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711. NUMERICAL DIFFERENTIATION OF ANALYTIC FUNCTIONS*

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1. Introduction. Consider a real valued analytic function of a complex variable $z \mapsto f(z)$, regular in a disc $|z|<r$. For numerical computation of derivatives of the function $x \mapsto f(x)$, for example at point $x=0$, we usually evaluate the function at points $x_k = kh$ $(k=0, \pm 1, \pm 2, \ldots)$ and then apply central finite differences. In order to obtain the results of high accuracy, we use high order finite differences. Thus, we are forced to extend the table of function values, so that we evaluate the function at points more and more far from $x=0$. An application of finite differences of the relatively high order causes a considerable accumulation on roundoff-errors, so that there exists an accuracy bound for the evaluation of derivatives. It should be noticed that the coefficients multiplying the function values in differentiation formulas are quite different for the central and the other abscissas [**1**]. Further, it is known that the numerical differentiation is an unstable process.

Analytic function $z \mapsto f(z)$ on the real axis becomes the function $x \mapsto f(x)$. The evaluation of the function $z \mapsto f(z)$ offers new information about the function $x \mapsto f(x)$. Thus we can effectivelly and with higher accuracy compute derivatives of the function $z \mapsto f(z)$ (i.e. $x \mapsto f(x)$), because we retain near $z=0$ (or $x=0$).

The numerical differentiation of analytic functions is treated in several papers [**2**–**4**]. In these papers the computation of derivatives is realized by applying the trapezoidal rule to the real part of $z \mapsto f(z)$, starting from the contour integral

(1) $$f^{(n)}(0)=\frac{n!}{2\pi i}\oint_C \frac{f(z)}{z^{n+1}}\,\mathrm{d}z,$$

where C is a closed contour surrounding the origin.

In the present paper we obtain formulas for numerical differentiation, introducing the special complex linear operators of finite differences, analogous with standard operators of numerical analysis. These formulas are also

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connected with the contour integral (1) and contain even number of points chosen on C.

2. Computation of the first derivative. Let us define the operator of finite central difference δ_θ by

$$\delta_\theta f(z) = f\left(z + \frac{h}{2} e^{i\theta}\right) - f\left(z - \frac{h}{2} e^{i\theta}\right), \tag{2}$$

where the function $z \mapsto f(z)$ is evaluated at symmetric points with respect to z, taken with complex increments. For $\theta = 0$ we obtain the standard central difference operator

$$\delta_0 f(z) = \delta f(z) = f\left(z + \frac{h}{2}\right) - f\left(z - \frac{h}{2}\right).$$

Since $E^s f(z) = f(z + sh)$ $(s \in \mathbf{C})$, where E is the shifting operator, we have

$$\delta_\theta = E^{\frac{1}{2} e^{i\theta}} - E^{-\frac{1}{2} e^{i\theta}}. \tag{3}$$

Using the well-known relationship $E = e^{hD}$, where D is the differentiation operator, operational equality (2) becomes

$$\delta_\theta = e^{\frac{1}{2} hDe^{i\theta}} - e^{-\frac{1}{2} hDe^{i\theta}} = 2 \operatorname{sh}\left(\frac{1}{2} h De^{i\theta}\right).$$

Developing the right hand side of this equality into the TAYLOR-series, we obtain

$$\delta_\theta = 2\left(\frac{hD}{2} e^{i\theta} + \frac{1}{3!}\left(\frac{hD}{2}\right)^3 e^{i3\theta} + \cdots\right) \tag{4}$$

$$= 2 \sum_{m=1}^{+\infty} \frac{1}{(2m-1)!} \left(\frac{hD}{2}\right)^{2m-1} e^{i(2m-1)\theta}.$$

