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Environmental Contamination and Toxicology

A Computer Program in Basic for Determining Probit and Log-Probit or Logit Correlation for Toxicology and Biology

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The probit function is widely used to model a logistic relationship between a stimulus and a quantal response in toxicology and biology. There are well known programs of this type for toxicology written in Fortran (Daum et al. 1966, Daum 1970, Russell et al. 1977 and Robertson et al. 1981) to run on minicomputers or main-frame computers. However, these programs are specifically intended for bio-assay and are not available for microcomputers.

The probit function may be appropriate for modeling other systems showing sigmoid relationships. The SAS (Statistical Analysis System) program has the probit function and will soon be available on IBM-PCs and compatibles, but will require a hard disk and 512 kilobytes of main memory. Many existing systems do not meet these specifications. The objective of this paper is to provide an additional means for determining two factor log-probit analysis. The BASIC programs presented here were developed using the probit equation and the tables published by Bliss (1935) and Finny (1952). These programs can be used as presented or adapted as subroutines within other application programs. There is no other available software offering the probit function for micro-computers to the best of our knowledge.

RESULTS AND DISCUSSION

The first program (PROPER) accepts values between 0.01 and 99.99 percent and transforms them to probit values or transforms probit values between 1.281 and 8.719 to percent values (Table 1). Examples of the input and output are shown in Table 2.

The second program (LOGPRO) accepts paired data and models the relationship between the pairs as

* Correspondence and reprint requests.

Table 1. Source listing of program PROPER

```
100 REM   PROGRAM  PROPER.BAS   VERSION 1.0  RELEASED 20 MAY 1985
110 REM   M. M. ABOU-SETTA, R. W. SORRELL, AND C. C. CHILDERS
250 ON ERROR GOTO 1020
260 REM CONSTANT
270  ININC = .001
280 REM PERCENT TO PROBIT TABLE
290  DIM PERCTB(17),PROBITB(17)
300  DATA  .01,1.2810,     .1,1.9098,  1,2.6737,  5,3.3551, 10,3.7184
310  DATA   20,4.1584,     30,4.4756, 40,4.7467, 50,5.0,    60,5.2533
320  DATA   70,5.5244,     80,5.8416, 90,6.2816, 95,6.6449, 99,7.3263
330  DATA 99.9,8.0902, 99.99,8.7190
340  FOR I=1 TO 17
350   READ PERCTB(I),PROBITB(I)
360  NEXT I
370 PRINT
380 PRINT " 1 - PERCENT TO PROBIT "
390 PRINT " 2 - PROBIT TO PERCENT "
400 INPUT "    ENTER  1  OR  2 :";DT
410 IF DT=1 OR DT=2 THEN 440
420 PRINT " INVALID SELECTION"
430 GOTO 400
440 INPUT " ENTER NUMBER OF VALUES TO BE TRANSFORMED (AN INTEGER) ";N
450   IF N<>INT(N) THEN 440
460   IF N=0 THEN 1090
470 DIM PV(N)
480 PRINT "   ENTER ";N;" VALUES (1 PER LINE, NO ZERO DATA) "
490 IF DT=1 THEN PRINT "        BETWEEN .01 AND 99.99"
500 IF DT=2 THEN PRINT "        BETWEEN 1.2810 AND 8.7190"
510 FOR C = 1 TO N
520  INPUT PV(C)
530  IF DT=1 AND (PV(C)>=.01 AND PV(C)<=99.99) THEN 570
540  IF DT=2 AND (PV(C)>=1.2810 AND PV(C)<=8.7190) THEN 570
550    PRINT " VALUE OUT OF RANGE, TRY AGAIN "
560    GOTO 520
570 NEXT C
580 IF DT=1 THEN PRINT TAB(4);"PERCENT";TAB(20);"PROBIT"
590 IF DT=2 THEN PRINT TAB(4);"PROBIT";TAB(20);"PERCENT"
600 FOR C = 1 TO N
610  REM      TRANSFORMING THE PROBIT VALUE TO PERCENT
620  IF DT=1 AND PV(C)<.01     THEN 780
630  IF DT=2 AND PV(C)<1.2810 THEN 780
640  FOR I = 1 TO 16
650   IF DT=1 AND (PV(C)<PERCTB(I) OR PV(C)>=PERCTB(I+1)) THEN 700
660   IF DT=2 AND (PV(C)<PROBITB(I) OR PV(C)>=PROBITB(I+1)) THEN 700
670   SUMIN = PERCTB(I)
680   START = PROBITB(I)
690   GO TO 800
700  NEXT I
710 REM UPPER LIMITS
720  IF DT<>1 OR PV(C)<>99.99 THEN 750
730   CALCPR = 8.7190
740   GOTO 970
750  IF DT<>2 OR PV(C)<>8.719 THEN 780
760   SUMIN = 99.99
770   GOTO 980
780  PRINT PV(C);" IS OUT OF RANGE"
790   GOTO 990
800 REM  INTEGRATE BY TRAPEZOIDAL RULE
810  IF DT=2 THEN 900
820   P1 = .3989422 * EXP(-(START - 5)^2 / 2) * 100
830   FOR CALCPR = START TO 10-ININC STEP ININC
840    IF SUMIN>=PV(C) THEN 970
850    P2 = .3989422 * EXP(-(CALCPR+ININC - 5)^2 / 2) * 100
860    SUMIN = SUMIN + (P1 + P2)/ 2 * ININC
870    P1=P2
880   NEXT CALCPR
890  GOTO 970
900    IF START>=PV(C) THEN 980
910   P1 = .3989422 * EXP(-(START - 5)^2 / 2) * 100
920   FOR CALCPR = START TO PV(C)-ININC STEP ININC
```

