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Letter to the editor

Lanczos' generalized derivative for higher orders

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Abstract

The method of differentiation by integration due to Lanczos is generalized to cover derivatives of arbitrary order. Umbral versions and further extensions are indicated.

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1. Lanczos' generalized derivative $\mathrm{D}_h f$, defined by [5]

$$\mathrm{D}_h f = (3/2h^3) \int_{-h}^{h} t f(x+t)\,\mathrm{d}t = (3/2h) \int_{-1}^{1} t f(x+ht)\,\mathrm{d}t, \tag{1}$$

is an approximation to the first derivative of $f(x)$, $\mathrm{d}f/\mathrm{d}x$ in the sense that

$$\mathrm{D}_h f = f'(x) + \mathrm{O}(h^2) \tag{2}$$

and is aptly called a method of "differentiation by integration".

Two recent notes examined its robustness (with respect to random errors on data) [3] and probabilistic overtones [4]. We report in this note, the analogue of (1) for *higher order derivatives*. In other words defining

$$\mathrm{D}_h^{(n)} f = h^{(-n)} \int_{-1}^{1} \rho_n(t) f(x+ht)\,\mathrm{d}t, \tag{3}$$

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we choose $\rho_n(t)$ that satisfies

$$\mathrm{D}_h^{(n)} f = f^{(n)}(x) + \mathrm{O}(h^2), \quad n = 1, 2, 3, \ldots \,. \tag{4}$$

Restricting the search to *polynomials*, we show in the next section that $\rho_n(t)$ is proportional to the familiar Legendre polynomials $P_n(t)$ [1]. Besides making a connection to Umbral (or operator) calculus [6,7], a formal operator representation for $\mathrm{D}_h^{(n)}$ can be given explicitly as a function of D where $\mathrm{D} = \mathrm{d}/\mathrm{d}x$. Further generalizations are also indicated.

The emphasis being on formal connections, our approach in this note is somewhat heuristic.

2. To identify $\rho_n(t)$ in (3) we employ the "brute force approach" based on finite difference representation or Taylor expansion [3]. Let us write, for a given n,

$$\begin{aligned} f(x+ht) &= f(x) + htf'(x) + \cdots + \frac{(h^n t^n)}{n!} f^{(n)}(x) \\ &\quad + \frac{(h^{(n+1)} t^{(n+1)})}{(n+1)!} f^{(n+1)}(x) + \frac{(h^{(n+2)} t^{(n+2)})}{(n+2)!} f^{(n+2)}(\theta). \end{aligned} \tag{5}$$

Substituting (5) in (3) and requiring that $\rho_n(t)$ satisfy the constraints

$$\int_{-1}^{1} \rho_n(t) t^m \,\mathrm{d}t = 0, \quad 0 \leqslant m < n \tag{6}$$

and

$$\int_{-1}^{1} \rho_n(t) t^n \,\mathrm{d}t = n!, \tag{7}$$

we deduce from the theory of orthogonal polynomials or otherwise that

$$\rho_n(t) = \gamma_n P_n(t), \tag{8}$$

where $P_n(t)$ is the Legendre polynomial and $\gamma_n = (\frac{1}{2})(1)(3)(5)\cdots(2n+1)$.

Observing that

$$\int_{-1}^{1} \rho_n(t) t^{n+1} \,\mathrm{d}t = 0 \tag{9}$$

and using (5)–(7) we can also conclude that

$$\mathrm{D}_h^{(n)} f = f^{(n)}(x) + \mathrm{O}(h^2). \tag{4$'$}$$

Thus, the nth derivative analogue of D_h is

$$\begin{aligned} \mathrm{D}_h^{(n)} &= (\gamma_n/h^n) \int_{-1}^{1} P_n(t) f(x+ht) \,\mathrm{d}t \\ &= (\gamma_n/h^{(n+1)}) \int_{-h}^{h} P_n\left(\frac{t}{h}\right) f(x+t) \,\mathrm{d}t \end{aligned} \tag{10}$$

with γ_n given by (9). For $n=1$, (10) reduces to (1), and for $n=2,3,\dots,$

$$\mathrm{D}_h^{(2)} f = (45/4h^5)\int_{-h}^{h}\left(t^2-\frac{h^2}{3}\right) f(x+t)\,\mathrm{d}t, \tag{10a}$$

$$\mathrm{D}_h^{(3)} f = (525/4h^7)\int_{-h}^{h} t\left(t^2-\frac{(3h^2)}{5}\right) f(x+t)\,\mathrm{d}t. \tag{10b}$$

3. It is easy to verify that D_h as defined in (1) is a delta operator [7] and an explicit representation for D_h and $\mathrm{D}_h^{(n)}$ in terms of the derivative operator $\mathrm{D}=(\mathrm{d}/\mathrm{d}x)$ is given below. Using the shift operator [7] form of Taylor expansion viz.,

$$f(x+t)=E_t f(x)=\mathrm{e}^{t\mathrm{D}} f(x) \tag{11}$$

in (10), it is seen that, formally,

$$\mathrm{D}_h^{(n)} f = (\gamma_n/h^n)\int_{-1}^{1} P_n(t)\mathrm{e}^{th\mathrm{D}} f(x)\,\mathrm{d}t. \tag{12}$$

Substituting the Neumann-type expansion [2]

$$\mathrm{e}^{\gamma z}=\sum_{n=0}^{\infty}(v+n)C_n^{(v)}(\gamma)\left(I_{\gamma+n}(z)\left(\frac{2}{z}\right)^{v}\right)\Gamma(v) \tag{13}$$

for the special case $v=\frac{1}{2}$; $C_n^{(1/2)}(\gamma)=P_n(\gamma)$, in (12) and noting the orthogonal property of $P_n(t)$, we deduce that

$$\mathrm{D}_h^{(n)}=(2\gamma_n/h^n)(f_n(h\mathrm{D})). \tag{14}$$

In (13), $I_v(z)$ and $C_n^{(v)}(\gamma)$ denote the modified Bessel function of the first kind and Gegenbauer polynomials [1,2] respectively, while in (14),

$$f_n(x)=\mathrm{I}_{n+1/2}(x)\sqrt{\frac{\pi}{2x}} \tag{15}$$

denotes the modified spherical Bessel functions [1].