Let us consider the equation $z^{2n} = 1$ $(n \in \mathbf{N})$. Its roots $z_k = e^{i\theta_k} = e^{i\frac{k\pi}{n}}$ $(k = 0, 1, \ldots, 2n-1)$ possess the following property (m is an integer):

$$\sum_{k=0}^{n-1} z_k^{2m} = \sum_{k=0}^{n-1} \left(e^{i\frac{2\pi m}{n}}\right)^k = \begin{cases} 0 & m \,(\mathrm{mod}\, n) \neq 0, \\ n & m \,(\mathrm{mod}\, n) = 0. \end{cases} \tag{5}$$

If we multiply (4) by $e^{-i\theta}$ and put $\theta = \theta_k$, it follows

$$e^{-i\theta_k} \delta_{\theta_k} = 2\left(\frac{hD}{2} + \frac{1}{3!}\left(\frac{hD}{2}\right)^3 e^{i2\theta_k} + \cdots + \frac{1}{(2m-1)!}\left(\frac{hD}{2}\right)^{2m-1} e^{i(2m-2)\theta_k} + \cdots\right).$$

By summing this equality with respect to k, from $k=0$ to $k=n-1$, using (5) we obtain

$$\sum_{k=0}^{n-1} e^{-i\theta_k} \delta_{\theta_k} = 2n\left(\frac{hD}{2} + \frac{1}{(2n+1)!}\left(\frac{hD}{2}\right)^{2n+1} + \frac{1}{(4n+1)!}\left(\frac{kD}{2}\right)^{4n+1} + \cdots\right) \tag{6}$$

$$= 2n \sum_{\nu=0}^{+\infty} \frac{1}{(2\nu n+1)!}\left(\frac{hD}{2}\right)^{2\nu n+1}.$$

From this equality we can find the differentiation operator in the form

$$D = \frac{1}{nh}\sum_{k=0}^{n-1} e^{-i\theta_k}\delta_{\theta_k} - \left(\frac{h}{2}\right)^{2n} \frac{D^{2n+1}}{(2n+1)!} - \left(\frac{h}{2}\right)^{4n} \frac{D^{4n+1}}{(4n+1)!} - \cdots, \tag{7}$$

i.e.

$$Df(z) = \frac{1}{nh}\sum_{k=0}^{n-1} e^{-i\theta_k}\delta_{\theta_k} f(z) + R_{1,n}, \tag{8}$$

with the error-term

$$R_{1,n} = -\left(\frac{h}{2}\right)^{2n} \frac{D^{2n+1} f(z)}{(2n+1)!} - \left(\frac{h}{2}\right)^{4n} \frac{D^{4n+1} f(z)}{(4n+1)!} - \cdots$$

Hence, for different values of n, we find practical formulas for numerical differentiation of analytic functions.

Introducing in (8) the expression for δ_θ, given by (2), and setting $\theta_k = \frac{k\pi}{n}$, we have

$$Df(z) = \frac{1}{nh}\sum_{k=0}^{n-1} e^{-i\frac{k\pi}{n}}\left(f\left(z+\frac{h}{2}e^{i\frac{k\pi}{n}}\right) - f\left(z-\frac{h}{2}e^{i\frac{k\pi}{n}}\right)\right) + R_{1,n}. \tag{9}$$

Remark 1. Let us prove that the sum in (9), divided by nh, representing an approximative value of the first order derivative, can be obtained using the trapezoidal rule for evaluation of the contour integral

$$f'(z) = \frac{1}{2\pi i} \oint_{|\zeta - z| = \frac{h}{2}} \frac{f(\zeta)}{(\zeta - z)^2}\, d\zeta.$$

By setting $\zeta = z + \frac{h}{2}e^{i\theta}$, we may rewrite this integral in the form

$$f'(z) = \frac{1}{\pi h}\int_0^{2\pi} e^{-i\theta} f\left(z + \frac{h}{2}e^{i\theta}\right) d\theta.$$