Table 1 continued.

```
930     P2 = .3989422 * EXP(-(CALCPR+ININC - 5)^2 / 2) * 100
940     SUMIN = SUMIN + (P1 + P2)/ 2 * ININC
950     P1 = P2
960   NEXT CALCPR
970 IF DT=1 THEN PRINT TAB(4);PV(C);TAB(20);INT(CALCPR*10000+.5)/10000
980 IF DT=2 THEN PRINT TAB(4);PV(C);TAB(20);INT(SUMIN*1000+.5)/1000
990 NEXT C
1000 PRINT
1010 GOTO 1090
1020 REM INPUT ERROR TRAP
1030 IF ERL<>400 AND ERL<>440 AND ERL<>520 THEN 1070
1040   PRINT " INVALID ENTRY, TRY AGAIN  ";
1050   RESUME
1070   PRINT " ERROR ";ERR;" OCCURRED AT LINE ";ERL
1080   RESUME 1090
1090 END
```

Table 2. Examples of input and output for PROPER.

```
 1 - PERCENT TO PROBIT
 2 - PROBIT TO PERCENT
    ENTER  1  OR  2 :? 1
 ENTER NUMBER OF VALUES TO BE TRANSFORMED (AN INTEGER) ? 5

    ENTER  5  VALUES (1 PER LINE, NO ZERO DATA)
        BETWEEN .01 AND 99.99
? .02
? .6
? 84.5
? 97
? 9.888

     PERCENT          PROBIT
      .02              1.46
      .6               2.4888
      84.5             6.0156
      97               6.8809
      9.888            3.7121

 1 - PERCENT TO PROBIT
 2 - PROBIT TO PERCENT
    ENTER  1  OR  2 :? 2
 ENTER NUMBER OF VALUES TO BE TRANSFORMED (AN INTEGER) ? 3

    ENTER  3  VALUES (1 PER LINE, NO ZERO DATA)
        BETWEEN 1.2810 AND 8.7190
? 1.2810
? 5.01
? 8.2135

     PROBIT           PERCENT
      1.281            .01
      5.01             50.399
      8.2135           99.934
```

log-probit (Table 3). The first value (X) is the stimulus and the second (Y) is the quantal response shown as a percent value. The output of this program can be stored in another file and contains the original input data and the transformed values (natural logarithms of the stimulus and probits of the response). The output also shows expected values so they can be used in plotting the relationship as linear (log-probit) or curvilinear (logit). The

