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Derivative Error Bounds for Lagrange Interpolation: An Extension of Cauchy's Bound for the Error of Lagrange Interpolation

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It is shown that for any $n+1$ times continuously differentiable function f and any choice of $n+1$ knots, the Lagrange interpolation polynomial L of degree n satisfies $\|f^{(n)}-L^{(n)}\| \leqslant \|\omega^{(n)}\|/(n+1)!\ \|f^{(n+1)}\|$, where $\|\ \|$ denotes the supremum norm. Further, this bound is the best possible. Applications of the above bound to the differencing formula are suggested. It is also shown that for $j=1, 2, ..., n-1$, $\|f^{(j)}-L^{(j)}\| \leqslant \|\omega^{(j)}\|/j!(n+1-j)!\ \|f^{(n+1)}\|$. This formula may be considered as a generalization of a formula due to Ciarlet, Schultz, and Varga (Numerical methods of high-order accuracy, *Numer. Math.* **9** (1967), 394–430) and may be compared to the conjectured best bound $\|f^{(j)}-L^{(j)}\| \leqslant \|\omega^{(j)}\|/(n+1)!\ \|f^{(n+1)}\|$.

STATEMENT OF THEOREMS

Let $f(x) \in C^{(n+1)}[a, b]$ and let $a \leqslant x_0 < x_1 < x_2 \cdots < x_n \leqslant b$. Let $L(x)$ be the nth order Lagrange polynomial satisfying

$$L(x_i) = f(x_i), \qquad i = 0, 1, ..., n. \tag{1.1}$$

The following theorem is attributed to Cauchy and is commonly found in elementary numerical analysis texts.

THEOREM 1. *Let L and f be as above. Then*

$$|f(x)-L(x)| \leqslant |\omega(x)|\,\frac{\|f^{(n+1)}\|}{(n+1)!}, \tag{1.2}$$

where $\omega(x) = (x-x_0)(x-x_1)\cdots(x-x_n)$ and where $\|\ \|$ denotes the supremum norm on $[a, b]$.

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Note 1. Most frequently, Theorem 1 is given with $x_0 = a$ and $x_n = b$. The slightly more general form given here follows from the same proof and is helpful in the proof of Theorem 3.

To see that the right hand side of (1.2) is the smallest possible, take $f(x) = \omega(x)$. Equality results for every x. From (1.2) it follows that

$$\|f - L\| \leqslant \|\omega\| \frac{\|f^{(n+1)}\|}{(n+1)!}. \tag{1.3}$$

Following Schoenberg [9], we will call this type of bound a Chebychev bound. Again, substitution of $\omega(x)$ for $f(x)$ shows that this bound is best possible.

Classically, Eqs. (1.2) and (1.3) have been the object of a good deal of study. For example, Chebyshev showed how to minimize $\|\omega(x)\|$ by choosing the knots $x_i = \arccos[(2i+1)/(2n+2)]$. Concerning $\|f^{(j)} - L^{(j)}\|$, generally only order of approximation results are given. The following conjecture is proposed.

CONJECTURE 1. Let f and L be as above. Then for all integers j, $0 \leqslant j \leqslant n$, the following holds

$$\|f^{(j)} - L^{(j)}\| \leqslant \|\omega^{(j)}\| \frac{\|f^{(n+1)}\|}{(n+1)!}. \tag{1.4}$$

If (1.4) is true, then by the substitution of $\omega(x)$ for $f(x)$, it is the best possible result. The conjecture can be justified numerically as will be discussed below.

Note 2. If Conjecture 1 is true then it also holds for the case of repeated roots, i.e., for Hermite interpolation.

