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Convergence of Numerical Differentiation

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Let D_0 be the functional given by $D_0 f = f'(0)$ on $C^1(-1, 1)$. Let Π_n be the set of polynomials of degree not exceeding n and let M_n be the polynomial interpolation to f at a given set of points $x_1, x_2, \ldots, x_n$. We approximate $D_0 f$ by $D_0 M_n f$. This is called a numerical differentiation formula. We study the pointwise convergence of $D_0 M_n$ to D_0 for two choices of the set of points: for equispaced points and for the extrema of the Chebycheff polynomials.

Let $C = C[-1, 1]$ be the Banach space of continuous real-valued functions on the interval $[-1, 1]$ with the Chebycheff norm and let C_i denote the space of i-times continuously differentiable functions. By numerical differentiation we mean the replacement of the derivative evaluated at the point zero

$$D_0 f = \frac{d}{dx} f \Big|_{x=0}$$

by the approximate expression

$$D_0 f \sim Ff = \sum_{i=1}^{n} \alpha_i f(x_i),$$

where $-1 \leqslant x_1 < x_2 < \cdots < x_n \leqslant 1$ and the α_i are real. This will be called a differentiation formula. The justification of the term "approximate" lies in our demand that $D_0 f = Ff$ for all polynomials f of degree not exceeding $n - 1$

$$FP = D_0 P, \qquad P \in \Pi_{n-1}.$$

Given the points x_i, this determines the coefficients α_i uniquely. In fact, if K is any functional defined for all polynomials and if x_i, $i = 1, \ldots, n$, are given, then the equality

$$KP = \sum_{i=1}^{n} \alpha_i P(x_i)$$

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for all $P \in \Pi_{n-1}$ determines the coefficients uniquely. Let $L_{n-1,j}(x_1, \ldots, x_n ; x)$ be the Lagrange interpolating polynomial:

$$L_j \in \Pi_{n-1},$$
$$L_j(x_1, \ldots, x_n ; x_i) = \delta_{ij}, \qquad i, j = 1, \ldots, n.$$

Then

$$\alpha_i = KL_i(x_1, \ldots, x_n ; \cdot). \tag{1}$$

We will consider two choices of the nodes $\{x_i\}$. The first is the easiest choice made using information neither on the functional to be approximated nor of the set on which the approximation is exact. This is

$$x_i = i/2m, \qquad i = 0, \pm 1, \ldots, \pm m. \tag{2}$$

The second choice is the set of extremal points of the Chebycheff polynomial of degree $2m - 1$, T_{2m-1}.

If we let

$$T_{2m-1}(x) = \cos\{(2m-1)\cos^{-1}x\}, \qquad -1 \leqslant x \leqslant 1,$$

and

$$\begin{aligned} x_i &= -\cos\frac{\pi(i+m)}{2m-1}, & i &= -m, -m+1, \ldots, -1, \\ x_0 &= 0, \\ x_i &= -\cos\frac{\pi(i+m-1)}{2m-1}, & i &= 1, 2, \ldots, m, \end{aligned} \tag{3}$$

then the x_i, $i \neq 0$, are the extrema of T_{2m-1} and

$$\begin{aligned} T_{2m-1}(x_i) &= (-1)^{i+m+1}, & i &= -m, \ldots, -1, \\ T_{2m-1}(x_i) &= (-1)^{i+m}, & i &= 1, \ldots, m. \end{aligned}$$

In either case, the functional

$$F_{2m} = \sum_{i=-m}^{m} \alpha_i L_{x_i}, \tag{4}$$

where the L_{x_i} are the point evaluation functionals, which reproduces D_0 exactly on Π_{2m}, has coefficients given by (1) if we replace K by D_0.

As a functional on C,

$$\| F_{2m} \| = \sum_{i=-m}^{m} | \alpha_i |.$$

It turns out that the choice of the Chebycheff extrema minimizes the norm of F_{2m} among all choices of nodes. As a consequence, this choice yields a differentiation formula which is the least sensitive to uncertainty in the given information $f(x_i)$. For more detail on this aspect see Pallaschke [4].

