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A note on Lanczos generalized derivative

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Abstract

Lanczos introduced an integral expression for calculating the derivative of a function, if this is continuous in the point x under analysis. Here we extend this expression to the case of a finite discontinuity at x.

key words. Lanczos Derivative; Method of Least Squares.

1. Introduction

Lanczos [1] used the Least Squares Method (MMC) of Gauss-Legendre to derive an integral expression that gives the derivative of a function, that is, derivation via integration [1-6]:

$$f'_L(x,\epsilon) = \frac{3}{2\epsilon}\int_{-\epsilon}^{\epsilon} t f(x+t)\ \mathrm{dt}\ , \tag{1}$$

and when $\epsilon \to 0$ tends to the ordinary derivative:

$$\lim_{\epsilon\to 0} f'_L(x,\epsilon) = f'(x). \tag{2}$$

The relation (1) is valid when $f(x)$ is continuous at x, which is shown in Sec. 2. In the literature we have not found explicitly, the corresponding generalization of (1) where $f(x)$ has a finite discontinuity; in Sec. 3 we obtain the generalization and (2) is replaced by [2]:

$$\lim_{\epsilon\to 0} f'_L(x,\epsilon) = \frac{1}{2}[f'_+(x) + f'_-(x)], \tag{3}$$

where $f'_+(x),\ f'_-(x)$) are the derivatives arising from the right and the left, respectively. We note that (3) also applies when in x there is no discontinuity of the function, but $f'_+(x)$ is different to $f'_-(x)$, which means that it is not derivable in the usual sense. The relation (3) reminds us a similar property of the Fourier series at a point of finite discontinuity [1]:

$$\lim_{n\to 0} f_n(x) = \frac{1}{2}[f_+(x) + f_-(x)]. \tag{4}$$

2. Lanczos derivative

Here we will indicate the main aspects of the construction of (1), useful in Sec. 3 for its generalization to a function with finite discontinuity at the point under study. Before testing (1), we check the validity of (2). The Taylor series gives the expression:

$$f(x+t) = f(x) + f'(x)t + \frac{1}{2}f''(x)t^2 + L, \tag{5}$$

that substituting in (1) implies:

$$f'_L(x,\epsilon) = f'(x) + \frac{\epsilon^2}{10}f'''(x) + L, \tag{6}$$

and thus (2) is immediate. In (6) we observe that as $\epsilon \to 0$ then is closer the equality between the two types of derivatives. We give three examples to illustrate the application of (1), taking $\epsilon = 10^{-4}$:

$$a) f(x) = \tan x, \qquad \text{then } f'(1) = \sec^2 1 = 3.42551882 \tag{7}$$

and the Lanczos derivative:

$$f'_L(1,10^{-4}) = \frac{3}{2}10^{12}\int_{-10^{-4}}^{10^{-4}} t\cdot\tan(1+t)\ \mathrm{dt} \ = 3.42551887$$

close enough to (7).

$$b) f(x) = |x|, \qquad \text{therefore } f'_-(0) = -1, \quad f'_+(0) = 1, \tag{8}$$

and from (1):

$$f'_L(1, 10^{-4}) = \frac{3}{2} 10^{12} \int_{-10^{-4}}^{10^{-4}} t \cdot |t| \text{ dt } = 0 \overset{(8)}{=} \frac{1}{2}[f'_-(0) + f'_+(0)],$$

in accordance with (3).

$$c) f(x) = \ln x, \qquad \text{so } f'(0.25) = 4, \tag{9}$$

such that:

$$f(0.25, 10^{-4}) = \frac{3}{2} 10^{12} \int_{-10^{-4}}^{10^{-4}} t \cdot \ln(0.25 + t) \text{ dt } = 4.00000012, \tag{6}$$

comparable to (9), etc.

