MATHEMATICS OF COMPUTATION, VOLUME 28, NUMBER 128
OCTOBER 1974, PAGES 1105–1115

Some Problems in Optimally Stable Lagrangian Differentiation

By Herbert E. Salzer

Abstract. In many practical problems in numerical differentiation of a function $f(x)$ that is known, observed, measured, or found experimentally to limited accuracy, the computing error is often much more significant than the truncating error. In numerical differentiation of the n-point Lagrangian interpolation polynomial, i.e., $f^{(k)}(x) \sim \Sigma_{i=1}^{n} L_i^{n(k)}(x) f(x_i)$, a criterion for optimal stability is minimization of $\Sigma_{i=1}^{n} |L_i^{n(k)}(x)|$. Let $L \equiv L(n, k, x_1, \ldots, x_n;\ x \text{ or } x_0) = \Sigma_{i=1}^{n} |L_i^{n(k)}(x \text{ or } x_0)|$. For x_i and *fixed* $x = x_0$ in $[-1, 1]$, one problem is to find the n x_i's to give $L_0 \equiv L_0(n, k, x_0) = \min L$. When the truncation error is negligible for any x_0 within $[-1, 1]$, a second problem is to find $x_0 = x^*$ to obtain $L^* \equiv L^*(n, k) = \min L_0 = \min \min L$. A third much simpler problem, for x_i equally spaced, $x_1 = -1, x_n = 1$, is to find $\bar{x}$ to give $\bar{L} \equiv \bar{L}(n, k) = \min L$. For lower values of n, some results were obtained on L_0 and L^* when $k = 1$, and on $\bar{L}$ when $k = 1$ and 2 by direct calculation from available tables of $L_i^{n(k)}(x)$. The relation of L_0, L^* and $\bar{L}$ to equally spaced points, Chebyshev points, Chebyshev polynomials $T_m(x)$ for $m \leqslant n - 1$, minimax solutions, and central difference formulas, considering also larger values of n, is indicated sketchily.

I. Introduction. One of the main problems in numerical differentiation is the loss in accuracy due to the size of the coefficients in the formulas that are used. Here, we are concerned with the differentiation of the n-point Lagrangian interpolation polynomial of the $(n-1)$th degree, i.e.,

$$f^{(k)}(x) = \sum_{i=1}^{n} L_i^{n(k)}(x) f(x_i) + R_n(x), \tag{1}$$

where

$$L_i^n(x) = \prod_{j=1, j\neq i}^{n} (x - x_j) \Big/ \prod_{j=1, j\neq i}^{n} (x_i - x_j), \tag{2}$$

for x and $x_i, i = 1(1)n$, within $[-1, 1]$. For a detailed discussion of the remainder

Received December 18, 1973.

AMS (MOS) subject classifications (1970). Primary 65D25; Secondary 65D05, 65G05.

Key words and phrases. Numerical differentiation, Lagrangian interpolation, optimally stable numerical differentiation, criteria for optimal stability, minimin and minimax solutions, Chebyshev points, Chebyshev polynomials, central difference formulas.

$R_n(x)$, see [1, pp. 154–162] or [2]; for optimization of $R_n(x)$ by the proper choice of x_i, see [3]. Here, $R_n(x)$ is assumed to be negligible, and we are interested in criteria to minimize $L \equiv L(n, k, x_1, \cdots, x_n; x \text{ or } x_0) = \Sigma_{i=1}^n |L_i^{n(k)}(x \text{ or } x_0)|$ by proper choice of x_i, $i = 1(1)n$. This is important when $f(x)$ is known, calculated, observed, measured, or found experimentally to a fixed number of decimals (e.g., in experimental physics, engineering, data reduction, physical chemistry, space sciences, trajectories, satellites in orbit, etc.). An explicit solution is known to the slightly related problem of finding x_i to minimize the maximum of L for variable x in $[-1, 1]$, namely $x_i = -\cos[(i-1)\pi/(n-1)]$, which is independent of k [4], [5], [6]. However, in many practical problems, for optimal stability in numerical differentiation at any particular point x, we may choose several more suitable locations of points (one of which involves a mini-min instead of mini-max), which is the subject of this present note.

