Exact multinomial probabilities for one-way contingency tables

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The following problems involve one-way contingency tables with theoretical expected population proportions: Twenty rats are given one trial in a T-maze, and we wish to test whether there is a preexperimental bias for one arm of the maze; a biologist samples a species of fish from a stream and wishes to know if the sample suggests an unequal sex ratio in the population; a coin is tossed 50 times, and we wish to test whether it is a "fair" coin. In the above examples, the theoretical population proportion of each cell is 0.5; however, it is easy to construct examples in which the theoretical proportions are other than 0.5. The data collected in these experiments are called Bernoulli trials, for which it is assumed that each score is independent of each other score and that the true population proportion remains constant throughout the data collection. In the statistical literature, two methods of answering the above experimental questions are described. One can perform an exact test based on the binomial distribution, or one may perform an approximate test based on the chi-square distribution (or a mathematically identical test based on the normal curve). Unfortunately, the exact test is rarely treated in sufficient detail, presumably because it requires a lot of calculation, particularly if the theoretical proportion is other than 0.5. In most textbook treatments, the binomial approach to these problems is used mainly as an introduction to the approximate solution, which is based on the fit of the continuous normal distribution to the discrete binomial distribution. Because the latter test is approximate, a correction for continuity is recommended when there are but two categories; the correction makes the approximation more conservative. We would argue that an approximate test should never be used in preference to an exact test, unless the computations required by the exact procedure are unduly onerous or the approximate test is so accurate that the alternate procedure provides little savings.

Type I Errors With Chi-Square. Since an exact test exists, it is possible to compute exactly the probability of a Type I error for the two-category chi-square test as follows. With a total sample size of N , there exist $N+1$ possible outcomes for the experiment: 0 and N , 1 and $N-1$, ..., N and 0, for categories 1 and 2, respectively. For each outcome, we can determine if the chi-square approximate test would be significant; if so, we

can compute the exact binomial probability of that outcome. The sum of the exact binomial probabilities of those tables leading to rejection of the null hypothesis with chi-square gives the actual Type I error rate for that test. Figure 1 presents the actual Type I error rates for a two-category chi-square test with $N = 20$ and $\alpha = 0.05$ (indicated by the horizontal line at that value in the figure). The solid line represents Type I errors for the uncorrected chi-square, and the broken line represents the corrected chi-square. The baseline represents various values of the true population proportion from 0 to 1. As can be seen, the approximation is quite rough, with particularly wild values for extreme population proportions; and it is clear that the continuity correction leads to a conservative test with true alpha of approximately one-half its nominal value, on the average. We submit that the chi-square test leaves much to be desired in terms of accuracy.

The Exact Binomial Test. Because the binomial test usually is described poorly in most statistics textbooks, and, when it is described, it is usually treated as a one-tailed test, a brief description of the test follows. First, one computes the binomial probability of the outcome that actually occurred, using the binomial distribution formula, $N!/[x!(N-x)!]p^x(1-p)^{N-x}$, where x is the observed frequency in category 1 and p is the theoretical population probability of category 1 membership. Next, one examines the binomial probabilities of all possible outcomes ($N+1$ of them) and sums the probabilities of all those outcomes as likely as or less likely than the actual outcome. This sum is the probability of the actual outcome or of a more extreme outcome's occurring by chance given the theoretical population proportion; if it is less than alpha, we reject the null hypothesis.

Figure 1. The actual probability of a Type I error (alpha) as a function of the theoretical proportion in the first category for a binomial population (two-category contingency table) with the total sample size equal to 20. The solid line represents the uncorrected chi-square, and the dotted line represents the chi-square corrected for continuity.

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Extension to the Multinomial Distribution. When there are more than two categories for a one-way contingency table with theoretical expected proportions, the exact test is based on the multinomial rather than on the binomial distribution. The formula for the multinomial distribution is $N!/(n_1!n_2! \dots n_k!)p_1^{n_1}p_2^{n_2} \dots p_k^{n_k}$, where k is the number of categories, p_i and n_i are the theoretical proportion and the observed frequency of category i , respectively, and the sum of n_i equals N . The number of possible tables that result in a total sample of N may be calculated by the formula $(N + k - 1)!/[N!(k - 1)!]$. The sum of the multinomial probabilities of all those tables whose likelihood is less than or equal to the original table provides the exact test. The test recommended for such data by statistics textbooks is again the approximate chi-square test, but with increased degrees of freedom, equal to the number of categories minus one.

The Program. Because the multinomial problem subsumes the binomial problem, the program was written to provide exact probabilities for one-way contingency tables with any number of categories using multinomial distribution (see Appendix). The user is queried interactively for the number of categories, the observed frequencies for each category, and the theoretical cell proportions. The program computes and displays the number of tables involved, and then accumulates and prints the multinomial probability. Because the number of tables that must be generated can be quite large, the program currently uses a cutoff at 5,000 tables, beyond which point the program recommends that the approximate chi-square test be used. Multinomial probabilities are computed by FUNCTION MP, which in turn calls FUNCTION FACL. The latter function computes factorials in $\log_e$ form; because the numerical values of the factorials required by the multinomial equation can become quite large, all calculations are done in log form, and only the final answer is transformed to a numerical value, if back-transformation is possible; otherwise, the probability is returned to zero. These functions may be useful to researchers who wish to construct multinomial confidence intervals, or to program other procedures involving this distribution.

