

## Optimal Numerical Differentiation Using Three Function Evaluations

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**Abstract.** Approximation of  $f'(x)$  by a difference quotient of the form

$$h^{-1}[a_1 f(x + b_1 h) + a_2 f(x + b_2 h) + a_3 f(x + b_3 h)]$$

is found to be optimized for a wide class of real-valued functions by the surprisingly asymmetric choice of  $\mathbf{b} = (b_1, b_2, b_3) = (1/\sqrt{3} - 1, 1/\sqrt{3}, 1/\sqrt{3} + 1)$ . The nearly optimal choice of  $\mathbf{b} = (-2, 3, 6)$  is also discussed.

**1. Introduction.** The problem of best approximating the derivative of a function at a single point using two values of the function is "best" solved by using the difference quotient

$$(1) \quad d_0(h) = \frac{f(x + \frac{1}{2}h) - f(x - \frac{1}{2}h)}{h}.$$

We consider the same problem using three values of the function and arrive at three different solutions by interpreting "best" in five different ways. Our best difference quotients are

$$(2) \quad d_1(h) = \frac{(3 - 2\sqrt{3})f(x + (\frac{1}{\sqrt{3}} + 1)h) + 4\sqrt{3}f(x + \frac{1}{\sqrt{3}}h) - (3 + 2\sqrt{3})f(x + (\frac{1}{\sqrt{3}} - 1)h)}{6h},$$

$$(3) \quad d_2(h) = \frac{f(x + h) + \omega^2 f(x + \omega h) + \omega f(x + \omega^2 h)}{3h},$$

where  $\omega = -\frac{1}{2} + \sqrt{3}i/2$  and  $\omega^2 = -\frac{1}{2} - \sqrt{3}i/2$  are the cube roots of 1, and

$$(4) \quad d_3(h) = \frac{32f(x + 3h) - 27f(x - 2h) - 5f(x + 6h)}{120h}.$$

Section 3 below was motivated by the kind suggestion of J. Lyness.

**2. Minimum Truncation Error.** Whenever we write  $f$ , we will mean either a complex-valued function of a complex variable or a real-valued function of a real variable. In the former case we assume that  $f$  is analytic near  $x$  and in the latter case that  $f$  is five times differentiable at  $x$ . The point  $x$  will be fixed and the variable  $h$  will be small. Our assumptions are chosen to guarantee (i) that  $f$  have at  $x$  a Taylor expansion to order  $h^4$  with error  $O(|h|^5)$  and (ii) that there be a bound for the modulus of  $f''''$  near  $x$ .

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Consider the general three-point difference quotient

$$(5) \quad d(h) = h^{-1} \sum_{i=1}^3 a_i f(x + b_i h) = d(\mathbf{a}, \mathbf{b})(h).$$

Substituting Taylor's theorem,

$$f(x + b_i h) = \sum_{j=0}^4 \frac{f^{(j)}(x)}{j!} h^j b_i^j + \frac{f^{(5)}(\xi_i)}{5!} h^5 b_i^5,$$

into (5) and interchanging the order of summation gives

$$(6) \quad \begin{cases} d(h) = \sum_{j=0}^4 c_j \frac{f^{(j)}(x)}{j!} h^{j-1} + O(h^4), \\ c_j = \sum_{i=1}^3 a_i b_i^j, \quad j = 0, 1, 2, 3, 4. \end{cases}$$

For  $d(h) \rightarrow f'(x)$  as  $h \rightarrow 0$ , we must have  $c_0 = 0$  and  $c_1 = 1$ . This motivates our first definition.

*Definition 1.* A three-point rule for the first derivative is a difference quotient  $d(\mathbf{a}, \mathbf{b})(h)$  of the form (5) where  $c_0 = \sum a_i = 0$  and  $c_1 = \sum a_i b_i = 1$ .

