Chi-Square Probability Function

$P(\chi^2|\nu)$ is defined as the probability that the observed chi-square for a correct model should be less than a value χ^2. (We will discuss the use of this function in Chapter 15.) Its complement $Q(\chi^2|\nu)$ is the probability that the observed chi-square will exceed the value χ^2 by chance *even* for a correct model. In both cases ν is an integer, the number of degrees of freedom. The functions have the limiting values

$$P(0|\nu) = 0 \qquad P(\infty|\nu) = 1 \tag{6.2.16}$$

$$Q(0|\nu) = 1 \qquad Q(\infty|\nu) = 0 \tag{6.2.17}$$

and the following relation to the incomplete gamma functions,

$$P(\chi^2|\nu) = P\left(\frac{\nu}{2}, \frac{\chi^2}{2}\right) = \texttt{gammp}\left(\frac{\nu}{2}, \frac{\chi^2}{2}\right) \tag{6.2.18}$$

$$Q(\chi^2|\nu) = Q\left(\frac{\nu}{2}, \frac{\chi^2}{2}\right) = \texttt{gammq}\left(\frac{\nu}{2}, \frac{\chi^2}{2}\right) \tag{6.2.19}$$

CITED REFERENCES AND FURTHER READING:

Abramowitz, M., and Stegun, I.A. 1964, *Handbook of Mathematical Functions*, Applied Mathematics Series, Volume 55 (Washington: National Bureau of Standards; reprinted 1968 by Dover Publications, New York), Chapters 6, 7, and 26.

Pearson, K. (ed.) 1951, *Tables of the Incomplete Gamma Function* (Cambridge: Cambridge University Press).

6.3 Exponential Integrals

The standard definition of the exponential integral is

$$E_n(x) = \int_1^\infty \frac{e^{-xt}}{t^n} dt, \qquad x > 0, \quad n = 0, 1, \dots \tag{6.3.1}$$

The function defined by the principal value of the integral

$$\mathrm{Ei}(x) = -\int_{-x}^\infty \frac{e^{-t}}{t}\, dt = \int_{-\infty}^x \frac{e^t}{t}\, dt, \qquad x > 0 \tag{6.3.2}$$

is also called an exponential integral. Note that $\mathrm{Ei}(-x)$ is related to $-E_1(x)$ by analytic continuation.

The function $E_n(x)$ is a special case of the incomplete gamma function

$$E_n(x) = x^{n-1}\Gamma(1-n, x) \tag{6.3.3}$$

We can therefore use a similar strategy for evaluating it. The continued fraction — just equation (6.2.6) rewritten — converges for all $x > 0$:

$$E_n(x) = e^{-x}\left(\frac{1}{x+}\;\frac{n}{1+}\;\frac{1}{x+}\;\frac{n+1}{1+}\;\frac{2}{x+}\cdots\right) \tag{6.3.4}$$

We use it in its more rapidly converging even form,

$$E_n(x) = e^{-x}\left(\frac{1}{x+n-}\;\frac{1\cdot n}{x+n+2-}\;\frac{2(n+1)}{x+n+4-}\;\cdots\right) \tag{6.3.5}$$

The continued fraction only really converges fast enough to be useful for $x \gtrsim 1$. For $0 < x \lesssim 1$, we can use the series representation

$$E_n(x) = \frac{(-x)^{n-1}}{(n-1)!}[-\ln x + \psi(n)] - \sum_{\substack{m=0\\ m\neq n-1}}^{\infty} \frac{(-x)^m}{(m-n+1)m!} \tag{6.3.6}$$

The quantity $\psi(n)$ here is the digamma function, given for integer arguments by

$$\psi(1) = -\gamma, \qquad \psi(n) = -\gamma + \sum_{m=1}^{n-1}\frac{1}{m} \tag{6.3.7}$$

where $\gamma = 0.5772156649\ldots$ is Euler's constant. We evaluate the expression (6.3.6) in order of ascending powers of x:

$$\begin{aligned} E_n(x) = &-\left[\frac{1}{(1-n)} - \frac{x}{(2-n)\cdot 1} + \frac{x^2}{(3-n)(1\cdot 2)} - \cdots + \frac{(-x)^{n-2}}{(-1)(n-2)!}\right] \\ &+ \frac{(-x)^{n-1}}{(n-1)!}[-\ln x + \psi(n)] - \left[\frac{(-x)^n}{1\cdot n!} + \frac{(-x)^{n+1}}{2\cdot(n+1)!} + \cdots\right] \end{aligned} \tag{6.3.8}$$

