

MEAN VALUE THEOREMS FOR GENERALIZED RIEMANN DERIVATIVES

J. M. ASH AND R. L. JONES

ABSTRACT. Let $x, e \geq 0, u_0 < \dots < u_{d+e}$, and $h > 0$ be real numbers. Let f be a real valued function and let $\Delta(h; u, w)f(x)h^{-d}$ be a difference quotient associated with a generalized Riemann derivative. Set $I = (x + u_0h, x + u_{d+e}h)$ and let f have its ordinary $(d - 1)$ st derivative continuous on the closure of I and its d th ordinary derivative $f^{(d)}$ existent on I . A necessary and sufficient condition that a difference quotient satisfy a mean value theorem (i.e., that there be a $\xi \in I$ such that the difference quotient is equal to $f^{(d)}(\xi)$) is given for $d = 1$ and $d = 2$. The condition is sufficient for all d . It is used to show that many generalized Riemann derivatives that are "good" for numerical analysis do not satisfy this mean value theorem.

1. Results. Let f be a real valued function of a real variable. The d th Riemann derivative of f is

$$R_d f(x) := \lim_{h \rightarrow 0} \frac{\sum_{i=0}^d \binom{d}{i} (-1)^{d-i} f(x + (-d/2 + i)h)}{h^d}.$$

The first two special cases

$$R_1 f(x) = \lim_{h \rightarrow 0} \frac{-f(x - h/2) + f(x + h/2)}{h}$$

and

$$R_2 f(x) = \lim_{h \rightarrow 0} \frac{f(x - h) - 2f(x) + f(x + h)}{h^2}$$

are the well-known symmetric and Schwarz derivatives [6, 10, 11].

The generalized Riemann derivative is

$$(1) \quad D_d(u, w)f(x) := \lim_{h \rightarrow 0} \frac{\Delta_d(h; u, w)f(x)}{h^d},$$

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where

$$(2) \quad \Delta_d(h; u, w)f(x) := \sum_{i=0}^{d+e} w_i f(x + u_i h);$$

here e is a nonnegative integer which we will call the *excess* and the w_i 's and u_i 's are *real* numbers. Here we insist upon the $d + 1$ consistency conditions

$$(3) \quad \sum w_i u_i^j = \begin{cases} 0, & j = 0, 1, \dots, d - 1, \\ d!, & j = d. \end{cases}$$

[1, 2, 7]. For notational convenience we will always assume $u_0 < u_1 < \dots < u_{d+e}$.

The most natural type of mean value theorem would say something like this. Let $I = [x + u_0 h, x + u_{d+e} h]$ where x and h are fixed. If $D_d f(t)$ exists for every $t \in I$, then there is a ξ interior to I with

$$\frac{\Delta_d(h; u, w)f(x)}{h^d} = D_d f(\xi).$$

But this is not even true for R_1 as the choices $x = -1$, $h = 3$, and $f(t) = |t|$ show [3].

It is possible that the only generalized Riemann derivative for which this mean value theorem holds is d/dx itself. A more fruitful set of mean value theorems are those of the following type.

STATEMENT $M(u, w)$. Fix x and h and set $I = [x + u_0 h, x + u_{d+e} h]$. If $f^{(d-1)}(t)$ is continuous on I and differentiable for all t interior to I , then there is a ξ interior to I with $\Delta_d(h; u, w)f(x)/h^d = f^{(d)}(\xi)$.

It is easy to see that any set of $d + 1$ distinct points $\mu = \{\mu_0, \dots, \mu_d\}$ has a unique d th derivative associated to it via the correspondence $\mu \rightarrow D_\mu$ where

$$D_\mu f(x) := \lim_{h \rightarrow 0} \sum_{i=0}^d d! \frac{[\prod_{j \neq i} (\mu_i - \mu_j)]^{-1} f(x + \mu_i h)}{h^d}$$

(see p. 182 of [1] or p. 12 of [3] for this). In particular, if $d = 1$ then the unique two point derivative at $\{\mu_0, \mu_1\}$ is

$$D_\mu f(x) = \lim_{h \rightarrow 0} \frac{f(x + \mu_1 h) - f(x + \mu_0 h)}{(\mu_1 - \mu_0)h}$$

and if $d = 2$ then the unique three point derivative at $\{\mu_0, \mu_1, \mu_2\}$ is

$$D_\mu f(x) = \lim_{h \rightarrow 0} \frac{1}{h^2} \left[\frac{2f(x + \mu_0 h)}{(\mu_0 - \mu_1)(\mu_0 - \mu_2)} + \frac{2f(x + \mu_1 h)}{(\mu_1 - \mu_0)(\mu_1 - \mu_2)} + \frac{2f(x + \mu_2 h)}{(\mu_2 - \mu_0)(\mu_2 - \mu_1)} \right].$$

