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NUMERICAL QUADRATURE METHODS OF ANALYTIC FUNCTIONS

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1. Introduction

Many methods exist for the evaluation of definite integrals. In a problem in which the integrand function is analytic and can by readily evaluated at points (other than singularities) in the complex plane, there is often scope for reformulating the problem in a manner to take advantage of there circumstances. Some of the possible approaches are described in ABRAMOWITZ [1] (reprinted in DAVIES and RABINOWITZ [2]) and in SMITH and LYNESS [7]. In this paper we describe three other useful transformations of the same nature.

One very straightforward approach to numerical quadrature on a finite interval is described in [6]. In its complete form this consists in determining the Taylor coefficients of the integrand function and integrating the Taylor series term by term. The Taylor coefficients are determined by discretising the Cauchy integral representation of the derivative. The advantages of this approach include its stability, the easy with which convergence may be observed or the error estimated, the iterative nature of the calculations and its simplicity for coding purposes. Since it provides an approximation to the primitive, it may be used for numerical indefinite integration within a finite interval.

However this method has several disadvantages. In cases when it can be used, it is two or three times as expensive as the corresponding Gaussian method (if the number of function values for this is known). But the major disadvantage is that it can be used only in situations in which the convergence of the underlying Taylor expansion can be assured. For example if there is a singularity near the integration interval, or if this interval is infinite, the direct use of this method becomes highly impracticable.

In the first section of this paper we give a direct extension of results obtained in [6] for the case of an analytical function in an annulus. The resulting integration method thus obtained has all advantages of the Lyness method. Meantime it is more elastic related to convergence interval and can be applied for example in the case of the integrand function having a singularity near the integration interval.

In the next two sections we describe simple transformations which can be used when the integrand is an analytical function. Their purpose is to replace the original problem by one amanable to the straightforward method.

2. A quadrature schema based on Laurent-series expansion

Let $f(z)$ be an analytical function in a domain which includes the smooth curve Γ. We shall attempt to evaluate numerically the integral

$$\int_\Gamma f(z)dz = \int_{z_1}^{z_2} f(z)dz, \tag{2.1}$$

z_1 and z_2 being the end points of the curve Γ (the origin is chosen so that we have $|z_1| = |z_2| = r$). We assume that the function $f(z)$ is holomorphic in an annular region whose centre is at the origin, which includes the curve Γ. Let R_1 be the radius of the inner circle and R_2 the radius of the external one. In the annulus the function $f(z)$ can be developed into Laurent-series

$$f(z) = \sum_{j=-\infty}^{+\infty} a_j z^j. \tag{2.2}$$

The coefficients a_j are given by

$$a_j = \frac{1}{2\pi i}\int_{C_r} \frac{f(\zeta)}{\zeta^{j+1}}\, d\zeta, \quad j = 0, \pm 1, \pm 2, \ldots \tag{2.3}$$

C_r being the circle of radius r, $(R_1 < r < R_2)$, with the center at the origin. Formula (2.3) can be also written under the form

$$r^j a_j = \frac{1}{2\pi}\int_0^{2\pi} f(re^{i\theta})\, e^{-ij\theta}\, d\theta \equiv \frac{1}{2\pi}\int_0^{2\pi} g(\theta)\, d\theta, \quad j = 0, \pm 1, \ldots \tag{2.4}$$

The series (2.2) converges uniformly on the circle C_r, and we have

$$f(r\, e^{i\theta}) = \sum_{j=-\infty}^{+\infty} a_j r^j e^{ij\theta}. \tag{2.5}$$

We shall estimate the coefficients a_j from relation (2.4) by using a numerical quadrature method. Since the integrand is a periodical function, one of the most efficient methods of numerical quadrature which can be used in this case is the trapezoidal rule

$$R^{[M,1]} g = \frac{1}{M}\sum_{j=1}^{M} g\left(\frac{2\pi}{M} j\right). \tag{2.6}$$

The resulting value for $r^k a_k$ is

$$r^k a_k^{(M)} = \sum_{j=1}^{M} f(r\, e^{2\pi i j/M})\, e^{-2\pi i jk/M}, \tag{2.7}$$

$$k = -(n-1), \ldots, -1, 0, 1, \ldots, m-1, \quad M = m + n - 1.$$

Numerical approximations of integrals like those appearing in (2.4) by the trapezoidal rule were considered in [3]. The author proved the convergence of the method and made the error analysis. In the following we shall rework this analysis by methods used in [6] in view of obtaining some relations useful for numerical quadrature schema developed below.

