High precision chi-square and normal curve integration

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The routine discussed in this paper determines chi-square and normal curve probabilities in a manner similar to a technique introduced by Wood and Wood (1985). Their program integrates the *t* density function to provide two-tailed *t* probabilities with five decimal place accuracy, up to a maximum of 115 df (*n*). The level of accuracy in their technique is achieved via an algorithm of Simpson's rule. The handling of the large maximum *n* without computer overflow is achieved by recognizing that, because *n* is integral in *t*, chi-square, and *F*, $\Gamma(n/2)$ is a factorial process. Because $f(t)$ contains $\Gamma[(n+1)/2]/\Gamma(n/2)$, common factorial factors are divided out before multiplication, thus reducing the magnitude of the two products and preventing overflow until *n* exceeds 115.

The routine presented here (see Appendix) achieves accurate results via application of the same swift algorithm of Simpson's rule in which the chi-square and normal density functions are divided into tiny segments. The areas are then determined and summed (Anton, 1981). Accuracy is provided to a minimum of five decimal places.

The range of numerical integration is not a problem with the normal curve, because this routine accurately finds any specified area bounded by $Z = -6$ and $Z = 6$, and having a probability within six decimal places. The range of integration becomes a problem with chi-square bounded by 0 and ∞ , and for which $\mu = n$ (Beyer, 1979, p. 522). Nevertheless, with one exception the program exactly evaluates all chi-squares having probabilities from .000001 to .999998 for $1 \leq n \leq 34$. Where $n = 3$, five place accuracy is maintained.

The Simpson's rule algorithm evaluates a standard version of chi-square (Beyer, 1979, p. 522) that is algebraically manipulated for programming purposes into the following form:

$$f(\chi^2) = \frac{1}{\sqrt{2^n} \cdot \Gamma(n/2)} \cdot \frac{(\sqrt{\chi^2})^{n-2}}{(\sqrt{e})^{\chi^2}}.$$

The left portion is the parametric component requiring only the number of degrees of freedom (*n*) for computation. The right component, having χ^{n-2} as its numerator, becomes exponentially large when both *n* and chi-square are large, and computer overflow results. Techniques em-

ployed in this program extend the usable range of chi-square and *n* before overflow occurs.

The program begins by presenting a menu to the user offering a chi-square probability, a normal curve area, or the end of work. If the user selects chi-square, the program requests the number of degrees of freedom. The logical path branches at this point according to *n*. For *n* = 1, 3, or 5, special subroutines exist. For all other values, a common path is taken beginning with the gamma function subroutine which evaluates $\Gamma(n/2)$. Using gamma, the parametric portion of $f(\chi^2)$ is then computed and assigned the variable name *P*.

The logical flow then branches to Line 1000 which begins a subroutine that sets the number of segments (*W*) into which the density function will be partitioned. All lines with 4-digit numbers are *W* setters. Generally *W* increases as function of *n* (*H* in the program) and chi-square (*U* in the program).

With *P* and *W* determined, the program begins the Simpson's rule algorithm which computes the area between zero and the user-entered chi-square. The significance figure, $1 - \text{Area}$, is also calculated. Finally the results are printed on the screen and the menu reappears.

For all degrees of freedom less than 20, except *n* = 1, the chi-square function is evaluated by Simpson's rule exactly as shown, because no overflow occurs for the maximum, usable values of *n* and chi-square. Specifically for *n* = 19 and $\chi^2 = 61.06947$, the computed probability is 0.999998 which is the limiting accuracy value of the routine. Beyond *n* = 19, however, special techniques are required to prevent overflow.