LEMMA 1. Let $u = (u_0, \dots, u_{d+e})$ and $w = (w_0, \dots, w_{d+e})$ be given and let D_j denote the unique generalized Riemann derivative associated with (u_j, \dots, u_{j+d}) , $j = 0, \dots, e$. Then the D associated with u and w is itself a generalized Riemann derivative if and only if there are p_j , $j = 0, \dots, e$, such that $\sum p_j = 1$ and $D = \sum p_j D_j$.

We will prove this in §2.

THEOREM. Let $D = D_d(u, w)$ be a d th generalized Riemann derivative.

- (i) If the p_i associated to D are all positive (so that D is a convex combination of the D_j 's), then the mean value theorem $M(u, w)$ holds.
- (ii) Conversely if $d = 1$ or $d = 2$ or $e = 1$, and if any p_i is negative, then Statement $M(u, w)$ is false.

The proof of (i) is easy. First if $e = 0$ then $p_0 = 1$ and indeed the Theorem is a well-established numerical analysis fact [8]. If $e > 0$ using this fact $e + 1$ times we have numbers ξ_i so that

$$s = \frac{\Delta_d(h; u, w)f(x)}{h^d} = \sum_{i=0}^e p_i f^{(d)}(\xi_i).$$

The right side is a convex combination of the numbers $\{f^{(d)}(\xi_0), \dots, f^{(d)}(\xi_e)\}$ and hence s lies between the smallest and the largest. But $f^{(d)} = (f^{(d-1)})'$ is an ordinary first derivative, hence is Darboux and therefore assumes the value s .

The proof of (ii) is longer so we will break it into three lemmas. These are contained in §2.

APPLICATIONS. 1. Using Taylor expansion techniques, it is easy to see that

$$\frac{\Delta_d(h; u, w)f(0)}{h^d} = \sum_{j=0}^p c_j \frac{f^{(j)}(0)}{j!} h^{j-d} + O(h^{p+1-d}),$$

where $p > d$ and $c_j = \sum_{i=1}^{d+e} w_i u_i^j$, $j = 0, 1, \dots, p$. To yield a generalized Riemann derivative, the c_j , $j = 0, \dots, d$, must satisfy the consistency conditions (3). In [5] a difference quotient based on $d + e$ points was defined to be optimal if in addition to the consistency conditions (3) we also have $c_j = 0$ for $j = d + 1, \dots, r$, with r as large as possible, $|c_{r+1}|$ as small as possible, and $|u_i - u_j| \geq 1$ for $i \neq j$. (The last condition is for normalization [5].)

With this definition of optimal, the above theorem implies that no optimal first or second derivative with positive excess has the mean value property. This will be proved at the end of §2.

2. From the Theorem it follows that the first derivative

$$\begin{aligned} &\lim_{h \rightarrow 0} \frac{-27f(x - 2h) + 32f(x + 3h) - 5f(x + 6h)}{120h} \\ &= \frac{9}{8} \left(\lim_{h \rightarrow 0} \frac{f(x + 3h) - f(x - 2h)}{5h} \right) - \frac{1}{8} \left(\lim_{h \rightarrow 0} \frac{f(x + 6h) - f(x + 3h)}{3h} \right) \end{aligned}$$

does not have the mean value property. This derivative is optimal in some senses for numerical approximation (see [4]).

3. The first derivative

$$\lim_{h \rightarrow 0} \frac{7f(x + 3h) - 13f(x + 4h) + 6f(x + 16h/3)}{h},$$

whose interesting properties were investigated by Patrick O'Conner, is an example of a derivative not having the mean value property (see [3, pp. 26, 17–18]; this derivative was discovered in [9]).

