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SOME FORMULAE FOR NUMERICAL DIFFERENTIATION AND INTEGRATION OF ANALYTIC FUNCTIONS

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1. Introduction

This paper is concerned with the numerical evaluation of derivatives and principal values of integrals from analytical functions. To compute the derivative of an analytical function we give a simpler deduction of formulae obtained by LYNESS [6]. Afterwords we give an extrapolation method to obtain more accurate numerical differentiation formulae. The iterative procedure based on extrapolation to the limit is superior to that given in [6]. We also describe how to derive formulae for numerical evaluation of residues at isolated singularities.

To evaluate the principal value integrals KUTT [5] derived Gauss type formulae computing the stations and the weights for some orders of the singularity. The method is cumbersome since it needs different stations and weights for every singularity. To avoid this difficulty we use the method of extraction of singularities [3]. This requires to evaluate some derivatives which can be made by formulae given previously. The resulting regular integrals can be computed by means of obvious mechanical quadrature rules. For Cauchy principal value integrals we refound the formulae due to PIESSENS [8] and HUNTER [4].

In the next section we consider the case that integrand has isolated singularities near the integration interval. We develop a formula based on Gauss—Chebyshev quadrature rule and on residue theorem. Again, to evaluate residues, use can be made of formulae given in section 2.

2. Numerical differentiation formulae

Let $f(z)$ be an analytical function without singularities in the neighbourhood $|z - z_0| < R$ of the point $z = z_0$. We have

$$(2.1)\qquad f(z) = f(z_0) + \frac{z - z_0}{1!} f'(z_0) + \ldots + \frac{(z - z_0)^m}{m!} f^{(m)}(z_0) + \ldots$$

Let $z_0 = z_0 + h \exp\left\{i\,\frac{2\pi j}{n}\right\}$; $(j = 0, 1, \ldots, n - 1)$ be the complex roots of the equation

$$(2.2)\qquad (z - z_0)^n = h^n$$

where $0 < h < R$.

The relation (2.1) gives

$$(2.3)\qquad \sum_{j=1}^{n} (z_j - z_0)^{-k} f(z_j) = \sum_{m=0}^{\infty} \frac{f^{(m)}(z_0)}{m!} \sum_{j=1}^{n} (z - z_j)^{-k+m}$$

But we have

$$(2.4)\qquad \sum_{j=1}^{n} (z_j - z_0)^{-k} = \begin{cases} 0 & \text{for } 1 \leqslant |k| \leqslant n - 1 \\ n & \text{for } k = 0 \\ nh^n & \text{for } k = n \end{cases}$$

and relation (2.3) becomes

$$(2.5)\qquad \sum_{j=1}^{n} (z_j - z_0)^{-k} f(z_j) = n\,\frac{f^{(k)}(z_0)}{k!} + n \sum_{m=1}^{\infty} h^{mn} \frac{f^{(k+mn)}(z_0)}{(k + mn)!} \qquad (k = 1, \ldots, n - 1)$$

Hence we obtain the numerical differentiation formulae

$$(2.6)\qquad f^{(k)}(z_0) = k!\,\frac{\sum\limits_{j=1}^{n} (z_j - z_0)^{-k} f(z_j)}{n} + E_{k,n} \qquad k = 1, 2, \ldots, n - 1$$

where

$$(2.7)\qquad E_{k,n} = -k! \sum_{m=1}^{\infty} h^{mn} \frac{f^{(k+mn)}(z_0)}{(k + mn)!}$$

is the error.

The formula (2.6) coincides with that given by LYNESS [6], by a more complicated way. The expression (2.7) puts into evidence the dependence of the error on h.

By using the value $f(z_0)$ we can give also an expression for $f^{(n)}(z_0)$. Thus from (2.2) and (2.3) we obtain

$$(2.8)\qquad \sum_{j=1}^{n} (z_j - z_0)^{-n} f(z_j) = nh^{-n} f(z_0) + n\,\frac{f^{(n)}(z_0)}{n!} + n \sum_{m=1}^{\infty} h^{mn} \frac{f^{((m+1)n)}(z_0)}{[(m + 1)n]!}$$

Hence

$$(2.9)\qquad f^{(n)}(z_0) = n!\,\frac{\sum\limits_{j=1}^{n} f(z_j) - n f(z_0)}{nh^n} + E_{n,n}$$

$$(2.10)\qquad E_{n,n} = -n! \sum_{m=1}^{\infty} h^{mn} \frac{f^{((m+1)n)}(z_0)}{[(m + 1)n]!}$$

The relations (2.6), (2.9) allow us to compute the derivatives to n-th order at the point z_0 by using $n + 1$ complex values of the function $f(z)$. If the restriction of the function $f(z)$ to the real axis is a real function the values of the function at points located in the lower half plane can be obtained from those from the upper half-plane and consequently the number of function evalutions reduces near to the half.