When *n* > 19, the density function is evaluated as follows:

$$f(\chi^2) = \frac{1}{\sqrt{2^n} \cdot \Gamma(n/2)} \cdot \frac{(\sqrt{\chi^2})^{n-20}}{(\sqrt{e})^{\chi^2}} (\sqrt{\chi^2})^{18},$$

so that the chi-square portion resolves to

$$\frac{\chi^{n-20}}{(\sqrt{e})^{\chi^2}} (\chi^{18}).$$

The effect is that for any *n* > 19, the right (i.e., χ^2) portion of the function still reduces to $\chi^{n-2}/(\sqrt{e})^{\chi^2}$, but for programming purposes an advantage has been achieved. Rather than directly computing χ^{n-2} which produces overflow when χ and *n* are large, this arrangement computes $\chi^{n-20}/(\sqrt{e})^{\chi^2}$ first. When that fraction is determined, it is then multiplied by χ^{18} . Without this modification, overflow occurs where *n* = χ^2 = 29; with it the range is extended up to *n* = χ^2 = 37. The gain of 8 df is not trivial, because each increase of 1 df results in an exponential increment in χ^{n-20} .

The *n* = 3 and *n* = 5 density functions were mentioned

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as special cases and are in the sense that their graphs exhibit extreme curvature. Because of this, many area segments are required for accurate probability determinations. Lines 1030-1035 set W for $n = 5$ and Lines 1040-1075 determine W for the curvy 3 df chi-square. These two functions also require double precision determinations of the parametric portion of $f(\chi^2)$, and these are written into the routine. The combination of a large number of segments and double precision parameters results in very slow running times.

A complication of numerical integration of $f(\chi^2)$ is that, when $n = 1$, $f(\chi^2)$ is asymptotic to the vertical axis and cannot be integrated from zero to a positive value. Resolution comes from the fact that $z^2 = \chi^2$ where $n = 1$, and the two roots of chi-square are the normal variates Z and $-Z$. A two-tailed test, therefore, of the unit normal distribution provides an exact significance test for one degree of freedom chi-squares. Thus when $\chi^2(n = 1)$ is entered, the positive square root is extracted and defined as Z. Simpson's rule is applied to determine the normal curve area between the $\mu = 0$ and Z. The area is doubled, yielding the area between $\chi^2 = 0$ and the user-entered value. Subtracting that area from one gives the significance test for the one degree of freedom chi-square.

Because the normal curve subroutine is an integral component of the chi-square program, a normal curve area-finding option has been included. When the user responds to the menu by selecting "Normal Curve," the computer presents instructions, which state that the routine finds the area between two Z scores. The algebraic value of the smaller Z is requested, followed by a request for the algebraic value of the larger. The normal curve area between the Z scores is displayed first and for purposes of hypothesis testing the total area beyond that subtended by the Z scores is also displayed. The user simply enters the negative of a Z involved in a significance test (e.g., Fisher's Z' for correlation) and then the positive value of Z: The two-tailed probability appears.

High accuracy is the primary priority of the routine and is achieved at some cost in running time, especially for the $n = 3$ and the $n = 5$ cases. Except for $n = 3$, results are accurate to six decimal places from $p = 0.000001$ to $p = 0.999998$, over the range from $n = 1$ to $n = 34$. Beyond 34 df, the accuracy continues, but the range is restricted by overflow; for example, $\chi^2 = 85$ with $n = 36$ is correctly assigned a probability of 0.999992, but when $\chi^2 = 89.324$ ($p = 0.999998$) is entered, overflow occurs. For the three degrees of freedom case, an enormous number of segments are required to provide five decimal place accuracy, and running times in the 5-20-min range are the rule. Even very small chi-squares run slowly. Accuracy is maintained, however, over the entire range from $p = 0.00001$ to $p = 0.99998$.

The accuracy of this program is so high that chi-square values taken from tables and having two, three, or even four decimal places when tested, often fail to result in the tabled probability figure. Three-digit tables, for example, cite $\chi^2 = 5.991$ as the $p = .05$ value for 2 df. The pro-

gram displays a significance figure $(1 - A)$ of 0.050012, for 5.991, and that is correct. When $\chi^2 = 5.991465$ is run, the figures $A = 0.950000$ and $1 - A = 0.050000$ appear.