QUESTION. Does the mean value theorem hold if $d \geq 3$, $e \geq 2$, and some p_i is negative? In particular, does the mean value theorem hold for the excess 2 third derivative $D := \frac{5}{8}D_0 - \frac{1}{4}D_1 + \frac{5}{8}D_2$, where for $i = 0, 1, 2$,

$$D_i := \lim_{h \rightarrow 0} \frac{f(x + ih) + 3f(x + [i + 1]h) - 3f(x + [i + 2]h) + f(x + [i + 3]h)}{h^3} \text{?}$$

2. Proofs.

PROOF OF LEMMA 1. Let p_0, \dots, p_e be real numbers with $\sum p_i = 1$. Let $u_0 < u_1 < \dots < u_{d+e}$ be $d + 1 + e$ real numbers. For $j = 0, \dots, e$, let D_j denote the unique generalized Riemann derivative based on $\{u_j, \dots, u_{d+j}\}$, and let $D = \sum_{i=0}^e p_i D_i$. Then a quick check of the consistency condition shows that D is also a d th derivative.

Conversely, if

$$D \sim \Delta = \sum_{j=0}^{d+e} w_j f(x + u_j h),$$

and

$$D_j \sim \Delta_j = \sum_{k=j}^{j+d} w_k f(x + u_k h) \text{ for } j = 0, 1, \dots, e$$

(recall $w_{kj} = d! [\prod_{l=j, l \neq k}^{j+d} (u_k - u_l)]^{-1}$), then $w_j = \sum_{i=0}^j p_i w_{j-i, i}$, $j = 0, \dots, e$. This allows the p_i 's to be found recursively as

$$p_0 := w_0/w_{00}, \quad p_j := \left(w_j - \sum_{i=0}^{j-1} p_i w_{j-1, i} \right) / w_{j, j}, \quad j = 1, 2, \dots, e.$$

Now let $Z = \Delta - \sum p_j \Delta_j$. We must show $Z = 0$. From the definition of the p_j 's, $Z = \sum_{j=e+1}^{e+d} c_j f(x + u_j h)$ for some numbers c_j . Testing Z on the functions $1, t, \dots, t^{d-1}$ at the point $x = 0$ and noting that D and all of the D_j satisfy the first d conditions in (3), we get $\sum c_j u_j^j = 0$, $j = 0, \dots, d - 1$. Since the Vandermonde matrix (u_j^i) is invertible, $Z = 0$. Applying Z to the function t^d at $x = 0$, noting that D and all D_j satisfy the last equation in (3), and that $Z = 0$, we get that $\sum p_i = 1$. Observe that the equations defining the p_j 's are quite explicit and simple.

LEMMA 2. Let $D = D_1(u, w)f(x)$ be a generalized first derivative, so that D has a unique representation as a linear combination of $e + 1$ two point first derivatives: $D = \sum_{j=0}^e p_j D_j$. If for some j , $p_j < 0$, then the mean value theorem fails.

PROOF. The proof will consist of constructing a function for which the mean value theorem fails. Define f inductively. Let $f(u_0) = 0$. Having defined $f(u_{i-1})$, set $f(u_i) = f(u_{i-1})$ if $p_{i-1} \leq 0$, and $f(u_i) = f(u_{i-1}) + (u_i - u_{i-1})$ if $p_{i-1} > 0$. Note f is not linear on $[u_0, u_{e+1}]$ since at least one p_j is negative and $\sum p_i = 1$.

We now extend the domain of f from $\{u_0, \dots, u_{e+1}\}$ to all of \mathbf{R} by making f linear on each interval $[u_i, u_{i+1}]$, $i = 1, \dots, e - 1$, linear on $(-\infty, u_1]$, linear on $[u_e, \infty)$, and continuous on \mathbf{R} . Since

$$\Delta_j(h; u)f(x) = \frac{f(x + u_{j+1}h) - f(x + u_jh)}{(u_{j+1} - u_j)h},$$

it follows that whenever $p_j \leq 0$ we have $\Delta_j(1; u)f(0) = 0$ and whenever $p_j > 0$ we have $\Delta_j(1; u)f(0) = 1$. Consequently $\Delta(1; u)f(0) = \sum p_j \Delta_j f(0) > 1$. Finally, round the corners of f to produce a differentiable function g with $g'(x) \leq 1$ for all x , but $\Delta(g) > 1$, so that the mean value theorem fails for g .

LEMMA 3. Let $D = D_2(u, w)f(x)$ be a generalized second derivative, so that D has a unique representation as a linear combination of $e + 1$ three point second derivatives, $D = \sum_{j=0}^e p_j D_j$. If for some j , $p_j < 0$, then the mean value theorem fails.

