Lanczo's Generalized Derivative

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1. INTRODUCTION. Is it possible to differentiate by integrating? A curious approximate differentiation rule of Cornelius Lanczos seems to adopt this oxymoronic approach. More orthodox finite difference rules for approximate differentiation arise naturally from the definition of the derivative. For example, replacing the limiting value in the definition of the derivative by the difference quotient at a small "finite difference" h gives the forward difference approximation:

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

and many other finite difference approximations can be developed by using higher order differences [**1**]. In this note we investigate a little-known, and at first sight ironical, approximation of the derivative that Lanczos called the "differentiation by integration" method [**4**, p. 324].

The method consists of computing the expression

$$D_h f(x) = \frac{3}{2h^3}\int_{-h}^{h} t f(x+t)\,dt \tag{1}$$

for a given small value of the parameter h, as an approximation of $f'(x)$; since $D_{-h}f(x) = D_h f(x)$, we may, and shall, take h to be positive. An application of Simpson's rule provides a connection between Lanczos' approximation and the more familiar symmetric difference approximation of the derivative. In fact, if $f \in C^4[x-h, x+h]$, then Simpson's rule [**1**, p. 257] gives

$$\int_{-h}^{h} t f(t+x)\,dt = \frac{h}{3}[-hf(x-h) + 0f(x) + hf(x+h)] + O(h^5)$$

and hence

$$D_h f(x) = \frac{f(x+h) - f(x-h)}{2h} + O(h^2).$$

On the other hand [**1**, p. 317],

$$\frac{f(x+h) - f(x-h)}{2h} = f'(x) + O(h^2)$$

and therefore

$$D_h f(x) = f'(x) + O(h^2).$$

This result can be obtained more directly from the Taylor approximation under the relaxed condition that $f \in C^3[x-H, x+H]$ for some $H > 0$:

$$f(x+t) = f(x) + f'(x)t + f''(x)t^2/2 + f'''(\theta_t)t^3/6$$

and hence

$$D_h f(x) = \frac{3}{2h^3}\int_{-h}^{h} tf(x+t)\,dt$$

$$= f'(x) + \frac{3}{2h^3}\int_{-h}^{h} f'''(\theta_t)\frac{t^4}{6}\,dt \tag{2}$$

$$= f'(x) + O(h^2). \tag{3}$$

In the next section we investigate the convergence of the Lanczos approximation under assumptions on f that are weaker than differentiability, thereby establishing that the Lanczos method defines a true generalized derivative. Furthermore, we show that the convergence behavior of the method is in a sense quite analogous to the convergence of Fourier series. Section 3 treats the effects of errors in the function values and gives a best possible uniform rate of convergence with respect to the error level in the function values.

2. A GENERALIZED DERIVATIVE. Suppose f is an integrable function on some interval $[a, b]$. Lanczos remarks that

$$\lim_{h \to 0} D_h f(x) \tag{4}$$

may exist even at points $x \in (a, b)$ "where a derivative in the ordinary sense does not exist." In the next proposition we show that (4) does indeed provide a generalized derivative. In fact, we show that the Lanczos method bears the same relationship to the *first* derivative that the Fourier partial sums bear to the *zeroth* derivative of a function [**2**, p. 75]. Namely, $D_h f(x)$ converges to the average value of the left and right hand derivatives at x, provided these one-sided derivatives exist. We use the following notation for the right and left derivatives, respectively:

$$f_R'(x) = \lim_{t \to 0^+} \frac{f(x+t) - f(x)}{t}, \quad f_L'(x) = \lim_{t \to 0^-} \frac{f(x+t) - f(x)}{t}.$$

Proposition 1. *If $f_R'(x)$ and $f_L'(x)$ exist, then*

$$\lim_{h \to 0} D_h f(x) = \frac{1}{2}(f_L'(x) + f_R'(x)).$$

Proof: According to the definition of the one-sided derivatives, for a given $\epsilon > 0$, there is s $\delta > 0$ such that

$$|f(x+t) - f(x) - f_R'(x)t| < \epsilon t \quad \text{if } 0 < t < \delta$$

and

$$|f(x+t) - f(x) - f_L'(x)t| < \epsilon |t| \quad \text{if } -\delta < t < 0.$$

Therefore, for $h > 0$,

$$\int_0^h tf(x+t)\,dt = \int_0^h t(f(x+t) - f(x) - f_R'(x)t) + t(f(x) + f_R'(x)t)\,dt$$

$$= \int_0^h t(f(x+t) - f(x) - f_R'(x)t)\,dt + \frac{h^2}{2}f(x) + \frac{h^3}{3}f_R'(x)$$

and similarly,

$$\int_{-h}^{0} tf(x+t)\,dt = \int_{-h}^{0} t(f(x+t) - f(x) - f_L'(x)t)dt - \frac{h^2}{2}f(x) + \frac{h^3}{3}f_L'(x).$$

