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ON THE NUMERICAL DIFFERENTIATION

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1. Let $-\infty < \alpha < x_0 < \beta < \infty$ and Y be the set of all functions $f:[\alpha,\beta] \to \mathbf{R}$ which are p-times differentiable at x_0. If $a = (a_1, a_2, \ldots, a_n)$, $b = (b_1, b_2, \ldots, b_n)$, $b_i \neq b_j$ for $i \neq j$, are arbitrary points in $\mathbf{R}^n$, $\frac{\alpha - x_0}{h} \leq b_k \leq \frac{\beta - x_0}{h}$, $k = 1, \ldots, n$, $h > 0$, let us consider *n-point differentiation formulas* of the following kind

(1) $$f^{(p)}(x_0) = d_n(f;a,b) + R_n(f),\ n \geq p+1 \geq 2,$$

where $d_n(.\,; a, b) : Y \to \mathbf{R}$ is a linear functional called the *n-point rule* for the pth derivative and is defined as

(2) $$d_n(f;a,b) := \frac{1}{h^p}\sum_{k=1}^{n} a_k f(x_k),\quad h > 0,\quad x_k := x_0 + hb_k .$$

The linear functional $R_n : Y \to \mathbf{R}$, $R_n(f) = f^{(p)}(x_0) - d_n(f;\, a,\, b)$ is the remainder. By denoting $e_k(t) = t^k$, we say that $d_n(.; a, b)$ belongs to the set $\mathcal{D}_m$ if and only if $d_n(e_k; a, b) = e_k^{(p)}(x_0)$, $k = 0, 1, \ldots, m$, and moreover $d_n(e_{m+1}; a, b) \neq \neq e_{m+1}^{(p)}(x_0)$. In other words, $\mathcal{D}_m$ contains all n-point rules which have the degree of exactness m. An n-point rule $d_n(.; a, b)$ is of *interpolatory type* if and only if

(3) $$d_n(f;a,b) = (L_{n-1}f)^{(p)}(x_0),$$

where

$$(L_{n-1}f)(x) = \sum_{k=1}^{n} l_k(x) f(x_k),\ l_k(x) = \frac{\Omega(x)}{(x - x_k)\Omega'(x_k)},\ \Omega(x) = \prod_{k=1}^{n}(x - x_k),$$

that is,

$$a = h^p\left(l_1^{(p)}(x_0), \ldots, l_n^{(p)}(x_0)\right).$$

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Though the following proposition is a very simple one, we have not found any references to it.

LEMMA 1. i) *An n-point rule $d_n(.;a,b)$ is of interpolatory type if and only if $d_n(g;a,b)=g^{(p)}(x_0)$ for any polynomial g of degree $\le n-1$.*

ii) *If $d_n(.;a,b)\in \mathcal{D}_m$, then $m\le n$.*

Proof. i) Suppose $d_n(.;a,b)$ is of interpolatory type. If g is an arbitrary polynomial of degree $\le n-1$, then from (3)

$$d_n(g;a,b)=g^{(p)}(x_0). \tag{4}$$

If (4) is satisfied, by choosing $g=l_k$, we find $a_k=h^p d_n(l_k;a,b)=h^p l_k^{(p)}(x_0)$, i.e., $d_n(.;a,b)$ is of interpolatory type.

ii) Let us assume $m\ge n+1$, and consider the polynomial $\Phi(x):=(x-x_0)\,\Omega(x)$. Observe that

$$R_n(\Omega)=\Omega^{(p)}(x_0) \quad\text{and}\quad R_n(\Phi)=p\Omega^{(p-1)}(x_0) \tag{5}$$

and, because Φ and Ω are of degree $\le m$, we must have $\Omega^{(p)}(x_0)=0$ and $\Omega^{(p+1)}(x_0)=0$. This is contradictory to the fact that Ω has distinct roots.

LEMMA 2. *If R_n is the remainder corresponding to an n-point rule of interpolatory type, then*

$$R_n(e_n)=\omega^{(p)}(0)h^{n-p}, \tag{6}$$

$$R_n(e_{n+1})=p\omega^{(p-1)}(0)h^{n-p+1}+\left((n+1)x_0+h\sum_{k=1}^{n}b_k\right)\omega^{(p)}(0)h^{n-p},$$

where $\omega(x)=\prod_{k=1}^{n}(x-b_k)$.

