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]:

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

(1)

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

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

(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]:

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

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]:

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

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:

\[ f(x + t) = f(x) + f'(x)t + \frac{1}{2} f''(x)t^2 + L, \]  

that substituting in (1) implies:

\[ f'_L(x, \epsilon) = f'(x) + \frac{\epsilon^2}{10} f'''(x) + L, \]  

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 \( \epsilon = 10^{-4} \):

\[ a)f(x) = \tan x, \quad \text{then } f'(1) = \sec^2 1 = 3.42551882 \]  
and the Lanczos derivative:

\[ f'_L(1, 10^{-4}) = \frac{3}{2} 10^{12} \int_{-10^{-4}}^{10^{-4}} t \cdot \tan(1 + t) \, dt = 3.42551887 \]
close enough to (7).

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

and from (1):

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

\[ \frac{1}{2} [f'_-(0) + f'_+(0)], \]

in accordance with (3).

\[ c) f(x) = \ln x, \quad \text{so } f'(0.25) = 4, \quad (9) \]

such that:

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

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 an empirical function tabulated in equidistant data, then he saw that with 5 points could fit a parabola through them, thus proposing the curve:

\[ y = a + bx + cx^2, \quad (10) \]

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

\[ y'(0) = b. \quad (11) \]

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 
\[
\sum_{k=-n}^{n} (a + bx_k + cx_k^2 - y_k)^2,
\]
and thus one of the resulting equations gives:

\[
a \sum x_k + b \sum x_k^2 + c \sum x_k^3 = \sum x_k y_k,
\]
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:

\[
b \int_{-\epsilon}^{\epsilon} t^2 \, dt = \int_{-\epsilon}^{\epsilon} t f(t) \, dt \therefore b = \frac{3}{2\epsilon^3} \int_{-\epsilon}^{\epsilon} t f(0 + t) \, dt,
\]
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 \( a_1 + b_1 x + c_1 x^2 \) via the MMC, obtaining equations similar to (12):

\[
na_1 + b_1 \sum x_k^2 + c_1 \sum x_k^2 = \sum y_k,
\]
\[
a_1 \sum x_k + b_1 \sum x_k^2 + c_1 \sum x_k^3 = \sum x_k y_k,
\]
\[
a_1 \sum x_k^2 + b_1 \sum x_k^3 + c_1 \sum x_k^4 = \sum x_k^2 y_k,
\]
recalling that the Lanczos derivative from the left is given by:

\[
f'_L(0, \epsilon) = b_1,
\]
such that

\[
\lim_{\epsilon \to 0} f'_L(0, \epsilon) = f'_L(0).
\]

When \( n \to \infty \) and \( h \to 0 \) in (14) the \( \sum \) become integrals and the system takes the form:
\[ a_1 - \frac{\epsilon}{2} b_1 + \frac{\epsilon}{3} c_1 = \frac{1}{\epsilon} \int_{-\epsilon}^{0} f(t) \, dt , \]

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

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

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

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

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 \( a_2 + b_2 x + c_2 x^2 \)):

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

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

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

obtaining \( b_2 \) which is the Lanczos derivative from the right:

\[ +f'_L(0, \epsilon) = \frac{12}{\epsilon^2} \int_{0}^{\epsilon} \left( -3 + \frac{16}{\epsilon} t - \frac{15}{\epsilon^2} t^2 \right) f(t) \, dt , \quad (20) \]

with the property:

\[ \lim_{\epsilon \to 0^-} +f'_L(0, \epsilon) = f'_+(0). \quad (21) \]

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

\[ \gamma f'_L(0, \epsilon) = -\gamma \frac{12}{\epsilon^2} \int_{0}^{\epsilon} \left( 3 - \frac{16}{\epsilon} u - \frac{15}{\epsilon^2} u^2 \right) f(\gamma u) \, du , \quad \gamma = \pm \quad (22) \]
then it is immediate its extension for arbitrary \( x \):

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

(23)

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

\[
f'_L(x, \epsilon) = \frac{1}{2} \left[ f'_L(x, \epsilon) + f'_L(x, \epsilon) \right] ,
\]

(24)

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

(25)

verifying (3).

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

\[
f(x) = \begin{cases} 
\tan x, & x \leq 1, \\
2x^2, & x > 1,
\end{cases}
\]

(26)

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

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

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

(27)

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

\[
-f'_L(1, \epsilon) = 3.42550001, \quad +f'_L(1, \epsilon) = 4.0010, \quad f'_L(1, \epsilon) = 3.71325000.
\]

(28)

and according \( \epsilon \) 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.
References


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