*Definition 2.* A three-point rule for the first derivative is of degree  $k$  if and only if  $d(\mathbf{a}, \mathbf{b})(h) = f'(0)$  for every polynomial  $f$  of degree  $k$ .

**LEMMA 1.** *A necessary and sufficient condition for the three-point rule to be of degree 3 is*

$$(7) \quad \begin{cases} c_0 = \sum a_i = 0, \\ c_1 = \sum a_i b_i = 1, \\ c_2 = \sum a_i b_i^2 = 0, \\ c_3 = \sum a_i b_i^3 = 0. \end{cases}$$

The proof of this is immediate from (6) above.

**LEMMA 2.** *No three-point rule is of degree 4. For a three-point rule to be degree 3, we must have all  $b_i$  distinct.*

*Proof.* For a rule to be of degree 4 would require  $c_2 = c_3 = c_4 = 0$ . Write this as a matrix equation

$$B\mathbf{a} = \begin{pmatrix} b_1^2 & b_2^2 & b_3^2 \\ b_1^3 & b_2^3 & b_3^3 \\ b_1^4 & b_2^4 & b_3^4 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}.$$

If all  $b_i \neq 0$ , then the Vandermonde-like matrix  $B$  is nonsingular, so  $\mathbf{a} = \mathbf{0}$ , contrary to  $c_1 = 1$ . If, say,  $b_3 = 0$ , the three equations  $c_2 = c_3 = 0$ ,  $c_1 = 1$  lead quickly to a similar contradiction.

Similarly, if, say,  $b_2 = b_3$ , we may as well combine  $a_2$  and  $a_3$ , which implies we are dealing with a two-point rule. As above, if both  $b_i \neq 0$ , the two equations  $c_2 = c_3 = 0$  force  $\mathbf{a}$  to be zero, contrary to  $c_1 = 1$ . The case of  $b_2 = b_3 = 0$  is treated similarly. Thus, for a three-point rule to be of degree 3, we must have all  $b_i$  distinct.

LEMMA 3. *The three-point rule  $d$  is of degree 3 if and only if*

$$(8) \quad b_1 b_2 + b_1 b_3 + b_2 b_3 = 0.$$

*Proof.* The first three equations in (7),  $c_0 = c_2 = 0$ ,  $c_1 = 1$ , may be written as a matrix equation

$$B\mathbf{a} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix},$$

where the Vandermonde matrix  $B$  is easily inverted. Substitute the result of this,

$$\mathbf{a} = [(b_2 - b_1)(b_3 - b_1)(b_3 - b_2)]^{-1}(b_2^2 - b_3^2, b_3^2 - b_1^2, b_1^2 - b_2^2),$$

into  $c_3 = 0$  to obtain (8).

*Definition 3.* A three-point rule  $d(\mathbf{a}, \mathbf{b})$  is said to be normalized if

$$\min\{|b_1 - b_2|, |b_1 - b_3|, |b_2 - b_3|\} = 1.$$

*Motivation for Definition 3.* The mapping  $h \rightarrow ch$  for a nonzero constant  $c$ , which may also be thought of as mapping  $(\mathbf{a}, \mathbf{b}) \rightarrow (c^{-1}\mathbf{a}, c\mathbf{b})$  while leaving  $h$  fixed, obviously does not change anything of substance. In other words, the set of three-point rules  $d(\mathbf{a}, \mathbf{b})(h)$  partitions into equivalence classes with  $d(\mathbf{a}, \mathbf{b}) \sim d(\mathbf{a}', \mathbf{b}')$  if there is a constant  $c$  such that  $\mathbf{a}' = c^{-1}\mathbf{a}$  and  $\mathbf{b}' = c\mathbf{b}$ . The quantity  $c_4(\mathbf{a}, \mathbf{b})$  is not a class invariant, for if  $d(\mathbf{a}, \mathbf{b}) \sim d(\mathbf{a}', \mathbf{b}')$ , where  $(\mathbf{a}', \mathbf{b}') = (\varepsilon^{-1}\mathbf{a}, \varepsilon\mathbf{b})$  with  $0 < \varepsilon < 1$ , we have

$$(9) \quad |c_4(\mathbf{a}', \mathbf{b}')| = \left| \sum (\varepsilon^{-1}a_i)(\varepsilon b_i)^4 \right| = \varepsilon^3 |c_4(\mathbf{a}, \mathbf{b})| < |c_4(\mathbf{a}, \mathbf{b})|.$$