Proof. Let Φ be defined as in the proof of Lemma 1. It is easy to observe that

$$e_n(x)=x^n=\Omega(x)+q_{n-1}(x),\ e_{n+1}(x)=\Phi(x)+e_n(x)\sum_{k=0}^{n}x_k+\hat{q}_{n-1}(x),$$

for some polynomials $q_{n-1}, \hat{q}_{n-1}$ of degree $\le n-1$.

Using (5), we find (6). □

THEOREM 1. *The following statements are equivalent:*

- $d_n(.;a,b)\in \mathcal{D}_n$;
- $a=(a_1,a_2,\dots,a_n)$ *is determined by*

$$a_k=\begin{cases}\dfrac{\omega^{(p+1)}(0)}{(p+1)\omega'(0)} & ;\ b_k=0,\ (p\ge 2),\\[2ex] \dfrac{p!}{b_k^{p+1}\omega'(b_k)}\displaystyle\sum_{s=p+1}^{n}\frac{b_k^s}{s!}\omega^{(s)}(0) & ;\ b_k\ne 0,\end{cases} \tag{7}$$

and the roots $b_1,b_2,\dots,b_n$ of $\omega(x)=\prod_{k=1}^{n}(x-b_k)$ are selected such that

$$\omega^{(p)}(0)=0 \ \text{and}\ \frac{\alpha-x_0}{h}\le b_k\le\frac{\beta-x_0}{h},\ k=1,2,\dots,n. \tag{8}$$

Proof. Suppose that $d_n(.;a,b)\in\mathcal{D}_n$ is true. Then, according to (6), we find (8) and observe that in this case $\omega^{(p-1)}(0)\ne 0$. At the same time, the n-point rule $d_n(.;a,b)$ being of interpolatory type, we get $a_k=h^p l_k^{(p)}(x_0)$, which may be written as in (7). □

In the following two sections we investigate the cases $p=1$ and $p=2$.

2. *Case $p=1$.* In order to make evident the differentiation formulas which are *optimal with respect to the degree of exactness*, i.e., $d_n(.;a,b)\in\mathcal{D}_n$, we use the results established in the above section. According to Theorem 1, for $p=1$ we must have $\omega(0)\ne 0$ and $\omega'(0)=0$, i.e.,

$$\frac{1}{b_1}+\frac{1}{b_2}+\dots+\frac{1}{b_n}=0. \tag{9}$$

This condition imposed on $b=(b_1,b_2,\dots,b_n)$ is also given in [4], and for $n=3$ see [1]. Moreover,

$$f'(x_0)=\frac{(-1)^{n-1}b_1b_2\dots b_n}{h}\sum_{k=1}^{n}\frac{f(x_0+hb_k)}{b_k^2\omega'(b_k)}+R_n^{\langle 1\rangle}(f), \tag{10}$$

where $b_1,b_2,\dots,b_n$ are arbitrary such that (9) is fulfilled, represents *all differentiation formulas from $\mathcal{D}_n$*. The case $n=3$ is studied in [1]. It may be noted that (10) is the same with

$$f'(x_0)=\frac{(-1)^{n-1}b_1b_2\dots b_n}{h}\left[b_1,b_2,\dots,b_n;\frac{f(x_0+ht)}{t^2}\right]+R_n^{\langle 1\rangle}(f),$$

where $[b_1,b_2,\dots,b_n;\phi]=[b_1,b_2,\dots,b_n;\phi(t)]$ denotes the divided difference of $\phi=\phi(t)$ at the distinct points $b_1,b_2,\dots,b_n$.