To see that this is so, consider the Newton representation for Lagrange or Hermite interpolation

$$L_n[f, x] = \sum_{k=0}^{n} f[x_0, x_1, ..., x_k](x - x_0)(x - x_1) \cdots (x - x_{k-1}), \tag{1.5}$$

where $f[x_0, x_1, ..., x_k]$ denotes the divided difference of the points $f(x_i)$, $i = 0, 1, ..., k$ and where the x_i are not necessarily distinct. As the divided difference over an arbitrary set of points with repetitions is the limit of divided differences of distinct points [10] it follows that any Hermite interpolation derivative can be expressed as the limit of a sequence of Lagrange interpolations. As the distinct roots coalesce, so also do the corresponding

$\omega^{(j)}$'s converge to the $\omega^{(j)}$ with repeated roots. The bound for the case of the coalesced roots therefore follows from the bound for distinct roots.

Several attempts have been made to prove Conjecture 1, most notably by Bojanov and Varma. The following special case will be shown here.

THEOREM 2. *Conjecture* 1 *holds for* $j=n$.

The proof follows from an identity due to Polya and used by Curry and Schoenberg [4]. For the derivatives $j=1, 2, ..., n-1$, $\|f^{(j)}-L^{(j)}\|$ can be bounded as follows.

THEOREM 3. *Let f and L be as above. Then*

$$\|f^{(j)}-L^{(j)}\| \leqslant \|\omega^{(j)}\| \frac{\|f^{(n+1)}\|}{j!(n+1-j)!}. \tag{1.6}$$

Letting $n+1=2k$ and considering two point Hermite interpolation as a limit as knots coalesce to 0 and 1, we have the case of Ciarlet, Schultz, and Varga [3] which can be considered as a special case of (1.6), where $\omega(x)=(x-a)^k(b-x)^k$. As in the case of Ciarlet, *et al.*, the proof extends the classical proof of Theorem 1.

PRELIMINARIES

The proof of Theorem 2 requires some machinery. The following facts are used in the proof. Let $L(x)=: L[f(x), x]$ be the Lagrange interpolation polynomial of degree n satisfying Eq. (1.1). Then we can employ the Lagrange representation

$$L(x)=\sum_{i=0}^{n} \frac{f(x_i)\,\omega(x)}{(x-x_i)\,\omega'(x_i)}. \tag{2.1}$$

Without loss of generality, we will prove Theorem 2 on the interval [0, 1]. Let $f(x) \in C^{(n+1)}[0, 1]$. Then by the Peano kernel representation (see [5])

$$f(x)-L(x)=\int_0^1 K(x, t)\frac{f^{(n+1)}(t)}{n!}\,dt, \tag{2.2}$$

where

$$\begin{aligned} K(x, t) &= (x-t)_+^n - L[(x-t)_+^n, x] \\ &= (x-t)_+^n - \sum_{i=0}^{n} \frac{(x_i-t)_+^n\,\omega(x)}{(x-x_i)\,\omega'(x_i)} \end{aligned}$$

and where

$$(x-t)_+^n = \begin{cases} (x-t)^n & \text{for } x-t \geqslant 0 \\ 0 & \text{for } x-t<0. \end{cases}$$

By putting $f(x) = \omega(x)/(n+1)!$ in (2.2), we obtain

$$\int_0^1 \frac{K(x, t)}{n!}\, dt = \frac{\omega(x)}{(n+1)!}. \tag{2.3}$$

Differentiating (2.2) j times, where $j \leqslant n$, we have

$$f^{(j)}(x) - L^{(j)}[f, x] = \int_0^1 K^{(j,0)}(x, t) \frac{f^{(n+1)}(t)}{n!}\, dt. \tag{2.4}$$

In particular, if (2.2) is differentiated n times, we have

$$f^{(n)}(x) - L^{(n)}[f, x] = \int_0^1 \left\{ (x-t)_+^0 - \sum_{i=0}^{n} \frac{(x_i - t)_+^n}{\omega'(x_i)} \right\} f^{(n+1)}(t)\, dt. \tag{2.5}$$