By picking  $\varepsilon$  very small, we can find arbitrarily small  $c_4$  without really changing anything. Some normalization is required to keep the vector  $\mathbf{b}$  from collapsing to  $\mathbf{0}$ .

In difference quotient (1) or in the standard difference quotient  $(f(x+h) - f(x))/h$ , a normalization has been achieved by expressing the error in powers of the distance between the two arguments. Set

$$\delta = \min\{|b_1 - b_2|, |b_1 - b_3|, |b_2 - b_3|\}$$

and rewrite the dominant error term in (6) as

$$(10) \quad c_4 \frac{f^{(4)}(x)}{4!} h^3 = \left( \frac{c_4}{\delta^3} \right) \frac{f^{(4)}(x)}{4!} (\delta h)^3 = G \frac{f^{(4)}(x)}{4!} (\delta h)^3.$$

A simple calculation as in (9) above shows that  $G = G(\mathbf{a}, \mathbf{b})$  is constant on each equivalence class.

LEMMA 4. *All three-point rules of degree 3 are of the form*

$$(11) \quad d(t) = \frac{t^3(t+2)f(x+(1+t)h) - (1+2t)f(x+t(1+t)h) - (t+1)^2(t^2-1)f(x-th)}{t(2t+1)(t+2)(t^2-1)h},$$

for some value of  $t$ , or are obtained from (11) by a transformation  $(\mathbf{a}, \mathbf{b}) \rightarrow (c^{-1}\mathbf{a}, c\mathbf{b})$ .

*Proof.* Select representatives from each equivalence class by setting  $b_1 = 1$ . Let  $t = b_2$ . From (8),  $b_3 = -t/(t+1)$ . Clear fractions by sending  $(\mathbf{a}, \mathbf{b}) \rightarrow ((1/(t+1))\mathbf{a}, (t+1)\mathbf{b})$ . Our representative quotient becomes (11).

**THEOREM 1.** *Let  $d$  be a normalized three-point rule of degree 3. Fix  $h$  and restrict  $\mathbf{a}$  and  $\mathbf{b}$  to be real. Then truncation error is minimized when  $d = d_1$ . (See Eq. (2).) This minimizing rule is unique up to the transformation  $(\mathbf{a}, \mathbf{b}) \rightarrow (-\mathbf{a}, -\mathbf{b})$ .*

*Proof.* Let  $d'(\mathbf{a}', \mathbf{b}')$  be any normalized three-point rule of degree 3. By Lemma 1, we have  $c_2(\mathbf{a}', \mathbf{b}') = c_3(\mathbf{a}', \mathbf{b}') = 0$ , so to minimize truncation error we must minimize  $|c_4(\mathbf{a}', \mathbf{b}')|$ . By Lemma 4, there is a real number  $t$  and an equivalent three-point rule  $d(t) = d(\mathbf{a}(t), \mathbf{b}(t))$  of the form (11). Since

$$|c_4(\mathbf{a}', \mathbf{b}')| = |c_4(\mathbf{a}', \mathbf{b}')/1^3| = |G(\mathbf{a}', \mathbf{b}')| = |G(\mathbf{a}, \mathbf{b})| = |c_4(\mathbf{a}, \mathbf{b})|/\delta^3,$$

where  $\delta = \min_{i \neq j} \{|b_i - b_j|\}$  (see (10)), we see that we must minimize  $|G(t)| = |c_4(\mathbf{a}(t), \mathbf{b}(t))|/\delta(\mathbf{b}(t))^3$  as  $t$  varies over  $\mathbf{R}$ .