Dividing segment $[0, 2\pi]$ by uniformly spaced abscissas into $2n$ equal parts, and using the trapezoidal rule, we have

$$f'(z) \approx \frac{1}{\pi h} \cdot \frac{\pi}{n} \left(f\left(z + \frac{h}{2}\right) + \sum_{k=1}^{2n-1} e^{-i\frac{k\pi}{n}} f\left(z + \frac{h}{2} e^{i\frac{k\pi}{n}}\right)\right). \tag{10}$$

Since

$$\sum_{k=n}^{2n-1} e^{-i\frac{k\pi}{n}} f\left(z + \frac{h}{2} e^{i\frac{k\pi}{n}}\right) = -\sum_{k=0}^{n-1} e^{-\frac{k\pi}{n}} f\left(z - \frac{h}{2} e^{i\frac{k\pi}{2}}\right),$$

relation (10) transforms to the required result

$$f'(z) \approx \frac{1}{nh} \sum_{k=0}^{n-1} e^{-i\frac{k\pi}{n}} \left(f\left(z + \frac{h}{2} e^{i\frac{k\pi}{n}}\right) - f\left(z - \frac{h}{2} e^{i\frac{k\pi}{n}}\right)\right),$$

which completes the proof.

3. Higher derivatives. We first deduce formulas for derivatives of odd order. Multiplying (4) by $e^{-i3\theta}$, we have

$$e^{-i3\theta} \delta_\theta = 2\left(\frac{hD}{2} e^{-i2\theta} + \frac{1}{3!}\left(\frac{hD}{2}\right)^3 + \frac{1}{5!}\left(\frac{hD}{2}\right)^5 e^{i2\theta} + \cdots\right)$$

$$= \sum_{m=1}^{+\infty} \frac{1}{(2m-1)!} \left(\frac{hD}{2}\right)^{2m-1} e^{i2(m-2)\theta}.$$

By setting $\theta = \theta_k$ and summing with respect to k from $k=0$ to $k=n-1$ $(n>1)$, we obtain

$$\sum_{k=0}^{n-1} e^{-i3\theta_k} \delta_{\theta_k} = 2n \left(\frac{1}{3!}\left(\frac{hD}{2}\right)^3 + \frac{1}{(2n+3)!}\left(\frac{hD}{2}\right)^{2n+3} + \cdots\right)$$

$$= 2n \sum_{\nu=0}^{+\infty} \frac{1}{(2\nu n+3)!} \left(\frac{hD}{2}\right)^{2\nu n+3}.$$

Hence, it follows that

$$D^3 f(z) = \frac{24}{nh^3} \sum_{k=0}^{n-1} e^{-i3\theta_k} \delta_{\theta_k} f(z) + R_{3,n},$$

where

$$R_{3,n} = -\frac{48}{h^3} \sum_{\nu=1}^{+\infty} \frac{1}{(2\nu n+3)!} \left(\frac{hD}{2}\right)^{2\nu n+3} f(z)$$

$$= -6\left(\left(\frac{h}{2}\right)^{2n} \frac{D^{2n+3} f(z)}{(2n+3)!} + \left(\frac{h}{2}\right)^{4n} \frac{D^{4n+3} f(z)}{(4n+3)!} + \cdots\right).$$

Generally, multiplying (4) by $e^{-i(2r-1)\theta}$, where $r \leq n$, setting $\theta = \theta_k$ and summing, we obtain

$$\sum_{k=0}^{n-1} e^{-i(2r-1)\theta_k} = 2n\left(\frac{1}{(2r-1)!}\left(\frac{hD}{2}\right)^{2r-1} + \frac{1}{(2r+2n-1)!}\left(\frac{hD}{2}\right)^{2n+2r-1} + \cdots\right)$$

$$= 2n \sum_{\nu=0}^{+\infty} \frac{1}{(2r+2\nu n-1)!}\left(\frac{hD}{2}\right)^{2r+2\nu n-1}.$$