It is another aspect, however, which is of primary interest to us, namely, the convergence of $F_{2m}(f)$ to $f'(o)$ as m increases.

Pallaschke, [3], has proved that the differentiation formula with the Chebycheff nodes (3) converges to $f'(o)$ for any f which is twice continuously differentiable. We will show here that this formula even converges for once differentiable functions. We then compare this behavior with that of the differentiation formula with equi-spaced nodes (2) which are worse behaved. It is shown that for equi-spaced nodes the formula also converges for three times continuously differentiable functions but diverges for at least one function not in this class.

The following three theorems represent our main results.

THEOREM 1. *Let*

$$F_{2m}(f) = \sum_{i=-m}^{m} \frac{d}{dx} L_{2m,i}(x_{-m}, \ldots, x_m ; x) |_{x=0} f(x_i), \tag{5}$$

where the x_i are the Chebycheff nodes (3). *Then for all $f \in C_1[-1, 1]$,*

$$F_{2m}(f) \to f'(0)$$

for $m \to \infty$.

THEOREM 2. *Let F_{2m} be given as above, however, with*

$$x_i = i/2m, \qquad i = -m, -m+1, \ldots, m.$$

Then

$$F_{2m}(f) \to f'(0)$$

for any f satisfying the Dini–Lipschitz condition for its derivative:

$$\omega(f', n^{-1}) \log n \to 0.$$

THEOREM 3. *Let F_{2m} be as in Theorem 2. Then there is some $f \in C_1[-1, 1]$, so that*

$$F_{2m}(f) \not\to f'(0).$$

One may resume these results in saying that the numerical differentiation formula for equi-spaced nodes is really worse than that for Chebycheff nodes but not so bad after all since it converges for functions satisfying a relatively weak condition on the derivative.

We begin a general analysis of these differentiation formulas following, in part, Pallaschke [3]. In the equi-spaced case,

$$\begin{aligned}\alpha_i &= \frac{d}{dx} L_{2m,i}(x_{-m}, \ldots, x_m ; x) \Big|_{x=0} \\ &= \frac{d}{dx} \prod_{\substack{j=-m \\ j\neq i}}^{m} \frac{(x - x_j)}{(x_i - x_j)} \Big|_{x=0} \\ &= -\left[\prod_{\substack{j=-m \\ j\neq i}}^{m} (x_i - x_j)\right]^{-1} \prod_{\substack{j=-m \\ j\neq 0,i}}^{m} x_j\end{aligned}$$

for $i \neq 0$, and $\alpha_0 = 0$.

Setting in the values for the nodes

$$\begin{aligned}\alpha_0 &= 0 \\ \alpha_i &= -\frac{m}{i} \prod_{\substack{j=-m \\ j\neq 0,i}}^{m} \frac{j}{i-j}, \qquad i \neq 0.\end{aligned} \tag{6}$$

For the case of Chebycheff nodes, we use the following representation of Lagrange interpolant to the function f at the Chebycheff nodes, which can be found in Rivlin [5].

$$\begin{aligned}M_{2m-1}(f: x) = (2m-1)^{-2}(1-x^2)\, T'_{2m-1}(x) \\ \times \Big\{ -\frac{1}{2}\frac{f(-1)}{(x+1)} - \frac{1}{2}\frac{f(1)}{(x-1)} + \sum_{j=-m+1}^{-1} (-1)^{j+1} \frac{f(x_j)}{(x-x_j)} \\ + \sum_{j=1}^{m-1} (-1)^j \frac{f(x_j)}{(x-x_j)} \Big\}.\end{aligned}$$