Substituting the values of  $\mathbf{a}(t)$  and  $\mathbf{b}(t)$ , as given in (11), into  $|c_4(\mathbf{a}, \mathbf{b})|$  reduces our problem to that of minimizing

$$(12) \quad |G(t)| = \frac{|t^2(t + 1)|^2}{\min\{|1 - t^2|, |2t + 1|, |t(t + 2)|\}^3} = \frac{|t^2(t + 1)|^2}{\delta(t)^3}.$$

Since  $t$  is real, we have

$$\delta(t) = \begin{cases} |t^2 - 1|, & -(\sqrt{3} + 1)/2 < t < -\sqrt{3} + 1, (\sqrt{3} - 1)/2 < t < \sqrt{3} + 1, \\ |t^2 + 2t|, & -(\sqrt{3} + 2) < t < -(\sqrt{3} + 1)/2, \sqrt{3} - 2 < t < (\sqrt{3} - 1)/2, \\ |2t + 1|, & -\infty < t < -(\sqrt{3} + 2), -\sqrt{3} + 1 < t < \sqrt{3} - 2, \sqrt{3} + 1 < t < \infty. \end{cases}$$

Substituting this into (12) and using the methods of elementary differential calculus on each interval yields that

$$\min_{t \in \mathbf{R}} |G(t)| = \frac{2}{9} \sqrt{3}$$

and that this minimum occurs at  $t = 1 + \sqrt{3}, 1 - \sqrt{3}, \frac{1}{2}(\sqrt{3} - 1), \frac{1}{2}(-\sqrt{3} - 1), \sqrt{3} - 2$ , and  $-\sqrt{3} - 2$ . All six values of  $t$  give equivalent difference quotients (the corresponding  $\mathbf{b}$  vectors are scalar multiples of one another). Normalizing the difference quotient corresponding to  $t = \frac{1}{2}(\sqrt{3} - 1)$  by sending  $(\mathbf{a}, \mathbf{b}) \rightarrow ((\sqrt{3}/2)\mathbf{a}, (2/\sqrt{3})\mathbf{b})$  produces difference quotient  $d_1$  (see (2)) as the unique (up to  $(\mathbf{a}, \mathbf{b}) \rightarrow (-\mathbf{a}, -\mathbf{b})$ ) normalized real three-point rule minimizing truncation error.

**THEOREM 2.** *Let  $d$  be a normalized three-point rule of degree 3. Fix  $h$  but allow all variables and functions to be complex-valued. Then truncation error is minimized when  $d = d_2$ . (See Eq. (3).) This minimizing rule is unique up to the transformations  $(\mathbf{a}, \mathbf{b}) \rightarrow (e^{-i\varphi}\mathbf{a}, e^{i\varphi}\mathbf{b})$ ,  $0 < \varphi < 2\pi$ .*

*Proof.* As in the proof of Theorem 1, we must minimize the function  $|G(t)|$  given in (12). Since  $t$  may be complex,

$$(13) \quad \delta(t) = \begin{cases} |t^2 - 1| & \text{on } A_1, \\ |t^2 + 2t| & \text{on } A_2, \\ |2t + 1| & \text{on } A_3, \end{cases}$$

where  $A_1$  is the union of the region enclosed by  $C_1 \cup C_3$  with the region enclosed by  $C_2 \cup C_4$ ,  $A_2$  is the reflection of  $A_1$  in the line  $\operatorname{Re} t = -\frac{1}{2}$ , and  $A_3 = \mathbb{C} - (A_1 \cup A_2)$ , where

$$C_1 = \left\{ -\frac{1}{2} + \frac{\sqrt{3}}{2} e^{i\theta}, 0 \leq |\theta| < \frac{\pi}{2} \right\},$$

$$C_2 = \left\{ -\frac{1}{2} + \frac{\sqrt{3}}{2} e^{i\theta}, \frac{\pi}{2} < |\theta| < \pi \right\},$$

$$C_3 = \left\{ 1 + \sqrt{3} e^{i\theta}, 0 \leq |\theta| < \frac{5}{6}\pi \right\},$$

$$C_4 = \left\{ 1 + \sqrt{3} e^{i\theta}, \frac{5}{6}\pi < |\theta| < \pi \right\}.$$