From (2.4) follows the pointwise bound

$$|f^{(j)}(x) - L^{(j)}[f, x]| \leqslant \int_0^1 |K^{(j,0)}(x, t)|\, dt \left\| \frac{f^{(n+1)}}{n!} \right\|. \tag{2.6}$$

The bound (2.6) is pointwise exact in the sense that

$$\int_0^1 \frac{|K^{(j,0)}(x, t)|}{n!}\, dt = \sup_{f \in C^{(n+1)}[0,1]} \left\{ \frac{|f^{(j)}(x) - L^{(j)}[f, x]|}{\|f^{(n+1)}\|} \right\}.$$

Thus determination of a pointwise exact bound is in theory possible by evaluating kernel expressions of the form of (2.6). Such an exact evaluation was given for two-point cubic and quintic Hermite interpolation by Birkhoff and Priver [1], by use of the symbolic manipulation package, MACSYMA. More generally, an APL program due to Howell and Diaa ([6], available on request), constructs and approximately integrates kernels for derivative error. By such efforts, Conjecture 1 can be verified for specific cases of interpolatory polynomials of a given degree and specified knots.

In order to prove the conjecture for the nth derivatives of Lagrange polynomials of degree n, we will use the following additional identities. Consider the kernel expression

$$M(t, x_0, x_1, \ldots, x_n) = \sum_{i=0}^{n} \frac{n(x_i - t)_+^{n-1}}{\omega'(x_i)} \tag{2.7}$$

used by Curry and Schoenberg [4] to develop properties of spline functions. Concerning M, they showed the following properties

(i) $M(t)>0$, if $0<t<1$;

(ii) $M(t)=0$ if $t\leqslant 0$ or $t\geqslant 1$;

(ii) $\int_0^1 M(t)\,dt=1$.

Proof of Theorem 2

It follows from (i) and (ii) that for $\alpha<\beta$ we have

$$0<\int_\alpha^\beta M(t, x_0, x_1, ..., x_n)\,dt$$

$$=-\sum_{i=0}^n \frac{(x_i-\beta)_+^n}{\omega'(x_i)}+\sum_{i=0}^n \frac{(x_i-\alpha)_+^n}{\omega'(x_i)}.$$

Hence,

$$N(t) \stackrel{\text{def}}{=} \sum_{i=0}^n \frac{(x_i-t)_+^n}{\omega'(x_i)} \tag{3.1}$$

is a monotone decreasing function and is strictly decreasing for $0<t<1$. From (2.5) we have

$$|f^{(n)}(x)-L^{(n)}[f, x]|\leqslant \int_0^1 \left|(x-t)_+^0-\sum_{i=0}^n \frac{(x_i-t)_+^n}{\omega'(x_i)}\right| dt\,\|f^{(n+1)}(t)\|.$$

$$\leqslant \int_0^1 |(x-t)_+^0-N(t)|\,dt\,\|f^{(n+1)}(t)\|. \tag{3.2}$$

Define

$$e_n(x)=:\int_0^1 |(x-t)_+^0-N(t)|\,dt=\int_0^x [1-N(t)]\,dt+\int_x^1 N(t)\,dt. \tag{3.3}$$

Thus $e_n'(x)=1-2N(x)$ and $e_n''(x)=\ -2N'(x)>0$. From this it follows that

$$\|e_n\|=\max\{e_n(0), e_n(1)\}=\max_{0\leqslant x\leqslant 1}\int_0^1 \frac{|K^{(n,0)}(x, t)|}{n!}\,dt. \tag{3.4}$$

From (2.3), we have

$$\int_0^1 \frac{K^{(n,0)}(x, t)}{n!}\,dt=\frac{\omega^{(n)}(x)}{(n+1)!}. \tag{3.5}$$