For $n=1$,

$$\mathrm{D}_h^{(1)}=\mathrm{D}_h=\left(\frac{2\gamma_1}{h}\right)\sqrt{\frac{\pi}{2h\mathrm{D}}}\,\mathrm{I}_{3/2}(h\mathrm{D})$$
$$=\left(\frac{3}{h}\right)\left[\frac{(\cosh h\mathrm{D}-\frac{\sinh h\mathrm{D}}{h\mathrm{D}})}{h\mathrm{D}}\right], \quad [1,\ \text{p. } 443]. \tag{16}$$

4. The above approach suggests that the choice of kernels $\rho_n(t)$ in (3) need not be restricted to polynomials. In fact, the following operators also perform the task of “differentiation by integration”.

$$\mathrm{D}_{h,\alpha}^{(n)} f = (\lambda_n/h^n)\int_{-1}^{1} C_n^{(\alpha)}(t)(1-t^2)^{\alpha-1/2} f(x+ht)\,\mathrm{d}t, \tag{17}$$

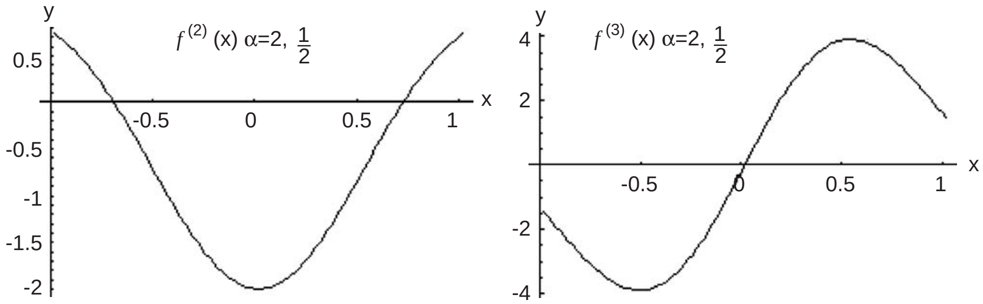

Fig. 1.

$$D_{h,\alpha}^{(1)} f = \left(2\frac{\alpha\lambda}{h}\right) \int_{-1}^{1} t(1-t^2)^{\alpha-1/2} f(x+ht)\,\mathrm{d}t \qquad \left(\alpha > -\frac{1}{2}\right) \tag{18}$$

can replace (10) and (1), and approximate $f^{(n)}x$ and $f'(x)$, respectively. In (17)

$$\lambda_n = \left(\frac{2^n(\alpha)_{n+1} n!}{(2\alpha)_n}\right)\left(\frac{\Gamma(\alpha)}{\Gamma(\alpha+\frac{1}{2})\sqrt{\pi}}\right), \tag{19}$$

where

$$(\alpha)_n = \frac{\Gamma(\alpha+n)}{\Gamma(\alpha)}. \tag{20}$$

In Fig. 1, the estimated values of the second and third derivatives of the function $f(x) = \exp(-x^2)$ calculated using (17) for the case of $\alpha = 2$, and $\alpha = \frac{1}{2}$ are plotted with their actual values. As is evident, the graphs are indistinguishable.

Calculations for a series of values of α yield a very similar result.

The operator connection, analogous to (14)–(16), is

$$D_{h,\alpha}^{(n)} = \left(\frac{2}{h}\right)^n \Gamma(\alpha+n+1)\left(I_{\alpha+n}(hD)\left(\frac{2}{hD}\right)^{\alpha}\right). \tag{21}$$

When $\alpha = \frac{1}{2}$, λ_n reduces to γ_n of (9) and the results of the previous section can be recovered. Again, the limit $\alpha \to 0$, where the Gegenbauer polynomials go over to Chebyshev polynomials, gives yet another option. For example,

$$D_{h,0}^{(n)} f = \left(\frac{(2^n)(n!)}{(\pi)(h^n)}\right) \int_0^{\pi} (\cos nt) f(x + h\cos t)\,\mathrm{d}t$$

comes under this category. Generalizations with respect to functions of several variables can also be made on the lines indicated here.

A final comment on the choice of the discretization parameter h is appropriate. On the basis of Eqs. (2) and (4), one would expect the approximations to improve as $h \to 0$, but a word of caution is in place. When the data are perturbed (random or systematic) such that $|f(x) - f^{\varepsilon}(x)| < \varepsilon$ (where $f^{\varepsilon}(x)$ is the perturbation), an optimal choice of h does not $h \to 0$, but has an order $\varepsilon^{(1/3)}$ [3]. This is particularly relevant when the integrals in (1) or (3) are not evaluated exactly (cf. Gaussian schemes).

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