Hence we obtain the general formula for numerical computation of derivatives of the odd order

$$D^{2r-1} f(z) = \frac{2^{2r-2}(2r-1)!}{nh^{2r-1}} \sum_{k=0}^{n-1} e^{-i(2r-1)\theta_k}\, \delta_{\theta_k} f(z) + R_{2r-1,n}, \tag{11}$$

where

$$R_{2r-1,n} = -(2r-1)! \sum_{\nu=1}^{+\infty} \frac{1}{(2\nu n+2r-1)!}\left(\frac{h}{2}\right)^{2\nu n} D^{2\nu n+2r-1} f(z) \tag{12}$$

and $r = 1, \ldots, n$.

REMARK 2. After the manner of (9), we can prove that (11) can be found by application of the trapezoidal rule to the contour integral

$$f^{(2r-1)}(z) = \square \oint\limits_{|\zeta - z| = \frac{h}{2}} \frac{f(\zeta)}{(\zeta - z)^{2r}}\, d\zeta.$$

To develop formulas for numerical computation of derivatives of the even order let us start from the complex averaging operator μ_θ, defined by

$$\mu_\theta f(z) = \frac{1}{2}\left(f\left(z + \frac{h}{2}e^{i\theta}\right) + f\left(z - \frac{h}{2}e^{i\theta}\right)\right).$$

We have

$$\mu_\theta = \frac{1}{2}\left(E^{\frac{1}{2}e^{i\theta}} + E^{-\frac{1}{2}e^{i\theta}}\right)$$

$$= \frac{1}{2}\left(e^{\frac{hD}{2}e^{i\theta}} + e^{-\frac{hD}{2}e^{i\theta}}\right) = \operatorname{ch}\left(\frac{hD}{2}e^{i\theta}\right)$$

$$= 1 + \frac{1}{2!}\left(\frac{hD}{2}\right)^2 e^{i2\theta} + \left(\frac{hD}{2}\right)^4 e^{i4\theta} + \cdots$$

i.e.

$$\mu_\theta = \sum_{m=0}^{+\infty} \frac{1}{(2m)!}\left(\frac{hD}{2}\right)^{2m} e^{im\theta}. \tag{13}$$

Multiplying (13) by $e^{-i2\theta}$ and then setting $\theta=\theta_k$ and summing with respect to k from $k=0$ to $k=n-1$ $(n>1)$, we obtain

$$\sum_{k=0}^{n-1} e^{-i2\theta_k}\mu_{\theta_k}=n\sum_{\nu=1}^{+\infty}\frac{1}{(2\nu n)!}\left(\frac{hD}{2}\right)^{2\nu n} \qquad (n>1). \tag{14}$$

In the special case $n=1$, we have

$$\mu_0=1+\sum_{\nu=1}^{+\infty}\frac{1}{(2\nu)!}\left(\frac{hD}{2}\right)^{2\nu},$$

where $\mu_0 f(z)=\frac{1}{2}\left(f\left(z+\frac{h}{2}\right)+f\left(z-\frac{h}{2}\right)\right)$.

From (14) we obtain the formula for numerical evaluation of the second derivative:

$$D^2 f(z)=\frac{8}{h^2}\sum_{k=0}^{n-1} e^{-i2\theta_k}\mu_{\theta_k} f(z)+R_{2,n}, \tag{15}$$

with the error-term

$$R_{2,n}=-2\sum_{\nu=2}^{+\infty}\frac{1}{(2\nu n)!}\left(\frac{h}{2}\right)^{2\nu n-2}D^{2\nu n}f(z), \tag{16}$$

where $n>1$.