The error introduced by using relation (2.6) can be estimated by „aliasing" [4]. Thus, since

$$R^{[M,1]} e^{ik\theta} = \begin{cases} 0 & \text{if } k/M \neq \text{integer or zero} \\ 1 & \text{if } k/M = \text{integer or zero} \end{cases}$$

by using relation (2.6) we have

$$r^k a_k^{(M)} = r^k a_k + r^{k-M} a_{k-M} + r^{k+M} a_{k+M} + + r^{k-2M} a_{k-2M} + r^{k+2M} a_{k+2M} + \ldots \tag{2.8}$$

Accordingly, formula (2.7) is exact if the function $f(z)$ is of the form

$$f(z) = P_{m+n-2}(z)/z^{n-1}, \tag{2.9}$$

$P_{m+n-2}(z)$ being an arbitrary polynomial of a degree at most equal to $m + n - 2$.

Moreover an iteration procedure can be given for determining the coefficient a_k. Thus, the use of the mid-point trapezoidal rule

$$R^{[m,0]} g = \frac{1}{M}\sum_{j=1}^{M} g\left(\frac{(2j-1)\pi}{M}\right),$$

leads to the following approximation of the coefficients a_k

$$r^k b_k^{(M)} = \frac{1}{M}\sum_{j=1}^{M} f\left(r e^{\frac{(2j-1)\pi i}{M}}\right) e^{-\frac{ik(2j-1)\pi}{M}}, \tag{2.10}$$

$$k = -(n-1), \ldots, -1, 0, 1, \ldots, (m-1).$$

This formula, like those above, is exact for the functions $f(z)$ of the form (2.9).

The relations

$$r^{k-M} a_{k-M}^{(M)} = r^{k+M} a_{k+M}^{(M)} = r^k a_k^{(M)},$$

$$r^{k-M} b_{k-M}^{(M)} = r^{k+M} b_{k+M}^{(M)} = -r^k b_k^{(M)},$$

$$k = -(n-1), \ldots, 1, 0, 1, \ldots, (m-1),$$

as well as the formula which results form (2.6) and (2.10)

$$R^{[2M,1]} g = \frac{1}{2} \{R^{[M,1]} g + R^{[M,0]} g\}$$

permit the obtaining of the following reccurence relations

$$r^k a_k^{(2M)} = \frac{1}{2} \{r^k a_k^{(M)} + r^k b_k^{(M)}\}, \quad -n+1 < k < m-1;$$

$$(2.11) \quad r^{k-M} a_{k-M}^{(2M)} = \frac{1}{2} \{r^k a_k^{(M)} - r^k b_k^{(M)}\}, \quad k = 1, 2, \ldots, m-1;$$

$$r^{k+M} a_{k+M}^{(2M)} = \frac{1}{2} \{r^k a_k^{(M)} - r^k b_k^{(M)}\}, \quad k = -1, -2, \ldots, -(n-1);$$

When these relations are used, account must be taken of the fact that we dispose of two arbitrary parameters (n and m) and hence we can increase either the number m of coefficients with positive subscripts or that of coefficients with negative subscript, or the number of boths sets of coefficients, function of the specific problem under consideration.

The convergence of this iteration procedure can be easily proved. Thus, from (2.3) we obtain the inequalities

$$|a_j| < M_2 R_2^{-j}, \; j > 0,$$

$$|a_j| < M_1 \; R_1^{-j}, \; j < 0,$$

where

$$M_j = \max_{z \in C_j} |f(z)| \qquad j = 1, 2.$$

The introduction of these inequalities into (2.8) leads to the estimation

$$(2.12) \quad |r^k a_k^{(M)} - r^k a_k| < M_2 \frac{\rho_2^{k+M}}{1-\rho_2^M} + M_1 \frac{\rho_1^{M-k}}{1-\rho_1^M},$$

where $\rho_2 = r/R_2$, $\rho_1 = R_1/r$. From relation (2.12) we have

$$\lim_{M \to \infty} r^k a_k^{(M)} = r^k a_k$$

The coefficients thus obtained permit to give the following rational approximation to the function $f(z)$

$$(2.13) \quad f^{[M]}(z) = \sum_{j=-(n-1)}^{m-1} a_j^{(M)} z^j$$

In order to estimate the error we write

$$f(z) - f^{[M]}(z) = \sum_{j=-(n-1)}^{m-1} (a_j - a_j^{(M)}) z^j + \sum_{\substack{j \leq n, \\ j \geq m.}} a_j z^j,$$

By using relations (2.8) and the Cauchy's inequalities we obtain

$$(2.14) \quad |f(z) - f^{[M]}(z)| \leq 2\left(M_1 \frac{\rho_1^n}{1-\rho_1} + M_2 \frac{\rho_2^m}{1-\rho_2}\right) \equiv \varepsilon.$$

This relation indicates that the function $f^{[M]}(z)$ constitutes a uniform approximation of the function $f(z)$ on the circle $|z| = r$.