Since $K^{(n,0)}(0, t) < 0$ and $K^{(n,0)}(1, t) > 0$, $0 < t < 1$, we have on recalling (3.3) the further equality

$$\|e_n\| = \max\left\{-\int_0^1 \frac{K^{(n,0)}(0, t)}{n!}\,dt, \int_0^1 \frac{K^{(n,0)}(1, t)}{n!}\,dt\right\}$$
$$= \max\left\{-\frac{\omega^{(n)}(0)}{(n+1)!}, \frac{\omega^{(n)}(1)}{(n+1)!}\right\}. \tag{3.6}$$

From (2.6), we have

$$\|f^{(n)} - L^{(n)}\| \leqslant \|e_n\|\ \|f^{(n+1)}\|$$
$$\leqslant \max\left\{-\frac{\omega^{(n)}(0)}{(n+1)!}, \frac{\omega^{(n)}(1)}{(n+1)!}\right\} \|f^{(n+1)}\|$$
$$\leqslant \frac{\|\omega^{(n)}\|}{(n+1)!}\ \|f^{(n+1)}\|. \tag{3.7}$$

This completes the proof of Theorem 2.

Proof of Theorem 3

We first show the theorem for the case of the first derivative, that is we show

$$\|f' - L'\| \leqslant \frac{\|\omega'\|}{n!}\ \|f^{(n+1)}\|. \tag{4.1}$$

Note first that there are at least n zeros $\eta_{i,1}$ of $f' - L'$, where for each i, $1 \leqslant i \leqslant n$, $x_i \leqslant \eta_{i,1} \leqslant x_{i+1}$. Define $\omega_1'(x) = \prod_{i=1}^n (x - \eta_{i,1})$. In this sense L' is an interpolatory polynomial of degree n. It follows from Theorem 1 (see Note 1) that for any x such that $a \leqslant x \leqslant b$

$$|f'(x) - L'(x)| \leqslant |\omega_1'(x)|\ \frac{\|f^{(n+1)}\|}{n!}. \tag{4.2}$$

For any given x, choose k depending on x such that $|x - x_k| = \min_{0 \leqslant i \leqslant n} |x - x_i|$. Such a k exists though there may be a choice. Denote $P_{x1}(t) = \omega(t)/(t - x_k) = \prod_{i \neq k} (t - x_i)$. Consider the case that $x_j < x < x_{j+1}$. We have that $x_0 < \eta_{1,1} < x_1 < \eta_{2,1} < x_2 \cdots < x_j < \eta_{j,1} < x_{j+1} < \cdots < x_{n-1} < \eta_{n,1} < x_n$, and k equaling either j or $j+1$. Then for $i = 1, 2, \ldots, j-1$, we have $|x - \eta_{i,1}| < |x - x_{i-1}|$. For $i = j$, we have $|x - \eta_{i,j}| < \max\{|x - x_j|, |x - x_{j+1}|\}$.

For $i=j+1, j+2, ..., n$, we have $|x-\eta_{i,1}|<|x-x_i|$. Then for the already fixed x, we have

$$|\omega_1'(x)| = \sum_{i=1}^{n} |x-\eta_{i,1}| \leqslant \left| \prod_{i \neq k} (x-x_i) \right| = |P_{x1}(x)|. \tag{4.3}$$

Similarly, (4.3) holds also for the case that x is chosen so that $x=x_j$ for some j, or for $a \leqslant x < x_0$, or for $x_n < x \leqslant b$ and thus for any fixed x, $a \leqslant x \leqslant b$.

Continuing to hold x arbitrary but fixed, we next compare $\max_{a \leqslant t \leqslant b}|P_{x1}(t)| = |P_{x1}(t_c)|$ to $|\omega'(t_c)|$. Of course, we do not know whether t_c is unique. We therefore make the comparison at all critical points of P_{x1}. We have

$$\omega'(t) = \frac{d}{dt}\left[(t-x_k) P_{x1}(t)\right] = P_{x1}(t) + (t-x_k) P'_{x1}(t). \tag{4.4}$$