Thus

$$\begin{aligned}&M'_{2m-1}(f; x)\,|_{x=0} \\ &= (2m-1)^{-2}\, T''_{2m-1}(0) \Big\{ \tfrac{1}{2}f(-1) - \tfrac{1}{2}f(1) + \sum_{j=-m+1}^{-1} (-1)^{j+1}\frac{f(x_j)}{-x_j} \\ &\quad + \sum_{j=1}^{m-1} (-1)^j \frac{f(x_j)}{-x_j}\Big\} \\ &\quad + (2m-1)^{-2}\, T'_{2m-1}(0) \Big\{ -\tfrac{1}{2}f(1) + \tfrac{1}{2}f(1) \\ &\quad - \sum_{j=-m+1}^{-1} (-1)^{j+1}\frac{f(x_j)}{x_j^2} \\ &\quad - \sum_{j=1}^{m-1} (-1)^j \frac{f(x_j)}{x_j^2}\Big\}.\end{aligned}$$

Since

$$\begin{aligned} T'_{2m-1}(0) &= (2m-1)(-1)^{m-1}, \\ T''_{2m-1}(0) &= 0, \\ M'_{2m-1}(f; x)\,|_{x=0} &= (2m-1)^{-1}(-1)^{m+1}\Big\{-\tfrac{1}{2}f(-1) + \tfrac{1}{2}f(1) \\ &\quad + \sum_{j=-m+1}^{-1} (-1)^j \frac{f(x^j)}{x_j^2} \\ &\quad + \sum_{j=1}^{m-1} (-1)^{j+1} \frac{f(x_j)}{x_j^2}\Big\}. \end{aligned}$$

Now we use the fact that $L_{2m-1,i}$ is a polynomial of degree $2m-1$ itself and so

$$M_{2m-1}(L_{2m-1}\,;\, x) = L_{2m-1,i}(x).$$

Since

$$L_{2m-1,i}(x_j) = \delta_{ij}$$

and since

$$\alpha_i = L'_{2m-1,i}(0),$$

we get

$$\begin{aligned} \alpha_{-m} &= \tfrac{1}{2}(2m-1)^{-1}(-1)^m, \\ \alpha_i &= (2m-1)^{-1}(-1)^i x_i^{-2} \qquad i = -m+1, -m+2,..., -1, \\ \alpha_0 &= 0, \\ \alpha_i &= (2m-1)^{-1}(-1)^{i+1}x_i^{-2}, \quad i = 1, 2,..., m-1, \\ \alpha_m &= \tfrac{1}{2}(2m-1)^{-1}(-1)^{m+1}. \end{aligned} \tag{7}$$

Now using (3), we have an explicit formula for F_{2m} :

$$\begin{aligned} F_{2m}(f) &= (2m-1)^{-1}\Big\{\tfrac{1}{2}(-1)^m f(-1) + \tfrac{1}{2}(-1)^{m+1} f(1) \\ &\quad + \sum_{i=-m+1}^{-1} (-1)^i \left[\cos\frac{\pi(i+m)}{2m-1}\right]^{-2} f\left[\cos\frac{\pi(i+m)}{2m-1}\right] \\ &\quad + \sum_{i=1}^{m-1} (-1)^{i+1} \left[\cos\frac{\pi(i+m+1)}{2m-1}\right]^{-2} f\left(\cos\frac{\pi(i+m+1)}{2m-1}\right)\Big\}. \end{aligned}$$

Note that we have interpolated from Π_{2m-1} because $L'_{2m-1,i}(0) = L'_{2m,i}(0)$ and so the numerical differentiation formulas from Π_{2m} and Π_{2m-1} are the same.

In order to prove Theorems 1 and 3, we consider not the functionals F_{2m} but rather the composition $F_{2m}S$ of F_{2m} with the operator of integration

$$Sf(x) = \int_{-1}^{x} f(t)\, dt.$$

We do this because of the following lemma:

LEMMA 4. *Let T_n be a sequence of functionals on $C[-1, 1]$. Then*

$$T_n(f) \to f'(0) \tag{8}$$

for all $f \in C_1$ if and only if

$$T_n P \to P'(0) \tag{9}$$

for any polynomial P and there exists an $M > 0$ such that

$$\| T_n S \| \leq M, \qquad n = 1, 2, \ldots . \tag{10}$$

Proof. Necessity: Let $f \in C$. Then $Sf \in C_1$. Thus

$$T_n(Sf) \to (Sf)'(0) = f(0).$$

An M satisfying (10) exists since point-wise boundedness implies uniform boundedness. Obviously (9) is satisfied also.