We have also:

$$\lim_{\substack{n \to \infty \\ m \to \infty}} f^{[M]}(z) = f(z)$$

uniformly on the circle mentioned above.

Performing the quadrature of the function $f^{[M]}(z)$ we obtain the following approximation to the primitive $F(z)$ of the function $f(z)$

$$(2.15) \quad F^{[M]}(z) = \sum_{\substack{j=-(n-1) \\ j \neq 1}}^{m-1} a_j^{(M)} \frac{z^{j+1}}{j+1} + a_{-1}^{(M)} \log z.$$

If the function $f(z)$ is a rational function of the form (2.9) the indefinite integration rule is exact. We have also

$$|F(z) - F^{[M]}(z)| \leq 2\pi\varepsilon,$$

provided both functions $F(z)$ and $F^{[M]}(z)$ have same value at a point on the circle. The recurrence relations (2.11) and formula (2.15) enables us to obtain an iterative quadrature scheme.

3. The indefinite integral of a function analytical on the real axis

Now let us assume that the real function $f(x)$ is the restriction to the Ox axis of the complex analytical function $f(z)$. We assume that all the singularities of the function lie within the circles

$$\left|z \pm \frac{1}{2}(p+q)\, i\right| = 0.5 \; (q-p); \; 0 < p < q$$

in the complex plane z.

We want to approximate $f(z)$ on the whole real axis Im $\{z\} = 0$. To this end we use the transformation

$$Z = \frac{z + ia}{z - ia},$$

which takes $z = x = \text{arctg}\,\frac{0}{2}$ (real axis from z plane) into $Z = e^{i0}$ (unity circle from Z plane). By this transformation the function $f(z)$ becomes the function

$$\Phi(Z) = f\left(ia\frac{Z+1}{Z-1}\right),$$

which takes real values on the circle $|Z| = 1$ and is analytic in an annulus $1 - \eta < r < 1 + \eta$. For the function $\Phi(Z)$ we can use the previous theory to obtain the approximation

$$\Phi^{[M]}(Z) = \sum_{j=-m}^{+m} a_j^{(M)} Z^j,$$

where $M = 2\,m + 1$. The coefficients $a_j^{(M)}$ result now from relation

$$a_k^{(M)} = \frac{1}{M}\left\{\sum_{j=1}^{M-1} f\left(a\,\text{ctg}\,\frac{2\pi j}{M}\right) e^{-2\pi ijk/M} + f(\infty)\right\}$$

(3.1)

$$a_{-k}^{(M)} = \bar{a}_k^{(M)},\quad k = 0,\ 1,\ 2,\ \ldots,\ m.$$

Taking the inverse transformation we obtain the following approximation of the function $f(x)$

$$f^{[M]}(x) = \sum_{j=-m}^{m} a_j^{(M)} \left(\frac{x + ia}{x - ia}\right)^j. \tag{3.2}$$

The primitive of this function approximates uniformly the primitive $F(x)$ of the function $f(x)$ over every finite interval of the real axis. Thus we have

$$F^{[M]}(x) = xf(\infty) - 4a \ln \rho \cdot \rho_1^{(M)} \cdot \sin \varphi_1^{(M)} + 4\varphi a \rho_1^{(M)} \cos \varphi_1^{(M)} -$$

(3.3)

$$- 2\sum_{j=2}^{m} \frac{(2a)^j}{j-1} \frac{\rho_j^{(M)}}{\rho^{j-1}} \cos\left\{j\frac{\pi}{2} + \varphi_j^{(M)} + (j-1)\varphi\right\},$$

where

$$x + ia = \rho e^{i\varphi};\quad 0 < \varphi < \pi;$$

$$\sum_{k=j}^{m} \binom{k}{j} a_k^{(M)} = \rho_j^{(M)} \cdot e^{i\varphi_j^{(M)}}.$$

Formula (3.2) is exact for the rational functions of the form

$$f(x) = \frac{P_{2m}(x)}{(x^2 + a^2)^m}.$$

Its use requires the evaluation of the function $f(x)$ at $2m$ points lying on the Ox axis. A discussion similar to that given in the preceding section can be used to prove that we have $\lim\limits_{m\to\infty} F^{[M]}(x) = F(x)$ over every finite interval of the real axis.

