

A NEW CLASS OF GENERALIZED LANCZOS DERIVATIVES

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Abstract In this note we introduce a family of linear operators D_k that contain a sequence of integrals expressions more general in form than the Lanczos Derivative (LD), and show that they all lead to the same limit. The standard LD is a particular case of this family, whose members are labeled by the value of a positive odd integer. The theory is applied to several special cases where the functions are not differentiable in the standard sense, and it is shown that the operators are well-behaved. In addition, we present another couple of operators $\mathcal{D}_\epsilon, \mathcal{D}_\epsilon^\dagger$ -also generalizations of LD-, that are gifted with parallel if not better properties. This fact allows us to claim that the structure of the ordinary LD can be extended in a natural manner by a more generic operator \mathcal{L}_ϵ , which includes a general analytic odd function $g(t)$ in the integrand. In the last part of the work we discuss a mechanism opposed to the Lanczos method, namely, integration by differentiation.

1 Introduction

In 1956 Lanczos [1] presented a non-standard mechanism to obtain the derivative of a function by means of a integral (differentiation by integration), inspired by the Least Squares Method. The Lanczos Derivative (LD) is given by

$$f'_L(x) = \frac{3}{2\epsilon^3} \int_{-\epsilon}^{\epsilon} tf(x+t)dt \quad (1.1)$$

For small ϵ . The history of this expression goes back to Cioranescu [2], Haslam-Jones[3], and Golay-Savitzky [4]. One of the main advantages of the ordinary LD resides in the fact that it allows to generalize the concept of the derivative for functions that are not well-behaved [5, 6], for example, functions which are perturbed by noise or which are only given in a sampled form. Groetsch [6], showed that LD is an extension of the standard derivative, and in fact converges to the average value of the right and left hand derivatives of a function, namely, $\lim_{\epsilon \rightarrow 0} f'_L(x) = (f'_+(x) + f'_-(x))/2$. Then, if these two derivatives exist at a given point x , LD will exist as well. Liebrock and Hicks [7] focused on the computational properties of the method with applications to astrophysics. Refs. [8, 9] provided generalizations to cover derivatives of arbitrary order, showing their close relationship with the Legendre polynomials. In [10] the statistical properties of the mechanism were investigated, in particular their relation with certain operators. Gordon [11], showed that an approach to differentiation based on least square lines to best fit rather than the secant lines leads in a natural manner to LD. The possible generalization of the Lanczos rule at points where $f(x)$ posses a finite discontinuity was investigated in [12]. Other mechanisms of differentiation based on Jacobi polynomials were developed in [13, 14, 15, 16, 17]. In this sense, a detailed and self-contained survey regarding the history of approximation formulas for n-th order derivatives by integrals involving orthogonal polynomials can be found in [18].

Expanding in a Taylor series the function $f(x+t)$ around x , it is straightforward to see that

$$f'_L(x) = \frac{3}{2\epsilon^3} \int_{-\epsilon}^{\epsilon} tf(x+t)dt = f'(x) + \frac{1}{10}\epsilon^2 f'''(x) + \dots \quad (1.2)$$

This shows that the Lanczos rule provides $f'(x)$ with an error of order ϵ^2 . In his work, Lanczos argues that this error, which he calls “noise”, can affect the analytical nature of $f(x)$, although at

the end it is balanced out due to their random character. Groetsch[6], analyzed in more detail the error of LD. He found that small errors in the function values are magnified by a factor of $3/2\epsilon$. This is not, however, a shortcoming of the method, rather, it seems inherent to the process of differentiation itself. It is interesting to note that the accuracy of LD is superior to the traditional derivative (TD), whose accuracy is only of order ϵ

$$\lim_{\epsilon \rightarrow 0} \frac{f(x + \epsilon) - f(x)}{\epsilon} = \lim_{\epsilon \rightarrow 0} \left(f'(x) + \frac{1}{2}\epsilon f''(x) + \dots \right) \tag{1.3}$$

Then, ironically LD is a better method than TD at least in terms of precision. However, the technique has also certain disadvantages or shortcomings, being one of them a lengthy computation that may become tedious in some cases. Our aim in this work is to show that the standard LD is not a mathematical oddity, rather, it belongs to a broader (infinite in fact) class of integrals that converge to $f'(x)$ when $\epsilon \rightarrow 0$.