The TRS-80 Model 4 microcomputer has a Z-80A microprocessor with a clock speed of 4 MHz, which gives running times ranging from 6 sec to 60 sec in all cases except $n = 3$ and $\chi^2 > 0.5$ and $n = 5$ and $\chi^2 \geq 17$. The latter run in 2 min, 8 sec, while the former are extremely slow. The program includes running times only for $n = 3$ and uses them as a guide. The program runs without modification on the IBM-PC and is noticeably faster than on the TRS-80. The limits at which overflow occurs are slightly higher on the IBM-PC.

On rare occasions a probability is required for larger values of n and chi-square than the present configuration affords. A significant expansion of the range of the program can be accomplished by rewriting Line 22 as follows.

```
22 Y = P * SQR(X^E/2.71828183#^X): Y = Y*SQR(X^18): RETURN
```

Using this expression, overflow first occurs with the $\chi^2 = n$ test at 44, and for $n = 40$, with this version of Line 22 overflow occurs at $\chi^2 = 78$ on the TRS-80 Model 4 computer. With the listed version, the limit is $\chi^2 = 15$ with $n = 40$. Because this version of Line 22 extracts two square roots rather than the one used in the Appendix, it runs a bit more slowly and on occasion introduces a one-unit error into the sixth decimal place. Users desiring only 5-place accuracy are advised that Line 22 should be replaced with the version above on a permanent basis.

Availability. A listing of the program can be obtained without charge from D. Louis Wood, Department of Psychology, University of Arkansas, 33rd Street and University Avenue, Little Rock, Arkansas 72204.

REFERENCES

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 BEYER, W. H. (Ed.). (1979). *C R C Standard Mathematical Tables* (25th ed.). Boca Raton, FL: C R C Press.
 WOOD, D. L., & WOOD, D. (1985). TINT: A Microsoft BASIC t integration program. *Behavior Research Methods, Instruments, & Computers*, 16, 479-480.

APPENDIX

Listing of Program for Chi-Square and Normal Curve Integration

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1 CLS
2 CLEAR:DEFINT J,H,M,W
3 P$="#####":P2$="#####":
4 PRINT"TYPE YOUR CHOICE BY NUMBER
  (1) Chi Square
  (2) Normal Curve
  (3) End"
5 C$=INKEY$:IF C$="" THEN 5
6 ON VAL(C$) GOTO 8,48,65,7
7 PRINT:PRINT"WRONG KEY PRESSED!":PRINT:GOTO 2
8 INPUT"ENTER df ";H:IF H>30 THEN DEFDBL D,S,T,X,Y,G
9 PRINT:INPUT"ENTER CHI SQUARE ";U:GOSUB 64
10 IF H=1 THEN Z=SQR(U):U=Z:L=0:W=90:GOTO 23
11 IF H<3 THEN 13 ELSE E=1:DEFDBL D,P,S,T,X,Y:P=.398942268#:P$="#####":
12 P2$="#####":GOSUB 1040:GOSUB 46:GOTO 32
13 IF H<5 THEN 15 ELSE E=3:DEFDBL D,P,S,T,X,Y:P=.132980756#:GOSUB 1030
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14 GOSUB 45:GOTO 32
15 GOSUB 37:P=1/(G*SQR(2*H)):GOSUB 1000:PRINT
16 IF H<20 THEN E=H-2:GOTO 32
17 E=H-20
18 D=U/W:S=0:T=0:X=0:GOSUB 22:S=S+Y:X=U:GOSUB 22:S=S+Y:M=W/2
19 FOR J=1 TO M:X=(2*J-1)*D:GOSUB 22:T=T+Y:NEXT:S=S+4*T:T=0:M=M-1
20 FOR J=1 TO M:X=2*J*D:GOSUB 22:T=T+Y:NEXT:S=S+2*T
21 A=D*S/3:GOTO 58
22 Y=P*SQR((X^E/2.71828183#^X)*X^18):RETURN
23 D=(U-L)/W:S=0:T=0:X=L:GOSUB 31:S=S+Y:X=U:GOSUB 31:S=S+Y:M=W/2
24 FOR J=1 TO M:X=L+(2*J-1)*D:GOSUB 31:T=T+Y:NEXT:S=S+4*T:T=0:M=M-1
25 FOR J=1 TO M:X=2*J*D:L:GOSUB 31:T=T+Y:NEXT:S=S+2*T
26 A=D*S/3:AR=2*A:ON VAL(C$) GOTO 58,27
27 PRINT"The Area Between Z Scores Is "USING P$;A
28 PRINT" "
29 PRINT"The Sum Of The Areas Beyond The Specified Z's Is "USING P$;1-A
30 PRINT" ":GOTO 2
31 Y=.398942/1.64872^(X*X):RETURN
32 D=U/W:S=0:T=0:X=0:GOSUB 36:S=S+Y:X=U:GOSUB 36:S=S+Y:M=W/2
33 FOR J=1 TO M:X=(2*J-1)*D:GOSUB 36:T=T+Y:NEXT:S=S+4*T:T=0:M=M-1
34 FOR J=1 TO M:X=2*J*D:GOSUB 36:T=T+Y:NEXT:S=S+2*T
35 A=S*D/3:GOTO 58
36 Y=P*SQR(X^E/2.71828183#^X):RETURN
37 IF H<5 THEN G=1:RETURN
38 G=1:IF H/2 >INT(H/2) THEN 40
39 M=H/2-1:FOR J=1 TO M:G=G*J:NEXT:RETURN
40 M=INT(H/2):M=2*M-1
41 FOR J=1 TO M STEP 2:G=G*J/2:NEXT
42 G=G*1.772454#:RETURN
43 PRINT" "
44 PRINT"THIS COMPUTATION IS SOMEWHAT SLOW !":RETURN
45 PRINT:PRINT"THIS COMPUTATION IS SLOW !":RETURN
46 PRINT"THIS COMPUTATION TAKES " RT " MINUTE S"
47 PRINT" ":RETURN
48 PRINT"NORMAL CURVE
49 PRINT" "