Table 3. Source listing of program LOGPRO.

```
100 REM   PROGRAM  LOGPRO.BAS   VERSION 1.0  RELEASED 13 MAY 1985
110 REM   M. M. ABOU-SETTA, R. W. SORRELL, AND C. C. CHILDERS
420 ON ERROR GOTO 2020
430 REM DEFINE CONSTANTS
440 S$ = " "
450 ININC = .001
460 FLAG = 0
470 REM PERCENT TO PROBIT TABLE
480  DIM PERCTB(17),PROBITB(17)
490  DATA  .01,1.2810,     .1,1.9098,  1,2.6737,  5,3.3551, 10,3.7184
500  DATA   20,4.1584,     30,4.4756, 40,4.7467, 50,5.0,     60,5.2533
510  DATA   70,5.5244,     80,5.8416, 90,6.2816, 95,6.6449, 99,7.3263
520  DATA 99.9,8.0902, 99.99,8.7190
530  FOR I=1 TO 17
540   READ PERCTB(I),PROBITB(I)
550  NEXT I
560 PRINT
570 PRINT " LOG-PROBIT CORRELATION BETWEEN TWO FACTORS"
580 PRINT " ENTER TITLE OF NO MORE THAN 70 CHARACTERS"
590 INPUT T$
600 T$ = "   " + T$
610 INPUT " ENTER NUMBER OF DATA POINTS (X,Y) ( >3 , INTEGER)";N
620   IF N<3 OR N<>INT(N) THEN 610
630 DIM PCENT(N),STIMULUS(N),LX(N),PY(N),EPROBY(N),EY(N)
640 PRINT "    ENTER ";N;" PAIRS OF VALUES: STIMULUS , REACTION"
650 PRINT "     STIMULUS AS A REAL NUMBER GREATER THAN 0"
660 PRINT "     REACTION AS .01 TO 99.99 PERCENT"
670 FOR C = 1 TO N
680 PRINT "         STIMULUS ";C;"= ";
690  INPUT STIMULUS(C)
700  IF STIMULUS(C)>0 THEN 730
710  PRINT " MUST BE A NUMBER GREATER THAN 0"
720  GOTO 680
730 PRINT "         REACTION ";C;"= ";
740  INPUT PCENT(C)
750  IF PCENT(C)>=.01 AND PCENT(C)<=99.99 THEN 780
760  PRINT " MUST BE A NUMBER NOT LESS THAN .01 OR GREATER THAN 99.99"
770  GOTO 730
780 NEXT C
790 PRINT
800 PRINT "              WORKING"
810 REM TRANSFORM STIMULUS TO LOG AND REACTION TO PROBIT
820 FOR C = 1 TO N
830  REM      TRANSFORM THE STIMULUS TO LOG AND ACCUMULATE
840   REM      SUM OF X AND SUM OF X SQUARED
850   LX(C) = LOG(STIMULUS(C))
860   SLX = SLX + LX(C)
870   SMLX2 = SMLX2 + (LX(C)^2)
880  REM      TRANSFORMING THE REACTION TO A PROBIT
890   IF PCENT(C)<.01 THEN 1000
900   FOR I = 1 TO 16
910    IF PCENT(C)<PERCTB(I) OR PCENT(C)>=PERCTB(I+1) THEN 950
920    ISUM = PERCTB(I)
930    BEGIN = PROBITB(I)
940    GO TO 1020
950  NEXT I
960  REM UPPER LIMITS
970   IF PCENT(C)<>99.99 THEN 1000
980   CALCPROB = 8.7190
990   GOTO 1100
1000  PRINT PCENT(C);" IS OUT OF RANGE"
1010   GOTO 2140
1020  REM  INTEGRATE BY TRAPEZOIDAL RULE UNTIL PERCENT VALUE IS REACHED
1030   P1 = .3989422 * EXP(-(BEGIN - 5)^2 / 2) * 100
1040  FOR CALCPROB = BEGIN TO 10-ININC STEP ININC
1050   IF ISUM>=PCENT(C) THEN 1100
1060   P2 = .3989422 * EXP(-(CALCPROB+ININC - 5)^2 /2) * 100
1070   ISUM = ISUM + (P1 + P2)/ 2 * ININC
1080   P1 = P2
1090  NEXT CALCPROB
```