II. Two Criteria for Optimality. One problem, for x fixed at x_0, is to determine $x_i \equiv x_i(x_0)$, $i = 1(1)n$, to obtain $L_0 \equiv L(n, k, x_0) = \min L$.(1) Then another problem is to determine the $x_0 = x^*$ that minimizes L_0 to $L^* \equiv L^*(n, k) = \min \min L$. Here, min min L is, of course, min L considered for the $n + 1$ variables x_0 and x_i. Questions about the uniqueness of the minimizing sets of x_i and x_0 will not be stressed here. We assume $x_0 \geqslant 0$, since for $x_0 < 0$ we change the variable to $x' = -x$. Since L^* is preferable to any other L_0, to find $f^{(k)}(x)$ by (1) for any particular $x = x_0$, the variable is shifted to $x' = x + x^* - x_0$, so that $x = x_0$ becomes $x' = x^*$, and $x = x_i - x^* + x_0$ becomes $x' = x_i \equiv x_i(x^*)$. This variable shift is permissible when $R_n(x^*)$ for the new $[-1, 1]$ interval is still negligible, which is usually the case, except near the end of the range of x. To obtain $f^{(k)}(x)$ for a succession of different x's, each of which is shifted to become x^*, requires $f(x)$ at different sets of points corresponding to $x_i \equiv x_i(x^*)$, $i = 1(1)n$, after the shift. This amount of computation is a reasonable price for the utmost in accuracy in $f^{(k)}(x)$, when $f(x)$ itself is of limited accuracy but readily available through observation, measurement or interpolation to that full limited accuracy.(2) When x_0 cannot be shifted to x^*, such as when (a) the entire range of x is too small, (b) x_0 is near or at the end of the range, or (c) a shift pushes the new interval $[-1, 1]$ to where it either includes or is too near a singularity of $f(x)$, then L_0 must suffice.

---

(1) T. J. Rivlin discovered a fundamental error in a paper of D. L. Berman [7] that gave, rather cryptically, a purportedly complete solution based upon the work of W. Markoff [8]. In several private communications, Rivlin verified the first of five parts of Berman's crucial Theorem 2 on pp. 13–14, discredited the other parts (giving also a counterexample), and subsequently stated that he was preparing for publication his own complete solution in which the x_i's cannot always be given explicitly.

(2) In connection with interpolation for $f(x)$, the number of points needed (which might lie in an interval different from $[-1, 1]$) may differ from n. Thus, in the extreme case where $f(x)$ is a critical table where no interpolation is necessary (in other words, $n = 1$ for interpolation), we still need $n > 1$ for numerical differentiation.

A somewhat simpler looking, but entirely equivalent, formulation of the L^* problem is to solve for x^* and x_i, $i = 1(1)n$, in $[-1, 1]$, where

$$(3)\qquad \sum_{i=1}^{n} A_i x_i^j = 0, \qquad j = 0(1)k-1,$$
$$= j(j-1)\cdots(j-k+1)x^{*j-k}, \quad j = k(1)n-1,$$

and

$$(3')\qquad \sum_{i=1}^{n} |A_i| = \text{minimum}.$$

In (3) and (3′), and also in (3a) and (3′a) below, $A_i \equiv L_i^{n(k)}(x^*)$.(3) Since the translation $x' = x - x^*$, $x_i' = x_i - x^*$, leaves $L_i^{n(k)}(x)$ unchanged, (3) and (3′) may be reformulated so that we always have $x'^* = 0$, and we must find x_i' and X, where x_i' is in the variable interval $[X, X+2]$ where X is in $[-2, 0]$, so that

$$(3\text{a})\qquad \sum_{i=1}^{n} A_i x_i'^j = k!, \quad j = k, \qquad j = 0(1)n-1,$$
$$= 0, \quad j \neq k,$$

and

$$(3'\text{a})\qquad \sum_{i=1}^{n} |A_i| = \text{minimum}.$$

III. Some Scattered Results. For L_0, at the endpoint $x_0 = 1$, for every n and k, $x_i = -\cos[(i-1)\pi/(n-1)]$, $i = 1(1)n$, which is independent of k, and

$$L_0 = T_{n-1}^{(k)}(1) = \overline{n-1}^2(\overline{n-1}^2 - 1^2)\cdots(\overline{n-1}^2 - \overline{k-1}^2)/1\cdot 3\cdots(2k-1).$$