The paper is organized as follows. In sec.2, we begin by introducing this family of operators D_k that depend on an odd integer number k , which contains the standard LD for $k = 1$. A remarkable characteristic of this class is that any integral that belong to it approximates to $f'(x)$ essentially with the same accuracy, of order ϵ^2 . We also discuss why the formula works for positive odd integers and why it cannot be extended to cover also the negative odds: The appearance of poles are unavoidable for negative values of k . In addition, subsec.2.4 is devoted to investigate the close relationship that exists among the LD and the odd functions; we show that the mechanism can be generalized for an arbitrary weight odd function $g(t)$ of its integrand, and we put some particular examples. Finally, in subsec.2.5 we focus on the opposite problem, namely, the introduction of a method for integration via differentiation. We warn the reader that, throughout this letter, we will deal essentially with continuous and analytical functions, although we will also study a couple of special cases where the functions are not differentiable (in the standard sense), and show that, even for such cases, the operators introduced are well-behaved. Nevertheless, the exhaustive application of the theory to such type of special functions is a task that we leave for a future work.

2 A General Class of Lanczos Operators, D_k

In this section, we will see that given a continuous and analytic real function $f(x)$ their derivative $f'(x)$ can be approximated by an arbitrary member of the following family of operators:

$$D_k f(x) \equiv \frac{k + 2}{2\epsilon^{k+2}} \int_{-\epsilon}^{\epsilon} t^k f(x + t) dt \quad \{k = 2t + 1 \mid t \in \mathbf{Z}^+\} \tag{2.1}$$

These operators are linear since they verify the property, $D_k(f + g) = D_k f + D_k g$. In particular, we establish the following proposition:

Proposition 2.1. *Suppose that f is a continuous and analytic function defined on a neighborhood of a point x . The operators given by (2.1) all lead to the same limit, namely:*

$$\lim_{\epsilon \rightarrow 0} \frac{k + 2}{2\epsilon^{k+2}} \int_{-\epsilon}^{\epsilon} t^k f(x + t) dt = f'(x) \quad \{k = 2t + 1 \mid t \in \mathbf{Z}^+\} \tag{2.2}$$

Let us make some comments before addressing their proof. First, k is here any positive odd integer, that labels and distinguishes between the different integrals that belong to the family. For negative odd integers, the operators (2.1) become pathological and ill-defined when $\epsilon \rightarrow 0$. We will analyze a special case of this type in a next subsection.

It is worth noting that LD is only a particular case of this general family of operators, and corresponds to $k = 1$. Indeed, the substitution of $k = 1$ in (2.1) provides

$$D_1 f(x) = \frac{3}{2\epsilon^3} \int_{-\epsilon}^{\epsilon} t f(x + t) dt = f'_L(x) \tag{2.3}$$

which agrees with Eq. (1.1). We proceed now to prove the previous proposition (2.1).

Proof. The assumed properties of the function $f(x)$ allow us to write an expansion for $f(x + t)$ based on the finite representation

$$f(x + t) = f(x) + f'(x)t + \frac{f''(x)}{2}t^2 + \dots = \sum_{n=0}^m \frac{f^{(n)}(x)}{n!}t^n + R_m(f) \tag{2.4}$$

Where $R_m(f)$ is the remainder term that vanishes as $m \rightarrow \infty$. Substituting this expansion in Eq. (2.1) yields

$$D_k f(x) = \frac{k + 2}{2\epsilon^{k+2}} \left(\sum_{n=0}^m \frac{f^{(n)}(x)}{n!(n + k + 1)} t^{n+k+1} \Big|_{-\epsilon}^{\epsilon} + \mathcal{R}_m \right) \quad \{k = 2t + 1 \mid t \in \mathbf{Z}^+\} \tag{2.5}$$

Where we have defined $\mathcal{R}_m \equiv \int_{-\epsilon}^{\epsilon} t R_m dt$. Notice that since k is a positive odd, the terms corresponding to even n cannot contribute to the sum. This is because all the subtractions $\epsilon^{n+k+1} - (-\epsilon)^{n+k+1}$ vanish identically in such cases. Then, taking into account this fact, the last sum will be equal to

$$\begin{aligned} D_k f(x) &= \frac{k + 2}{2\epsilon^{k+2}} \left(\sum_{n=0}^m \frac{f^{(n)}(x)}{n!(n + k + 1)} t^{n+k+1} \Big|_{-\epsilon}^{\epsilon} + \mathcal{R}_m \right) = \frac{k + 2}{2\epsilon^{k+2}} \left(f'(x) \frac{2\epsilon^{k+2}}{k + 2} + f^{(3)}(x) \frac{2\epsilon^{4+k}}{3!(k + 4)} + f^{(5)}(x) \dots \right) \\ &= f'(x) + f^{(3)}(x) \frac{\epsilon^2(k + 2)}{3!(k + 4)} + f^{(5)}(x) \frac{\epsilon^4(k + 2)}{5!(k + 6)} + \dots \end{aligned} \tag{2.6}$$

Thus, from the last result it follows that, $\lim_{\epsilon \rightarrow 0} D_k f(x) = f'(x)$, which provides the desired result. □