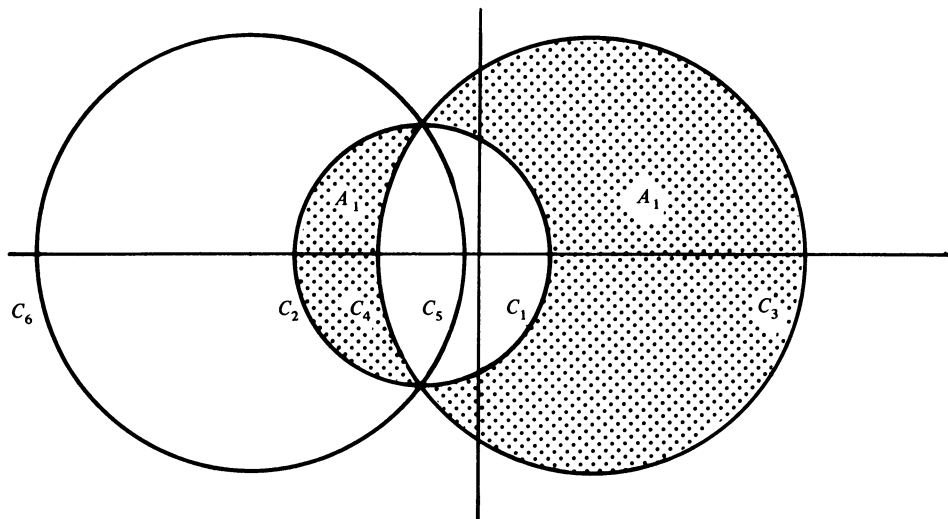


FIGURE 1

The shaded area in Figure 1 is  $A_1$ . Substitute (13) into (12), use the maximum modulus theorem on  $(G(t))^{-1}$  to see that the minimum of  $G$  must occur on one of the three circles of Figure 1, and use the method of elementary calculus on each circle, treating  $G$  as the appropriate function of  $\theta$  on each  $C_i$ . The result is

$$\min_{t \in \mathbb{C}} |G(t)| = \frac{1}{9} \sqrt{3}$$

and that the minimum occurs at  $t = \omega$  and  $\omega^2$ . Again, the corresponding difference quotients are equivalent; in fact, both are equivalent to difference quotient  $d_2$  (see (3)). Notice that, for any nonzero complex constant  $c = \rho e^{i\varphi}$ , the mapping  $(\mathbf{a}, \mathbf{b}) \rightarrow (c^{-1}\mathbf{a}, c\mathbf{b})$ , gives an equivalent best complex three-point rule minimizing truncation error. Thus the “obvious” best three-point rule here is any one obtained by letting  $\mathbf{b}$  be the three vertices of any equilateral triangle centered at  $x$ . (The word “obvious” is in quotes since the corresponding symmetric choice was not the best one in the real case above.)