Generally, multiplying (13) by $e^{-i2r\theta_k}$ $(r=1,\ldots,n)$, setting $\theta=\theta_k$ and summing with respect to k, it follows that

$$\sum_{k=0}^{n-1} e^{i2r\theta_k}\mu_{\theta_k}=n\sum_{\nu=0}^{+\infty}\frac{1}{(2r+2\nu n)!}\left(\frac{hD}{2}\right)^{2r+2\nu n} \qquad (r<n). \tag{17}$$

For $r=n$ we have

$$\sum_{k=0}^{n-1}\mu_{\theta_k}=n\left(1+\sum_{\nu=0}^{+\infty}\frac{1}{(2n(1+\nu))!}\left(\frac{hD}{2}\right)^{2n(1+\nu)}\right). \tag{18}$$

Using (17), the formula for derivatives of the even order is

$$D^{2r}f(z)=\frac{(2r)!}{n}\frac{2^{2r}}{h^{2r}}\sum_{k=0}^{n-1} e^{-i2r\theta_k}\mu_{\theta_k}f(z)+R_{2r,n}, \tag{19}$$

where

$$R_{2r,n}=-(2r)!\sum_{\nu=1}^{+\infty}\frac{1}{(2r+2\nu n)!}\left(\frac{h}{2}\right)^{2\nu n}D^{2r+2\nu n}f(z)$$

and $r=1,\ldots,n-1$.

In the special case $r=n$, from (18) we obtain

$$D^{2n}f(z)=\frac{(2n)!\,2^{2n}}{h^{2n}}\left(\frac{1}{n}\sum_{k=0}^{n-1}\mu_{\theta_k}f(z)-f(z)\right)+R_{2n,n}, \tag{20}$$

where

$$R_{2n,n} = -(2n)! \sum_{\nu=1}^{+\infty} \frac{1}{(2n(1+\nu))!} \left(\frac{h}{2}\right)^{2\nu n} D^{2n(1+\nu)} f(z).$$

REMARK 3. The expression $\frac{1}{n} \sum_{\nu=1}^{+\infty} \mu_{\theta_k} f(z)$ in (20) is the arithmetic mean of the function $z \mapsto f(z)$ evaluated at the $2n$ points $z + \frac{h}{2} e^{i\frac{k\pi}{n}}$ $(k=0, 1, \ldots, 2n-1)$. Therefore for the purpose of simplicity we can use (20) for evaluation of derivatives of even order. We can deduce the more general formula

$$f^{(n)}(z) = \frac{n!}{h^n}\left(\frac{1}{n}\sum_{k=0}^{n-1} f(z + he^{i\frac{2\pi k}{n}}) - f(z)\right) + R_{n,n},$$

where

$$R_{n,n} \approx -\frac{n!}{(2n)!} h^n f^{(2n)}(z).$$

REMARK 4. Formulas for derivatives of even order can also be derived by iterating with the operator δ_θ. Starting from (3) we have

$$\delta_\theta{}^2 = E^{e^{i\theta}} + E^{-e^{i\theta}} - 2 = e^{hDe^{i\theta}} + e^{-hDe^{i\theta}} - 2$$

$$= 2\left(\frac{D^2 h^2}{2!} e^{i2\theta} + \frac{D^4 h^4}{4!} e^{i4\theta} + \cdots + \frac{D^{2m} h^{2m}}{(2m)!} e^{i2m\theta} + \cdots\right).$$

Using the same procedure given above we obtain, for instance,

$$\sum_{k=0}^{n-1} e^{-i2\theta_k} \delta_{\theta_k}{}^2 = 2n\left(\frac{D^2 h^2}{2!} + \frac{D^{2n+2} h^{2n+2}}{(2n+2)!} + \frac{D^{4n+2} h^{4n+2}}{(4n+2)!} + \cdots\right),$$

and from this a formula for the second derivative readily follows.