Now let us assume that the function $f(x)$ has singularities on the real axis outside the interval $[c,\ d]$ where its primitive is to be calculated. We shall perform the change of variable

$$x' = \left(\frac{x - c}{d - x}\right)^{\frac{1}{2}};\quad \alpha' = \left(\frac{\alpha - c}{d - \alpha}\right)^{\frac{1}{2}};\quad \beta' = \left(\frac{\beta - c}{d - \beta}\right)^{\frac{1}{2}},$$

which yields

$$\int_{\alpha}^{\beta} f(x)\ \mathrm{d}x = \int_{\alpha'}^{\beta'} f\left(\frac{dx'^2 + c}{1 + x'^2}\right) \frac{2x'(d - c)}{(1 + x'^2)^2}\, dx'.$$

The new function

$$g(x') = f\left(\frac{dx'^2 + c}{1 + x'^2}\right) \frac{2x'(d - c)}{(1 + x'^2)^2}$$

has no singularities on the real axis. In addition, since in the argument of the function f the variable x' intervenes only by its square, it follows that the use of formula (3.2) implies the evaluation of the function $f(x)$ only at m points.

The theory above can be used for obtaining numerical quadrature formulas for integrals with weighting factors. Thus, using the approximation (3.2) to $f(x)$ we obtain the following quadrature formula

$$\int \frac{f(x)}{x^2 + a^2}\,\mathrm{d}x = \frac{a_0^{(M)}}{a}\text{arctg}\,\frac{x}{a} - \frac{1}{a}\sum_{j=1}^{m} (2a)^j \frac{\hat{\rho}_j(M)}{\rho^j} \times$$

(3.4)

$$\times \sin\left(j\varphi + j\frac{\pi}{2} - \hat{\varphi}_j^{(M)}\right) + R_M,$$

where

$$\sum_{k=j}^{m} \binom{k}{j} a_k^{(M)} \cdot k^{-1} = \hat{\rho}_j^{(M)} e^{i\hat{\varphi}_j^{(M)}}$$

and R_M denotes the truncation error.

The above quadrature rule is exact for same class of functions such as formula (3.3). It constitutes an approximation for the primitive valid on the whole real axis and is useful for evaluating slowly convergent integrals. If the integration interval coincides with the Ox axis the numerical quadrature formula (3.4) reduces to the TAN rule considered in [8].

To estimate the error R_M we can write

$$R_M = \left| \int_0^{} \frac{f(x) - f^{[M]}(x)}{x^2 + a^2} dx \right| \leqslant \max_{x \in R} |f(x) - f^{[M]}(x)| \int_0^{x} \frac{dx}{x^2 + a^2} < \varepsilon \frac{\pi}{a}$$

Thus, we get $\lim\limits_{m \to \infty} R_M = 0$.

As an application we shall estimate the integral

$$I_1 = \int_0^c \frac{2x + 5}{(x+1)^2 (x+4)^2} \exp\left\{\frac{1}{(x+1)(x+4)}\right\} dx, \qquad c > 0.$$

This quadrature can be analytically performed and gives

$$I_1 = \exp\left\{\frac{1}{(c+1)(c+4)}\right\}.$$

Since the integrand has singularities on the negative real axis, the use of formulas (3.3) or (3.4) requires the preliminary change of variable $x = x'^2$. Using formula (3.2) with $m = 10$, we have obtained results of relative accuracy 10^{-6} for values of c ranging from 0,5 to 64. On the other hand, using the Gauss-Legendre ten point formula, we need different abscises for each value of c. For values of c less than 4 the accuracy is greater about 10^{-7}, but for the larger values of c this accuracy degrades being 10^{-1} at $c = 64$. When formula (3.4) was applied results of relative accuracy 10^{-6} were obtained for values of c ranging form 0,5 to 10^{20}.