On the other hand, Eq. (2.6) implies the compact formula

$$D_k f(x) \equiv \frac{k + 2}{2\epsilon^{k+2}} \int_{-\epsilon}^{\epsilon} t^k f(x+t) dt = \sum_{n=1}^{\infty} \frac{(k + 2) f^{(2n-1)}(x)}{(2n - 1)!(k + 2n)} \epsilon^{2(n-1)} = \sum_{n=1}^{\infty} a_n(k) f^{(2n-1)}(x) \epsilon^{2(n-1)} \tag{2.7}$$

where we have defined the coefficients $a_n(k)$ as,

$$a_n(k) \equiv \frac{k + 2}{(2n - 1)!(k + 2n)} \tag{2.8}$$

This formula will show to be useful in the next subsections.

2.1 Some examples. The operator D_3 . Comparison with D_1

We have shown in the previous section that $f'_L(x) = D_1 f(x)$, namely, LD corresponds to the first case (with respect to the possible values of k) within the class of functions (2.1). However, it would be very interesting to compare Lanczos' integral with other members of their own family of operators, for example, with the function that corresponds to the following odd integer, namely, $k = 3$. Then, we refer to the function $D_3 f(x)$, that according to (2.1) is given by

$$D_3 f(x) = \frac{5}{2\epsilon^5} \int_{-\epsilon}^{\epsilon} t^3 f(x + t) dt \tag{2.9}$$

What about its accuracy? Using Eqs.(2.6) and (2.7), we can see that this function also provides a very good approximation to $f'(x)$

$$D_3 f(x) = \frac{5}{2\epsilon^5} \int_{-\epsilon}^{\epsilon} t^3 f(x + t) dt = f'(x) + \frac{5}{42} \epsilon^2 f^{(3)}(x) + \dots \tag{2.10}$$

Thus, the error of the approximation to the derivative is similar to the standard LD (1.2), with a small numerical variation. Indeed, Lanczos' function gives, $D_1 f(x) \simeq f'(x) + 0, 1\epsilon^2 f^{(3)}(x)$, while $D_3 f(x)$ provides nearly the same result, i.e, $D_3 f(x) \simeq f'(x) + 0, 119\epsilon^2 f^{(3)}(x)$. This is

remarkable, indeed Eq.(2.6) implies that the accuracy is of the same order ϵ^2 for all the members of the family, although the lowest coefficient $a_2(k)$ of the class corresponds to the Lanczos function. The reason resides in the fact that the second-order coefficient $a_2(k) = (k + 2)/6(k + 4)$ that multiplies ϵ^2 , reaches their minimum value for $k = 1$, corresponding precisely to the standard LD (D_1). Indeed, note that $a_2(k)$ increases with k : $a_2(1) = 1/10$, $a_2(3) = 5/42$, $a_2(5) = 7/54$, $a_2(7) = 9/66$, and so on. However, the grow of $a_2(k)$ with k is very slow, and in the limit of large k , their value tends to stabilize around $1/6$. In Fig.(1) we plot the values of the coefficient $a_2(k)$ for a range of operators D_k .

Let us now study how D_3 and the generic operator D_k behave over some special cases of