We then have

$$\begin{aligned}
D_h f(x) &= \frac{3}{2h^3}\int_{-h}^{h} tf(x+t)\,dt \\
&= \frac{3}{2h^3}\int_{-h}^{0} t(f(x+t) - f(x) - f_L'(x)t)\,dt + \frac{1}{2}f_L'(x) \\
&\quad + \frac{3}{2h^3}\int_{0}^{h} t(f(x+t) - f(x) - f_R'(x)t)\,dt + \frac{1}{2}f_R'(x),
\end{aligned}$$

so, if $0 < h < \delta$, then

$$\begin{aligned}
&\left| D_h f(x) - \frac{1}{2}(f_L'(x) + f_R'(x)) \right| \\
&\quad \le \frac{3}{2h^3}\left(\int_{-h}^{0} |t||f(x+t) - f(x) - f_L'(x)t|\,dt \right. \\
&\qquad\qquad \left. + \int_{0}^{h} t|f(x+t) - f(x) - f_R'(x)t|\,dt \right) \\
&\quad \le \frac{3}{2h^3}\epsilon\int_{-h}^{h} t^2\,dt = \epsilon.
\end{aligned}$$

Since $D_h f(x) = D_{-h} f(x)$, we therefore have

$$\lim_{h\to 0} D_h f(x) = \frac{1}{2}(f_L'(x) + f_R'(x)).$$

■

In particular, we see that if f is differentiable at x, then

$$\lim_{h\to 0} D_h f(x) = f'(x).$$

However, the limit may exist even at points where f is not differentiable. For example, if $f(x) = |x|$, then

$$\lim_{h\to 0} D_h f(0) = 0$$

by Proposition 1, while $f'(0)$ does not exist.

Lanczos suggests that formula (4) may be useful in cases where one desires an approximate derivative of a function contaminated by noise, since "noise is a typically nonanalytic phenomenon which destroys the analytical nature of the true $f(x)$." In the next section we show that formula (4) has no particular advantage when handling noisy functions, although it can give satisfactory results if used properly, and we provide an analysis of the behavior of Lanczos' approximate derivative when the function is corrupted by error.

3. ERROR EFFECTS. Before proceeding with the analysis, it is useful to get some feel for the process by performing some modest experiments. Fortunately, modern software, such as MATLAB™, makes this an easy job. As a simple test case we use the function $f(x) = e^{x^2}$ for $-1 \le x \le 1$. The integral we wish to compute is

$$\frac{3}{2h^3}\int_{-h}^{h} te^{(x+t)^2}\,dt = \frac{3}{2h}\int_{-1}^{1} ue^{(x+hu)^2}\,du. \tag{5}$$

In a simple MATLAB program this quantity was computed for $h = .001$ at 101 equally spaced values $x \in [-1, 1]$ by using an eight point Gauss-Legendre quadrature rule to approximate the integrals. The resulting Lanczos approximate derivative and the true derivative are plotted on the same axes in Figure 1.

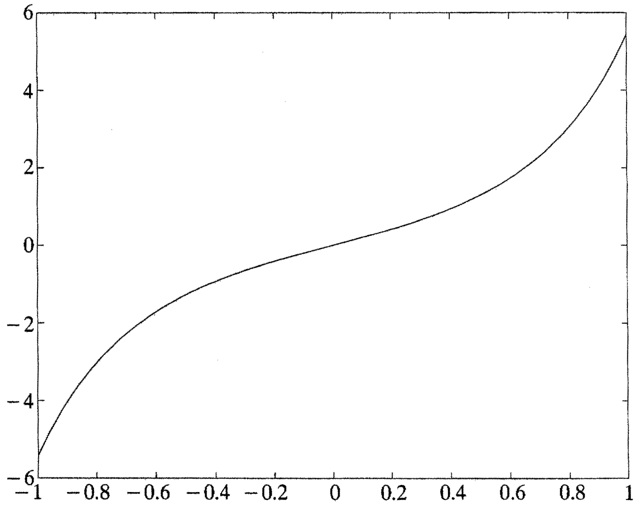

Figure 1

Don't be surprised if you see only one graph—the Lanczos approximation is so good that the approximate derivative virtually overlies the true derivative.