4. Numerical integration scheme based on the residue theorem

Let us estimate the integral

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

where $f(x)$ is the restriction to the real axis of an analytical function in the complex plane $z = x + iy$, without singularities on the segment $[a, b]$. We consider the function

$$h(z) = \frac{1}{i\pi} f(z) \cdot \log \frac{z - b}{z - a}. \tag{4.1}$$

This is an analytical function in the complex plane which has the cut $[a, b]$ on the real axis. The values of the real part of the function $h(z)$ on the Ox axis are

$$\operatorname{Re}\{h(z)\} = \begin{cases} 0 & x < a;\ x > b, \quad y = 0 \\ f(x) & a < x < b, \quad y = +0 \\ -f(x) & a < x < b, \quad y = -0 \end{cases} \tag{4.2}$$

We apply the residue theorem to the function $h(z)$ for the domain bounded by the cut indicated above and by a circle of radius R which includes this cut. If in this domain the function $h(z)$ has only isolated singular points, we have

$$2 \int_a^b f(x)\, dx + \int_{C_R} h(z)\, dz = 2\pi i \sum_{(j)} \operatorname{Rez}\{h(z),\ \alpha_j\}. \tag{4.3}$$

The sum which appears in the right-hand side of this relation extends to all singular points α_j of the function $h(z)$ in the considered domain. If $z = z^{(0)} + Re^{i\theta}$ is the equation of te circle C_R, from (4.3) we get

$$\int_a^b f(x) dx = \frac{1}{2i} \int_0^{2\pi} h(z^{(0)} + Re^{i\theta}) Re^{i\theta} + d\theta + \pi i \sum_{(j)} \operatorname{Rez}\{h(z),\ \alpha_j\}. \tag{4.4}$$

The residues which appear in this relation can be analytically estimated [5], and the integral in the right-hand side of relation (4.4) can be numerically approximated. As the integrand is a periodical function formula (2.6) can be used for its estimation. In this formula we set $M = 2m$ and assume that z_0 is real.

Since on the axis OX the function $f(z)$ assumes real values, we have $f(z) = f(\bar{z})$. Consequently, the application of this formula requires only $m-1$ evaluations of the complex function $f(z)$ and two evaluation of the real function $f(x)$. Finally, we get

$$\int_a^b f(x) dx = \pi i \sum_{(j)} \operatorname{Rez}\left\{f(z) \log \frac{z-b}{z-a};\ \alpha_j\right\} - \frac{1}{m}\left\{\sum_{j=1}^{m-1} (z_j - z^{(0)}) \times \right.$$
$$\left. \times f(z_j) \log \frac{z_j - b}{z_j - a} + \frac{z_0 - z^{(0)}}{2} f(z_0) \log \frac{z_0 - b}{z_0 - a} + \frac{z_m - z^0}{2} f(z_m) \log \frac{z_m - b}{z_m - a}\right\}, \tag{4.5}$$

where

$$z_j = z^{(0)} + Re^{ij\pi/m}, \qquad j = 0, 1, \ldots, m.$$

The error resulting from the use of formula (4.5) can be expressed by relation (2.12) where $k = 0$ and

$$M_j = \max_{z \in C_j} |h(z)|.$$

This relation shows that the error is the smaller the more remote is the circle C_R from the singularities of the function $h(z)$. This gives a criterion for the choice of this circle.

Relation (4.5) can be extended to the calculation of finite part integrals. Likewise, it can be successfully used to the problem of quadrature close to an unintegrable singularity.

As an example of application of the method described above, we shall try to evaluate numerically the integral

$$I_2 = \int_A^{\frac{1}{2}} \frac{dx}{\sin^2 \pi x},$$

which was also considered in [6].

The function

$$f(z) = \frac{1}{\sin^2 \pi z}$$

has second order poles at the points $z = 0$, has second order poles at the has second order poles at the points $z = 0, \pm 1, \pm 2, \ldots$ We choose the circle $C_R \equiv \{z = 0{,}2 + 0{,}5\, e^{i\theta}\}$. Inside this circle the function $h(z)$ has a second order pole at the origin with the residue

$$\text{Rez}\,\{h(z),\ z = 0\} = \frac{1}{i\,\pi^3} \cdot \frac{1 - 2A}{A}.$$

The results of calculation indicate that this method gives results of an order of accuracy comparable with that given in [6], that is a relative error of about 10^{-12}.

6. Conclusions

The theory of complex variable functions can be successfully applied to problems of numerical analysis for analytical functions. The results obtained in [6] can be extended to the case of holomorphic functions in an annular region.

The formulas for the indefinite integral obtained on the basis of this generalization prove to be particularly efficient in all examples considered.

Likewise, the use of the residue theorem combined with the numerical quadrature formula for periodical functions to the quadrature scheme (4.5) which is also efficient for analytical functions.

All the integration rules obtained can be successfully used due to their iterative aspect and analytic simplicity.

The quadrature formulas (2.15), (3.3), (3.4) are also advantageous in that they permit one to obtain expressions for the primitive functions at no significant additional cost. A drewback of all formulas given is that they can be applied only to analytical functions.

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