Requirements. The program is written in single-precision FORTRAN IV and runs on a DEC-20 computer. Because the program is interactive, the input and output are through the computer terminal. Several nonstandard FORTRAN statements are used to make the program run efficiently on the DEC system. Users with other systems will probably need to modify the assignment of logical units, READ statements with an "*" in place of the usual format statement number (this causes free format on the DEC), and format statements that end with the symbol "\$," which causes the cursor to remain at the end of the line on the DEC. The run time is roughly proportional to the number of tables that must be generated. With 5,000 required tables, the DEC-20 computer uses about 2.5 sec of CPU time for each solution.

Program Availability. A listing of the program may be obtained at no charge from William P. Dunlap, Department of Psychology, Tulane University, New Orleans, Louisiana 70118.

APPENDIX FORTRAN Code for Exact Multinomial Probabilities

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C COMPUTES THE MULTINOMIAL (EXACT) PROBABILITY FOR A 1 X K
C CONTINGENCY TABLE
      DIMENSION C(20),P(20),T(20),TL(17)
      COMMON TL
      OPEN (UNIT=5,DEVICE='TTY')
      OPEN (UNIT=6,DEVICE='TTY')
C CREATE TABLE OF LOG FACTORIALS FOR NUMBERS LESS THAN 18
      FL=0.
      DO 1 I=2,17
        A=I
        FL=FL+A*LOG(A)
      1 TL(I)=FL
C ENTER PROBLEM PARAMETERS
      2 WRITE(6,3)
      3 FORMAT('/' ENTER THE NUMBER OF CELLS (0 TO STOP) - ', $)
      READ(5,*)K
      IF(K.EQ.0)STOP
      WRITE(6,4)
      4 FORMAT('/' ENTER THE OBSERVED FREQUENCIES')
      XN=0.
      DO 6 I=1,K
        WRITE(6,5) I
      5 FORMAT(' CELL(' ,I2,') -- ', $)
      READ(5,*)C(I)
      6 XN=XN+C(I)
      KMO=K-1
      7 WRITE(6,8)
      8 FORMAT('/' DO THE CELLS HAVE EQUAL EXPECTED PROPORTIONS (Y OR N)
      9 ' ? ', $)
      READ(5,9)ANS
      FORMAT(A1)
      IF(ANS.EQ.'N') GOTO 11
      XK=K
      PC=1./XK
      DO 10 I=1,K
      10 P(I)=PC
      GOTO 15
      11 WRITE(6,12)
      12 FORMAT('/' ENTER THEORETICAL CELL PROPORTIONS')
      GP=0.
      DO 13 I=1,K
        WRITE(6,5) I
      13 GP=GP+P(I)
      IF(ABS(GP-1.).LT.0.001)GOTO 15
      14 WRITE(6,14)
      14 FORMAT('/' THEORETICAL PROPORTIONS DONT SUM TO 1; TRY AGAIN')
      GOTO 11
      15 PRBC=0.
C COMPUTE NUMBER OF POSSIBLE TABLES
      CNT=1.
      DO 16 I=1,KMO
        XI=I
      16 CNT=CNT*(XN+XI)/XI
      WRITE(6,17) CNT
      17 FORMAT('/' THE NUMBER OF POSSIBLE TABLES IS ',F12.0)
      IF(CNT.LT.5000.)GOTO 19
      18 WRITE(6,18)
      18 FORMAT(' MAXIMUM PERMITTED BY PROGRAM AT PRESENT IS 5000/'
      2 ' ' USE CHI-SQUARE APPROXIMATE TEST')
      GOTO 2
      19 CONTINUE
      PA=PM(C,P,K,XN)
C -- START GENERATING ALL POSSIBLE TABLES
      DO 20 I=1,KMO
        T(I)=0.
      20 KK=2
      S=0.
      DO 23 I=1,KMO
        S=S+T(I)
      23 IF(S.GT.XN) GOTO 24
        T(K)=XN-S
        PT=PM(T,P,K,XN)
        IF((PT-PA)/PA.LT.0.00001) PRBC=PRBC+PT
        T(1)=T(1)+1.
        GOTO 22
      24 DO 25 I=1,KMO
        IF(T(I).GE.XN) GOTO 27
      25 CONTINUE
        T(KK)=T(KK)+1.
        KMO=KK-1
        DO 26 I=1,KMO
          T(I)=0.
        26 GOTO 22
      27 IF(I.EQ.KMO) GOTO 29
        KK=I+1
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      T(KK)=T(KK)+1.
      DO 28 J=1,I
28    T(J)=0.
      GOTO 21
29    CONTINUE
      WRITE(6,30) PRBC
30    FORMAT(/' EXACT CUMULATIVE MULTINOMIAL PROBABILITY = ',F10.6)
      GOTO 2
      END
C
      FUNCTION PM(C,P,K,XN)
C  COMPUTES THE MULTINOMIAL PROBABILITY OF A K-CATEGORY TABLE
C  WITH FREQUENCIES IN C AND PROBABILITIES IN P
      DIMENSION C(1),P(1)
      PM=0.
      PML=FACL(XN)
      DO 1 I=1,K
1    PML=PML-FACL(C(I))*ALOG(P(I))*C(I)
      IF(PML.GT.-70.)PM=EXP(PML)
      RETURN
      END

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C
      FUNCTION FACL(A)
C  -- RETURNS WITH THE NATURAL LOG OF THE FACTORIAL OF A
C  -- TABLE LOOK UP BELOW 18 - STIRLINGS APPROX. ABOVE
      DIMENSION TL(17)
      COMMON TL
      FACL=0.
      IF(A.LE.1.)RETURN
      IF(A.GT.17.)GOTO 1
      I=A
      FACL=TL(I)
      RETURN
1    FACL=.918938533+.ALOG(A)*(A+.5)-A+1./(.12.*A)
      RETURN
      END

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