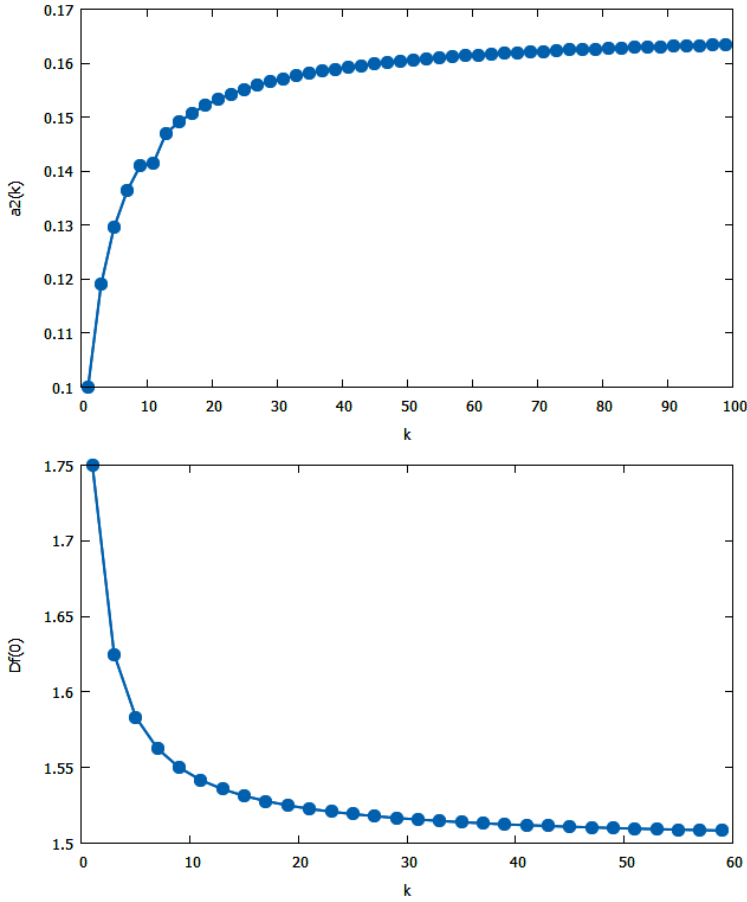


Figure 1. Behavior of the second-order coefficient $a_2(k)$ and representation of $D_k\theta(0)$ for several operators of the class. The asymptotic behavior is $a_2(k) \rightarrow 1/6$ and $D_k\theta(0) \rightarrow 3/2$

non-differentiable (in the usual sense) functions.

Example 2.2. Suppose α and β are two different real numbers. Let us define a function f such that

$$f(x) = \begin{cases} \alpha x & \text{if } x \leq 0 \\ \beta x & \text{if } x > 0. \end{cases} \tag{2.11}$$

Then

$$D_3f(0) = \frac{5}{2\epsilon^5} \int_{-\epsilon}^0 \alpha t^4 dt + \frac{5}{2\epsilon^5} \int_0^\epsilon \beta t^4 dt = \frac{\beta + \alpha}{2} \tag{2.12}$$

The last example illustrates that the Derivative $D_3f(x)$ can exist even when the ordinary derivative does not exist, and the result is the same for all the members of the family $D_kf(x)$.

$$D_kf(0) = \frac{k + 2}{2\epsilon^{k+2}} \int_{-\epsilon}^0 \alpha t^{k+1} dt + \frac{k + 2}{2\epsilon^{k+2}} \int_0^\epsilon \beta t^{k+1} dt = \frac{\beta + \alpha}{2} \tag{2.13}$$

As a corollary, we have the automatic application to the Absolute Value Function $f(x) = |x|$, which is non-differentiable in the ordinary sense at $x = 0$. Indeed, note that if we select the particular values $\alpha = -1, \beta = 1$, the function of our example becomes

$$f(x) = \begin{cases} -x & \text{if } x \leq 0 \\ x & \text{if } x > 0. \end{cases} \tag{2.14}$$

This the definition of the function $f(x) = \text{abs}(x)$. Then, substituting $\alpha = -1, \beta = 1$ into Eq. (2.13), we see that $D_k|x|_{x=0} = 0$. Notice again that the result is independent of k and therefore remains the same for a generic operator D_k of the class. Indeed, since the previous functions posses Derivatives that yield the same output regardless the particular operator chosen, let us continue now by introducing an special type of function with a discontinuity point and whose Generalized Derivatives evaluated at such point exist and depend explicitly on k .

Example 2.3. Let ϵ be a positive real parameter, and let us define an step function $\theta(x)$ such that

$$\theta(x) = \begin{cases} 0 & \text{if } x \leq 0 \\ \epsilon & \text{if } x > 0. \end{cases} \tag{2.15}$$

$$D_k\theta(0) = \frac{k+2}{2\epsilon^{k+2}} \int_{-\epsilon}^0 t^{k+1} dt + \frac{k+2}{2\epsilon^{k+2}} \int_0^\epsilon t^k(\epsilon+t) dt = \frac{3k+4}{2k+2} \tag{2.16}$$

Then, the Generalized Derivatives D_k may exist even at points of discontinuity. For several members of the class the values at the discontinuity are $D_1\theta(0) = 7/4, D_3\theta(0) = 13/8, D_5\theta(0) = 19/12$, and so on. Notice that $D_k\theta(0) \rightarrow 3/2$ as $k \rightarrow \infty$. In Fig.(1) we plot the values of the Generalized Derivatives of $\theta(x)$ at $x = 0$ as function of k .