Now we shall show how Lanczos [1] obtained (1) by the celebrated Gauss-Legendre MMC. Cornelius Lanczos wanted to calculate, for example in $x = 0$, the derivative of and empirical function tabulated in equidistant data, then he saw that with 5 points could fit a parabola through them, thus proposing the curve:

$$y = a + bx + cx^2, \tag{10}$$

whose coefficients were obtained via the MMC, and in doing with b because it is clear that:

$$y'(0) = b. \tag{11}$$

In other words, $f'_L(0, \epsilon)$ is the derivative of this parabola when the number n of data tends to infinity and the separation h between them approaches to zero, all this happening in the vicinity $[-\epsilon, \epsilon]$, $\epsilon << 1$, about $x = 0$, and the empirical function approaches to a continuous function.

In applying the technique of MMC seek $a,\ b,\ c$ that minimize the mean square error $\sum_{k=-n}^{n}\left(a+bx_k+cx_k^2-y_k\right)^2$, and thus one of the resulting equations gives:

$$a\sum x_k+b\sum x_k^2+c\sum x_k^3=\sum x_k y_k, \tag{12}$$

but x_k but x_k are distributed symmetrically about the origin, then it is clear that $\sum x_k=\sum x_k^3=0$ canceling the coefficients a and c in (12), and assuming $n\to\infty$ and $h\to 0$, the relation (12) involve:

$$b\int_{-\epsilon}^{\epsilon} t^2\ \mathrm{dt}\ =\int_{-\epsilon}^{\epsilon} tf(t)\ \mathrm{dt}\ \ \therefore b=\frac{3}{2\epsilon^3}\int_{-\epsilon}^{\epsilon} tf(0+t)\ \mathrm{dt}\ , \tag{13}$$

and if instead of $f_L'(0,\epsilon)$ we had been interested in $f_L'(x,\epsilon)$ then would have been (1), q.e.d. It is important to note the significance of the MMC in the derivation of the Lanczos formula.

3. Lanczos derivative for a discontinuous function

It is now natural to ask by the expression for $f_L'(0,\epsilon)$ at a point where the function has a finite discontinuity. First we consider the left side of $x=0$, where equidistant data conform to the parabola $a_1+b_1x+c_1x^2$ via the MMC, obtaining equations similar to (12):

$$\begin{aligned} na_1+b_1\sum x_k^2+c_1\sum x_k^2&=\sum y_k,\\ a_1\sum x_k+b_1\sum x_k^2+c_1\sum x_k^3&=\sum x_k y_k,\\ a_1\sum x_k^2+b_1\sum x_k^3+c_1\sum x_k^4&=\sum x_k^2 y_k, \end{aligned} \tag{14}$$

recalling that the Lanczos derivative from the left is given by:

$$f_L'(0,\epsilon)=b_1, \tag{15}$$

such that

$$\lim_{\epsilon\to 0} f_L'(0,\epsilon)=f_-'(0). \tag{16}$$

When $n\to\infty$ and $h\to 0$ in (14) the $\sum$ become integrals and the system takes the form:

$$a_1 - \frac{\epsilon}{2}b_1 + \frac{\epsilon}{3}c_1 = \frac{1}{\epsilon}\int_{-\epsilon}^{0} f(t)\ \mathrm{dt}\ ,$$

$$-\frac{1}{2}a_1 + \frac{\epsilon}{3}b_1 - \frac{\epsilon}{4}c_1 = \frac{1}{\epsilon^2}\int_{-\epsilon}^{0} tf(t)\ \mathrm{dt}\ , \tag{17}$$

$$\frac{1}{3}a_1 - \frac{\epsilon}{4}b_1 + \frac{\epsilon}{4}c_1 = \frac{1}{\epsilon^3}\int_{-\epsilon}^{0} t^2 f(t)\ \mathrm{dt}\ ,$$

where we can solve b_1, that in union of (15) implies:

$$f'_L(0,\epsilon) = \frac{12}{\epsilon^2}\int_{-\epsilon}^{0}\left(3 + \frac{16}{\epsilon}t + \frac{15}{\epsilon^2}t^2\right) f(t)\ \mathrm{dt}\ , \tag{18}$$

which, based on (16), approaches to $f'_-(0)$ when $\epsilon \to 0$. So (18) permits to calculate, through a process of integration, the derivative of $f(x)$ from left at $x = 0$.