### 3. Roundoff Error.

*Motivation for Theorem 3.* In the previous section, evaluations were assumed to be exact. Here we assume that each computation of the function  $f$  may be in error

by as much as  $\pm \epsilon$  where  $\epsilon$  is a small fixed positive quantity. From (5), we see that this generates a roundoff error bounded by

$$E_R = \frac{(|a_1| + |a_2| + |a_3|)\epsilon}{h} = \frac{A\epsilon}{h}.$$

Fix a difference quotient satisfying (7). From (6) and (7), we see that the dominant term in the truncation error is  $c_4 f^{(4)}(x)(4!)^{-1}h^3$  which is dominated by

$$(14) \quad E_T = \frac{|c_4|f_4h^3}{4!},$$

where  $f_4 = \sup\{|f^{(4)}(y)| : y \text{ is near } x\}$ . Define the overall error  $E$  by  $E = E_T + E_R$ . Elementary calculus shows the  $h$  which makes  $E$  smallest to be given by

$$(15) \quad \begin{cases} h = \left(\frac{8A\epsilon}{|c_4|f_4}\right)^{1/4}, & \text{for which } h \text{ we have} \\ E = \frac{2^{5/4}}{3}(A^3|c_4|)^{1/4}f_4^{1/4}\epsilon^{3/4}. \end{cases}$$

**THEOREM 3.** *Let  $d$  be a normalized three-point rule of degree 3. Fix  $h$  and restrict  $\mathbf{a}$  and  $\mathbf{b}$  to be real. Then overall error is minimized when  $d = d_1$ . (See Eq. (2).) This minimizing rule is unique up to the transformation  $(\mathbf{a}, \mathbf{b}) \rightarrow (-\mathbf{a}, -\mathbf{b})$ .*

*Proof.* From (15) it follows that we have to minimize  $A^3|c_4|$ . (Note that  $(\mathbf{a}, \mathbf{b}) \rightarrow (c^{-1}\mathbf{a}, c\mathbf{b})$  sends  $A \rightarrow |c|A$ ,  $|c_4| \rightarrow |c|^{-3}|c_4|$ , so that this quantity is constant over each equivalence class.)

Assume  $\mathbf{a}$ ,  $\mathbf{b}$ , and  $t$  are real. Then

$$\begin{aligned} A^3|c_4| &= \left(\sum |a_i|\right)^3 \sum a_i b_i^4 \\ &= \left(\frac{|t^3(t+2)| + |2t+1| + |(t+1)^2(t^2-1)|}{|t(2t+1)(t+2)(t^2-1)|}\right)^3 t^2(t+1)^2 \\ &= \begin{cases} 8t^8/|(t+1)[(2t+1)(t-1)]^3|, & -1 \leq t \leq -\frac{1}{2}, 1 \leq t < \infty, \\ 8(t+1)^8/|t[(2t+1)(t+2)]^3|, & -\infty < t \leq -2, -\frac{1}{2} \leq t < 0, \text{ and} \\ 8/|t(t+1)[(t+2)(t-1)]^3|, & -2 \leq t < -1, 0 < t < 1. \end{cases} \end{aligned}$$

By elementary calculus we have

$$\min_{t \in \mathbf{R}} A^3|c_4| = \left(\frac{2}{3}\right)^3 \cdot 2^4$$

and that this minimum occurs at  $t = 1 + \sqrt{3}$ ,  $1 - \sqrt{3}$ ,  $\frac{1}{2}(\sqrt{3} - 1)$ ,  $\frac{1}{2}(-\sqrt{3} - 1)$ ,  $\sqrt{3} - 2$ , and  $-\sqrt{3} - 2$ . Thus rule  $d_1$  also minimizes the overall error  $E$  among all real normalized three-point rules.

**THEOREM 4.** *Let  $d$  be a normalized three-point rule of degree 3. Fix  $h$  but allow all variables and functions to be complex-valued. Then overall error is minimized when  $d = d_2$ . (See Eq. (3).) This minimizing rule is unique up to the transformations  $(\mathbf{a}, \mathbf{b}) \rightarrow (e^{-i\varphi}\mathbf{a}, e^{i\varphi}\mathbf{b})$ ,  $0 < \varphi < 2\pi$ .*

*Proof.* Let  $z = 2t + 1$ . As in the proof of Theorem 3, we must minimize  $A^3|c_4| = F(z)$  where

$$(16) \quad F(z) = \frac{1}{16} \left( \frac{|z-1|^3|z+3| + 16|z| + |z+1|^3|z-3|}{|z(z^2-9)|} \right)^3 \frac{1}{|z^2-1|}.$$