2.2 Pathological behavior for negative values of k . Divergences

Due to the fact that the formula (2.1) gives satisfactory results for any k positive odd, it seems natural to investigate their possible extension to cover the negative odd values as well . Nevertheless, in such cases the integrals (2.1) turn out to be pathological and ill-defined when $\epsilon \rightarrow 0$, containing besides a certain number of poles. For example, let us pay attention to the first case, namely, $k = -1$. The function $D_{-1}(x)$ is defined by the integral

$$D_{-1}f(x) = \frac{1}{2\epsilon} \int_{-\epsilon}^\epsilon \frac{f(x+t)}{t} dt \tag{2.17}$$

And expanding the function $f(x+t)$ we obtain

$$\begin{aligned} D_{-1}f(x) &= \frac{1}{2\epsilon} \int_{-\epsilon}^\epsilon \frac{f(x+t)}{t} dt = \frac{1}{2\epsilon} \int_{-\epsilon}^\epsilon \left(\frac{f(x)}{t} + f'(x) + \frac{f''(x)}{2}t + \frac{f^{(3)}(x)}{3!}t^2 + \dots \right) dt \\ &= \frac{1}{2\epsilon} \int_{-\epsilon}^\epsilon \frac{f(x)}{t} dt + f'(x) + \frac{1}{18}f^{(3)}(x)\epsilon^2 + \dots \end{aligned} \tag{2.18}$$

The problem lies in the first term, because not only the Riemann integral here does not exist (the antiderivative of $1/t$ is $\ln|t|$), but also blows up when $\epsilon \rightarrow 0$. This destroys the rest of the well-behaved expansion. For $k = -3$ the situation does not improve

$$D_{-3}f(x) = -\frac{\epsilon}{2} \int_{-\epsilon}^\epsilon \frac{f(x+t)}{t^3} dt = \frac{f'(x)}{\epsilon^2} - \frac{f''(x)}{2} \epsilon \int_{-\epsilon}^\epsilon \frac{dt}{t} - \frac{f^{(3)}(x)}{3!} \epsilon^2 + \dots \tag{2.19}$$

Now the pathological term remains, but as $\epsilon \rightarrow 0$ the divergence persists and even worsens. In general, the divergence will worsen if k becomes more negative. Then, the family of well-behaved functions $D_k f(x)$ that converge to $f'(x)$ when $\epsilon \rightarrow 0$, are those where the values of k are constrained to the positive odd integers, as we have shown in the previous subsections.

2.3 Properties of D_k and higher-order derivatives

Proposition 2.4 (Leibniz Rule). *Let f and g be a couple of continuous and analytic real functions defined on a neighborhood of a point x . The product rule of the standard differential calculus is recovered by $D_k(f \cdot g)$ when $\epsilon \rightarrow 0$, namely:*

$$\lim_{\epsilon \rightarrow 0} D_k(f \cdot g) = f'g + fg' \quad \{k = 2t + 1 \mid t \in \mathbf{Z}^+\} \quad (2.20)$$

Proof. From Eq.(2.1) we have

$$\begin{aligned} D_k(f \cdot g) &= \frac{k+2}{2\epsilon^{k+2}} \int_{-\epsilon}^{\epsilon} t^k f(x+t)g(x+t)dt = \frac{k+2}{2\epsilon^{k+2}} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{f^{(n)}(x)g^{(m)}(x)}{n!m!} \int_{-\epsilon}^{\epsilon} t^{k+n+m} dt \\ &= \frac{k+2}{2\epsilon^{k+2}} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{f^{(n)}(x)g^{(m)}(x)}{n!m!} \frac{1}{n+m+k+1} \left(\epsilon^{n+m+k+1} - (-\epsilon)^{n+m+k+1} \right) \end{aligned} \quad (2.21)$$

Since k is odd, the only terms that do not vanish are those for which $n+m$ is also an odd integer. It is therefore clear that the previous sum acquires the form

$$\begin{aligned} D_k(f \cdot g) &= \frac{k+2}{2\epsilon^{k+2}} \left(fg' \frac{2\epsilon^{k+2}}{k+2} + f'g \frac{2\epsilon^{k+2}}{k+2} + \frac{\epsilon^{k+4}}{(k+4)} (f'g'' + f''g') + \frac{\epsilon^{k+4}}{3(k+4)} (fg^{(3)} + f^{(3)}g) + \dots \right) \\ &= f'g + fg' + \frac{k+2}{k+4} \epsilon^2 \left(\frac{1}{2} (f'g'' + f''g') + \frac{1}{6} (fg^{(3)} + f^{(3)}g) \right) + \dots \end{aligned} \quad (2.22)$$

We conclude that $\lim_{\epsilon \rightarrow 0} D_k(f \cdot g) = f'g + fg'$ \square

It is important to note that the standard product rule and even the more general involving the Lanzcos Derivatives, namely, $D_k(f \cdot g) = gD_k f + fD_k g$ are only valid for analytic functions, otherwise these rules are not satisfied. For example, let us evaluate $D_k \theta^2(x)$, where $\theta(x)$ is the step function defined in (2.15)

$$D_k \theta(x)^2 = \frac{k+2}{2\epsilon^{k+2}} \int_{-\epsilon}^0 t^{k+1} dt + \frac{k+2}{2\epsilon^{k+2}} \int_0^{\epsilon} t^k (\epsilon+t)^2 dt = \frac{1}{2} + \frac{\epsilon}{2} \left(\frac{k+2}{k+1} + \frac{k+2}{k+3} + 1 \right) \quad (2.23)$$

The details are left to the reader, but it is not difficult to see that this result does not match with $2\theta D_k \theta$, namely, $D_k \theta^2 \neq 2\theta D_k \theta$. Therefore, the argument given for example in Ref. ([11]) for the standard LD (D_1) is also true for the complete class of operators D_k .