Table 3 continued.

```
1100  PY(C) = CALCPROB
1110  REM  FIND SUM OF Y, SUM OF Y SQUARED, AND SUM OF XY
1120   SPY = SPY + PY(C)
1130   S2PY = S2PY + (PY(C)^2)
1140   SUMLXPY = SUMLXPY + (LX(C)*PY(C))
1150 NEXT C
1160 REM FIND R-SQUARED, Y-INTERCEPT, AND SLOPE OF REGRESSION LINE
1170  RSQUARE=(SUMLXPY-SLX*SPY/N)^2/(S2PY-SPY^2/N)*(SMLX2-SLX^2/N)
1180  NTERCEPT = (SMLX2*SPY-SUMLXPY*SLX)/(N*SMLX2-SLX^2)
1190  LSLOPE = (N*SUMLXPY-SPY*SLX)/(N*SMLX2-SLX^2)
1200 REM      CALCULATING THE EXPECTED REACTION VALUES
1210 FOR C = 1 TO N
1220  EPROBY(C) = NTERCEPT+LSLOPE*(LOG(STIMULUS(C)))
1230  FOR I = 1 TO 16
1240   IF EPROBY(C)<PROBITB(I) OR EPROBY(C)>=PROBITB(I+1) THEN 1280
1250   ISUM = PERCTB(I)
1260   BEGIN = PROBITB(I)
1270   GO TO 1350
1280  NEXT I
1290  REM UPPER LIMITS
1300   IF EPROBY(C) = 8.7190 THEN ISUM = 99.99
1310   IF EPROBY(C) > 8.7190 THEN ISUM = 100
1320   IF EPROBY(C) < 1.2810 THEN ISUM = 0
1330   FLAG = 1
1340   GOTO 1430
1350  REM  INTEGRATE BY TRAPEZOIDAL RULE
1360   P1 = .3989422 * EXP(-(BEGIN - 5)^2 / 2) * 100
1370  FOR CALCPROB = BEGIN TO EPROBY(C)-ININC STEP ININC
1380   IF BEGIN>=EPROBY(C) THEN 1430
1390   P2 = .3989422 * EXP(-(CALCPROB+ININC - 5)^2 / 2) * 100
1400   ISUM = ISUM + (P1 + P2)/ 2 * ININC
1410   P1 = P2
1420  NEXT CALCPROB
1430  EY(C) = ISUM
1440 NEXT C
1450 PRINT
1460 REM OUTPUT TO SCREEN AND FILE
1470 L1$= " LOG-PROBIT CURVE REGRESSION AND CORRELATION"
1480 L2$= "      X            Y         LOGe X     "
1481 R2$= "PROBIT    EXPECTED   EXPECTED"
1490 L3$= " (STIMULUS) (REACTION%)
1491 R3$= "  Y         PROBIT         Y"
1500  PRINT
1510  PRINT L1$
1520  PRINT
1530  PRINT T$
1540  PRINT
1550  PRINT L2$;R2$
1560  PRINT L3$;R3$
1570  PRINT
1580  FOR C = 1 TO N
1590   PRINT TAB(2);STIMULUS(C);TAB(13);PCENT(C);
1600   PRINT TAB(24);INT(LX(C)*10000+.5)/10000;
1610   PRINT TAB(35);INT(PY(C)*10000+.5)/10000;
1620   PRINT TAB(46);INT(EPROBY(C)*10000+.5)/10000;
1630   PRINT TAB(57);INT(EY(C)*1000+.5)/1000
1640  NEXT C
1650   PRINT
1660   PRINT " PROB Y = ";NTERCEPT;" + ";LSLOPE;" LOGe X"
1670   PRINT
1680   PRINT " R-SQUARED =";RSQUARE
1690   PRINT
1700  IF FLAG=0 THEN 1730
1710   PRINT " EXPECTED Y OF 0 OR 100 IS AN ESTIMATION"
1720   PRINT "  DUE TO EXTREME EXPECTED PROBIT VALUES."
1730   PRINT
1740  PRINT " IF OUTPUT IS TO BE SAVED IN A FILE, ENTER FILENAME"
1750  INPUT " IF NOT, PRESS RETURN ";FILE$
1760  IF FILE$="" THEN 2140
```

