NUMERICAL DIFFERENTIATION OF ANALYTIC FUNCTIONS

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Earlier D. D. Tošić obtained an infinite series representation for the central difference operator $\delta_{\theta} f(z) = f\left(z + \frac{1}{2}he^{i\theta}\right) - f\left(z - \frac{1}{2}he^{i\theta}\right)$, and used it to derive an n-point interpolation formula for the derivative f'(z) of an analytic function f(z). In this paper we give a direct proof of the n-point interpolation formula for f'(z) with an error term $R_{1,n}$ expressed in integral form. Various other formulae are also included.

D. D. Tošić in [1] has shown that the operator

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

admits the representation

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

and this formula is used to obtain the numerical differentiation formula

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

where the error term $R_{1,n}$ is given by the series

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

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In this note a direct approach to the derivation of (1) and (2) is given with an integral form for the error term $R_{1,n}$ in (2), together with a finite series plus error term form for (1). Various other formulae are also derived. We begin with the algebraic identity

$$\frac{1}{t-z-\zeta} = \frac{1}{t-z} + \frac{\zeta}{(t-z)^2} + \dots + \frac{\zeta^m}{(t-z)^{m+1}} + \frac{\zeta^{m+1}}{(t-z)^m(t-z-\zeta)},$$

and differentiation with respect to ζ gives

$$\frac{1}{(t-z-\zeta)^2} = \frac{1}{(t-z)^2} + \dots + \frac{m\zeta^{m-1}}{(t-z)^{m+1}} + \frac{\zeta^m \left[(m+1)(t-z) - m\zeta \right]}{(t-z)^m (t-z-\zeta)^2}.$$

This, together with the CAUCHY integral formulae

$$\frac{f^{(k)}(z)}{k!} = \frac{1}{2\pi i} \oint \frac{f(t)}{(t-z)^{k+1}} dt, \qquad (k=1,2,\dots,m),$$

then gives us

(3)
$$f'(z+\zeta) = f'(z) + \zeta f''(z) + \dots + \frac{\zeta^{m-1} f^{(m)}(z)}{(m-1)!} + \frac{1}{2\pi i} \oint_{C} \frac{f(t) \zeta^{m} [(m+1)(t-z) - m\zeta]}{(t-z)^{m} (t-z-\zeta)^{2}} dt,$$

where c is a circle centre z and is such that $\zeta + z$ lies inside c. Using

$$\delta_{\theta} f(z) = \int_{-\frac{h}{2}e^{i\theta}}^{\frac{h}{2}e^{i\theta}} f'(z+\zeta) d\zeta$$

and (3) with m = 2r - 1, we deduce the finite series plus error term form for (1), namely

(4)
$$\delta_{\theta} f(z) = 2 \sum_{\nu=1}^{r} \frac{1}{(2\nu - 1)!} \left(\frac{he^{i\theta}}{2} \right)^{2\nu - 1} f^{(2\nu - 1)}(z) + R_{2r - 1}(\theta, h, z),$$

where

$$R_{2r-1}(\theta, h, z) = \frac{1}{2\pi i} \int_{-\frac{h}{2}e^{i\theta}}^{\frac{h}{2}e^{i\theta}} \oint_{c} \frac{f(t)\zeta^{2r-1} \left[2r(t-z) - (2r-1)\zeta\right]}{(t-z)^{2r-1}(t-z-\zeta)^{2}} dt d\zeta$$

and c is a circle centre z and radius greater than $\frac{|h|}{2}$.

Note 1. To obtain (1) we simply use the infinite series

$$\frac{1}{(t-z-\zeta)^2} = \frac{1}{(t-z)^2} + \frac{2\zeta}{(t-z)^3} + \dots + \frac{m\zeta^{m-1}}{(t-z)^{m+1}} + \dots$$

and integrate term-by-term as above.

