, and regression analysis, two pages of MathCAD output are shown (Figure 1). A problem from one of the popular physical chemistry textbooks is used as an example. The question is to calculate the dissociation energy of one of the excited states of the dioxygen molecule, using the wavenumbers of the Schumann–Runge band system in the UV. The power of MathCAD is well illustrated, showing the use of vectors in regression analysis, the ability to plot two graphs on the same grid, and the use of different types of regression analyses as well as the numerical integration procedure. The execution time for the whole program was 22 s on a Copam XT IBM compatible 10-MHz PC without a mathematical coprocessor. The time needed for the same calculation on a Copam AT IBM compatible 10-MHz PC, fitted with a 80287 mathematical coprocessor, was 2.5 s.

The text on these two pages is rather compressed only to save space. In actual practice, much more space can be introduced to make the document more readable. It is also possible to print documents that are wider than 80 columns by using the horizontal wraparound option of MathCAD. It is also possible to "hide" intermediate tables and calculations beyond the right border of the screen—an option that is very handy for reference purposes and for seeing trends developing in calculated numbers. This makes MathCAD very useful for report and paper writing, and it is suggested that MathCAD ought to make itself indispensable to students and researchers alike, provided enough time is spent to learn how to use it to its full capacity.

This example refers to Problem 18.24 of P.W.Atkins, Physical Chemistry, Second Edition,Oxford University Press,1982. The series of lines in the UV spectrum of the exited state of the oxygen molecule can be used to calculate the dissociation energy of the molecule in this state. The differences in the wave numbers of these lines are plotted against the quantum number of the lower level involved in the transition and extrapolated to the x-axis. The value of the integral under the line gives the dissociation energy. The data are given in the vectors x and y below, where the x's are numbers and the y's wave numbers. The MathCAD option of units was not used here.

Defining the number of vector elements:

$i := 0 \,..\, 13$

Defining the data vectors of dimension 14 for the 14 data points:

$$x := \begin{bmatrix} 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \end{bmatrix} \qquad y := \begin{bmatrix} 662.8 \\ 643.6 \\ 619.6 \\ 590.4 \\ 564.4 \\ 536.2 \\ 497.4 \\ 464.8 \\ 436.4 \\ 381.8 \\ 343.1 \\ 304.2 \\ 253.0 \\ 210.3 \end{bmatrix}$$

The vector x holds the vibrational quantum number of the lower level from which the transition takes place.

The vector y holds the difference between the transition wave numbers of two adjacent spectral lines.

Calculation of the linear regression line:

$\mathrm{corr}(x,y) = -0.993$

$m := \mathrm{slope}(x,y) \qquad b := \mathrm{intercept}(x,y)$

$\mathrm{linear}(x) := m \cdot x + b$

$m = -35.151$

$$\int_0^{20} \mathrm{linear}(x)\, dx = 6.837 \cdot 10^3$$

$b = 693.34$

Extrapolate linear regression line to where it cuts the x-axis:

$v := 1 \,..\, 20$

$Xa(v) := m \cdot v + b$

$$\int_0^{20} Xa(v)\, dv = 6.837 \cdot 10^3$$

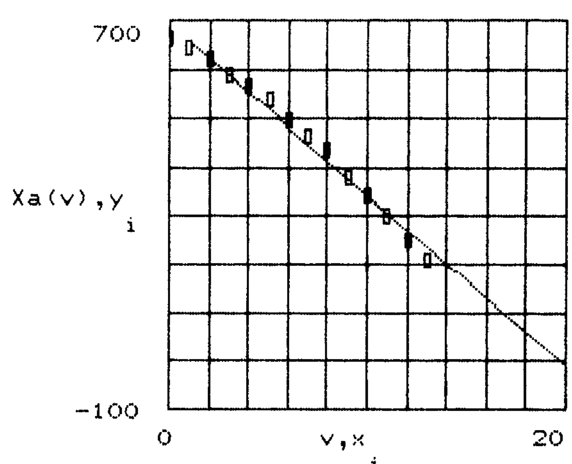

FIGURE 1. Linear regression. The square points show the experimentally-obtained differences in wave numbers between adjacent spectral lines. v and x are the quantum numbers of the lower level of each transition.

THE QUADRATIC FIT TO THE EXPERIMENTAL POINTS.