We address now how to appropriately introduce the higher-order operators, i.e. higher orders Generalized Derivatives $D_k^{(n)}$

Proposition 2.5. *Let f be a continuous and analytic function defined on a neighborhood of a point x . Then*

$$\lim_{\epsilon \rightarrow 0} D_k^{(2)} f(x) = f''(x) \quad \{k = 2t + 1 \mid t \in \mathbf{Z}^+\} \quad (2.24)$$

Proof. We begin by noting that

$$D_k^{(2)} f(x) = \frac{k+2}{2\epsilon^{k+2}} \int_{-\epsilon}^{\epsilon} t^k D_k f(x+t) dt \quad (2.25)$$

Using the expansion in powers of ϵ given by means of Eq. (2.7), we obtain

$$\begin{aligned} D_k^{(2)} f(x) &= \frac{k+2}{2\epsilon^{k+2}} \int_{-\epsilon}^{\epsilon} t^k D_k f(x+t) dt = \frac{k+2}{2\epsilon^{k+2}} \sum_{n=1}^{\infty} a_n(k) \epsilon^{2(n-1)} \int_{-\epsilon}^{\epsilon} t^k f^{(2n-1)}(x+t) dt \\ &= \frac{k+2}{2\epsilon^{k+2}} \sum_{n=1}^{\infty} \sum_{m=0}^{\infty} a_n(k) \epsilon^{2(n-1)} \frac{f^{(2n+m-1)}(x)}{m!} \int_{-\epsilon}^{\epsilon} t^{k+m} dt \end{aligned} \quad (2.26)$$

Following an equivalent reasoning employed previously, we can compute the leading terms of this expansion which turn out to be

$$D_k^{(2)} f(x) = \frac{k+2}{2\epsilon^{k+2}} \left(a_1(k) f''(x) \frac{2\epsilon^{k+2}}{k+2} + f^{(4)}(x) \epsilon^{k+4} \left(\frac{a_1(k)}{3(k+4)} + \frac{2a_2(k)}{k+2} \right) + \dots \right) \quad (2.27)$$

The coefficients $a_1(k)$ and $a_2(k)$ can be computed by virtue of Eq. (2.8) which provides, $a_1(k) = 1$, $a_2(k) = \frac{k+2}{6(k+4)}$. Hence we finally obtain the result

$$D_k^{(2)} f(x) = f''(x) + f^{(4)}(x) \frac{k+2}{3(k+4)} \epsilon^2 + \dots \quad (2.28)$$

□

It is possible to write from Eq.(2.25) a full integral representation of $D_k^{(2)}$, which turns out to be

$$D_k^{(2)} f(x) = \frac{k+2}{2\epsilon^{k+2}} \int_{-\epsilon}^{\epsilon} t^k D_k f(x+t) dt = \frac{(k+2)^2}{4\epsilon^{2k+4}} \int_{-\epsilon}^{\epsilon} \int_{-\epsilon}^{\epsilon} (t_1 t_2)^k f(x+t_1+t_2) dt_1 dt_2 \quad (2.29)$$

On the other hand, an iterative process allows to define the n-esime Generalized Lanczos Derivative $D_k^{(n)} f(x)$ by means of the recursive formula

$$D_k^{(n)} f(x) = \frac{k+2}{2\epsilon^{k+2}} \int_{-\epsilon}^{\epsilon} t^k D_k^{(n-1)} f(x+t) dt \quad \{k = 2t + 1 \mid t \in \mathbf{Z}^+\} \quad (2.30)$$

And their explicit integral representation is given by

$$D_k^{(n)} f(x) = \frac{(k+2)^n}{2^n \epsilon^{n(k+2)}} \int_{-\epsilon}^{\epsilon} \int_{-\epsilon}^{\epsilon} \dots \int_{-\epsilon}^{\epsilon} \prod_{r=1}^n t_r^k f\left(x + \sum_{r=1}^n t_r\right) dt_1 dt_2 \dots dt_n \quad \{k = 2t + 1 \mid t \in \mathbf{Z}^+\} \quad (2.31)$$