PROOF. Let D be given with some $p_j < 0$. Fix $x = 0$ and $h = 1$. Let $\Delta_j := \sum_{i=j}^{j+2} \omega_{ij} f(u_i)$ and $\Delta := \sum \omega_j f(u_j)$ so that $\Delta = \sum p_j \Delta_j$. Let $\mathcal{P} = \{j: p_j > 0\}$ and $\mathcal{N} = \{j: p_j < 0\}$. Then $\sum_{j \in \mathcal{P}} p_j + \sum_{j \in \mathcal{N}} p_j = 1$, so $\sum_{j \in \mathcal{N}} p_j < 0$ implies $\sum_{j \in \mathcal{P}} p_j > 1$.

We prove Lemma 3 by constructing a function f satisfying $\Delta > 1$ and $f''(x) \leq 1$ for all $x \in [u_0, u_{e+2}]$. The function f will be created by rounding the corners of a continuous, piecewise twice differentiable function g .

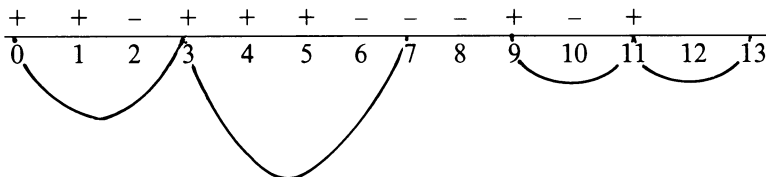


FIGURE 1

To understand how g is constructed in general first consider an example (Figure 1). In Figure 1 the point labeled 4 is u_4 , and the + sign above the 4 indicates that p_4 is positive, etc. The function g is defined by

$$g(x) = \begin{cases} .5(x - u_0)(x - u_3), & u_0 \leq x \leq u_3, \\ .5(x - u_3)(x - u_7), & u_3 \leq x \leq u_7, \\ 0, & u_7 \leq x \leq u_9, \\ .5(x - u_9)(x - u_{11}), & u_9 \leq x \leq u_{11}, \\ .5(x - u_{11})(x - u_{13}), & u_{11} \leq x \leq u_{13}. \end{cases}$$

Observe that $g''(x) \in \{0, 1\}$ when $x \notin \{u_3, u_7, u_9, u_{11}\}$.

We have $\Delta_0 = \Delta_1 = \Delta_3 = \Delta_4 = \Delta_5 = \Delta_9 = \Delta_{11} = 1$. To see this note for example that from the viewpoint of $\Delta_4 = \omega_{44}g(u_4) + \omega_{54}g(u_5) + \omega_{64}g(u_6)$ the function g “is” the quadratic polynomial $.5(x - u_3)(x - u_7)$ and $\Delta_4(.5x^2 + \dots) = (.5x^2 + \dots)'' = 1$. Similarly $\Delta_7 = 0$. Next observe that the line joining $(u_2, g(u_2))$ to $(u_4, g(u_4))$ passes below the point $(u_3, g(u_3)) = (u_3, 0)$ so the quadratic q interpolating these three points has negative second derivative. Since $g = q$ from the viewpoint of $\Delta_2 = \Delta_2(u_2, u_3, u_4)$, it follows that $\Delta_2 < 0$. Similarly, Δ_6, Δ_8 , and Δ_{10} are also negative. Totalling up,

$$\Delta = \sum_{i \in \{0, 1, 3, 4, 5, 9, 11\}} p_i \Delta_i + \sum_{j \in \{2, 6, 7, 8, 10\}} p_j \Delta_j > \sum_{i \in \{0, 1, 3, 4, 5, 9, 11\}} p_i$$

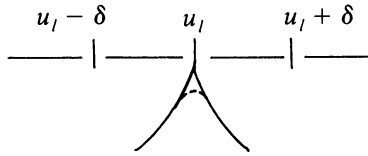


FIGURE 2

since in the first sum each $\Delta_i = 1$, while in the second sum each $p_j < 0$ and each $\Delta_j \leq 0$. Hence $\Delta > \sum_{i \in \mathcal{P}} p_i > 1$.

We now show how to construct such a function g whenever \mathcal{N} is not empty. We suggest that the reader test the construction on the above example to see how it works.