Proof. Applying (1) to $T_{n-1}^{(k)}(1)$, since $|T_{n-1}(x)| \leq 1$, $T_{n-1}^{(k)}(1)$ is a lower bound for L at $x_0 = 1$, for *any* x_i, i.e., $T_{n-1}^{(k)}(1) \leq L_0$. But $T_{n-1}^{(k)}(1)$ is also an upper bound for L when $x_i = -\cos[(i-1)\pi/(n-1)]$, $i = 1(1)n$, for *any* x_0 in $[-1, 1]$, by the minimax property [4], [5], [6], i.e., $L_0 \leq L$ for $x_i = -\cos[(i-1)\pi/(n-1)]$, at $x_0 = 1, \leq T_{n-1}^{(k)}(1)$. The last two statements together imply $L_0 = T_{n-1}^{(k)}(1)$, $x_i = -\cos[(i-1)\pi/(n-1)]$, $i = 1(1)n$. Q.E.D. That $x_i = -\cos[(i-1)\pi/(n-1)]$ are also the points for optimally stable extrapolatory differentiation, as well as extrapolation, when $k \geq 0, x_0 > 1$, follows from

$$\sum_{i=1}^{n} |L_i^{n(k)}(x_0)| = \left| \sum_{i=1}^{n} (-1)^i L_i^{n(k)}(x_0) \right| = T_{n-1}^{(k)}(x_0) = L_0,$$

the last because $T_{n-1}^{(k)}(x_0)$ is a lower bound for every L.

The preceding results for x within $[1, \infty]$ are special cases of Berman's Theorem 2, part 1, [7] which states that for $x_i = -\cos[(i-1)\pi/(n-1)]$ and x_0

(3) Elsewhere A_i denotes $L_i^{n(k)}(x_0)$ for whatever x_0 is under discussion.

within any of the intervals $(-\infty, \xi_1)$, (η_j, ξ_{j+1}), $j = 1(1)n-2-k$, (η_{n-1-k}, ∞), where $L_1^{n(k)}(\eta_i) = 0$, $L_n^{n(k)}(\xi_i) = 0$, $i = 1(1)n-1-k$, we have $L = L_0 = |T_{n-1}^{(k)}(x_0)|$. From the interlacing of the ξ_j with the η_j, $\xi_j < \eta_j$, it can be shown that for $n-k$ odd, the interval $(\eta_{(n-1-k)/2}, \xi_{(n+1-k)/2})$ includes 0, so that at $x_0 = 0$, $L = L_0 = |T_{n-1}^{(k)}(0)|$. In particular, $x_i = -\cos[(i-1)\pi/(n-1)]$ gives L_0, when $k = 1$, for x_0 within $[½, 1]$ when $n = 3$, within $[0, 0.1076]$ or $[0.7743, 1]$ when $n = 4$, and within $[0.3223, 0.4446]$ or $[0.8723, 1]$ when $n = 5$, and when $k = 2$, for x_0 within $[1/3, 1]$ when $n = 4$, and within $[0, 0.1319]$ or $[0.6319, 1]$ when $n = 5$.

For L_0, at $x_0 = 0, k = 1$, a lower bound is $n - 2\,(n-1)$ for odd (even) n, since $|T'_m(0)| = m$ when m is odd. As will be shown further on, this bound (seen above to be assumed for every even n) is assumed also for $n = 3$ and 5, is approached closely for small odd $n > 5$, and to within a factor of 2½ for odd $n \sim 101$. For general k, $L_0 \geqslant (=) k!\cdot|\text{coefficient of } x^k|$ in $T_{n-2}(x)\ (T_{n-1}(x))$ for n and k of the same (opposite) parity.

For $k = 1, n = 3, 4$ and 5, we may note also the following:

For $L^*, k = 1, n = 2$: $x^* =$ any point in $[-1, 1]$, $x_1 = -1, x_2 = 1, A_1 = -½, A_2 = ½, L^* = 1$. For $L^*, k = 1, n = 3$: $x^* = 0, x_1 = -1, x_2 =$ any $\neq -1$ or 1, $x_3 = 1, A_1 = -½, A_2 = 0, A_3 = ½, L^* = 1$. That we cannot improve $L^* = 1$, for $n = 2$ or 3, is seen from $f(x) = x$, where for any choice of x_0, x_i within $[-1, 1]$,

$$1 = |f'(x_0)| = \left|\sum_{i=1}^{n} L_i^{n\prime}(x_0)x_i\right| \leqslant \sum_{i=1}^{n} |L_i^{n\prime}(x_0)|.$$

This inequality is an illustration of the following general property that gives lower bounds to L^*, namely, $L^* \geqslant \max|P_m^{(k)}(x^*)|$ of all polynomials $P_m(x)$ of degree $m \leqslant n-1$, where $|P_m(x)| \leqslant 1$ for x in $[-1, 1]$. Thus far we have used only the Chebyshev polynomials $T_m(x)$ for $P_m(x)$.