Now we blend a little noise into the simulation by perturbing the function values with uniform random errors of magnitude $\le .01$ (about one percent) before applying the approximation formula. The results appear in Figure 2.

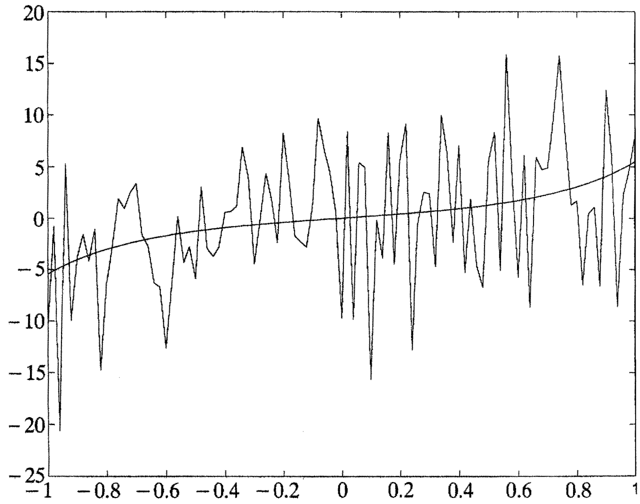

Figure 2

The difference is certainly eye catching, but not particularly surprising. The small errors in the function values are filtered through the integral in (5) and magnified by the factor $3/2h$, leading to large errors in the approximate derivative. This is not a deficiency in the method, but rather a manifestation of the inherent instability of the differentiation process itself **[3]**. To paraphrase Cassius, the fault, dear reader, is not in the method, but in ourselves—or more precisely, in our application of the method. A simple analysis suggests that a more intelligent application of the method can lead to more satisfactory results.

To get some idea of the effect of data errors, suppose f is bounded and has three bounded derivatives on some interval I containing the point x. Suppose further, that f^ϵ is some bounded integrable perturbation of f satisfying

$$|f(t) - f^\epsilon(t)| \leq \epsilon \tag{6}$$

for all $t \in I$, where ϵ is a known error bound. Then by (2)

$$\begin{aligned} |D_h f^\epsilon(x) - f'(x)| &\leq |D_h f(x) - f'(x)| + |D_h f^\epsilon(x) - D_h f(x)| \\ &\leq \frac{M}{10}h^2 + \frac{3}{2h^3}\int_{-h}^{h} |t|\epsilon\, dt \\ &= \frac{M}{10}h^2 + \frac{3}{2}\frac{\epsilon}{h}, \end{aligned}$$

where M is a bound for the magnitude of the third derivative.

This type of bound is the Scylla and Charybdis of numerical analysis for unstable problems. The first term (the *truncation* error) goes to zero as $h \to 0$, while the second term (the *stability* error) blows up as $h \to 0$. Clearly, some compromise is needed and the computational Odysseus would do well to steer a midcourse between these two numerical hazards by balancing the two terms with a parameter choice of the form $h = \text{constant} \times \epsilon^{1/3}$. Such a parameter choice gives

$$|D_h f^\epsilon(x) - f'(x)| = O(\epsilon^{2/3}). \tag{7}$$

In particular, if the example is rerun using the parameter $h = \epsilon^{1/3}$, instead of the unreasonably small parameter that produced Figure 2, we get the much more satisfactory result shown in Figure 3.

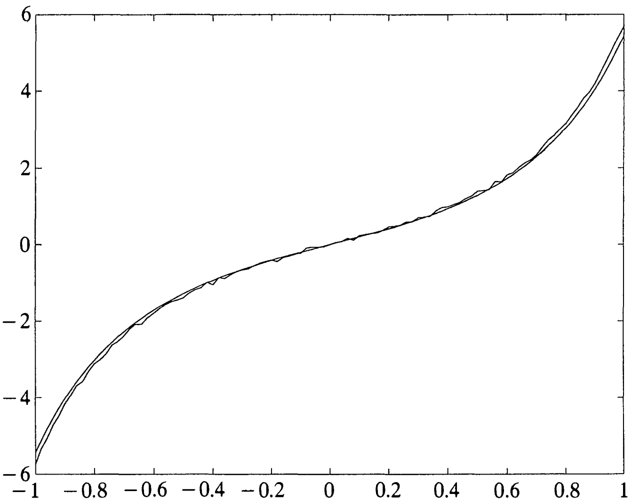

Figure 3

This brings up a final question. Is the rate of convergence $O(\epsilon^{2/3})$ given in (7) best possible? To be more precise, is it possible to squeeze out a better rate of the form $o(\epsilon^{2/3})$? Our next proposition shows that this is possible only in trivial special cases, namely when f is a quadratic polynomial. We consider the polynomials of degree at most two to be a trivial case because D_h produces the exact derivative when applied to such polynomials.

