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Mapping an Arbitrary Range into (—1, 1) with a Side Condition: Application to Numerical Quadratures

There exist powerful techniques[1] for numerically evaluating $\int_{-1}^{1} dt\, g(t)$ by use of

$$\int_{-1}^{1} dt\; g(t) \approx \sum_i U_i g(t_i). \tag{1}$$

One technique, for example, is the use of Gauss-Legendre quadratures for which tables of weights, U_i, and roots, t_i, are widely available.[2] The purpose of this communication is to extend these techniques to integrals $\int_a^b dx\, f(x)$ by mapping (a, b) onto $(-1, 1)$.

In an optimum quadrature formula, contributions from each integration point should be of the same order of magnitude. Use of the mapping described here allows an approach to this optimum condition that has been found useful and efficient in actual applications.

The mapping used is[3]

$$x = c_1 + c_2(1 + \beta)/(1 - \beta t), \tag{2}$$

where points x in the range (a, b) map onto points in the range $(-1, 1)$ subject to the constraints that $a \to -1$, $b \to 1$, and $m \to 0$. The value m is an arbitrary point in the range (a, b). Freedom of choice of m is the feature of this mapping which makes it particularly attractive. As will now be shown, this mapping is satisfactory for all ranges (a, b) with the exception of the doubly infinite range $(-\infty, \infty)$. This latter range can be broken into multiple ranges, to any one of which the mapping of Eq. (2) is applicable. The quantities c_1, c_2, β, can be evaluated in terms of a, b, m, by solving the equations containing the constraints of the mapping, namely,

$$\begin{aligned} a &= c_1 + c_2 \\ m &= c_1 + c_2(1 + \beta) \\ b &= c_1 + c_2(1 + \beta)/(1 - \beta). \end{aligned} \tag{3}$$

The result is that

$$\begin{aligned} x &= \frac{1}{2\beta}\left[-(b - a) + \beta(b + a) + \frac{(b - a)(1 - \beta^2)}{(1 - \beta t)}\right] \\ \beta &= [(b + a) - 2m]/(b - a). \end{aligned} \tag{4}$$

Equation (4) is now used to obtain the required quadrature formula

$$\int_a^b dx\; f(x) = \int_{-1}^{1} dt\; g(t) \approx \sum_i U_i g(t_i) = \sum_i W_i f(x_i),$$

where

$$\begin{aligned} x_i &= \frac{1}{2\beta}\left[-(b - a) + \beta(b + a) + \frac{(b - a)(1 - \beta^2)}{(1 - \beta t_i)}\right] \\ W_i &= [U_i(b - a)(1 - \beta^2)]/2(1 - \beta t_i)^2 \\ \beta &= [(b + a) - 2m]/(b - a). \end{aligned} \tag{5}$$

Inspection of Eqs. (5) shows that $-1 \leq \beta \leq 1$, and that in case that $\beta = 0, 1, -1$, limiting forms must be taken.

(i) $\beta = 0$. This corresponds to $b + a = 2m$, i.e., m is the midpoint of the range. The appropriate limiting forms of Eqs. (5) are

$$\begin{aligned} \lim_{\beta \to 0} x_i &= [(b + a) + (b - a)t_i]/2 \\ \lim_{\beta \to 0} W_i &= U_i(b - a)/2. \end{aligned} \tag{6}$$

(ii) $\beta = 1$. This corresponds to b infinite (either positive

or negative), and the required limiting forms are

$$\lim_{\beta \to 1} x_i = [m(1 + t_i) - 2at_i]/(1 - t_i)$$

$$\lim_{\beta \to 1} W_i = 2U_i(m - a)/(1 - t_i)^2. \tag{7}$$

It will be noted that if the point $t = 1$ is used, the product $W_i f(x_i)$ cannot be computed directly; rather, a further limit must be taken.

(iii) $\beta = -1$. This corresponds to a infinite (either positive or negative), with the limiting forms

$$\lim_{\beta \to -1} x_i = [m(1 - t_i) + 2bt_i]/(1 + t_i)$$

$$\lim_{\beta \to -1} W_i = 2U_i(b - m)/(1 + t_i)^2. \tag{8}$$

If the point $t = -1$ is used then, as in the previous case, a further limit must be taken.

In conclusion, we note that in specific applications it may be necessary to break the integration range into more than one part and apply the formulas developed above to each part separately in order to obtain a satisfactory quadrature formula. We have written a versatile computer subroutine (in FAP for the IBM 7090) to provide such formulas using Gauss-Legendre quadratures for the variable t. This subroutine is available on request to the authors.

References and footnotes

1. See for example, V. I. Krylov, *Approximate Calculation of Integrals*, Macmillan Co., New York, 1962.
2. P. Davis and P. Rabinowitz, *J. Res. Natl. Bur. Std.* (U.S.) **56**, 35 (1956); **60**, 613 (1958).
3. We arrived at this mapping by generalizing a transformation used by A. C. Wahl, P. E. Cade and C. C. J. Roothaan, *J. Chem. Phys.* **41**, 2578 (1964). The formulas corresponding to $\beta = 0, 1, -1$, had previously been used by one of us (A.D.M.) in computer programs reported in *J. Chem. Phys.* **32**, 1595 (1960).

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