Similarly, the system for the right side of the discontinuity in $x = 0$ we have (adjusting to the parabola $a_2 + b_2 x + c_2 x^2$):

$$a_2 = \frac{\epsilon}{2}b_2 + \frac{\epsilon^2}{3}c_2 = \frac{1}{\epsilon}\int_{0}^{\epsilon} f(t)\ \mathrm{dt}\ ,$$

$$\frac{1}{2}a_2 + \frac{\epsilon}{3}b_2 + \frac{\epsilon^2}{4}c_2 = \frac{1}{\epsilon^2}\int_{0}^{\epsilon} tf(t)\ \mathrm{dt}\ , \tag{19}$$

$$\frac{1}{3}a_2 + \frac{\epsilon}{4}b_2 + \frac{\epsilon}{5}c_2 = \frac{1}{\epsilon^3}\int_{0}^{-\epsilon} t^2 f(t)\ \mathrm{dt}\ ,$$

obtaining b_2 which is the Lanczos derivative from the right:

$${}_+f'_L(0,\epsilon) = \frac{12}{\epsilon^2}\int_{0}^{\epsilon}\left(-3 + \frac{16}{\epsilon}t - \frac{15}{\epsilon^2}t^2\right) f(t)\ \mathrm{dt}\ , \tag{20}$$

with the property:

$$\lim_{\epsilon \to 0}\ {}_- + f'_L(0,\epsilon) = f'_+(0). \tag{21}$$

Relationships (18) and (20) can be grouped in the form:

$${}_\gamma f'_L(0,\epsilon) = -\gamma\frac{12}{\epsilon^2}\int_{0}^{\epsilon}\left(3 - \frac{16}{\epsilon}u - \frac{15}{\epsilon^2}u^2\right) f(\gamma u)\ \mathrm{du}\ , \quad \gamma = \pm \tag{22}$$

then it is immediate its extension for arbitrary x:

$$ {}_{\gamma}f'_L(x,\epsilon) = -\gamma \frac{12}{\epsilon^2} \int_0^{\epsilon} \left(3 - \frac{16}{\epsilon} u - \frac{15}{\epsilon^2} u^2 \right) f(x+\gamma u)\ \mathrm{du}\ , \quad \gamma = \pm \tag{23} $$

Finally, according to (3) and in analogy to the Fourier series, the Lanczos derivative at x is defined as:

$$ f'_L(x,\epsilon) = \frac{1}{2}[{}_{-}f'_L(x,\epsilon) +_{-} f'_L(x,\epsilon)], \tag{24} $$

$$ = \frac{6}{\epsilon^2} \int_0^{\epsilon} \left(3 - \frac{16}{\epsilon} u + \frac{15}{\epsilon^2} u^2 \right) [f(x-u) - f(x+u)]\ \mathrm{du}\ , \tag{25} $$

verifying (3).

As an example of (23), ... ,(25) we consider the function:

$$ f(x) = \begin{cases} = \tan x, & x \leq 1, \\ 2x^2, & x > 1, \end{cases} \tag{26} $$

then $f_-(1) = 1.5574 \neq f_+(1) = 2$, besides:

$$ f'_-(1) = \sec^2 1 = 3.42551882,\ \ f'_+(1) = 4, $$

$$ \frac{1}{2} \left[f'_-(1) - f'_+(1) \right] = 3.71275941 \tag{27} $$

If we choose $\epsilon = 10^{-4}$, from (23), ..., (26) it follows that:

$$ {}_{-}f'_L(1,\epsilon) = 3.42550001,\ \ {}_{+}f'_L(1,\epsilon) = 4.0010,\ \ f'_L(1,\epsilon) = 3.71325000. \tag{28} $$

and according ϵ is smaller then the values (28) is closer to (27). Relationships (23) and (25), which we have not found explicitly in the literature, are the Lanczos derivatives for a function with a finite discontinuity. Thus (1) and (2) are special cases of (25) and (3), respectively. Emphasizing that in all these expressions the derivatives are calculated using the integration process.

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