For $n = 3$, any $x_0, (x_1, x_2, x_3) = (-1, 0, 1)$, $A_1 = x_0 - ½, A_2 = -2x_0, A_3 = ½ + x_0$. When $x_0 \geqslant ½, L = 4x_0 \geqslant L_0$ must be L_0, since for $T_2(x) = 2x^2 - 1$, $T_2'(x_0) = 4x_0 \leqslant L_0$.(4) When $x_0 < ½, L = 1 + 2x_0 > 4x_0$, which tells us no more than the already known $L_0 \geqslant 1$ for x_0 in $[0, ¼]$ and $L_0 \geqslant 4x_0$ for x_0 in $[¼, ½]$.

For $n = 4, x_0 = 0, L_0 = 3$, the x_i being the Chebyshev points $-\cos[(i-1)\pi/3]$, $i = 1(1)4$, or $(-1, -½, ½, 1)$ for which the corresponding A_i are $(1/6, -4/3, 4/3, -1/6)$. That 3 is best is seen from $T_3(x) = 4x^3 - 3x$, and $|T_3'(0)| = 3$.(5) This is an illustration of where, for $x_0 = 0$, Chebyshev spacing for x_i is better than equal spacing(6) for which $L = 3.5$. However, L^* for $n = 4$ is

(4) Cf. same result in 4th preceding paragraph.

(5) Cf. same result in 5th preceding paragraph.

(6) In "equal spacing" it is always understood that $x_1 = -1$ and $x_n = 1$.

less than 3, because for equal spacing of x_i, $L = 2.16...$ for $x_0 = 0.48$ (see Schedule I). That 2.16 is within 12.5% of L_0 for $x_0 = 0.48$ follows from $L_0 \geqslant T_2'(0.48) = 1.92$. From $T_2(x)$ and $T_3(x)$ it is also apparent that any improvement over 2.16 for L^* must take place *before* $T_2'(x_0) = 4x_0 = 2.16$ and *after* $|T_3'(x_0)| = |3 - 12x_0^2| = 2.16$, or (approximately) $0.265 \leqslant x_0 \leqslant 0.54$.

For $n = 5, x_0 = 0, L_0 = 3$, which is attained for equally spaced x_i, i.e., $(-1, -½, 0, ½, 1)$, and $A_i = (1/6, -4/3, 0, 4/3, -1/6)$, and that no improvement is possible is seen again from $|T_3'(0)| = 3$. Here Chebyshev spacing, $x_i = -\cos[(i-1)\pi/4], i = 1(1)5$, for $x_0 = 0$, gives the appreciably larger $L = 3.83$; trying the other Chebyshev points $x_i = -\cos[(2i-1)\pi/10], i = 1(1)5$, which do not include the endpoints of $[-1, 1]$, we get, surprisingly enough, $L = 3.40$.

IV. First Derivative at Midpoint, n **Large.** Around $x_0 = 1$, as n increases, L becomes prohibitively large for x_i equally spaced. By comparison, when the x_i are either of the Chebyshev points $-\cos[(i-1)\pi/(n-1)]$ or $-\cos[(2i-1)\pi/2n]$, L is tremendously reduced. Thus, for $n = 100, k = 1$, the reduction is from the neighborhood of 10^{28} or more, to around 10^4. We have just noted, in the preceding paragraph, for $n = 5, k = 1, x_0 = 0$, that Chebyshev spacing for x_i is not quite so good as equal spacing. Then for very large odd n, say, $n = 101$, for which Chebyshev spacing is so vastly better at the endpoint, it is also of interest to make a similar comparison for $k = 1$, at $x_0 = 0$. We calculate L by finding $L_i^{101\prime}(0)$ as the coefficient of x in $L_i^{101}(x)$, as given in (2).

(a) Equal spacing, $x_i = -1 + (i-1)/50$: Taking into account the oddness of $\Pi_{i=1}^{101}(x - x_j)$, and $L_{102-i}^{101\prime}(0) = -L_i^{101\prime}(0)$, we find that $L = 2 \times 50 \times 50!^2 \times \Sigma_{i=1}^{50} 1/i(i+50)!(50-i)!$, which is around 225. (See also VI, 2nd paragraph.)