Create second variable:x-squared:

$$x2 := \overrightarrow{\left[x^{2}\right]}$$

Create X matrix:

$$X_{i,0} := 1 \qquad X^{<1>} := x \qquad X^{<2>} := x2$$

$$b := \left(X^{T}\cdot X\right)^{-1}\cdot\left(X^{T}\cdot y\right)$$

$$b = \begin{bmatrix} 664.238 \\ -20.6 \\ -1.119 \end{bmatrix} \qquad \begin{matrix} b0 \\ b1 \\ b2 \end{matrix}$$

Fitted curve up to transition 14:

$$quad(x) := b_0 + b_1\cdot x + b_2\cdot x^{2}$$

Extrapolate the quadratic regression line to where it intersects the x-axis and compare it with the values from Atkins:

$$v := 0 \,..20$$

$$Xb(v) := b_0 + b_1\cdot v + b_2\cdot v^{2}$$

Xb(14)	= 156.451	160.4 ATKINS
Xb(15)	= 103.391	110.0
Xb(16)	= 48.093	57.0
Xb(17)	= -9.445	0.0

$$\int_{0}^{17} Xb(v)\, dv = 6.482\cdot 10^{3}$$

$$Xb(16.838485) = 7.08\cdot 10^{-6}$$

$$\int_{0}^{16.838485} Xb(v)\, dv = 6.483\cdot 10^{3}$$;Atkins:6835 wave numbers.

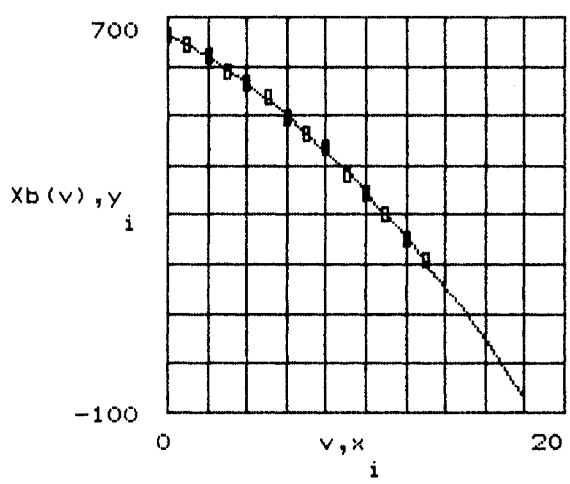

FIGURE 2. The polinomial regression fit to the same experimental data. The line is extrapolated to the x-axis.

The value of the integral may be improved marginally by enforcing the value of Xb(17)=0.0, since fractional quanta cannot occur. If this is done by changing the 1st statement to i:0 ..14, and by enlarging the vectors x and y by one, adding the elements 17 and 0, respectively, the value of the integral becomes 6501 wave numbers and the extrapolated regression line has a value of -2.057 at x=17.

Figure 1. Illustration of some MathCAD options.

There are some criticisms, though. MathCAD does not store the calculated data, tables, and graphs when a program is saved. Hence, every time a program is recalled, MathCAD has to recalculate all the information and redraw all the graphs. This is, naturally, a wasteful process. The graphical construction of the tabular grid is also time-consuming, especially when scrolling up or down through a calculation. It would, indeed, be helpful if the user could choose whether the tabular grid is needed in any particular calculation or not. It would also be advantageous to have other kinds of tabular choices to suit the individual applications. The text editor is not as extensive as one would like (for instance, it proved elusive to use sub- and superscripts in text regions), but no real problems were experienced.

MathCAD has an extensive HELP menu that can be called up at any stage of the proceedings through the F1 function key. The screen can be split without any trouble, so that two documents can be viewed and edited at the same time and text and other blocks can be freely transferred between the two documents. It is, for instance, convenient to open a library file in which often-used formulas, etc., are stored and are then transferred to the working document through the split screen and paste operations. There is also a SEARCH command for editing purposes. The editor is easy to learn and to use. The color graphics of MathCAD make graphs very easy to read since they are displayed in contrasting colors.

MathCAD publishes a regular *User's Journal* (Vol. 2, No. 1 has been published for the winter term of 1988). This journal contains many hints and applications that may be of use for the different users and is distributed to all registered users. The cited number contains information on MathCAD art (drawing a swirl in the complex plane), news about new printer drivers, new ways to analyze data, and a very good introduction to linear and nonlinear regression using any curve of the form

$$y = a + b^*f1(x) + c^*f2(x)$$

where $f1(x)$ could be functions like x, $(1/x)$, $\sin(x)$, $\cos(x)$ $\exp(x)$, or any other function handled by the program. In addition, there is news about a new MathCAD User Forum that is to start on CompuServe. *User's Journal* forms an attractive addition to the MathCAD package.

Summarizing, MathCAD[2] is a mathematical calculation and graphical package that can be very useful to chemists, especially for those engaged in teaching or writing textbooks, or to students who have to work out computational and graphical problems and laboratory notebooks.

REFERENCES AND NOTES

(1) Gregory, R. T.; Karney, D. L. *A Collection of Test Matrices for Testing Computational Algorithms*; Wiley-Interscience: New York, 1969.
(2) MathCAD, developed by MathSoft, Inc., 1 Kendall Square, Cambridge, MA 02139.