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NOTE

The Numerical Evaluation of Principal-Value Integrals

In this note we point out that principal value integrals may be evaluated with the same ease as ordinary integrals, provided that the integration region is symmetric, and that suitable quadrature rules are used. In fact, it is even possible to evaluate principal value integrals with computer routines written for ordinary integrals. The technique described below was developed to evaluate principal value integrals arising in the three-particle collision problem [1].

We consider the principal value integral

$$\boldsymbol{P}\int_{-1}^{1} f(x)\,dx \equiv \boldsymbol{P}\int_{-1}^{1} \frac{g(x)}{x}\,dx, \tag{1}$$

where $f(x)$ is an analytic function with a simple pole at the origin, so that $g(x) = xf(x)$ is regular at the origin. On using

$$\boldsymbol{P}\int_{-1}^{1} \frac{1}{x}\,dx = 0,$$

we obtain the well known result

$$\boldsymbol{P}\int_{-1}^{1} f(x)\,dx = \int_{-1}^{1} \frac{g(x) - g(0)}{x}\,dx. \tag{2}$$

The right-hand side of (2) is an ordinary integral, since the integrand has the finite value $g'(0)$ at the origin.

Equation (2) expresses the principal value integral as an ordinary integral, so that formally the problem is solved. Some caution is required, however, in numerical quadrature based on (2), for if a grid point falls near the origin then errors in $g(x)$ and $g(0)$ are magnified by the large factor $1/x$, and may produce large errors in the result. In extreme cases rounding errors in $g(x)$ and $g(0)$ may even lead to complete loss of significance in the result.

The simplest way to keep the grid points away from the pole, and so minimise these errors, is to use a symmetric even-order quadrature rule. Specifically, we consider a symmetric $2n$-point rule, with abscissas at $\pm x_i (i = 1,\ldots, n)$ and corresponding weights w_i, so that the rule for an arbitrary regular function $F(x)$ is

$$\int_{-1}^{1} F(x)\, dx \approx \sum_{i=1}^{n} w_i[F(x_i) + F(-x_i)]. \tag{3}$$

If we apply this rule to the right-hand side of (2), the contributions from the second term of (2) cancel, and on using $g(x)/x = f(x)$ we obtain

$$P \int_{-1}^{1} f(x)\, dx \approx \sum_{i=1}^{n} w_i[f(x_i) + f(-x_i)], \tag{4}$$

which has exactly the same structure as (3). It follows that we can treat the principal-value integral as though it were an ordinary integral, provided that the quadrature rule is symmetric about the pole. Rounding errors are not a serious problem in (4). For example, if $g(x) \equiv 1$, and if the rounding errors in $g(x_i)$ and $g(-x_i)$ are ϵ_i and δ_i, respectively, then the resulting error in (4) is

$$\sum_{i=1}^{n} (\epsilon_i - \delta_i)\, w_i/x_i \approx (\epsilon_1 - \delta_1)\, w_1/x_1 .$$

To a first approximation, the error is independent of n, since x_1 and w_1 approach zero together as n increases.

The most attractive quadrature rules for this purpose are probably the even-order Gaussian rules, and these were in fact used in the calculations of [1], with the same computer routine handling both principal-value and ordinary integrals. It frequently happens, of course, that the integration region is not symmetric about the pole. The integration region may then be divided into a symmetric region about the pole, and a second region remote from the pole, in which ordinary methods may be used.

Reference

1. I. H. Sloan, *Phys. Rev.* **165**, 1587 (1968).

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