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Adaptive Gaussian Quadrature

Function subprograms `GAUSS`, `DGAUSS` and `QGAUSS` compute, to an attempted specified accuracy, the value of the integral

$$I = \int_A^B f(x)dx\,.$$

The quadruple-precision version `QGAUSS` is available only on computers which support a `REAL*16` Fortran data type.

Structure:

`FUNCTION` subprograms
User Entry Names: `GAUSS`, `DGAUSS`, `QGAUSS`
Files Referenced: `Unit 6`
External References: `MTLMTR` (N002), `ABEND` (Z035), user-supplied `FUNCTION` subprogram

Usage:

In any arithmetic expression,

`GAUSS(F,A,B,EPS)`, `DGAUSS(F,A,B,EPS)` or `QGAUSS(F,A,B,EPS)`

has the approximate value of the integral I.

`F`	Name of a user-supplied `FUNCTION` subprogram, declared `EXTERNAL` in the calling program. This subprogram must set `F(X)` $= f($`X`$)$.
`A,B`	End-points of integration interval. Note that `B` may be less than `A`.
`EPS`	Accuracy parameter (see **Accuracy**).

`GAUSS` is of type `REAL`, `DGAUSS` is of type `DOUBLE PRECISION`, `QGAUSS` is of type `REAL*16`, and the arguments `F`, `A`, `B`, `EPS` and `X` (in `F`) have the same type as the function name.

Method:

For any interval $[a,b]$ we define $g_8(a,b)$ and $g_{16}(a,b)$ to be the 8-point and 16-point Gaussian quadrature approximations to

$$\int_a^b f(x)dx$$

and define

$$r(a,b) = \frac{|g_{16}(a,b) - g_8(a,b)|}{1 + |g_{16}(a,b)|}.$$

Then, with G = `GAUSS` or `DGAUSS`,

$$G = \sum_{i=1}^{k} g_{16}(x_{i-1}, x_i),$$

where, starting with $x_0 = A$ and finishing with $x_k = B$, the subdivision points x_i $(i = 1, 2, \ldots)$ are given by

$$x_i = x_{i-1} + \lambda(B - x_{i-1}),$$

with λ equal to the first member of the sequence $1, \frac{1}{2}, \frac{1}{4}, \ldots$ for which $r(x_{i-1}, x_i) < \texttt{EPS}$. If, at any stage in the process of subdivision, the ratio

$$q = \left| \frac{x_i - x_{i-1}}{B - A} \right|$$

is so small that $1 + 0.005q$ is indistinguishable from 1 to machine accuracy, an error exit occurs with the function value set equal to zero.

Accuracy:

Unless there is severe cancellation of positive and negative values of $f(x)$ over the interval $[A, B]$, the argument `EPS` may be considered as specifying a bound on the *relative* error of I in the case $|I| > 1$, and a bound on the *absolute* error in the case $|I| < 1$. More precisely, if k is the number of sub-intervals contributing to the approximation (see Method), and if

$$I_{abs} = \int_A^B |f(x)| dx,$$

then the relation

$$\frac{|G - I|}{I_{abs} + k} < \texttt{EPS}$$

will nearly always be true, provided the routine terminates without printing an error message. For functions f having no singularities in the closed interval $[A, B]$ the accuracy will usually be much higher than this.

Error handling:

Error `D103.1`: The requested accuracy cannot be obtained (see **Method**). The function value is set equal to zero, and a message is written on `Unit 6` unless subroutine `MTLSET` (N002) has been called.

Notes:

Values of the function $f(x)$ at the interval end-points A and B are not required. The subprogram may therefore be used when these values are undefined.

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