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Are micro-computers growing up?

Review of: Tallarida, R.J. & R.B. Murray (1981). Manual of pharmacologic calculations with computer programs. – Berlin, Heidelberg, New York, Springer, 150 pp., DM 33.

1.0 Contents

This book presents a number of computer programs for analysing pharmacological data. Although primarily intended for pharmaceuts, many of these programs are also applicable in different fields of the biological sciences. The following programs are included:

1 dosage and concentration: drug stock solution;
2 mean, standard deviation, and confidence limits;
3–7 linear regression: standard, lines through origin, analysis, test for parallelism, construction of parallel lines;
8–9 dose-response: graded, quantal;
10 relative potency;
11–13 dissociation constant: agonists, partial agonist, perturbation methods;
14–16 pA2 analysis: schild plot, time-dependent method, constrained plot;
17–19 enzyme kinetics: Michaelis-Menten equation, competitive inhibition, noncompetitive inhibition;
20 first-order drug decay;
21 Scatchard plot;
22 Henderson-Hasselbach equaation;
23 exponential growth and decay;
24 constant infusion with first-order elimination;
25 multiple intravenous injections;
26 area under curve: Simpson's rule and trapezoidal rule;
27 analysis of variance;
28–29 t-test: grouped data, paired data;
30 chi-square test;
31 Dunnett's test;
32 Mann-Whitney test;
33 method of Litfield and Wilcoxon: confidence limits of ED50.

The book is divided into two parts which are roughly equal in size. The initial part discusses the pharmacological background and the mathematical and statistical equations for each algorithm. The second part presents a listing of the corresponding computer programs.

These programs are written in BASIC.

Each analysis is adstructed with a small example. First it is used in the background part. The same example is also presented in a sample session preceding each program listing.

All programs are available on floppy disc or casette for Radio Shack model I, model III, and Apple micro-computers with at least 16K memory.

2.0 General impact

The first appearance of well-documented program packages for micro-computers seems to me an interesting and inspiring phenomenon. It may well indicate the further penetration of small and cheap micros; not only for the amateur, not only for dedicated applications, but also for general purpose applications in the scientific fields. Assuming a further increase in power – especially in memory – in micros, I expect implementation of powerful program packages like SPSS, BMDP, SAS, etc. for micro-computers in the near future. The newest micro-computer generation with core of 0.5M and upwards should be able to handle such packages easily.

However, this book clearly shows the state of the art nowadays: micro. The choice and implementation of the treated programs shows a useful, but very basic package for analyses. For example univariate statistics are restricted to means, standard deviation, and standard error only. Not included are median, modus, quartiles, frequency-plot, and the like, although these are especially useful when non-normal distributions are present.

3.0 Documentation part

The presentation is very lucid and easily understandable. Layout and typography together with a generous use of graphs facilitate a fast understanding.

No proofs or formula derivations are presented, but just the bare essentials. This is, in my opinion, exactly the requirement for a good program documentation.

Hardly any literature is referred to. This is not surprising because the presented programs are so basic, and the used algorithms so straightforward (regardless of their numeric reliability) that they can be found in any undergraduate/graduate textbook.

As seems 'good' practice in program packages, nowhere is treatment given to numerical reliability. This is a serious shortcoming, especially in small micro-computers with a very limited worth length. For example univariate analysis with normal precision on a TRS/80 model I of the sample '7 9 10 10 11 13' yields the proper values of 10 and 2 for the mean and standard deviation. However, the sample '7.000 7.002 7.003 7.004 7.006' returns 7.003 and 1.99986E-3 instead of 7.003 2E-3 and '7.000000 7.000001 . . . 7.000006' returns 7.0 and 2.3554E-6 instead of 7.000003 and 2E-6. These results improve considerably when the single precision is changed into double precision.

The suppletion of 12 tables is surprising in a book with computer programs. What is their use? Granted that some of these tables are only replaceable by

fairly complicated computer programs. But if they are useful – and some of these tables certainly are – so will be inclusion of the computer algorithm. And the reasons for inclusion of a table for common logs, a table for natural logs, powers of e, and a table with squares and square roots utterly elude my understanding.

4.0 Program part

The presentation is clear and comprehensible. Each program listing is preceded by a brief instructive sample session.

It is a pity, however, that the programs are written in BASIC. I think we have to put up with the fact that BASIC still is the most widely applied language for micro-computers today. Given the abominable structure facilities of BASIC the programs are nevertheless frequently – although regrettably not always – written in a fairly lucid style. The design of most programs is modular with superfluous use of GOSUBs. Their layout is moderately good and mostly shows the scope of loops properly. There are however also very clumsy constructions included.

For example: it takes some time to discover the scope of the J-loop in:

```
11210 PZ$ = STRING$(9,45): PRINT: FOR J = 1 TO L STEP 2
. . .
11230 FOR I = 1 TO N(J)
. . .
11260 NEXT I, J
```

Another example of bad programming style:

Compare the well-written program S23:

```
23030 GOSUB 23100: REM          input
23040 GOSUB 23200: REM          process
23050 GOSUB 23900: REM          output
23060 RETURN
```

with program S24:

```
24030 GOSUB 24100: REM          input
24040 GOSUB 24800: REM          output
23050 RETURN
```

this program seems to lack any process, unless one looks at

```
24100 GOSUB 24110: GOSUB 24170:     RETURN
      input part       process part
```

Another clumsy aspect in the design is the INPUT-part. Observations are entered by hand one by one, which is fine for a small dataset, but very irritating if several analyses are required of one, fairly extensive, dataset.

5.0 Conclusion

As a final remark: this book is an interesting publication. It seems a forerunner for more mature program packages yet to come. As a documentation aid for the programs, it is very worthwhile; it is clear and quickly understandable. The program package itself is still on a 'micro'-level. Its main use will be as an aid for rather basic analyses of 'clean' data for the lowest classes of graduate students.

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