2.4 Other generalizations of the Lanczos mechanism.

Let us conclude the discussion concerning the generalized LD by showing how, apart from the whole family of operators D_k , there exist other natural generalizations of the Lanczos mechanism. Indeed, we are going to study a couple of cases that are apparently not related, and then we will show that the similarities among these functions with the standard LD are not a mere coincidence. Rather, they all belong to a common mathematical structure. This will allow us to construct the more general LD, an operator that we will denote as \mathcal{L}_ϵ , built by a generic weight function $g(t)$ of their integrand with specific parity properties. Let us start by defining the following operator \mathcal{D}_ϵ .

$$\mathcal{D}_\epsilon f \equiv \frac{3}{2\epsilon^3} \int_{-\epsilon}^{\epsilon} \sin(t) f(x+t) dt \quad (2.32)$$

This function also provides an excellent approximation to $f'(x)$. We omit the details of the proof, since are very similar to those employed throughout this work and therefore do not add anything substantially new. Indeed, the reader may verify that

$$\mathcal{D}_\epsilon f(x) = \frac{3}{2\epsilon^3} \int_{-\epsilon}^{\epsilon} \sin(t) f(x+t) dt = f'(x) + \frac{\epsilon^2}{10} (f'''(x) - f'(x)) + \dots \quad (2.33)$$

If we compare this result with that of the standard LD (D_1) given by Eq.(1.2), we can see that the precision provided by the function (2.32) is at least even if not better (depending on the sign of f'). Indeed, notice that in those special cases where $f' = f'''$ at a given point, the first correction of order ϵ^2 vanishes and the error decreases to $\mathcal{O}(\epsilon^4)$ or beyond. The fact that Eq.(2.32) also converges to $f'(x)$ is not a mere coincidence. Indeed, let us exchange the function $\sin(t)$

of the integrand by another odd function; for example, instead we can select their hyperbolic counterpart, i.e, $\sinh(t)$ and define an operator $\mathcal{D}_\epsilon^\dagger$ such that

$$\mathcal{D}_\epsilon^\dagger f(x) \equiv \frac{3}{2\epsilon^3} \int_{-\epsilon}^\epsilon \sinh(t)f(x+t)dt = f'(x) + \frac{\epsilon^2}{10} (f'''(x) + f'(x)) + \dots \tag{2.34}$$

It is natural to wonder if all that is valid for the odd functions $t, t^k, \sin(t), \sinh(t)$ will be valid as well for a generic odd function of the integrand. Indeed, let us define a weight function $g(t)$ such that, $g(-t) = -g(t)$, continuous and analytic on a neighborhood of $t = 0$. We define a Generalized Lanczos Derivative, such that

$$\mathcal{L}_\epsilon f(x) \equiv \frac{3}{2\epsilon^3} \int_{-\epsilon}^\epsilon g(t)f(x+t)dt. \tag{2.35}$$

If $g(t)$ is an odd and analytic weight function its expansion is given by the finite Taylor representation

$$g(t) = \sum_{m=0}^{m'} g^{(2m+1)}(0) \frac{t^{2m+1}}{(2m+1)!} + R_{m'}(g) \tag{2.36}$$

Where $g^{(2m+1)}(0)$ denotes the $(2m+1)$ -esime derivative of the weight function $g(t)$ and $R_{m'}(g)$ is a remainder term that vanishes as $m' \rightarrow \infty$. Substituting this expansion in Eq. (2.37) we obtain the result

$$\mathcal{L}_\epsilon f(x) = \frac{3}{2\epsilon^3} \int_{-\epsilon}^\epsilon g(t)f(x+t)dt = g'(0)f'(x) + \frac{\epsilon^2}{10} (g'(0)f'''(x) + f'(x)g'''(0)) + \mathcal{O}(\epsilon^4) \tag{2.37}$$

And therefore, $\lim_{\epsilon \rightarrow 0} \mathcal{L}_\epsilon f(x) = g'(0)f'(x)$ which shows that $\mathcal{L}_\epsilon f(x)$ provides for small ϵ the first derivative with a normalization or weight given by the factor $g'(0)$. For the particular case $g(t) = t$ (the standard LD) this normalization obviously reduces to 1, providing the exact first derivative. Indeed, particularizing Eq. (2.37) for different odd weight functions, namely, $g(t)=t, \sin(t)$, and $\sinh(t)$ we automatically recover the results for the standard LD $f'_L(D_1), \mathcal{D}_\epsilon$, and $\mathcal{D}_\epsilon^\dagger$ given by Eqs. (1.2), (2.33) and (2.34), respectively. On the other hand, for the special case $g(t) = t^k, k \in 2\mathbb{Z}^+ + 1$, the dependence on ϵ needs to be corrected, namely, the term $3/2\epsilon^3$ must be replaced by the more general factor $(k+2)/2\epsilon^{k+2}$, since for $g(t) = t^k$ all the derivatives at $t = 0$ vanish up to the k -esime order. This is precisely the case of the family of operators D_k that we presented in the beginning of this letter.