With r = 1 in (4) we have

$$e^{-i\theta}\delta_{\theta}f(z) = hf'(z) + \frac{e^{-i\theta}}{2\pi i} \int_{-\frac{h}{2}e^{i\theta}}^{\frac{h}{2}e^{i\theta}} \oint_{c} \frac{f(t)\zeta[2(t-z)-\zeta]}{(t-z)(t-z-\zeta)^{2}} dt d\zeta,$$

and setting $\theta = \theta_k = \frac{k\pi}{n}$ gives, on summing over $k = 0, 1, \dots, n-1$,

$$\sum_{k=0}^{n-1} e^{-i\theta_k} \delta_{\theta_k} f(z) = nhf'(z) + \sum_{k=0}^{n-1} \frac{e^{-i\theta_k}}{2\pi i} \int_{-\frac{h}{2}e^{i\theta_k}}^{\frac{h}{2}e^{i\theta_k}} \oint_c \frac{f(t)\zeta \left[2(t-z) - \zeta\right]}{(t-z)(t-z-\zeta)^2} dt d\zeta,$$

so that

$$Df(z) = \frac{1}{nh} \sum_{k=0}^{n-1} e^{-i\theta_k} \delta_{\theta_k} f(z) - \frac{1}{nh} \sum_{k=0}^{n-1} \frac{e^{-i\theta_k}}{2\pi i} \int_{-\frac{h}{2}e^{i\theta_k}}^{\frac{h}{2}e^{i\theta_k}} \oint_c \frac{f(t)\zeta \left[2(t-z) - \zeta\right]}{(t-z)(t-z-\zeta)^2} dt d\zeta,$$

which is (2) with a new form for the remainder $R_{1,n}$.

For higher derivatives of odd order we have

(5)
$$D^{2r-1}f(z) = \frac{2^{2r-2}(2r-1)!}{nh^{2r-1}} \sum_{k=0}^{n-1} e^{-i(2r-1)\theta_k} \delta_{\theta_k} f(z) + R_{2r-1,n},$$

where the error term $R_{2r-1,n}$ is given in integral form. To obtain (5) we simply set $\theta = \theta_k$ in (4), multiply through by $e^{-i(2r-1)\theta_k}$ and sum over $k = 0, 1, \ldots, n-1$; the error term $R_{2r-1,n}$ then takes the form

$$R_{2r-1,n} = -\frac{2^{2r-2}(2r-1)!}{nh^{2r-1}} \sum_{k=0}^{n-1} e^{-i(2r-1)\theta_k} R_{2r-1}(\theta_k,h,z).$$

Next, we turn to the operator

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

which, in [1], is shown to admit the representation

(6)
$$\mu_{\theta} = \sum_{m=0}^{\infty} \frac{1}{(2m)!} \left(\frac{hD}{2}\right)^{2m} e^{i2m\theta},$$

and is used to obtain the numerical differentiation formula

(7)
$$D^{2r}f(z) = \frac{(2r)! \, 2^{2r}}{nh^{2r}} \sum_{k=0}^{n-1} e^{-i2r\theta_k} \mu_{\theta_k} f(z) + R_{2r,n},$$

where the error term $R_{2r,n}$ is given by the series

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

for r = 1, 2, ..., n - 1. In case r = n, the corresponding formulae are

(8)
$$D^{2n}f(z) = \frac{(2n)! \, 2^{2n}}{h^{2n}} \left[\frac{1}{n} \sum_{k=0}^{n-1} \mu_{\theta_k} f(z) - f(z) \right] + R_{2n,n}$$

and

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

We now give a finite series plus error term form for (6) and indicate how (6) may be derived directly. In addition, (7) is derived with an integral form for the error term $R_{2r,n}$ (r = 1, 2, ..., n) and the case r = n is dealt with in similar fashion. We begin with the identity

$$\frac{t-z}{(t-z)^2-\zeta^2} = \frac{1}{(t-z)} + \frac{\zeta^2}{(t-z)^3} + \dots + \frac{\zeta^{2\nu}}{(t-z)^{2\nu+1}} + \frac{\zeta^{2\nu+2}}{(t-z)^{2\nu+1}} \left[(t-z)^2 - \zeta^2 \right].$$

This, together with

$$\mu_{\theta} f(z) = \frac{1}{4\pi i} \oint_{c} f(t) \left(\frac{1}{t - z - \frac{h}{2} e^{i\theta}} + \frac{1}{t - z + \frac{h}{2} e^{i\theta}} \right) dt$$
$$= \frac{1}{2\pi i} \oint_{c} \frac{f(t)(t - z)}{(t - z)^{2} - \frac{h^{2}}{4} e^{i2\theta}} dt$$

and $\zeta = \frac{h}{2}e^{i\theta}$ gives, on using the Cauchy integral formulae,

(9)
$$\mu_{\theta} f(z) = \sum_{m=0}^{\nu} \left(\frac{h e^{i\theta}}{2} \right)^{2m} \frac{f^{(2m)}(z)}{(2m)!} + R_{2\nu}(\theta, h, z)$$

which is (6) in finite series plus error term form, where the error term is given by

$$R_{2\nu}(\theta, h, z) = \frac{1}{2\pi i} \oint \frac{1}{(t-z)^{2\nu+1} \left[(t-z)^2 - \frac{h^2}{4} e^{i2\theta} \right]} \left(\frac{he^{i\theta}}{2} \right)^{2\nu+2} f(t) dt$$

and c is a circle centre z and radius greater than $\frac{|h|}{2}$.