The first square bracket is omitted when $n = 1$. This method of evaluation has the advantage that for large n the series converges before reaching the term containing $\psi(n)$. Accordingly, one needs an algorithm for evaluating $\psi(n)$ only for small n, $n \lesssim 20 – 40$. We use equation (6.3.7), although a table look-up would improve efficiency slightly.

Amos [1] presents a careful discussion of the truncation error in evaluating equation (6.3.8), and gives a fairly elaborate termination criterion. We have found that simply stopping when the last term added is smaller than the required tolerance works about as well.

Two special cases have to be handled separately:

$$\begin{aligned} E_0(x) &= \frac{e^{-x}}{x} \\ E_n(0) &= \frac{1}{n-1}, \qquad n > 1 \end{aligned} \tag{6.3.9}$$

The routine expint allows fast evaluation of $E_n(x)$ to any accuracy EPS within the reach of your machine's word length for floating-point numbers. The only modification required for increased accuracy is to supply Euler's constant with enough significant digits. Wrench [2] can provide you with the first 328 digits if necessary!

```
FUNCTION expint(n,x)
INTEGER n,MAXIT
REAL expint,x,EPS,FPMIN,EULER
PARAMETER (MAXIT=100,EPS=1.e-7,FPMIN=1.e-30,EULER=.5772156649)
   Evaluates the exponential integral E_n(x).
   Parameters: MAXIT is the maximum allowed number of iterations; EPS is the desired rel-
   ative error, not smaller than the machine precision; FPMIN is a number near the smallest
   representable floating-point number; EULER is Euler's constant γ.
INTEGER i,ii,nm1
REAL a,b,c,d,del,fact,h,psi
nm1=n-1
if(n.lt.0.or.x.lt.0..or.(x.eq.0..and.(n.eq.0.or.n.eq.1)))then
    pause 'bad arguments in expint'
else if(n.eq.0)then                  Special case.
    expint=exp(-x)/x
else if(x.eq.0.)then                 Another special case.
    expint=1./nm1
else if(x.gt.1.)then                 Lentz's algorithm (§5.2).
    b=x+n
    c=1./FPMIN
    d=1./b
    h=d
    do 11 i=1,MAXIT
        a=-i*(nm1+i)
        b=b+2.
        d=1./(a*d+b)                 Denominators cannot be zero.
        c=b+a/c
        del=c*d
        h=h*del
        if(abs(del-1.).lt.EPS)then
            expint=h*exp(-x)
            return
        endif
    enddo 11
    pause 'continued fraction failed in expint'
else                                 Evaluate series.
    if(nm1.ne.0)then                 Set first term.
        expint=1./nm1
    else
        expint=-log(x)-EULER
    endif
    fact=1.
    do 13 i=1,MAXIT
        fact=-fact*x/i
        if(i.ne.nm1)then
            del=-fact/(i-nm1)
        else
            psi=-EULER               Compute ψ(n).
            do 12 ii=1,nm1
                psi=psi+1./ii
            enddo 12
            del=fact*(-log(x)+psi)
        endif
        expint=expint+del
        if(abs(del).lt.abs(expint)*EPS) return
    enddo 13
```

```
    pause 'series failed in expint'
endif
return
END
```

A good algorithm for evaluating Ei is to use the power series for small x and the asymptotic series for large x. The power series is

$$\mathrm{Ei}(x) = \gamma + \ln x + \frac{x}{1 \cdot 1!} + \frac{x^2}{2 \cdot 2!} + \cdots \tag{6.3.10}$$

where γ is Euler's constant. The asymptotic expansion is

$$\mathrm{Ei}(x) \sim \frac{e^x}{x}\left(1 + \frac{1!}{x} + \frac{2!}{x^2} + \cdots\right) \tag{6.3.11}$$