Let j_1 be the smallest index in \mathcal{P} . Let $g(x) = 0$ for $x \in [u_0, u_{j_1}]$. If \mathcal{N} has any numbers larger than j_1 , let $k_1 = \min\{n \in \mathcal{N} \mid n > j_1\} + 1$; otherwise let $k_1 = e + 2$. Let $g(x) = .5(x - u_{j_1})(x - u_{k_1})$ for $x \in [u_{j_1}, u_{k_1}]$. If \mathcal{P} has any members $\geq k_1$, let j_2 be the least one; otherwise let $j_2 = e + 2$. Let $g(x) = 0$ for $x \in [u_{k_1}, u_{j_2}]$. If \mathcal{N} has any members larger than j_2 , let $k_2 = \min\{n \in \mathcal{N} \mid n > j_2\} + 1$; otherwise let $k_2 = e + 2$. Let $g(x) = .5(x - u_{j_2})(x - u_{k_2})$ on $[u_{j_2}, u_{k_2}]$. Proceed inductively. The process terminates when some j_i or $k_i = e + 2$. The process does terminate since $j_i < k_i \leq j_{i+1}$.

Having constructed g , we now show that $\Delta(g) > 1$. It suffices to show that $\Delta_i \leq 0$ if $p_i \in \mathcal{N}$ and $\Delta_i = 1$ if $p_i \in \mathcal{P}$, for then

$$\Delta = \sum_{i \in \mathcal{P}} p_i \Delta_i + \sum_{i \in \mathcal{N}} p_i \Delta_i \geq \sum_{i \in \mathcal{P}} p_i \Delta_i = \sum_{i \in \mathcal{P}} p_i > 1.$$

Let $l \in \mathcal{N}$. Then either $l \leq j_1 - 1$, $l \in [k_\nu - 1, j_{\nu+1})$ for some ν , or $l > j_p$ where j_p is the largest member of \mathcal{P} . If $l \leq j_1 - 2$ or $l \in [k_\nu - 1, j_{\nu+1} - 1)$ or $l \in [j_p + 2, e]$, then $g(u_e) = g(u_{e+1}) = g(u_{e+2}) = 0$ and $\Delta_l = 0$. If $l = j_1 - 1$ or $j_{\nu+1} - 1$, then $g(u_e) \leq 0$, $g(u_{e+1}) = 0$, and $g(u_{e+2}) < 0$ so that the quadratic q passing through the three points $(u_k, g(u_k))$, $k = e, e + 1, e + 2$, is concave, whence $\Delta_e = q'' < 0$. Finally if $l = j_p + 1$, $g(u_e) < 0$, $g(u_{e+1}) = g(u_{e+2}) = 0$ so that $\Delta_l < 0$.

If now $l \in \mathcal{P}$, then g agrees with a quadratic of the form $q(x) = .5(x - \alpha)(x - \beta)$ at $x = u_l, u_{e+1}$, and u_{e+2} so that $\Delta_l = q'' = 1$.

Let $\epsilon_0 = \Delta - 1$. We now construct f as a twice differentiable perturbation of g . Any point of (u_0, u_{e+2}) where g'' does not exist is of the form u_l where either (i) $l \in \{j_\nu\} \cap \{k_\nu\}$ (u_3 and u_{11} in the example), (ii) $l \in \{k_\nu\} \setminus \{j_\nu\}$ (u_7 in the example), or (iii) $l \in \{j_\nu\} \setminus \{k_\nu\}$ (u_9 in the example).

In case (i), g looks like the solid curve in Figure 2.

Let f be a rounded version of g on $[u_l - \delta, u_l + \delta]$ (the dotted curve in Figure 2). Then on $[u_l - \delta, u_l + \delta] \cap \{x: f(x) \neq g(x)\}$ the slope of f decreases steadily so $f'' < 0$. Pick δ so small that

$$(1) \quad -f(u_l) < \frac{\epsilon_0}{2e|w_l|}$$

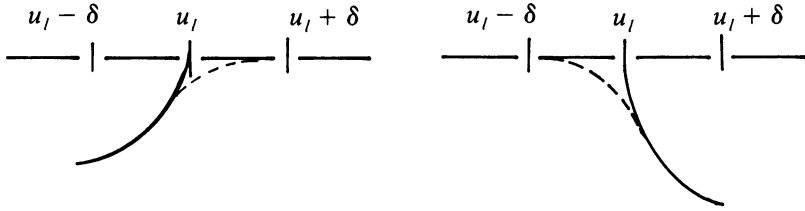


FIGURE 3

and also so small that

$$(2) \quad \delta < \frac{1}{2} \min\{u_l - u_{l-1}, u_{l+1} - u_l\}.$$

Cases (ii) and (iii) are similar. The pictures are given in Figure 3.