To obtain more accurate formulae we can increase the number n of points. Thus by doubling the number of points we obtain formulae with the error of O (h^{2n}) order at the price of more n function evaluations.

Alternatively we can use the extrapolation to the limit [2]. Let

$$(2.11)\qquad D_k^{(0)}(h) = k!\,\frac{\sum\limits_{j=1}^{n} (z_j - z_0)^{-k} f(z_j)}{n} \qquad (k = 1, 2, \ldots, n - 1)$$

We have

$$(2.12)\qquad f^{(k)}(z_0) = D_k^{(0)}(h) - h^n k!\,\frac{f^{(k+n)}(z_0)}{(k + n)!} - k! \sum_{m=2}^{\infty} h^{mn} \frac{f^{(k+mn)}(z_0)}{(k + mn)!}$$

$$(2.13)\qquad f^{(k)}(z_0) = D_k^{(0)}\left(\frac{h}{2}\right) - \frac{h^n}{2^n} k!\,\frac{f^{(k+n)}(z_0)}{(k + n)!} - k! \sum_{m=2}^{\infty} \frac{h^{mn}}{2^{mn}} \frac{f^{(k+mn)}(z_0)}{(k + mn)!}$$

and hence

$$(2.14)\qquad f^{(k)}(z_0) = D_k^{(1)}\left(\frac{h}{2}\right) + k! \sum_{m=2}^{\infty} \frac{1 - 2^{(1-m)n}}{2^n - 1} h^{mn} \frac{f^{(k+mn)}(z_0)}{(k + mn)!}$$

where

$$(2.15)\qquad D_k^{(1)}\left(\frac{h}{2}\right) = \frac{2^n D_k^{(0)}\left(\frac{h}{2}\right) - D_k^{(0)}(h)}{2^n - 1} \qquad (k = 1, \ldots, n - 1)$$

The truncation error in formula (2.15) is about 2^n times smaller than that given by relation (2.7) corresponding to $2n$ points. The extrapolation process can be continuated. Thus the formula

$$D_k^{(m)}\left(\frac{h}{2j}\right) = \frac{2^{nj} D_k^{(m-1)}\left(\frac{h}{2^j}\right) - D_k^{(m-1)}\left(\frac{h}{2^{j-1}}\right)}{2^{nj} - 1}; \qquad (k = 1, \ldots, n-1) \tag{2.16}$$

$$j = 1, 2, \ldots$$
$$m = 1, 2, \ldots, j$$

gives the approximation $D_k^{(m)}$ to $f^{(k)}(z_0)$ with error of order $O(h^{n(m+1)}/2^{mn})$.

For $k = n$ the relations (2.15), (2.16) are still valid with the initialization

$$D_n^{(0)}(h) = n!\,\frac{\sum_{j=1}^{n} f(z_j) - nf(z_0)}{n\,h^n} \tag{2.17}$$

The obtained formulae can be used to determine the residue of an analytical function at a polar singularity. Thus if $z = z_0$ is a l'th order pole for the function $g(z)$ we have

$$\text{Rez}\,\{g(z), z_0\} = \frac{1}{(l-1)}\left\{\frac{d^{(l-1)}}{d z^{l-1}}(z - z_0)^l g(z)\right\}_{z=z_0} \tag{2.18}$$

and this derivative can be estimated by using the above mentioned relations.