Sufficiency: Assume (9) and (10) and let $P = SQ$, where Q is a polynomial. Then

$$(T_n S)Q = T_n P \to P'(0) = Q(0).$$

By the Banach–Steinhaus theorem again, we may conclude that

$$(T_n S)g \to g(0)$$

for any $g \in C$, since the polynomials are dense in C. But any $f \in C_1$ may be written as $f = Sg$ for some $g \in C$, so that

$$T_n f \to g(0) = f'(0).$$

In considering the convergence of differentiation formulas, we can thus, by using Lemma 4, restict ourselves to the functionals $T_n S$. Note also that this lemma is independent of the nodes.

Now, also for both our choices of nodes

$$\begin{aligned}(F_{2m}S)f &= \sum_{\substack{i=-m \\ i \neq 0}}^{m} \alpha_i (Sf)(x_i) = \sum_{\substack{i=-m \\ i \neq 0}}^{m} \alpha_i \int_{-1}^{x_i} f(t)\, dt \\ &= \sum_{i=-m+1}^{-1} \int_{x_{i-1}}^{x_i} \Bigl(\sum_{\substack{j=i \\ j \neq 0}}^{m} \alpha_j \Bigr) f(t)\, dt \\ &\quad + \sum_{i=2}^{m} \int_{x_{i-1}}^{x_i} \Bigl(\sum_{j=i}^{m} \alpha_j \Bigr) f(t)\, dt \\ &\quad + \int_{x_{-1}}^{x_1} \Bigl(\sum_{j=1}^{m} \alpha_j \Bigr) f(t)\, dt\end{aligned}$$

and so

$$\| F_{2m}S \| = \sum_{i=-m+1}^{-1} (x_i - x_{i-1}) \left| \sum_{\substack{j=i \\ j\neq 0}}^{m} \alpha_j \right|$$

$$+ (x_1 - x_{-1}) \left| \sum_{j=1}^{m} \alpha_j \right| + \sum_{j=1}^{m} (x_i - x_{i-1}) \left| \sum_{j=i}^{m} \alpha_j \right|.$$

Now since the F_{2m} are exact on Π_{2m},

$$F_{2m}(1) = \sum_{i=-m}^{m} \alpha_i = 0.$$

From (6) and (7), we see that

$$\alpha_{-j} = -\alpha_j .$$

Because

$$x_{-j} = -x_j ,$$

$$\| F_{2m}S \| = 2 \left\{ x_1 \left| \sum_{j=1}^{m} \alpha_j \right| + \sum_{i=2}^{m} (x_i - x_{i-1}) \left| \sum_{j=i}^{m} \alpha_j \right| \right\}. \tag{11}$$

We want to continue with exact formulas for $\| F_{2m}S \|$. To do this, we show that

$$\sigma\left(\sum_{j=i}^{m} \alpha_j \right) = \sigma(\alpha_i) = (-1)^{i+1}, \qquad i = 1, 2,..., m.$$

First we observe that for Chebycheff nodes,

$$| \alpha_j | > | \alpha_{j+1} |, \qquad j = 1, 2,..., m - 1,$$

and that the α_j alternate in sign. This is clear from (6). For the equi-spaced case, we consider

$$\frac{\alpha_{i+1}}{\alpha_i} = - \left(\frac{i}{i+1} \right) \left(\frac{n-i}{n+i+1} \right).$$

Since both factors of the right hand side are smaller than one, here also the α_j decrease in absolute value with increasing j and alternate in sign.

