2.18 Digamma or $\psi$ Function

A. Purpose
The procedures described here compute the digamma or $\psi$ function defined by $\psi(z) = d[\ln \Gamma(z)]/dz = \Gamma'(z)/\Gamma(z)$. Additional procedures, not necessary for simplest usage, are provided to specify unusual options or retrieve error estimates.

B. Usage

B.1 Program Prototype, Single Precision

REAL U, X, SPSI
EXTERNAL SPSI

Assign a value $x$ to X, and obtain $U = \psi(x)$ by using

\[ U = \text{SPSI}(X) \]

B.2 Argument Definitions

X [in] The argument of the function, $x$ above.

B.3 Program Prototype, Single Precision, Specify Unusual Options

REAL TOL, XERR
INTEGER MSGOFF

Assign values to TOL, XERR and MSGOFF, and specify options for SPSI by using

\[ \text{CALL SPSIK}(\text{TOL}, \text{XERR}, \text{MSGOFF}) \]

B.4 Argument Definitions

TOL [in] Relative error tolerance for $\psi(x)$. When positive, it indicates relative error tolerance. When negative or zero, it indicates the default, equal to the square root of the round-off level, $\sqrt{\rho}$, should be used. $\rho$ is the smallest number such that the floating point representation of $1.0 + \rho \neq 1.0$. TOL only affects the threshold for producing error messages; it does not affect the accuracy of computation.

XERR [in] If non-negative, XERR provides the estimated relative error in X. If negative, XERR indicates the default error estimate for X, the round-off level, $\rho$, should be used.

MSGOFF [in] MSGOFF is added onto the error message level before an error message is produced by using the error message processor described in Chapter 19.2.

If SPSIK is not called, the effect is as though CALL SPSIK (0.0, −1.0, 0) had been executed.

B.5 Program Prototype, Single Precision, Determine Error Estimate

REAL ERR, IERFLG

Retrieve the relative error committed by the last call to SPSI, and the internal error indicator, by using

\[ \text{CALL SPSIE}(\text{ERR}, \text{IERFLG}) \]

B.6 Argument Definitions

ERR [out] reports the relative error committed by the last call to SPSI. If SPSI has not been called, ERR is returned with the value $-1$.

IERFLG [out] reports the value of the internal error flag. If SPSI has not been called, or if computation on the last call to SPSI was completely successful, IERFLG is returned with the value zero. See Section E below for discussion of non-zero values of IERFLG.

B.7 Modifications for Double Precision

Change the REAL statements to DOUBLE PRECISION and change the first letter of the procedure names from S to D. One must declare DPSI to be DOUBLE PRECISION, as its default type would be REAL.

C. Examples and Remarks

See DRDPSI and ODDPSI for an example of the usage of DPSIK, DPSI and DPSIE.

For $x \geq 0$, $\psi(x)$ is a monotone increasing function of $x$. $\psi(x)$ has singularities for $x = 0$ or $x$ a negative integer. See [1] for a discussion of other properties of $\psi(x)$. 
D. Functional Description

The computational methods used in SPSI were developed by L. Wayne Fullerton of Los Alamos National Scientific Laboratory. The methods include rational Chebyshev expansions, recurrences, and a reflection formula.

When $X > 0$ SPSI estimates the relative error in $\psi(X)$ is the round-off level. Otherwise, SPSI computes an estimate for the relative error in $\psi(X) = (\text{relative error in } X) \times |X| \times |\psi'(X)| / |\psi(X)|$, with $\psi'(X)$ approximated by $\pi^2 \cot^2 \pi X$. When $X < 0$ and $X$ is approximately an integer, or $\psi(X)$ is approximately zero, the error will be large. When $X << 0$ and $2X$ is not approximately an integer, SPSI may underestimate the error it committed.

References


E. Error Procedures and Restrictions

If SPSI estimates the specified error tolerance is not satisfied (because $x$ is too near a negative integer), $\psi(x)$ is computed, but an error message is issued by using the error message processor described in Chapter 19.2, with LEVEL = 1 + MSGOFF, where MSGOFF is zero unless specified by a call to SPSIK at some time before calling SPSI. The IERFLG output from SPSIE will be $-3$.

If SPSI is called with $X$ zero or a negative integer, $\psi(x)$ is not defined, and an error message is issued by using the error message processor described in Chapter 19.2, with LEVEL = 2 + MSGOFF. If error termination is suppressed by calling SPSIK with a negative value of MSGOFF, or by calling the ERMSET procedure described in Chapter 19.2, the function value will be zero, and the IERFLG output from SPSIE will be 1 if $X$ is zero, or 2 if $X$ is a negative integer.

F. Supporting Information

All code is written in ANSI Standard Fortran 77.

The program units SPSI, SPSIB, SPSIE and SPSIK communicate by way of a common block /SPSIC/. The program units DPSI, DPSIB, DPSIE and DPSIK communicate by way of a common block /DPSIC/.

Entry Required Files

| DPSI | AMACH, DCSEVL, DERM1, DERV1, DINITS, DPSI, ERFIN, ERMSG, IERM1, IERV1 |
| DPSIE | AMACH, DCSEVL, DERM1, DERV1, DINITS, DPSI, ERFIN, ERMSG, IERM1, IERV1 |
| DPSIK | AMACH, DCSEVL, DERM1, DERV1, DINITS, DPSI, ERFIN, ERMSG, IERM1, IERV1 |
| SPSI | AMACH, ERFIN, ERMSG, IERM1, IERV1, SCSEVL, SERM1, SERV1, SINITS, SPSI |
| SPSIE | AMACH, ERFIN, ERMSG, IERM1, IERV1, SCSEVL, SERM1, SERV1, SINITS, SPSI |
| SPSIK | AMACH, ERFIN, ERMSG, IERM1, IERV1, SCSEVL, SERM1, SERV1, SINITS, SPSI |

program DRDPSI

 Minor change in format for C conversion.

 Changes to use M77CON

 Original Code

 replaces "?": DR?PSI, ?PSI, ?PSIE

double precision E, P, DPSI, X
integer I, IE
external DPSI
print ' ( ' ' X DPSI(X) FLAG EST.ABS.ERR' ' )'
x = -4.5d0

 do 10 i = 1, 14
   p = dpsi(x)
   call dpsie ( e , i e )
   print ' (2x , 2 g14 . 8 , i4 , 2 x , g14 . 8 )' , x , p , i e , e*abs(p)
   x = x + 1.0d0
10 continue
stop
end

ODDPSI

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