If $z = z_0$ is an essential singularity of the function $g(z)$ we have in a neighbourhood $|z - z_0| < R$ of this point.

$$g(z) = \sum_{j=-\infty}^{\infty} c_j (z - z_0)^j. \tag{2.19}$$

hence

$$\sum_{j=1}^{n} (z_j - z_0) g(z_j) = nc_{-1} + n\sum_{k=1}^{\infty} c_{nk-1} h^{nk} + n\sum_{k=1}^{\infty} \frac{c_{-nk-1}}{h^{nk}} \tag{2.20}$$

We obtain finally the formula

$$\text{Rez}\,\{g(z), z_j\} \equiv c_{-1} = \frac{\sum_{j=1}^{n} (z_j - z_0)\,g(z_j)}{n} + E_n \tag{2.21}$$

$$E_n = -\sum_{k=1}^{\infty}\left(c_{nk-1} h^{nk} + \frac{c_{-nk-1}}{h^{nk}}\right) \tag{2.22}$$

The form of the error make impossible to develope on, an extrapolation process. Consequently in order to obtain more accurate values for c_{-1} we must use the itterative procedure based on formula (2.21) by doubling the number of points z_j.

3. Numerical evaluation of principal value integrals

Let us consider the finite part integral

$$I = \int_a^b \frac{w(x) f(x)}{(x - x_0)^m}\,dx \qquad x_0 \in (a, b); \qquad m \in \mathbf{N} \tag{3.1}$$

$w(x)$ being a positive and continue weight function and $f(z)$ a holomorphic function in a domain including the segment $[a, b]$.

We shall put

$$I = \int_a^b \frac{w(x)}{(x - x_0)^m}\left\{f(x) - f(x_0) - \ldots - \frac{(x - x_0)^{m-1}}{(m-1)!} f^{(m-1)}(x_0)\right\} dx + \tag{3.2}$$
$$+ \sum_{j=0}^{m-1} \frac{f^{(j)}(x_0)}{j!} \int_a^b \frac{w(x)}{(x - x_0)^m}\,dx.$$

The first integral in relation (3.2) is a regular one and can be performed by using the standard quadrature rules; the second one will be analiticaly estimated. The derivatives in relation (3.2) for functions with a complicated analytical expression will be aproximated by using the methods given in the previous section.

Further on we consider two particular cases.

a) If $w(x) = 1$, $a = -1$, $b = 1$, we obtain

$$\int_{-1}^{1} \frac{f(x)}{(x - x_0)^m}\,dx = \sum_{r=1}^{n} H_r \frac{f(x_r)}{(x_r - x_0)^m} - \tag{3.3}$$
$$- \sum_{j=0}^{m-2} \frac{f^{(j)}(x_0)}{j!}\left\{\sum_{r=1}^{n} H_r \frac{1}{(x_r - x_0)^{m-j}} + \frac{1}{(1 - x_0)^{m-j-1}} + \frac{(-1)^{m-j}}{(1 + x_0)^{m-j-1}}\right\} +$$
$$+ \frac{f^{(m-1)}(x_0)}{(m-1)!}\left\{\ln\frac{1 - x_0}{1 + x_0} - \sum_{r=1}^{n} \frac{H_r}{x_r - x_0}\right\} + R_{m,n}$$

where $x_1, x_2, \ldots, x_n$ are the zeros of the Legendre polynomial $P_n(x)$ and H_j the corresponding weights. By R_n we denoted the remainder.

For $m = 1$ we have the formula for evaluation of Chauchy principal value

$$\int_{-1}^{1} \frac{f(x)}{x - x_0}\, dx = \sum_{r=1}^{n} H_r \frac{f(x_r)}{x_r - x_0} + f(x_0)\left\{\ln \frac{1 - x_0}{1 + x_0} - \sum_{r=1}^{n} \frac{H_r}{x_r - x_0}\right\} + R_{1,n} \tag{3.4}$$

For $x_0 = 0$ and n even the formula (3.4) coincide, due to the symmetry of points $x_1, \ldots, x_n$, with Piessens formula

$$\int_{-1}^{1} \frac{f(x)}{x}\, dx = \sum_{r=1}^{n} H_r \frac{f(x_r)}{x_r} + R_{1,n} \tag{3.5}$$

Likewise for n old from (3.4) we obtain the formula

$$\int_{-1}^{1} \frac{f(x)}{x}\, dx = H_1 f'(0) + \sum_{r=2}^{n} H_r \frac{f(x_r)}{x_r} + R_{1,n} \tag{3.6}$$

given by HUNTER [4].