By re-grouping,

$$\sum_{j=i}^{m} \alpha_j = (\alpha_i + \alpha_{i+1}) + (\alpha_{i+2} + \alpha_{i+3}) + \cdots,$$

one sees that

$$\sigma\left(\sum_{j=i}^{m} \alpha_j\right) = \sigma(\alpha_i) = (-1)^{i+1}, \qquad i > 0, \tag{12}$$

and

$$|\alpha_i + \alpha_{i+1}| \leqslant \left|\sum_{j=i}^{m} \alpha_j\right| \leqslant |\alpha_i|. \tag{13}$$

Thus we can write

$$\| F_{2m}S \| = 2\left\{x_1 \sum_{j=1}^{m} \alpha_j + \sum_{i=2}^{m} (x_i - x_{i-1})(-1)^{i+1} \sum_{j=i}^{m} \alpha_j\right\}. \tag{14}$$

We are now ready for the

Proof of Theorem 3

Now $x_i = 1/2m$ so that

$$\begin{aligned}
\| F_{2m}S \| &= \frac{1}{m}\left\{\sum_{j=1}^{m} \alpha_j + \sum_{i=2}^{m} (-1)^{i+1} \sum_{j=i}^{m} \alpha_j\right\} \\
&= \frac{1}{m} \sum_{i=1}^{m} (-1)^{i+1} \sum_{j=i}^{m} \alpha_j \\
&= \frac{1}{m} \sum_{j=1}^{m} \alpha_j \left(\sum_{k=1}^{j} (-1)^{i-1}\right) \\
&= \frac{1}{m} \sum_{j=1}^{m} \alpha_j \frac{1}{2} (1 + (-1)^{j+1}) \\
&= \frac{1}{m} (\alpha_1 + \alpha_3 + \cdots + \alpha_m \text{ or } \alpha_{m-1}).
\end{aligned}$$

The last term is α_m or α_{m-1} depending on which ever index is odd.

Note that this formula is exact. It enables us to obtain upper and lower bounds on $\| F_{2m}S \|$.

Obviously

$$\sum_{\substack{i \text{ odd} \\ i>0}} |\alpha_i| < \tfrac{1}{2} \| F_{2m} \|.$$

Since $|\alpha_i| > |\alpha_{i+1}|$,

$$\sum_{\substack{i>0 \\ i \text{ odd}}} |\alpha_i| > \sum_{\substack{i>0 \\ i \text{ even}}} |\alpha_i|$$

and because

$$\tfrac{1}{2} \| F_{2m} \| = \sum_{i>0} | \alpha_i |$$

$$\sum_{\substack{i>0 \\ i \text{ odd}}} | \alpha_i | > \tfrac{1}{4} \| F_{2m} \|.$$

Upper and lower bounds for $\| F_{2m}S \|$ are thus

$$(4m)^{-1} \| F_{2m} \| \leqslant \| F_{2m}S \| \leqslant (2m)^{-1} \| F_{2m} \|.$$

From the explicit formula for α_i,

$$\alpha_i = (-1)^{i+1} \frac{m}{i} \frac{m(m-1) \cdots (m-i+1)}{(m+1)(m+2) \cdots (m+i)},$$

it follows that for fixed i,

$$\left| \frac{\alpha_i}{m} \right| \to i^{-1}$$

as $m \to \infty$. It follows immediately that

$$\frac{1}{m} \| F_{2m} \| \to \infty \qquad \text{as } m \to \infty.$$

From Lemma 4, we may conclude that there exists an $f \in C_1$ for which

$$F_{2m} f \nrightarrow f'(0)$$

which concludes the proof.

Proof of Theorem 1

Using (13) and (14),

$$\| F_{2m}S \| \leqslant 2 \left\{ x_1 \alpha_1 + \sum_{i=2}^{m} | x_i - x_{i-1} | \, | \alpha_i | \right\}$$

$$< 2 \left\{ \frac{1}{(2m-1)\, x_1} + \sum_{i=2}^{m} \frac{(x_i - x_{i-1})}{(2m-1)\, x_i^2} \right\}$$

$$= \frac{2}{2m-1} \left\{ x_1^{-1} + \sum_{i=2}^{m} \frac{x_i - x_{i-1}}{x_i^2} \right\}.$$

Since x^{-2} falls monotonely,

$$\sum_{i=2}^{m} \frac{x_i - x_{i-1}}{x_i^2} \leqslant \int_{x_1}^{x_m} \frac{dx}{x^2} = x_1^{-1} - 1.$$