Again we get $f'' < 0$ on $[u_l - \delta, u_l + \delta] \cap \{x: f(x) \neq g(x)\}$ in both cases. Again we choose δ small enough to force (1) and (2). Define $f(x) = g(x)$ on the remainder of $[u_0, u_{e+2}]$. Then $f''(x) \leq 1$ everywhere on (u_0, u_{e+2}) and f' is continuous on $[u_0, u_{e+2}]$ (with the usual convention that $f'(u_0) := f'^+(u_0)$, $f'(u_{e+2}) := f'^-(u_{e+2})$). However $\Delta(f) = \Delta(g) - \sum w_l f(u_l) > (1 + \epsilon_0) - \sum(\epsilon_0/2e)$ where the sum is over the discontinuities of g'' . Since there are at most e such u_l 's, it follows that $\Delta(f) > 1 + \epsilon_0/2 > 1$ and hence $\Delta(f) \notin \text{Range}(f'') \subseteq (-\infty, 1]$. Therefore the mean value theorem fails for this f .

LEMMA 4. Let $D = D_d(u, w)f(x)$ be a generalized d th derivative with excess 1, where $u_0 < \dots < u_{d+1}$, so that D has a unique representation as a linear combination of two $d + 1$ point d th derivatives, $D = p_0 D_0 + p_1 D_1$. If one p_j is negative, then the mean value theorem is false for D .

PROOF. Let D_0 be the unique d th derivative based on $\{u_0, \dots, u_d\}$ and D_1 the one based on $\{u_1, \dots, u_{d+1}\}$. Let $D = p_0 D_0 + p_1 D_1$. Fix $x_0 = 0$, $h = 1$, and let Δ , Δ_0 , and Δ_1 be the respective corresponding differences. First suppose $p_0 < 0$. Let $f = (x - u_1)^d/d!$ on $[u_1, u_{d+1}]$, and $f(x) = 0$ on $[u_0, u_1]$. Now

$$\Delta_0 \left(\frac{1}{d!} (x - u_1)^d \right) = \frac{d!}{\prod_{i=1}^d (u_0 - u_i)} \cdot \frac{1}{d!} (u_0 - u_1)^d + \dots$$

has positive first term since $\text{sgn}(\prod_{i=1}^d (u_0 - u_i)) = \text{sgn}((u_0 - u_1)^d)$, while

$$\Delta_0(f) = \frac{d!}{\prod_{i=1}^d (u_0 - u_i)} f(u_0) + \dots$$

has 0 first term. Since all other terms are equal, $\Delta_0(f) < \Delta_0((x - u_1)^d/d!) = 1$. Write $\Delta_0(f) = 1 - \eta$ where $\eta > 0$. Then $\Delta(f) = p_0(1 + \eta) + p_1(1) = p_0 + p_1 - p_0\eta = 1 - p_0\eta > 1$ since $p_0 < 0$ and $\eta > 0$. However, for $x \neq u_1$,

$$f^{(d)}(x) = H(x - u_1) = \begin{cases} 0, & x < u_1, \\ 1, & x > u_1. \end{cases}$$

We must smooth f . Let

$$H_\epsilon(x) = \begin{cases} 0, & x < 0, \\ x/\epsilon, & 0 \leq x \leq \epsilon, \\ 1, & x > \epsilon. \end{cases}$$

Then let

$$f_\epsilon(x) = \int_0^{x-u_1} \frac{(x-u_1-t)^{d-1}}{(d-1)!} H_\epsilon(t) dt.$$

If $x \in [u_0, u_{d+1}]$,

$$|f(x) - f_\epsilon(x)| \leq \int_0^\epsilon \frac{(x-u_1-t)^{d-1}}{(d-1)!} dt = O(\epsilon),$$

so that if ϵ is small enough, $\Delta(f_\epsilon) > 1$. However, $f_\epsilon^{(d)}(x) = H_\epsilon(x - u_1)$ has range contained in $[0, 1]$, so the mean value theorem fails for p_0 negative.

If p_0 is nonnegative, then $p_1 < 0$. In this case let $f(x) = (x - u_d)^d/d!$ on $[u_0, u_d]$ and $f(x) = 0$ on $[u_d, u_{d+1}]$. As above, $\Delta(f) > 1$, $f^{(d)}(x) \in \{0, 1\}$ for $x \neq u_\alpha$, and a smoothed version of f then becomes the required counterexample.