Table 3 continued.

```
1770  OPEN FILE$ FOR OUTPUT AS #1
1780  PRINT #1, S$
1790  PRINT #1, L1$
1800  PRINT #1, S$
1810  PRINT #1, T$
1820  PRINT #1, S$
1830  PRINT #1, L2$;R2$
1840  PRINT #1, L3$;R3$
1850  PRINT #1, S$
1860  FOR C = 1 TO N
1870  PRINT #1, TAB(2);STIMULUS(C);TAB(13);PCENT(C);
1880  PRINT #1, TAB(24);INT(LX(C)*10000+.5)/10000;
1890  PRINT #1, TAB(35);INT(PY(C)*10000+.5)/10000;
1900  PRINT #1, TAB(46);INT(EPROBY(C)*10000+.5)/10000;
1910  PRINT #1, TAB(57);INT(EY(C)*1000+.5)/1000
1920  NEXT C
1930  PRINT #1, S$
1940  PRINT #1, " PROB Y = ";NTERCEPT;" + ";LSLOPE;" LOGe X"
1950  PRINT #1, S$
1960  PRINT #1, " R-SQUARED =";RSQUARE
1970  PRINT #1, S$
1980  IF FLAG=0 THEN 2140
1990   PRINT #1," EXPECTED Y OF 0 OR 100 IS AN ESTIMATION"
2000   PRINT #1,"  DUE TO EXTREME EXPECTED PROBIT VALUES."
2010  GOTO 2140
2020 REM ERROR TRAPS
2030 REM FILE OPEN ERRORS
2040 IF ERL <> 1770 THEN 2070
2050  PRINT " ERROR OPENING FILE ";FILE$
2060  RESUME 1740
2070 REM INPUT ERRORS
2080 IF ERL=590 OR ERL=610 OR ERL=690 OR ERL=740 OR ERL=1750 THEN 2120
2090 REM OTHER ERRORS
2100  PRINT " ERROR ";ERR;" OCCURED AT LINE ";ERL
2110  RESUME 2140
2120 PRINT " INVALID ENTRY, TRY AGAIN  ";
2130  RESUME
2140 END
```

output contains the determination factor (R-squared) of the data. An example of the input and output of the program LOGPRO is shown in Table 4.

The two programs were written in "generic" BASIC for portability. More efficient code could increase speed and decrease program size for a specific computer. The programs will run with no modification on DEC VAX minicomputers in VAX-11 BASIC, on IBM-PC microcomputers and compatibles and on the Radio Shack Model 100 with 32K of main memory. The output of LOGPRO will be difficult to read on the 40 column screen of the Model 100 and should be saved in a file and printed.

The accuracy of these programs is to plus or minus one integration step (.001) for probits. More accuracy could be obtained by decreasing the step size but this would also increase running time.

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Table 4. Example of input and output for LOGPRO.

```
 LOG-PROBIT CORRELATION BETWEEN TWO FACTORS
 ENTER TITLE OF NO MORE THAN 70 CHARACTERS
? Sample data for LOGPRO
 ENTER NUMBER OF DATA POINTS (X,Y) ( >3 , INTEGER)? 10

   ENTER  10  PAIRS OF VALUES: STIMULUS , REACTION
    STIMULUS AS A REAL NUMBER GREATER THAN 0
    REACTION AS .01 TO 99.99 PERCENT
        STIMULUS  1 = ? 20
        REACTION  1 = ? .02
        STIMULUS  2 = ? 40
        REACTION  2 = ? .03
        STIMULUS  3 = ? 60
        REACTION  3 = ? 5.1
        STIMULUS  4 = ? 80
        REACTION  4 = ? 14.3
        STIMULUS  5 = ? 100
        REACTION  5 = ? 46.7
        STIMULUS  6 = ? 120
        REACTION  6 = ? 47.1
        STIMULUS  7 = ? 140
        REACTION  7 = ? 82
        STIMULUS  8 = ? 160
        REACTION  8 = ? 87
        STIMULUS  9 = ? 180
        REACTION  9 = ? 85.5
        STIMULUS  10 = ? 200
        REACTION  10 = ? 89
             WORKING


  LOG-PROBIT CURVE REGRESSION AND CORRELATION

   Sample data for LOGPRO

     X            Y          LOGe X     PROBIT     EXPECTED    EXPECTED
 (STIMULUS)  (REACTION%)                  Y        PROBIT         Y

   20          .02         2.9957      1.46       .8061        0
   40          .03         3.6889      1.569      2.4783       .583
   60          5.1         4.0943      3.3651     3.4565       6.131
   80          14.3        4.382       3.9334     4.1505       19.778
   100         46.7        4.6052      4.9177     4.6889       37.775
   120         47.1        4.7875      4.9277     5.1287       55.093
   140         82          4.9416      5.9156     5.5006       69.159
   160         87          5.0752      6.1266     5.8227       79.458
   180         85.5        5.193       6.0586     6.1069       86.577
   200         89          5.2983      6.2266     6.3611       91.317

  PROB Y = -6.42113  +  2.4125  LOGe X

  R-SQUARED = .943429

  EXPECTED Y OF 0 OR 100 IS AN ESTIMATION
   DUE TO EXTREME EXPECTED PROBIT VALUES.

  IF OUTPUT IS TO BE SAVED IN A FILE, ENTER FILENAME
  IF NOT, PRESS RETURN ? sample.lis
```

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