In the case $m = 2$, $x_0 = 0$ and n even the relation (3.5) gives also a simple formula:

$$\int_{-1}^{1} \frac{f(x)}{x^2}\, dx = \sum_{r=1}^{n} H_r \frac{f(x_r)}{x_r^2} - f(0)\left\{2 + \sum_{r=1}^{n} \frac{H_r}{x_r^2}\right\} + R_{2,n} \tag{3.7}$$

b) For $w(x) = (1 - x^2)^{-1/2}$, $a = -1$, $b = 1$, we have

$$\int_{-1}^{1} \frac{f(x)\, dx}{\sqrt{1 - x^2}\,(x - x_0)^m} = \frac{\pi}{n} \sum_{r=1}^{n} \frac{f(x_r)}{(x_r - x_0)^m} - \frac{\pi}{n} \sum_{j=0}^{m-1} \frac{f^{(j)}(x_0)}{j!} \sum_{r=1}^{n} \frac{1}{(x_r - x_0)^{m-j}} + R_{m,n} \tag{3.8}$$

where $x_r = \cos((2r - 1)\pi/2n)$.

To avoid the difference of two close numbers we shall put in (3.8) x_j as being the n distinct numbers $x_j^* = \cos\left(\theta_0 + \frac{(2j - 1)\pi}{2n}\right) (j = 1, \ldots, 2n)$ where $x_0 = \cos\theta_0$.

For $m = 1$ we have

$$\int_{-1}^{1} \frac{f(x)\, dx}{\sqrt{1 - x^2}\,(x - x_0)} = \frac{\pi}{n} \sum_{r=1}^{n} \frac{f(x_r) - f(x_0)}{x_r - x_0} + R_{1,n} \tag{3.9}$$

In all this formulae the remainder can be evaluated as in the case of the absence of singularities since the integrand in (3.2) is a regular function for $x = x_0$.

4. Numerical quadrature formulae for a function which has isolated singularities near the integration interval

Let L be a closed contur enclosing the interval $[-1, 1]$ and $f(z)$ an analytical function in the domain enclosed by the curve L and having in this domain isolated singularities at the points $z_1, z_2, \ldots, z_m$. We denote by $t_1, t_2, \ldots, t_n$ the zeros of the Chebyshev polynomial $T_n(t)$. We have

$$f(t) = \sum_{j=1}^{n} \frac{T_n(t) f(t_j)}{(t - t_j)\, T_n'(t_j)} - \sum_{j=1}^{m} \frac{1}{2\pi i} \int_{L_j} \frac{T_n(t) f(z) dz}{(z - t)\, T_n(z)} + \frac{1}{2\pi i} \int_{L} \frac{T_n(t) f(z) dz}{(z - t)\, T_n(z)} \tag{4.1}$$

L_j being the cercle $|z - z_j| = \varepsilon$.

From relation (4.1) we obtain

$$\int_{-1}^{1} \frac{f(t)}{\sqrt{1 - t^2}}\, dt = \frac{\pi}{n} \sum_{j=1}^{n} f\left(\cos \frac{(2j - 1)\pi}{2n}\right) + \sum_{j=1}^{m} \frac{1}{2\pi i} \int_{L_j} \frac{f(z)}{T_n(z)}\, dz \int_{-1}^{1} \frac{T_n(t)\, dt}{\sqrt{1 - t^2}\,(t - z)} + \frac{1}{2\pi i} \int_{L} \frac{f(z)}{T_n(z)}\, dz \int_{-1}^{1} \frac{T_n(t)\, dt}{\sqrt{1 - t^2}\,(t - z)}. \tag{4.2}$$

We can write

$$T_n(z) = \frac{1}{2}\left[(z + \sqrt{z^2 - 1})^n + (z + \sqrt{z^2 - 1})^{-n}\right] \tag{4.3}$$

$$q_n^*(z) = \int_{-1}^{1} \frac{T_n(t)\, dt}{\sqrt{1 - t^2}\,(z - t)} = \frac{\pi}{\sqrt{z^2 - 1}\,(z + \sqrt{z^2 - 1})^n} \tag{4.4}$$

with $-\pi < \arg(z \pm 1) \leqslant \pi$.