Let t_c be such that $P_{x1}(t_c) = \max_{a \leqslant t \leqslant b}|P_{x1}(t)|$. Then either by (4.4)

$$0 = P'_{x1}(t_c) \Rightarrow \omega'(t_c) = P_{x1}(t_c) \tag{4.5}$$

or $t_c = a$ or $t_c = b$. If we can show that for $t \leqslant x_0$ and $t \geqslant x_n$

$$|P_{x1}(t)| \leqslant w'(t)|, \tag{4.6}$$

we will have demonstrated for the arbitrary fixed x that

$$\|P_{x1}\| \overset{\text{def}}{=} \sup_{a \leqslant t \leqslant b} |P_{x1}(t)| \leqslant \|\omega'\| \overset{\text{def}}{=} \sup_{a \leqslant t \leqslant b} |\omega'(t)|. \tag{4.7}$$

To show (4.6) define (recalling (4.4))

$$Q(t) = \omega'(t) - P_{x1}(t) = (t-x_k) P'_{x1}(t) \tag{4.8}$$

a polynomial of degree n with all its n zeros inside $[x_0, x_n]$. We can express ω' and P_{x1} in terms of their respective n roots

$$\omega'(t) = (n+1) \prod_{i=0}^{n-1} (t-\eta_i), \qquad x_0 < \eta_i < x_n \text{ (for all } i)$$

$$P_{x1}(t) = \prod_{i=0}^{n-1} (t-\xi_i), \qquad x_0 \leqslant \xi_i \leqslant x_n \text{ (for all } i).$$

Thus $\lim_{t \to \infty}(\omega'(t)/P_{x1}(t)) = n+1$. Since there are no zeros of $Q(t)$ for $t > x_n$, we must have $\omega'(t)/P_{x1}(t) > 1$ for $t > x_n$. Thus $|\omega'(x_n)| \geqslant |P_{x1}(x_n)|$. A similar argument applies when $t < x_0$.

Summing up the argument, we string together the inequalities (4.2)–(4.5), (4.7). For arbitrary x, $a \leqslant x \leqslant b$ (where in the intermediate inequality we take $|x-x_k|$ minimal for the given x),

$$\begin{aligned}|f'(x)-L'(x)| &\leqslant |\omega_1'(x)| \frac{\|f^{(n+1)}\|}{n!}\\ &\leqslant |P_{x1}(x)| \frac{\|f^{(n+1)}\|}{n!}\\ &\leqslant |P_{x1}(t_c)| \frac{\|f^{(n+1)}\|}{n!}\\ &\leqslant |\omega'(t_c)| \frac{\|f^{(n+1)}\|}{n!},\end{aligned}$$

where t_c is a critical point such that $|P_{x1}|$ attains its maximum.

Hence, for all x, $a \leqslant x \leqslant b$, we have

$$|f'(x)-L'(x)| \leqslant \|\omega'\| \frac{\|f^{(n+1)}\|}{n!}. \tag{4.9}$$

This completes the case for the first derivative.

For the case of the jth derivative, $1 \leqslant j \leqslant n$, fix x arbitrary in $[a, b]$. We have analogous to (4.2),

$$|f^{(j)}(x)-L^{(j)}(x)| \leqslant |\omega_j^{(j)}(x)| \frac{\|f^{(n+1)}\|}{(n+1-j)!}, \tag{4.10}$$

where $\omega_j^{(j)}(x) = \prod_{i=1}^{n+1-j} (x-\eta_{i,j})$ and where $\eta_{i,j}$ are such that $f^{(j)}(\eta_{i,j}) = L^{(j)}(\eta_{i,j})$ and $x_i < \eta_{i,j} < x_{i+j}$. For the given x, we can choose consecutive knots $x_k, x_{k+1}, ..., x_{k+j-1}$ so that $P_{xj}(t) \overset{\text{def}}{=} \prod_{i \neq k, k+1, ..., k+j-1} (t-x_i)$ and

$$|\omega_j^{(j)}(x)| \leqslant |P_{xj}(x)|. \tag{4.11}$$

For the particular fixed x, we then construct a string of intermediate monic polynomials, P_{xm}, where for each m, $0 \leqslant m \leqslant j$,

$$P_{xm}(t)(t-x_{k+m-1}) = P_{xm-1}(t)$$

is a monic polynomial of degree $n+1-m$ and where $P_{x0}(t) = \omega(t)$.