Inspired by the results of Section 2 (see Theorem 2), we were able to guess that the minimum would occur for  $t = \omega$  and  $\omega^2$ , which correspond to  $z = \sqrt{3}i$  or  $z = -\sqrt{3}i$ , where  $F = 1$ . Because of the symmetries  $F(z) = F(\bar{z}) = F(-z)$ , it suffices to show that  $F > 1$  at every point of the first quadrant,  $\mathbf{C}_+$ , except  $\sqrt{3}i$ . Let  $r = |z|$ . For  $z \in \mathbf{C}_+$  and  $a \geq 0$ , we have  $|z+a| \geq r$ , so, from (16),

$$F(z) \geq \frac{1}{16} \left( \frac{(r-1)^3r + 16r + r^3(r-3)}{r(r^2+9)} \right)^3 \frac{1}{r^2+1} = g(r).$$

Direct calculation shows  $g' > 0$  on  $[9, \infty)$  and  $g(9) > 1$ , reducing the domain of investigation to  $\mathbf{C}_+ \cap \{|z| \leq 9\} = D$ . Finally, a combination of evaluating  $F$  on the points of a mesh containing  $D$ , together with bounding  $\text{grad } F$  away from the singularities  $z = 0, 1, 3$ , shows  $F > 1$  away from  $\sqrt{3}i$ , while a Taylor expansion of  $F$  about  $\sqrt{3}i$  shows  $F > 1$  on the remainder of  $D \setminus \{\sqrt{3}i\}$ . Thus three-point rule  $d_2$  also minimizes the overall error  $E$  among all normalized three-point rules.

#### 4. A Third Rule and Some Remarks.

*Motivation for the Third Rule* (see (4)). Estimating the first derivative from an equally spaced table adds the constraint that all three  $b_i$  be integers. Under these conditions it is clear from formula (11) that the rule given by (4) is best in a number of ways. It is best among integer three-point rules of degree 3 with respect to (i) minimizing  $\max\{b_i\} - \min\{b_i\}$ , (ii) minimizing  $\sum b_i^2$ , (iii) minimizing  $\sum |b_i|$ , et cetera.

*History of Three-Point Rules.* Essentially all real three-point rules appearing in the literature have been only of degree 2. (However, compare [3, p. 217].) The most prevalent of these is  $(-3f(x) + 4f(x+h) - f(x+2h))/2h$ ; see [1]. The complex rule (with  $\mathbf{b} = (1, \omega, \omega^2)$ ) seems to be well known; see [2].

*Comparison of Three-Point Rules.* In Table 1 below,  $f_4$  is a bound for the modulus of the fourth derivative near  $x$ . All derivatives have been normalized to make  $\min|b_i - b_j| = 1$ .

Observe that the overall error for the rule  $d_3$  is only slightly worse than that of the rule  $d_1$ . (By Theorem 3 it must be worse.)

*Generalizations.* 1. If we use  $p > 3$  points in our approximating rule, the most we can hope to achieve is

$$(17) \quad c_1 = 1, \quad c_0 = c_2 = \cdots = c_p = 0.$$

This follows from a simple linear algebra argument like the one found in Lemma 2. Such a difference quotient is easily found in the complex case by letting  $\mathbf{b}$  be the  $p$ th roots of unity and solving the Vandermonde system,

$$c_1 = 1, \quad c_0 = c_2 = \cdots = c_{p-1} = 0,$$

for **a**. Such a quotient appears in [2]. The last equation in (17) holds automatically from the  $p$ -periodicity. The same result holds in the real case. If  $p$  is even, one simply finds the appropriate linear combination of  $f(x + h) - f(x - h), f(x + 2h) - f(x - 2h), \dots, f(x + ph/2) - f(x - ph/2)$ . This process is essentially Romberg extrapolation. If  $p$  is odd, more delicate arguments are required, but Eqs. (17) can still be satisfied.