In connection with the remainder $R_n^{(1)}$, some considerations were made by H. E. Salzer [4]. We shall prove the following

THEOREM 2. *If* $f \in C^{(n+1)}[\alpha, \beta]$, *then there exists a point* Θ, $\Theta \in (\alpha, \beta)$, *such that*

$$R_n^{(1)}(f) = (-1)^n h^n b_1 b_2 \ldots b_n \frac{f^{(n+1)}(\Theta)}{(n+1)!}. \tag{11}$$

Proof. If $z_1, z_2, \ldots, z_m$ are distinct points from $[\alpha, \beta]$, we denote by

$$(H_n f)(x) := H_n(\underbrace{z_1, \ldots, z_1}_{k_1}, \underbrace{z_2, \ldots, z_2}_{k_2}, \ldots, \underbrace{z_m, \ldots, z_m}_{k_m}; f; x), \ (k_1 + \ldots + k_m = n+1)$$

the unique polynomial of degree $\le n$ which satisfies

$$(H_n f)^{(j)}(z_\nu) = f^{(j)}(z_\nu), \ j = 0, 1, \ldots, k_\nu - 1; \ \ \nu = 1, 2, \ldots, m,$$

i.e., the Hermite interpolation polynomial. Further we use that

$$f(x) - (H_n f)(x) = (x - z_1)^{k_1} \ldots (x - z_m)^{k_m} \frac{f^{(n+1)}(\xi)}{(n+1)!}, \tag{12}$$

with $\xi \in (\alpha, \beta)$. Defining

$$g(x) = f(x) - H_n(x_0, x_0, x_2, \ldots, x_n; f; x),$$

we get from (10)

$$R_n^{(1)}(f) = R_n^{(1)}(g) = g'(x_0) - \frac{(-1)^{n-1} b_1 b_2 \ldots b_n}{h} \sum_{k=1}^{n} \frac{g(x_k)}{\omega'(b_k) b_k^2} =$$

$$= \frac{(-1)^{n-1} b_1 b_2 \ldots b_n}{h} \frac{g(x_1)}{\omega'(b_1) b_1^2},$$

and (12) completes this proof. □

The remainder of some differentiation formulas was also investigated by H. Brass [3].

Let us give some numerical examples: For $n = 4$, $H > 0$, we have

$$f'(x_0) = \frac{1}{6H}\left(f(x_0 - H) - 8f\left(x_0 - \frac{H}{2}\right) + 8f\left(x_0 + \frac{H}{2}\right) - f(x_0 + H)\right) + \frac{H^4}{480} f^{(5)}(\Theta_1),$$

with $f \in C^{(5)}[x_0 - H, x_0 + H]$, $x_0 - H < \Theta_1 < x_0 + H$.

Another formula is

$$f'(x_0) = \frac{1}{H}\left(\frac{1}{260} f(x_0 + H) - \frac{1152}{221} f\left(x_0 - \frac{H}{12}\right) + \frac{72}{5} f\left(x_0 + \frac{H}{6}\right) - \frac{625}{68} f\left(x_0 + \frac{H}{5}\right)\right) - \frac{H^4}{43200} f^{(5)}(\Theta_2),$$

for $f \in C^{(5)}\left[x_0 - \frac{H}{12}, x_0 + H\right]$, $x_0 - \frac{H}{12} < \Theta_2 < x_0 + H$.

In the following numerical example let us consider $n = 2m$ in (10). According to [2], the *truncation error* is minimized for $b_k = \frac{H}{2h}(2k - 2m - 1) = \frac{H}{h} w_{k,m}$. From (10) the desired differentiation formula is

$$f'(x_0) = \frac{c_m}{H} \sum_{k=1}^{m} (-1)^{m+1-k} \binom{2m}{k} \frac{k}{(w_{k,m})^2} \left(f(x_0 + w_{k,m} H) - f(x_0 - w_{k,m} H)\right) + (-1)^m c_m H^{2m} \frac{f^{(2m+1)}(\xi)}{(2m+1)},\tag{13}$$

where $c_m := \frac{1}{4^{2m}} \binom{2m}{m}$ satisfies $\frac{1}{4^m \sqrt{m\pi + \frac{\pi}{2}}} \le c_m \le \frac{1}{4^m \sqrt{m\pi}}$.

It is supposed that $f \in C^{(2m+1)}[\alpha, \beta]$ and $0 < \left(m - \frac{1}{2}\right) H \le \min(x_0 - \alpha, \beta - x_0)$. Further, with $m = 3$, $H = 2h$ in (13), we find

$$f'(x_0) = \frac{1}{128}\left(3[x_0 - 5h, x_0 + 5h; f] - 25[x_0 - 3h, x_0 + 3h; f] + 150[x_0 - h, x_0 + h; f]\right) - \frac{5}{112} h^6 f^{(7)}(\xi),$$

where $f \in C^{(7)}[\alpha, \beta]$, $0 < h \le \frac{1}{5} \min(x_0 - \alpha, \beta - x_0)$.