PROOF FOR APPLICATION 1. Let $\Delta(h; u, w)f(x) = \sum_{i=1}^n w_i f(x + u_i h)$ be the difference associated to an optimal first derivative based on $n \geq 3$ points. From [5] we have that if $n = 2k$, $k = 2, 3, \dots$, then the optimal choice of u is $u = -(k - \frac{1}{2}), -(k - \frac{3}{2}), \dots, -\frac{1}{2}, \frac{1}{2}, \dots, k - \frac{1}{2}$; while if $n = 2k + 1$, $k = 1, 2, 3, \dots$, then the optimal choice of u is $u = (\alpha_n - k, \alpha_n - k + 1, \dots, \alpha_n + k)$ where $\frac{1}{2} < \alpha_n < \frac{1}{2} + 1/4n$, $n = 3, 5, 7, \dots$. Fix n . Let

$$R_1(x) := \prod_{i=2}^n (x - u_i) \quad \text{and} \quad R_2(x) := (x - u_1) \prod_{i=3}^n (x - u_i).$$

On the one hand, logarithmic differentiation of R_j and the fact that the optimal choice of u satisfies identity $\sum u_i^{-1} = 0$ (see [5, p. 157]) yield $R'_j(0) = u_j^{-1} \prod_{i \neq j} (-u_i)$, $j = 1, 2$; while on the other hand from $\Delta(1; u, w)R_j(0) = R'_j(0)$, $j = 1, 2$ (see [5]), we have $R'_j(0) = w_j R_j(u_j)$, $j = 1, 2$. This yields formulas for w_1 and w_2 in terms of k . From these and the proof of Lemma 1 we get

$$\frac{p_2}{p_1} = 1 + \frac{w_2}{w_1} = 1 - \left(\frac{u}{u+1} \right) (n-1),$$

where $u = -k + \frac{1}{2}$ when k is even and $\alpha_n - k$ when k is odd. This is easily shown to be negative. Since one of $\{p_1, p_2\}$ must be negative, by the Theorem of §1 each optimal n point first derivative, $n \geq 3$, fails to satisfy a mean value theorem.

For the second derivative case let $\Delta = \sum_{i=1}^n w_i f(x + u_i h)$ be the difference associated to an optimal second derivative based on $n \geq 4$ points. Again using the results from [5] we have if $n = 2k + 1$, $k = 2, 3, \dots$, then the optimal choice of u is $u = (-k, -k + 1, \dots, k - 1, k)$; while if $n = 2k$, $k = 2, 3, 4, \dots$, then the optimal choice of u is $u = (\beta_n - k, \beta_n - k + 1, \dots, \beta_n + k - 1)$ where $\beta_4 = 1.145$, $\beta_6 = 1.085$, and $1 < \beta_n < 1 + 1/2n$, $n = 8, 10, \dots$

Computing $(\log R_j)''$ and using the fact that the optimal choice of u satisfies the identity $\sum_{i \neq j} (u_i u_j)^{-1} = 0$ (see [5, pp. 162–163]), we obtain

$$R_j''(0) = \frac{2 \prod_{i=1}^n (-u_i) (u_j \sum_{i=1}^n u_i^{-1} - 1)}{u_j^3 \prod_{i \neq j} (u_j - u_i)}, \quad j = 1, 2.$$

On the other hand from $\Delta(1; u, w)R_j(0) = R_j''(0)$ we have $R_j''(0) = w_j R_j(u_j)$, $j = 1, 2$. This yields formulas for w_1 and w_2 in terms of u . From these and the proof of Lemma 1 we get

$$\frac{p_2}{p_1} = 2 + \frac{w_2}{w_1} = 2 - (n - 1) \left(\frac{u}{u + 1} \right)^3 \left(\frac{1 - (u + 1) \sum_{i=1}^n u_i^{-1}}{1 - u \sum_{i=1}^n u_i^{-1}} \right),$$

where $u = -k$ if n is odd and $u = \beta_n - k$ if k is even. It can now be shown that $p_2/p_1 < 0$. (To do this, we needed three cases: n odd, n even and at least 6, and $n = 4$.) Again finish by applying the Theorem of §1.

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MATHEMATICAL SCIENCES DEPARTMENT, DEPAUL UNIVERSITY, CHICAGO, ILLINOIS 60614