(b) Chebyshev spacing, $x_i = -\cos[(i-1)\pi/100]$: Here

$$\left|\prod_{j=1,j\neq i}^{101} (x - x_i)\right| = |(x^2 - 1)U_{99}(x)/2^{99}(x - x_i)|,$$

where $U_n(x) = \sin(n+1)\theta/\sin\theta, x = \cos\theta$, is the Chebyshev polynomial of the second kind [9, p. 156], and $|1/\Pi_{j=1,j\neq i}^{101}(x_i - x_j)| = 2^{99}/100$ for $i \neq 1, 101$, $= 2^{98}/100$ for $i = 1, 101$ [9, p. 157]. The coefficient of x in $U_{99}(x)$ is -100, so that after division and summation, noting that $L_{51}^{101\prime}(0) = 0$, we get

$$L = 2 \cdot 100 \cdot \frac{2^{99}}{100} \cdot \frac{1}{2^{99}} \sum_{i=1}^{50}{}' 1/\cos[(i-1)\pi/100]$$

($i = 1$ term in Σ' is halved) $= 2\Sigma_{i=1}^{\prime 50} \sec[(i-1)\pi/100]$, which is close to 300.

(c) Chebyshev spacing, $x_i = -\cos[(2i-1)\pi/202]$: The absolute value of the coefficient of x in the numerator of (2) is $101/2^{100}|x_i|$, and

$$\left| 1 \Big/ \prod_{j=1, j \neq i}^{101} (x_i - x_j) \right| = 2^{100} \sin[(2i-1)\pi/202]/101,$$

so that $L = 2\Sigma_{i=1}^{50} \tan[(2i-1)\pi/202]$, which is approximately 260.

Thus, neither of the Chebyshev spacings is as good as equal spacing, for which $L \sim 225$, if not actually L_0, is at worst less than 2½ times $L_0 \geqslant 99 = L_0$ for $n = 100$. Comparison of this $L \sim 225 \geqslant L^*$ with the Chebyshev point minimax of 10^4 shows that min min/min max $< 1/44$.(7)

V. **Optimality for Equal Spacing, with Schedules.** A drastic but practical simplification of the L^* problem, which reduces the number of variables from $n + 1$ to just one, is to specify the x_i, $i = 1(1)n$, to be equally spaced, and to find the point $x = \bar{x}$ giving $\min L = \bar{L}$. There is evidence throughout this article, for both smaller and larger n, to indicate that $\bar{L}$ may not be too far from L^* (e.g., in the preceding discussion for $n = 101, k = 1$, at $x_0 = 0$, where L cannot be reduced by more than 56% even by varying all 101 points x_i, but where the shift of x_0 from endpoint to center reduces L, substantially for Chebyshev spacing, but spectacularly for equal spacing of the x_i's). Answers to the $\bar{L}$ problem, for $k = 1$ and 2, for the lower values of n, were found readily with the aid of two published tables which give (in a slightly different notation) $L_i^{n(k)}(x)$ as functions of $p = (x - x_{[(n+1)/2]})/h$(8) and $h =$ the tabular interval $x_{i+1} - x_i$ [10], [11].

In Schedule I, we give for $k = 1$ and $n = 3(1)7, \bar{x}, L_i^{n\prime}(\bar{x})$ for $x_i = -1 + 2(i-1)/(n-1), i = 1(1)n, \bar{L}$, and for comparison, $L_1 =$ the largest L, which is at $x = 1$. These values were obtained by a direct calculation from [10], $\bar{x}$ given exactly (approximately) for n odd (even). The $L_i^{n\prime}(\bar{x})$ (as well as $L_i^{n\prime\prime}(\bar{x})$ in Schedule II) is given exactly for the argument $\bar{x}$, even where that $\bar{x}$ is an approximate value for the true $\bar{x}$.

It is of interest to note in Schedule I that $\bar{x}$ is at 0 when n is odd, but considerably away from 0 when n is even. In fact, at $x = 0, L$ for $n = 4$ and 6 is 3.5 and 6.21, respectively, which is appreciably larger than $\bar{L}$. Since $n = 4$ is the least n for which L^* is not yet known, an attempt was made (just by hand calculation) to improve the $\bar{L} = 2.16$ by varying the equally spaced locations of the x_i's, but without any success. For $n = 5$, if there should happen to be an $L^* <$

(7) A similar comparison, $n = 101, x_0 = 0, x_i$ equally spaced, but for $k = 2$, for which L is approximately $2.2 \cdot 10^4$, may be made with the Chebyshev minimax of $10^4(10^4 - 1)/3$. But knowing here that for $x_i = -\cos[(i-1)\pi/100], L = L_0 = |T''_{100}(0)| = 10^4$, we may infer that min min/min max $< (1/3) \cdot 10^{-3}$.