We have finaly

$$\int_{-1}^{1} \frac{f(t)}{\sqrt{1 - t^2}}\, dt = \frac{\pi}{n} \sum_{j=1}^{n} f\left(\cos \frac{(2j - 1)\pi}{2n}\right) - 2\pi \sum_{j=1}^{m} \operatorname{Rez}\left\{\frac{f(z)}{\sqrt{z^2 - 1}\,[(z + \sqrt{z^2 - 1})^{2n} + 1]};\ z_j\right\} + R_n \tag{4.5}$$

where

$$R_n = \frac{1}{2\pi i} \int_{L} \frac{f(z)\, q_n^*(z)}{T_n(z)}\, dz \tag{4.6}$$

In relation (4.5) the residues can be evaluated by means of relations (2.18) or (2.21).

The remainder (4.6) can be estimated by using the method employed in [1]. One can give similar numerical quadrature formulae based on Gauss—Legendre method.

5. Numerical examples

The computation of the examples given bellow was performed on a Hewlett-Packard 9825B calculator.

a) $$I(y) = \int_0^1 \frac{dx}{\sqrt{x}\,(x - y^2)} = \frac{1}{y} \ln \frac{1-y}{1+y}, \quad 0 < y < 1$$

In the same way as in [5] we have put

$$I(y) = \int_0^{\varepsilon} \frac{dx}{\sqrt{x}\,(x - y^2)} + \int_{\varepsilon}^1 \frac{dx}{\sqrt{x}\,(x - y^2)}.$$

For the first integral the change of variable $x = \varepsilon t^2$ was performed. Afterwords, both integrals were calculated with the aid of the ten points Gauss—Legendre formula. We have taken $\varepsilon = 0.2$ and have calculated the principal value integral by using the formulae (3.4). The obtained value $I(0.6) = -2.310490599$ has nine correct significant digits. In [5] by using 44 function evaluations and double precision computation ten correct significant digite were obtained.

b) $$I(y) = \int_0^1 \frac{dx}{\sqrt{x}\,(x - y^2)^3} = \frac{4}{y^5} \ln \frac{1-y}{1+y} + \frac{3 - 5y^2}{4y^4(1 - y^2)^2}; \; 0 < y < 1.$$

To compute this integral we have used the same method as above (with $\varepsilon = 0.25$) and the formula (3.3) for the principal value integral. The derivatives in this relation were obtained by using the relation (2.6) with $n = 4$ and $h = 0.025$. Both regular integrals were evaluated by means of ten points Gauss—Legendre formula. We have obtained $I(0.7) = -1.668503578$ with seven correct significant digits. The total number of function evaluations was 24; this are favorable comparated with the result given in [5] where eight correct significant digits were obtained at the price of 44 function evaluations.

c) $$I(\lambda, y) = \int_{-1}^{1} \frac{(1 - x^2)^{-1/2}\,dx}{(x^2 + y^2)(\lambda - x)} = \frac{\pi\lambda}{y\sqrt{1 + y^2}\,(y^2 + \lambda^2)}; \quad |\lambda| < 1$$

This integral has a singularity at $x = \lambda$ and for small value of y it possess a polar singularity near the integration interval. It was conside-

red in [7]. For beginning the integral was computed by using formula (3.9) for $y = 5$, 0.1 and $\lambda = 0.25$ and 0.99. The resultad errors for some value of n are included in the table bellow

n	$I(0.25, 5) = 1.22916112 \cdot 10^{-3}$	$I(0.99, 5) = 4.69556191 \cdot 10^{-3}$
	Error	Error
2	$-2.4 \cdot 10^{-7}$	$-9 \cdot 10^{-7}$
3	$2.31 \cdot 10^{-9}$	$9 \cdot 10^{-9}$
4	$-2.31 \cdot 10^{-11}$	$-9 \cdot 10^{-11}$
5	$2.7 \cdot 10^{-13}$	$9 \cdot 10^{-14}$

n	$I(.25, 0.1) = 107.793156$	$I(0.99, 0.1) = 31.256858$
	Error	Error
11	26.97	7.82
15	11.355	3.29
19	4.96	1.44
23	2.20	0.64

The obtained results for $j = 5$ are better than those from [7] with two to six order of magnitudes. For $y = 0.1$ the accuracy is affected by the presence of the pole near the integration interval. In order to prove the accuracy in this case we combined the results of section 3 (formula (3.9)) with those given in section 4 (formula (4.5)). The resultated error in evaluation of $I(0.25, 0.1)$ and $I(0.99, 0.1)$ are of order 10^{-9} even for small values of n ($n = 2, 4, \ldots$).

R E F E R E N C E S

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