Hence

$$\| F_{2m} S \| \leqslant \frac{2}{2m-1} \left\{ \frac{2}{x_1} - 1 \right\} \leqslant \frac{4}{(2m-1)\, x_1}.$$

Now

$$x_1 = -\cos \frac{m\pi}{2m-1} = \sin \frac{\pi}{2(2m-1)}.$$

For $0 \leqslant x \leqslant \frac{1}{2}$,

$$\sin x \geqslant x - x^3/6$$

from which

$$x_1^{-1} \leqslant \frac{2(2m-1)}{\pi} \left[1 - \frac{\pi^2}{24(2m-1)^2} \right]^{-1} \leqslant \frac{4(2m-1)}{\pi}.$$

Thus

$$\| F_{2m} S \| \leqslant \frac{16}{\pi}$$

which together with Lemma 4 proves Theorem 1.

To prove Theorem 2, we find an upper bound for $\| F_{2m} \|$. We can use the previous formulas for α_i in the case of equi-spaced nodes to obtain

$$\alpha_1 = \frac{m^2}{m+1}$$

and

$$\begin{aligned} | \alpha_i | &\leqslant \left| \frac{\alpha_i}{\alpha_{i-1}} \cdot \frac{\alpha_{i-1}}{\alpha_{i-2}} \cdots \frac{\alpha_2}{\alpha_1} \right| \\ &\leqslant \frac{i-1}{i} \cdot \frac{i-2}{i-1} \cdots \frac{1}{2} \cdot \alpha_1 \\ &= \frac{1}{i} \frac{m^2}{m+1}, \qquad i \geqslant 1. \end{aligned}$$

Thus

$$\| F_{2m} \| = \sum_{i=-m}^{m} | \alpha_i | \leqslant 2m \log m$$

and so

$$\| F_{2m}S \| \leqslant (2m)^{-1} \| F_{2m} \| \leqslant \log m.$$

Now we may use the triangle inequality in the usual way

$$\begin{aligned} \| F_{2m}f - f' \| &= \| F_{2m}Sf' - f' \| \\ &\leqslant \| F_{2m}S(f' - P_{2m-1})\| + \| P_{2m-1} - f' \| \\ &\leqslant \{\| F_{2m}S \| + 1\} \| P_{2m-1} - f' \|. \end{aligned}$$

Thus

$$\begin{aligned} \| F_{2m}f - f' \| &\leqslant \{\| F_{2m}S \| + 1\} \cdot \inf_{P_{2m-1}} \| f' - P_{2m-1} \| \\ &\leqslant E_{2m-1}(f')(\log m + 1). \end{aligned}$$

If f' satisfies the Dini–Lipschitz condition, then $F_{2m}f$ converges to f'.

In concluding, it is perhaps of interest to compare these results, which show convergence at a point, with a recent result of Haverkamp [1] who analysed the uniform convergence of the differentiation formula for Chebycheff nodes. He obtained

THEOREM 5. *Let $P_{2m}(f)$ be the polynomial in Π_{2m} which interpolates f at the Chebycheff nodes. Then for $f \in C_1$*

$$\| f' - P'_{2m}(f)\| \leqslant 4[\ln 2m + 2]\, E_{2m-1}(f'),$$

where

$$E_n(f) = \min_{P \in \Pi_n} \| f - P \|$$

is the degree of approximation to f from Π_n and $\| \cdot \|$ is the uniform norm.

If we know that $f' \in \text{Lip}\, \alpha$ for some $\alpha > 0$, then

$$E_n(f') \leqslant Mn^{-\alpha}$$

for some $M > 0$. Thus $P'_{2m}(f)$ converges to f' uniformly, If, however, nothing is known about f' other than that is continuous, $P'_{2m}(f)$ need not converge to f' since $E_{2m}(f')$ may decrease arbitrarily slowly. Theorem 1 shows that even for arbitrary functions in C_1, convergence at a point is possible.

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