(8) Just here, [$\cdots$] denotes the nearest integer.

Schedule I

n	$\bar{x}$	i	x_i	$L_i^{n'}(\bar{x})$	$\bar{L}$	L_1
3	0	1	−1	−1/2	1	4
		2	0	0		
		3	1	1/2		
4	0.48	1	−1	0.2137	2.16	10
		2	−1/3	−1.0611		
		3	1/3	−0.0189		
		4	1	0.8663		
5	0	1	−1	1/6	3	21.33...
		2	−1/2	−4/3		
		3	0	0		
		4	1/2	4/3		
		5	1	−1/6		
6	0.252	1	−1	−3.74792 805/48	4.494	42.66...
		2	−3/5	26.97658 025/48		
		3	−1/5	−95.84104 050/48		
		4	1/5	−1.25707 950/48		
		5	3/5	80.87059 975/48		
		6	1	−7.00113 195/48		
7	0	1	−1	−1/20	5.5	83.2
		2	−2/3	9/20		
		3	−1/3	−9/4		
		4	0	0		
		5	1/3	9/4		
		6	2/3	−9/20		
		7	1	1/20		

$\bar{L} = 3$, it would be for x_i unequally spaced, and at $x^* \neq 0$ because (as shown before) L_0, at $x_0 = 0$, is also 3.

In Schedule II, we give, for $k = 2$ and $n = 4(1)9, \bar{x}, L_i^{n''}(\bar{x}), \bar{L}$ and L_1, all readily calculated from [11]. The results for $n = 4$ are exact (and infinite in number), while $\bar{x}$ for $n = 5(1)9$ is given approximately, more roughly for $n = 8$ and 9, where the tabular interval for p in [11] is 0.1 instead of 0.01 for $n = 5(1)7$. There is no problem for $n = 3$, since for any x_0, $L_1^{3''}(x_0) = L_3^{3''}(x_0) = 1, L_2^{3''}(x_0) = -2$, and $L = \bar{L} = 4$ $(= L_0 = L^*$ from $T_2''(x) = 4)$.

Schedule II

n	$\bar{x}$	i	x_i	$L_i^{n''}(\bar{x})$	$\bar{L}$	L_1
4	any x_0 in [0, 1/9]	1	−1	$9(1-3x_0)/8$	4.5	27
		2	−1/3	$9(9x_0-1)/8$		
		3	1/3	$9(-9x_0-1)/8$		
		4	1	$9(3x_0+1)/8$		
5	0.455	1	−1	2(−0.7457)/3	10.9828	106.66...
		2	−1/2	2(3.5228)/3		
		3	0	2(−0.0942)/3		
		4	1/2	2(−7.3972)/3		
		5	1	2(4.7143)/3		
6	0.064	1	−1	−5.8837/12	19.8325	333.33...
		2	−3/5	40.2535/12		
		3	−1/5	−1.6770/12		
		4	1/5	−102.6530/12		
		5	3/5	78.7415/12		
		6	1	−8.7813/12		
7	0.27	1	−1	0.28201 94537 5	32.296	918.4
		2	−2/3	−2.10932 82225 0		
		3	−1/3	6.58379 93062 5		
		4	0	−0.17230 40750 0		
		5	1/3	−13.12289 31937 5		
		6	2/3	9.28202 57775 0		
		7	1	−0.74331 90462 5		
8	1/35	1	−1	49(0.04469 2)/9	50.105	2348
		2	−5/7	49(−0.41594 4)/9		
		3	−3/7	49(1.79863 2)/9		
		4	−1/7	49(−0.72572 0)/9		
		5	1/7	49(−2.92878 0)/9		
		6	3/7	49(2.70496 8)/9		
		7	5/7	49(−0.53105 6)/9		
		8	1	49(0.05320 8)/9		
9	1/5	1	−1	−6.88605 44/63	71.33	5721
		2	−3/4	66.40312 32/63		
		3	−1/2	−288.63313 92/63		
		4	−1/4	710.85629 44/63		
		5	0	179.69011 20/63		
		6	1/4	−1775.55087 36/63		
		7	1/2	1275.79002 88/63		
		8	3/4	−175.90394 88/63		
		9	1	14.23445 76/63		