The lower limit for the use of the asymptotic expansion is approximately $|\ln \mathtt{EPS}|$, where EPS is the required relative error.

```
      FUNCTION ei(x)
      INTEGER MAXIT
      REAL ei,x,EPS,EULER,FPMIN
      PARAMETER (EPS=6.e-8,EULER=.57721566,MAXIT=100,FPMIN=1.e-30)
C        Computes the exponential integral Ei(x) for x > 0.
C        Parameters: EPS is the relative error, or absolute error near the zero of Ei at x = 0.3725;
C        EULER is Euler's constant γ; MAXIT is the maximum number of iterations allowed; FPMIN
C        is a number near the smallest representable floating-point number.
      INTEGER k
      REAL fact,prev,sum,term
      if(x.le.0.) pause 'bad argument in ei'
      if(x.lt.FPMIN)then                 Special case: avoid failure of convergence test be-
        ei=log(x)+EULER                      cause of underflow.
      else if(x.le.-log(EPS))then        Use power series.
        sum=0.
        fact=1.
        do 11 k=1,MAXIT
          fact=fact*x/k
          term=fact/k
          sum=sum+term
          if(term.lt.EPS*sum)goto 1
        enddo 11
        pause 'series failed in ei'
1       ei=sum+log(x)+EULER
      else                               Use asymptotic series.
        sum=0.                           Start with second term.
        term=1.
        do 12 k=1,MAXIT
          prev=term
          term=term*k/x
          if(term.lt.EPS)goto 2          Since final sum is greater than one, term itself ap-
          if(term.lt.prev)then               proximates the relative error.
            sum=sum+term                 Still converging: add new term.
          else
            sum=sum-prev                 Diverging: subtract previous term and exit.
            goto 2
          endif
        enddo 12
2       ei=exp(x)*(1.+sum)/x
      endif
```

```
return
END
```

CITED REFERENCES AND FURTHER READING:

Stegun, I.A., and Zucker, R. 1974, *Journal of Research of the National Bureau of Standards*, vol. 78B, pp. 199–216; 1976, *op. cit.*, vol. 80B, pp. 291–311.

Amos D.E. 1980, *ACM Transactions on Mathematical Software*, vol. 6, pp. 365–377 [1]; also vol. 6, pp. 420–428.

Abramowitz, M., and Stegun, I.A. 1964, *Handbook of Mathematical Functions*, Applied Mathematics Series, Volume 55 (Washington: National Bureau of Standards; reprinted 1968 by Dover Publications, New York), Chapter 5.

Wrench J.W. 1952, *Mathematical Tables and Other Aids to Computation*, vol. 6, p. 255. [2]

6.4 Incomplete Beta Function, Student's Distribution, F-Distribution, Cumulative Binomial Distribution

The incomplete beta function is defined by

$$I_x(a,b) \equiv \frac{B_x(a,b)}{B(a,b)} \equiv \frac{1}{B(a,b)} \int_0^x t^{a-1}(1-t)^{b-1}dt \qquad (a,b>0) \tag{6.4.1}$$

It has the limiting values

$$I_0(a,b)=0 \qquad I_1(a,b)=1 \tag{6.4.2}$$

and the symmetry relation

$$I_x(a,b)=1-I_{1-x}(b,a) \tag{6.4.3}$$

If a and b are both rather greater than one, then $I_x(a,b)$ rises from "near-zero" to "near-unity" quite sharply at about $x=a/(a+b)$. Figure 6.4.1 plots the function for several pairs (a,b).

The incomplete beta function has a series expansion

$$I_x(a,b) = \frac{x^a(1-x)^b}{aB(a,b)}\left[1+\sum_{n=0}^{\infty}\frac{B(a+1,n+1)}{B(a+b,n+1)}x^{n+1}\right], \tag{6.4.4}$$

but this does not prove to be very useful in its numerical evaluation. (Note, however, that the beta functions in the coefficients can be evaluated for each value of n with just the previous value and a few multiplies, using equations 6.1.9 and 6.1.3.)

The continued fraction representation proves to be much more useful,

$$I_x(a,b) = \frac{x^a(1-x)^b}{aB(a,b)}\left[\frac{1}{1+}\frac{d_1}{1+}\frac{d_2}{1+}\cdots\right] \tag{6.4.5}$$