4. Examples. Equalities (11), (19) and (20), together with corresponding error-terms, for $n=2$ and $z=0$ transform to practical formulas for numerical evaluation of the first four derivatives of the function $x \mapsto f(x)$ at $x=0$. Thus

$$f'(0) = \frac{1}{2h}\left(f\left(\frac{h}{2}\right) - f\left(-\frac{h}{2}\right) - i\left(f\left(i\frac{h}{2}\right) - f\left(-i\frac{h}{2}\right)\right)\right)$$
$$-\left(\frac{h}{2}\right)^4 \frac{f^{(5)}(0)}{5!} - \left(\frac{h}{2}\right)^8 \frac{f^{(9)}(0)}{9!} - \cdots; \tag{21}$$

$$f''(0) = \frac{2}{h^2}\left(f\left(\frac{h}{2}\right) + f\left(-\frac{h}{2}\right) - \left(f\left(i\frac{h}{2}\right) + f\left(-i\frac{h}{2}\right)\right)\right)$$
$$-2\left(\frac{h}{2}\right)^4 \frac{f^{(6)}(0)}{6!} - 2\left(\frac{h}{2}\right)^8 \frac{f^{(10)}(0)}{10!} - \cdots; \tag{22}$$

$$f'''(0)=\frac{12}{h^3}\left(f\left(\frac{h}{2}\right)-f\left(-\frac{h}{2}\right)+i\left(f\left(i\frac{h}{2}\right)-f\left(-i\frac{h}{2}\right)\right)\right) \tag{23}$$

$$-6\left(\frac{h}{2}\right)^4\frac{f^{(7)}(0)}{7!}-6\left(\frac{h}{2}\right)^8\frac{f^{(11)}(0)}{11!}-\cdots;$$

$$f^{(4)}(0)=\frac{96}{h^4}\left(f\left(\frac{h}{2}\right)+f\left(-\frac{h}{2}\right)+f\left(i\frac{h}{2}\right)+f\left(-i\frac{h}{2}\right)-4f(0)\right) \tag{24}$$

$$-24\left(\frac{h}{2}\right)^4\frac{f^{(8)}(0)}{8!}-24\left(\frac{h}{2}\right)^8\frac{f^{(12)}(0)}{12!}-\cdots$$

An examination of the first term in each of the error expressions, which are the main parts of the errors, shows a curious behaviour under the condition that the higher derivatives are approximately equal i.e., $f^{(5)}(0)\approx f^{(6)}(0)\approx\ldots$, which is true for $x\mapsto e^x$. We find

$$R(2,\ 2)\approx\frac{1}{3}R(1,\ 2),\quad R(3,\ 2)\approx\frac{1}{7}R(1,\ 2),\quad R(4,\ 2)\approx\frac{1}{14}R(1,\ 2).$$

Thus for a fixed number of points if we compute higher derivatives, their accuracy increases. Such property of differentiation formulas is quite different than the property of corresponding formulas in the real domain.

For the purposes of simplicity consider the function $x\mapsto e^x$ at $x=0$. This is very convenient since all derivatives are equal to unity.

Results of numerical evaluation of f', f'', f''' and $f^{(4)}$ by (21) — (24) to ten significant figures are presented in the following table.

h	f'	f''	f'''	$f^{(4)}$
2	1.00833 6089	1.00277 8329	1.00119 0627	1.00059 5288
1	1.00052 0844	1.00017 3613	1.00007 4405	1.00003 7203
0.5	1.00003 2552	1.00001 0851	1.00000 4650	1.00000 2328
0.25	1.00000 2035	1.00000 0678	1.00000 0291	1.00000 0168

If we further decrease h, the errors reach minimum and then increase, which indicates that roundoff errors appear to be significant.

An analysis of the practical application of our formulas will be given in [5].

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NUMERIČKO DIFERENCIRANJE ANALITIČKIH FUNKCIJA

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U radu je iznet razvoj praktičnih formula za numeričko diferenciranje analitičkih funkcija. U tom cilju razvijeni su kompleksni operatori: operator centralne razlike δ_θ i usrednjavajući operator μ_θ. Pomoću veze ovih operatora sa operatorom D, izveden je niz formula za numeričko diferenciranje. Ove formule se mogu efikasno primeniti na realne funkcije.