TABLE 1

	$\begin{matrix} \text{a} \\ \text{b} \end{matrix}$	Truncation Error (see (14))	Overall Error (see (15))
$d_0$ (see (1))	$\begin{matrix} 1 & & -1 \\ \text{-----} & & \text{-----} \\ 1/2 & & -1/2 \end{matrix}$	$\frac{f_3 h^2}{3!} \doteq .167 f_3 h^2$	$\frac{1}{2} 3^{2/3} f^{1/3} \epsilon^{2/3} \doteq 1.04 f_3^{1/3} \epsilon^{2/3}$
$d_1$ (see (2))	$\begin{matrix} \frac{3-2\sqrt{3}}{6} & \frac{4\sqrt{3}}{6} & \frac{-3-2\sqrt{3}}{6} \\ \text{-----} & \text{-----} & \text{-----} \\ \frac{1}{\sqrt{3}} + 1 & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} - 1 \end{matrix}$	$\frac{2}{9} \sqrt{3} \frac{f_4}{4!} h^3 \doteq .016 f_4 h^3$	$\frac{8}{3^{7/4}} f_4^{1/4} \epsilon^{3/4} \doteq 1.17 f_4^{1/4} \epsilon^{3/4}$
$d_2$ (see (3))	$\begin{matrix} \frac{1}{\sqrt{3}} & \frac{\omega^2}{\sqrt{3}} & \frac{\omega}{\sqrt{3}} \\ \text{-----} & \text{-----} & \text{-----} \\ \frac{1}{\sqrt{3}} & \frac{\omega}{\sqrt{3}} & \frac{\omega^2}{\sqrt{3}} \end{matrix}$	$\frac{1}{9} \sqrt{3} \frac{f_4}{4!} h^3 \doteq .008 f_4 h^3$	$\frac{2^{5/4}}{3} f_4^{1/4} \epsilon^{3/4} \doteq .793 f_4^{1/4} \epsilon^{3/4}$
$d_3$ (see (4))	$\begin{matrix} \frac{32}{40} & & \frac{-27}{40} & & \frac{-5}{40} \\ \text{-----} & & \text{-----} & & \text{-----} \\ \frac{3}{3} & & \frac{-2}{3} & & \frac{6}{3} \end{matrix}$	$\frac{4}{3} \cdot \frac{f_4}{4!} h^3 \doteq .056 f_4 h^3$	$\frac{16}{3(375)^{1/4}} f_4^{1/4} \epsilon^{3/4} \doteq 1.21 f_4^{1/4} \epsilon^{3/4}$

2. Pass now to the  $d$ th derivative,  $d > 2$ . To approximate  $f^{(d)}(x)$  we now need  $p > d + 1$ . As above, we choose **(a, b)** in such a way that  $d(h)$  is an approximation to the  $d$ th derivative, i.e., that  $c_0 = c_1 = \dots = c_{d-1} = 0, c_d = d!$  (see (6)) and that as many higher order terms be 0 as possible. Again the kind of argument used in Lemma 2 shows that we may hope for  $c_{d+1} = c_{d+2} = \dots = c_{d+p-1} = 0$  at most. As in the preceding generalization 1, we may achieve this in the complex case by letting the components of **b** be the  $p$ th roots of unity. In the real case, however, we *cannot* always do as well. For example, let  $d = 2$  and  $p = 3$ . Here

$$\frac{2}{3} [f(x + h) + \omega f(x + \omega h) + \omega^2 f(x + \omega^2 h)] / h^2 = f''(x) + \frac{1}{60} f^{(5)}(x) h^3 \dots$$

so  $c_0 = c_1 = c_3 = c_4 = 0, c_2 = 2$ , as desired, while an easy calculation shows this system to be insoluble with **a** and **b** real.



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