Note 2. To obtain the representation formula (6) we use the infinite series

$$\frac{t-z}{(t-z)^2-\zeta^2} = \frac{1}{(t-z)} + \frac{\zeta^2}{(t-z)^3} + \dots + \frac{\zeta^{2\nu}}{(t-z)^{2\nu+1}} + \dots,$$

and integrate term-by-term as above.

Setting $\theta = \theta_k = \frac{k\pi}{n}$ and $\nu = r$ in (9), and multiplying through (9) by $e^{-i2r\theta_k}$ $(r = 1, 2, \dots, n-1)$ and summing over $k = 0, 1, 2, \dots, n-1$ (n > 1) gives

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

and so

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

where

$$R_{2r,n} = -\frac{(2r)!}{n} \sum_{k=0}^{n-1} \frac{h^2 e^{i2\theta_k}}{8\pi i} \oint \frac{f(t)}{(t-z)^{2r+1} \left[(t-z)^2 - \frac{h^2}{4} e^{i2\theta_k} \right]} dt.$$

In case r = n we have

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

and so

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

giving

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

where

$$R_{2n,n} = -\frac{(2n)!}{n} \sum_{k=0}^{n-1} \frac{h^2 e^{i2\theta_k}}{8\pi i} \oint_c \frac{f(t)}{(t-z)^{2n+1} \left[(t-z)^2 - \frac{h^2}{4} e^{i2\theta_k} \right]} dt$$

which is (8) with a new form for the error term $R_{2n,n}$.

In conclusion, we prove that

(10)
$$\sum_{k=0}^{n-1} e^{-i2\theta_k} \delta_{\theta_k}^2 = 2n \left(\frac{h^2 D^2}{2!} + \frac{h^{2n+2} D^{2n+2}}{(2n+2)!} + \cdots + \frac{h^{2np+2} D^{2np+2}}{(2np+2)!} \right) + R_{2np+2,n},$$

and indicate how the formula

(11)
$$\sum_{k=0}^{n-1} e^{-i2\theta_k} \delta_{\theta_k}^2 = 2n \left(\frac{h^2 D^2}{2!} + \frac{h^{2n+2} D^{2n+2}}{(2n+2)!} + \frac{h^{4n+2} D^{4n+2}}{(4n+2)!} + \cdots \right)$$

may be established.

Now

$$\delta_{\theta}^{2} f(z) = f(z + he^{i\theta}) + f(z - he^{i\theta}) - 2f(z)$$
$$= \int_{0}^{he^{i\theta}} (f'(z + \zeta) - f'(z - \zeta)) d\zeta$$

and using (3) with 2m in place of m we have

$$\delta_{\theta}^{2} f(z) = \int_{0}^{he^{i\theta}} \left(2\zeta f''(z) + \frac{2\zeta^{3} f^{(4)}(z)}{3!} + \dots + \frac{2\zeta^{2m-1} f^{(2m)}(z)}{(2m-1)!} \right) d\zeta$$

$$+ \frac{1}{2\pi i} \int_{0}^{he^{i\theta}} \oint_{c} \frac{f(t) \cdot 4\zeta^{2m+1} \left[(m+1)(t-z)^{2} - m\zeta^{2} \right]}{(t-z)^{2m} \left[(t-z)^{2} - \zeta^{2} \right]^{2}} dt d\zeta$$

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

$$+ R_{2m}(\theta, h, z).$$

Setting $m=np+1,\ \theta=\theta_k=\frac{k\pi}{n}$ and summing over $k=0,1,\ldots,n-1$ after multiplying through by $e^{-i2\theta_k}$, we get

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

which is (10).

Note 3. To obtain (11) we use the infinite series

$$f'(z + \zeta) = f'(z) + \zeta f''(z) + \frac{\zeta^2}{2!} f'''(z) + \cdots$$

in place of (3) and proceed as above.

REFERENCES

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