3. *Case* $p = 2$ *and* $b_1 = 0$. For the sake of brevity, we put

$$r_n = -\sum_{k=2}^{n} \frac{1}{b_k^2}, \quad v(x) = \frac{\omega(x)}{x}.$$

From (7) with $b_1 = 0$ it is seen that the formula

$$(14)\qquad f''(x_0)=\frac{1}{h^2}\left(r_n\cdot f(x_0)+2(-1)^n b_2b_3\dots b_n\sum_{k=2}^{n}\frac{f(x_0+hb_k)}{b_k^3 v'(b_k)}\right)+R_n^{\langle 2\rangle}(f),$$

with $\frac{1}{b_2}+\frac{1}{b_3}+\dots+\frac{1}{b_n}=0$, has the degree of exactness equal to n.

THEOREM 3. *If* $f\in C^{(n+1)}[\alpha,\beta]$, *then there exists a point* η, $\eta\in(\alpha,\beta)$, *such that*

$$(15)\qquad R_n^{\langle 2\rangle}(f)=2(-1)^{n-1}h^{n-1}b_2b_3\dots b_n\frac{f^{(n+1)}(\eta)}{(n+1)!}.$$

Proof. Let us start with

$$h(x)=f(x)-H_n(x_0,x_0,x_0,x_3,x_4,\dots,x_n;f;x)$$

and observe that

$$h(x_0)=0,\ h'(x_0)=0,\ h''(x_0)=0,\ h(x_3)=\dots=h(x_n)=0.$$

Further, from (14),

$$(16)\qquad R_n^{\langle 2\rangle}(f)=R_n^{\langle 2\rangle}(h)=2(-1)^{n-1}\frac{b_2b_3\dots b_n}{h^2}\frac{h(x_2)}{b_2^3 v'(b_2)}$$

and (12) enables us to write

$$h(x_2)=(x_2-x_0)^3(x_2-x_3)\dots(x_2-x_n)\frac{f^{(n+1)}(\eta)}{(n+1)!}=h^{n+1}v'(b_2)b_2^3\frac{f^{(n+1)}(\eta)}{(n+1)!},$$

which completes, together with (16), the proof. □

Now one can give the following numerical example: Let us consider $n=2m+1$; then we get from (14) the differentiation formula

$$(17)\qquad f''(x_0)=\frac{2}{H^2}\left(c_m\sum_{k=1}^{m}(-1)^{m+k-1}\binom{2m}{k}\frac{k}{\left(k-m-\frac{1}{2}\right)^3}\times\right.$$

$$\left.\times\left(f\left(x_0+\left(k-m-\frac{1}{2}\right)H\right)+f\left(x_0-\left(k-m-\frac{1}{2}\right)H\right)\right)-4f(x_0)\sum_{k=1}^{m}\frac{1}{(2k-1)^2}\right)+$$

$$+(-1)^m c_m H^{2m}\frac{f^{(2m+2)}(\xi_2)}{(2m+1)(m+1)},$$

where $c_m:=\frac{1}{4^{2m}}\binom{2m}{m}$, $f\in C^{(2m+2)}[\alpha,\beta]$ and $0<\left(m-\frac{1}{2}\right)H\le\min(x_0-\alpha,\beta-x_0)$, $\xi_2\in(\alpha,\beta)$. Further, with $m=4$ in (17), we find

$$f''(x_0)=\frac{1}{512}\left(1225\left[x_0-\frac{H}{2},x_0,x_0+\frac{H}{2};f\right]-245\left[x_0-\frac{3H}{2},x_0,x_0+\frac{3H}{2};f\right]+\right.$$

$$\left.+49\left[x_0-\frac{5H}{2},x_0,x_0+\frac{5H}{2};f\right]-5\left[x_0-\frac{7H}{2},x_0,x_0+\frac{7H}{2}\right]\right)+\frac{7H^8}{294912}f^{(10)}(\xi_2),$$

where $f\in C^{(10)}[\alpha,\beta]$, $0<H\le\frac{2}{7}\min(x_0-\alpha,\beta-x_0)$.

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