We may note, from Schedule II, that for $n = 4, \bar{L} = 4\frac{1}{2}$ cannot be too far from $L^* \geqslant 4$. For $n = 5, \bar{L} = 10.9828$ is very close to L_0 for $x_0 = \bar{x} = 0.455$, since $L_0 \geqslant T_3''(0.455) = 10.92$. Also, for $L^* \leqslant \bar{L}$, the x^* must lie in the interval $[0.228, 0.458]$, which is apparent from $T_3''(x) = 24x > 10.9828$ when $x > 0.458$ and $|T_4''(x)| = |96x^2 - 16| > 10.9828$ when $x < 0.228$. Comparing $\bar{x}$ for $k = 1$ with $\bar{x}$ for $k = 2$, the schedules show the latter close to 0, for n even (not exactly at 0 as for $k = 1, n$ odd), and close to $\bar{x}$ for $k = 1$ in the $(n - 1)$-point formula, for n odd.

VI. More Points, Higher Derivatives. To find an approximate $\bar{x}$ and $\bar{L}$ for k or n outside the range of Schedules I and II, we may refer to the tables in [12] which give the exact values of $L_i^{n(k)}(x_j)$ (i.e., only at tabular points), for $k = 1(1)n - 1$, $n = 3(1)7$, and $k = 1(1)4$, $n = 9, 11$. The smallest $L \sim \bar{L}$ is not at the most central value of x_i for these values of k and n in [12] which are not included in Schedules I and II: $k = 4, n = 7, \bar{x} \sim x_5 = 1/3; k = 4, n = 9, \bar{x} \sim x_6 = 1/4; k = 2, n = 11, \bar{x} \sim x_8 = 2/5; k = 4, n = 11, \bar{x} \sim x_7 = 1/5$.

It is interesting to note from [12] that for $k = 1, n = 9$ and 11, $x_0 = 0$, we obtain $L = 8.33$ and 11.42, which are within 20% and 27% of $L_0 \geqslant |T_7'(0)| = 7$ and $T_9'(0) = 9$ respectively. For odd $n = 2m + 1, k = 1, x_0 = 0$, it may also be shown from (5) below and [13] that $L = m\Sigma_{i=1}^m 1/i$, so that

$$L/(n - 2) = (m/(2m - 1)) \sum_{i=1}^{m} 1/i \geqslant L/L_0.$$

From [12], for $n = 11, k = 2(4), L$ is around 171 $(2.48 \cdot 10^4)$ at $x_0 = 0$, and down to around 156 $(1.85 \cdot 10^4)$ at $x_0 = 1/5$, considerably better than the minimax $L = 3300$ $(8.24 \cdot 10^5)$ for $x_i = -\cos[(i - 1)\pi/10], i = 1(1)11$; but since at $x_0 = 0$ it is known that $L_0 = |L_{10}''(0)| = 100$ $(|L_{10}^{(4)}(0)| = 0.96 \cdot 10^4)$, min min/min max may be expected to be $< 1/33(85)$.

VII. Central Difference Formulas for Large n. Even though in some preceding examples, for various n, and the x_i equally spaced, the L would not have been improved appreciably, even if we had obtained $L = L_0$ at the same point x_0 by changing all the x_i, still the drop from L to L^*, by varying x_0 with the x_i, could be considerably greater. However, at present, pending further specific information on L_0 and L^*, and the accompanying x_i and $L_i^{n(k)}(x_0)$, especially for large n, for many practical problems we might choose $x_0 = 0, x_i$ equally spaced, and find that the limits to the tolerance in L would not be exceeded. In employing $x_0 = 0$, x_i equally spaced, for $n > 11$, computing or using the $L_i^{n(k)}(0)$ becomes cumbersome, and it is more convenient to choose an odd $n = 2m + 1$ and employ numerical differentiation formulas in terms of central differences δ_0^{2r}, for k even, and mean central differences $\mu\delta_0^{2r-1}$, for k odd, as far as the term $r = m$ [13]. These formulas have the advantages of consisting of terms with small factors and varying with n

only in their end terms. They are given by

$$(4)\qquad f^{(k)}(x_0) \cong \frac{1}{h^k} \sum_{r=(k+1)/2}^{m} A_{2r-1}^{k}\,\mu\delta_0^{2r-1}, \qquad k \text{ odd},$$
$$\cong \frac{1}{h^k} \sum_{r=k/2}^{m} A_{2r}^{k}\,\delta_0^{2r}, \qquad k \text{ even},$$