Proposition 2. *Suppose f is bounded and has three continuous bounded derivatives on some open interval I, and that $h(\epsilon) \to 0$ as $\epsilon \to 0$. If for each bounded integrable function f^ϵ satisfying* (6) *we have*

$$\left|D_{h(\epsilon)} f^\epsilon(x) - f'(x)\right| = o(\epsilon^{2/3})$$

for all $x \in I$, then f is a polynomial of degree at most two on I.

Proof: Suppose $f'''(x) > 0$ for some $x \in I$. Then there is a $\delta > 0$ and an $H > 0$ such that

$$f'''(s) \geq \delta > 0 \quad \text{if } x - H \leq s \leq x + H.$$

Suppose $0 < h(\epsilon) < H$ and let $\eta(t) = \epsilon$ for $t \geq x$, and $\eta(t) = 0$, otherwise. Then

$$D_h \eta(x) = \frac{3\epsilon}{2h^3} \int_0^h t\, dt = \frac{3\epsilon}{4h}.$$

Now let $f^\epsilon(t) = f(t) + \eta(t)$. Then (6) is satisfied.

By Taylor's Theorem, we have

$$f(x+t) = f(x) + f'(x)t + f''(x)\frac{t^2}{2} + \int_x^{x+t} f'''(s)\frac{(x+t-s)^2}{2}\, ds$$

and therefore

$$D_h f(x) - f'(x) = \frac{3}{2h^3}\int_{-h}^{h} t f(x+t)\, dt - f'(x)$$

$$= \frac{3}{2h^3}\int_{-h}^{h} t \int_x^{x+t} f'''(s)\frac{(x+t-s)^2}{2}\, ds\, dt.$$

But, for $0 < h < H$,

$$\frac{3}{2h^3}\int_0^h t \int_x^{x+t} f'''(s)\frac{(x+t-s)^2}{2}\, ds\, dt \geq \frac{3\delta}{2h^3}\int_0^h t \int_x^{x+t} \frac{(x+t-s)^2}{2}\, ds\, dt = \frac{\delta}{20}h^2,$$

and

$$\frac{3}{2h^3}\int_{-h}^{0} t \int_x^{x+t} f'''(s)\frac{(x+t-s)^2}{2}\, ds\, dt$$

$$\geq \frac{3\delta}{2h^3}\int_{-h}^{0} (-t) \int_{x+t}^{x} \frac{(x+t-s)^2}{2}\, ds\, dt = \frac{\delta}{20}h^2.$$

Therefore,

$$D_h f^\epsilon(x) - f'(x) = D_h f(x) - f'(x) + D_h \eta(x) \geq \frac{\delta}{10}h^2 + \frac{3}{4}\frac{\epsilon}{h}.$$

Since

$$\left| D_{h(\epsilon)} f^{\epsilon}(x) - f'(x) \right| = o(\epsilon^{2/3}),$$

we then have

$$\frac{\delta}{10} h^2(\epsilon) + \frac{3}{4} \frac{\epsilon}{h(\epsilon)} = o(\epsilon^{2/3})$$

and therefore

$$\frac{\delta}{10} \left(\frac{h(\epsilon)}{\epsilon^{1/3}} \right)^2 + \frac{3}{4} \left(\frac{\epsilon^{1/3}}{h(\epsilon)} \right) \to 0$$

as $\epsilon \to 0$, which is clearly impossible. A similar argument shows that for no $x \in I$ is $f'''(x) < 0$. Therefore, $f'''(x) = 0$ for all $x \in I$, so f is a quadratic polynomial on I. ■

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REFERENCES

1. K. E. Atkinson, *An Introduction to Numerical Analysis*, Second Edition, Wiley, New York, 1989.
2. R. V. Churchill and J. W. Brown, *Fourier Series and Boundary Value Problems*, Fourth Edition, McGraw-Hill, New York, 1987.
3. C. W. Groetsch, Differentiation of approximately specified functions, *Amer. Math. Monthly* **98** (1991), 847–850.
4. C. Lanczos, *Applied Analysis*, Prentice-Hall, Englewood Cliffs, N.J., 1956.

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