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50 PRINT"This Program Computes Areas Under The Unit Normal Curve Between Two"
51 PRINT"User Supplied Z Scores.":PRINT
52 PRINT"FOR NEGATIVE INFINITY LET Z = -6 ;USE Z = 6 TO INDICATE ";
53 PRINT"POSITIVE INFINITY."
54 PRINT:INPUT"Enter The Smaller Z Algebraically ";L
55 PRINT:INPUT"Enter The Larger Z Algebraically ";U
56 IF L<0 AND U>0 AND ABS(U-L)>6 THEN W=90 ELSE W=52
57 GOSUB 64:GOTO 23
58 PRINT
59 CLS:IF H=1 THEN A=AR
60 PRINT"The Area Between Zero And Chi Square Is "USING P$;A
61 PRINT"The Probability Of Chance Occurrence Of A Larger Chi Square Is ";
62 PRINT USING P2$;1-A
63 PRINT" ":GOTO 2
64 PRINT:PRINT"C O M P U T I N G !":RETURN
65 END
1000 IF H<10 AND U>25 THEN W=480:GOSUB 43:RETURN
1005 IF H<10 AND U>15 THEN W=320:GOSUB 42:RETURN
1010 IF H<12 AND U>10 THEN W=110:RETURN
1015 IF H<31 AND U<31 THEN W=60:RETURN
1020 IF H<31 AND U<71 THEN W=300:GOSUB 42:RETURN
1025 W=480:GOSUB 43:RETURN
1030 IF U<17 THEN W=576 ELSE W=1200
1035 RETURN
1040 IF U<.5 THEN W=640:RT=.85:RETURN
1045 IF U<4 THEN W=3600:RT=4.8:RETURN
1050 IF U<6 THEN W=4800:RT=6.5:RETURN
1055 IF U<8 THEN W=6400:RT=8.33:RETURN
1060 IF U<9.4 THEN W=7520:RT=10:RETURN
1065 IF U<11.4 THEN W=9200:RT=16.1:RETURN
1070 IF U<16.3 THEN W=12000:RT=20.82:RETURN
1075 W=18000:RT=23.59:RETURN

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