Differentiating $j+1-m$ times gives

$$(j+1-m)\, P_{xm}^{(j-m)}(t) + (t-x_{k+m-1})\, P_{xm}^{(j+1-m)}(t) = P_{xm-1}^{(j+1-m)}(t),$$

where $(j+1-m)\, P_{xm}^{(j-m)}(t)$ is a polynomial of degree $n+1-j$ with leading coefficient $(j+1-m)(n+1-m)!/(n+1-j)!$ compared to the leading coefficient $(n+2-m)!/(n+1-j)!$ of the polynomial $P_{xm-1}^{(j+1-m)}(t)$ of the same degree $n+1-j$. This gives a ratio $(n+1-j)/(j+1-m) > (n+1-j)/(n+1-m) \geqslant 1$ of the leading coefficients. Comparing all critical points, we have by the same logic as for the first derivative case the inequality

$$\|P_{xm}^{(j-m)}\| \leqslant \frac{\|P_{xm-1}^{(j+1-m)}\|}{j+1-m}. \tag{4.12}$$

Applying (4.10), (4.11), and inductively (4.12), we have for fixed x and j

$$\begin{aligned}
|f^{(j)}(x) - L^{(j)}(x)| &\leqslant |\omega_j^{(j)}(x)| \frac{\|f^{(n+1)}\|}{(n+1-j)!} \\
&\leqslant |P_{xj}(x)| \frac{\|f^{(n+1)}\|}{(n+1-j)!} \\
&\leqslant \|P_{xj}\| \frac{\|f^{(n+1)}\|}{(n+1-j)!} \\
&\leqslant \frac{\|P_{x0}^{(j)}\|}{j!} \frac{\|f^{(n+1)}\|}{(n+1-j)!} \\
&= \frac{\|\omega^{(j)}\|}{j!} \frac{\|f^{(n+1)}\|}{(n+1-j)!},
\end{aligned} \tag{4.13}$$

which is the desired result.

Applications

The nth derivative $L^{(n)}$ of the Lagrange interpolant satisfying (1.1) is merely the nth divided difference of f times $n!$, i.e.,

$$L^{(n)} = n! f[x_0, x_1, ..., x_n].$$

As such $L^{(n)}$ is frequently used as an approximation for $f^{(n)}$. The bound on $\|f^{(n)} - L^{(n)}\|$ is therefore of some interest. Suppose that $\|f^{(n+1)}\| \leqslant 1$. Then by Theorem 2 we have

$$\|f^{(n)} - L^{(n)}\| \leqslant \frac{\|\omega^{(n)}\|}{(n+1)!} \tag{5.1}$$

and we can minimize $\|f^{(n)} - L^{(n)}\|$ by choosing x_i to minimize $\|\omega^{(n)}\|$.

Differentiating (2.1) we have

$$\frac{\omega^{(n)}(x)}{(n+1)!} = x - \sum_{i=0}^{n} \frac{x_i}{n+1}. \tag{5.2}$$

$\|\omega^{(n)}\|$ will be minimized when $\sum_{i=0}^{n} x_i/(n+1) = (b+a)/2$, that is when the average of the differenced points is in the middle of the interval. Thus minimization of $\|f^{(n)} - L^{(n)}\|/\|f^{(n+1)}\|$ on an interval, $a \leqslant x \leqslant b$ can be accomplished by any knot choices symmetric about the interval midpoint.

For other derivatives, the bound in terms of $\|\omega^{(j)}\|$ indicates the desirability of using knots chosen so that $\omega^{(j)}$ has roots as the Chebychev nodes.

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