where $h = x_{i+1} - x_i$. In our notation, after adjusting the range of x_i to $[-1, 1]$, x_0 in (4) is the central argument $x_{m+1} = 0$, and the right member of (4) is identical with the right member of (1) without $R_n(x)$, for $x = 0$. From (4), we find

$$(5)\qquad L = \frac{1}{h^k} \sum_{r=(k+1)/2}^{m} |A_{2r-1}^{k}| \cdot {}_{2r-1}C_r, \qquad k \text{ odd},$$
$$= \frac{1}{h^k} \sum_{r=k/2}^{m} |A_{2r}^{k}| \cdot 2^{2r}, \qquad k \text{ even}.$$

To prove (5), we obtain the coefficients of $f(x_i)$ on the right side of (4), using the coefficients of $f(x_i)$ in $\mu\delta_0^{2r-1}$ and δ_0^{2r}, and taking into account the alternation with r in the signs of A_{2r-1}^k and A_{2r}^k.

In (4) and (5), the formulas for odd k may be expected to give an L that is closer to L^* than for even k (cf. Schedules I and II, and [12]). For even k, it appears that a better L than that from (4) and (5) is had by differentiating Stirling's interpolation formula [1, pp. 67–68] and setting $x = 1.8/(n-1)$ instead of 0, to obtain a formula for $f^{(k)}(1.8/(n-1))$ in terms of both $\mu\delta_0^{2r-1}$ and δ_0^{2r}.

941 Washington Avenue
Brooklyn, New York 11225

1. L. M. MILNE-THOMSON, *Calculus of Finite Differences,* Macmillan, London, 1933.

2. J. F. STEFFENSEN, *Interpolation*, Williams and Wilkins, Baltimore, Md., 1927, pp. 60–68.

3. H. E. SALZER, "Optimal points for numerical differentiation," *Numer. Math.,* v. 2, 1960, pp. 214–227. MR 22 # 658.

4. D. L. BERMAN, "The solution of an extremal problem of the theory of interpolation," *Dokl. Akad. Nauk SSSR,* v. 87, 1952, pp. 167–170. (Russian) MR **14**, 542.

5. T. J. RIVLIN, *An Introduction to the Approximation of Functions,* Blaisdell, Waltham, Mass., 1969, pp. 117–118. MR **40** #3126.

6. R. J. DUFFIN & A. C. SCHAEFFER, "A refinement of an inequality of the brothers Markoff," *Trans. Amer. Math. Soc.,* v. 50, 1941, pp. 517–528. MR **3**, 235.

7. D. L. BERMAN, "The solution of an extremal problem of the theory of interpolation," *Izv. Vysš. Učebn. Zaved. Matematika* (43), v. 6, 1964, pp. 10–14. (Russian) MR **30** #632.

8. W. MARKOFF, "*Über* Polynome, die in einem gegebenen Intervalle möglichst wenig von Null abweichen," *Math. Ann.,* v. 77, 1916, pp. 213–258 (translated from the Russian, St. Petersburg Acad., 1892).

9. H. E. SALZER, "Lagrangian interpolation at the Chebyshev points $x_{n,\nu} \equiv \cos(\nu\pi/n)$, $\nu = 0(1)n$; some unnoted advantages," *Comput. J.,* v. 15, 1972, pp. 156–159; ibid., v. 16, 1973, pp. 190, 382. MR **47** #4414.

10. H. E. SALZER, *Table of Coefficients for Obtaining the First Derivative Without Differences,* Nat. Bur. Standards, Washington, D. C., Appl. Math. Ser., no. 2, 1948, 20 pp. MR **10**, 69.

11. H. E. SALZER & P. T. ROBERSON, *Table of Coefficients for Obtaining the Second Derivative Without Differences,* Convair-Astronautics, San Diego, Calif., 1957, 25 pp. MR 19, 689.

12. W. G. BICKLEY, "Formulae for numerical differentiation," *Math. Gaz.,* v. 25, 1941, pp. 19–27. MR **2**, 240.

13. H. E. SALZER, "Coefficients for numerical differentiation with central differences," *J. Math. Phys. Mass. Inst. Tech.,* v. 22, 1943, pp. 115–135. MR **5**, 50.