2.5 Integration by differentiation

In this last part we are going to investigate an opposed method to the Lanczos mechanism. As is well known, in general it turns out to be more complicated to integrate than to differentiate (at least in the standard sense). Indeed, differentiation is a simpler process from the technical point of view while integration requires in most cases the employment of numerical methods. Then, it would be interesting to investigate alternative ways of integration, for example, the apparently contradictory integration by differentiation, which is the opposed mathematical mechanism to the generalized Lanczos method that we discussed in the first part of this work. The existence of a technique for integrating by differentiating could open new ways to think about old problems in multiple branches of mathematics and theoretical physics. In this sense, we believe that it never hurts to have new mathematical tools. Let us begin by introducing the following proposition

Proposition 2.6. *Let f be a real-valued continuous and analytic function defined on the closed and bounded interval $[-\epsilon, \epsilon], \epsilon \in \mathbb{R}$. Their Riemann integral may be computed by the equivalent prescription*

$$\int_{-\epsilon}^\epsilon f(x)dx = \lim_{t \rightarrow 0} f\left(\frac{d}{dt}\right) \left(\frac{2 \sinh(\epsilon t)}{t}\right) \tag{2.38}$$

Proof. Since $f(x)$ is continuous on the closed and bounded interval $[-\epsilon, \epsilon]$ then is Riemann integrable. We start by noting that

$$f(x) = \lim_{t \rightarrow 0} f\left(\frac{d}{dt}\right) e^{tx} \tag{2.39}$$

This identity is always valid as long as $f(x)$ is analytic. Thus, the integration with respect to x provides

$$\int f(x)dx = \int \lim_{t \rightarrow 0} f\left(\frac{d}{dt}\right)e^{tx} dx = \lim_{t \rightarrow 0} f\left(\frac{d}{dt}\right) \int e^{tx} dx = \lim_{t \rightarrow 0} \left(f\left(\frac{d}{dt}\right)\frac{e^{tx}}{t} + h(t) \right) \tag{2.40}$$

Since this is a indefinite integral, we should add to the result a constant, or more generically in this case, a function $h(t)$. Thus, the symmetric definite integral gives

$$\int_{-\epsilon}^{\epsilon} f(x)dx = \lim_{t \rightarrow 0} \left(f\left(\frac{d}{dt}\right)\frac{e^{tx}}{t} + h(t) \right) \Big|_{-\epsilon}^{\epsilon} = \lim_{t \rightarrow 0} f\left(\frac{d}{dt}\right)\left(\frac{e^{t\epsilon} - e^{-t\epsilon}}{t}\right) = \lim_{t \rightarrow 0} f\left(\frac{d}{dt}\right)\left(\frac{2 \sinh(t\epsilon)}{t}\right) \tag{2.41}$$

□

We underline that $f(d/dt)$ should be understood as a differential operator. For example, for the particular case of an analytic function that admits a MacLaurin expansion, namely, $f(t) = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} t^n$, the operator $f(d/dt)$ will acquire the form

$$f\left(\frac{d}{dt}\right) = f(0) + f'(0)\frac{d}{dt} + \frac{f''(0)}{2}\frac{d^2}{dt^2} + \dots = \sum_{n=0}^m \frac{f^{(n)}(0)}{n!} \frac{d^n}{dt^n} + \mathcal{R}_m(f(d/dt)) \tag{2.42}$$

Where \mathcal{R}_m is a remainder operator. Notice that (2.42) is linear since, $f(d/dt)(g + h) = f(d/dt)g + f(d/dt)h$. On the other hand, once established the proof of proposition (2.6), let us give a quick example of application with a random test function to see how the method works. For instance, we can select $f(t) = t^n$, whose symmetric definite integral provides, $\int_{-\epsilon}^{\epsilon} t^n dt = 2\frac{\epsilon^{n+1}}{n+1}$ for even n . (and zero for odd n). We begin with the infinite Taylor representation of the hyperbolic function $\sinh(\epsilon t)$

$$\sinh(\epsilon t) = \sum_{m=1}^{\infty} \frac{(\epsilon t)^{2m-1}}{(2m-1)!} \tag{2.43}$$

Then, the differential operator $f(d/dt)$ acting on the function $\sinh(\epsilon t)/t$ that appears on the left hand side of (2.38) acquires the form

$$f\left(\frac{d}{dt}\right)\left(\frac{2 \sinh(\epsilon t)}{t}\right) = 2 \frac{d^n}{dt^n} \sum_{m=1}^{\infty} \frac{\epsilon^{2m-1} t^{2m-2}}{(2m-1)!} = \begin{cases} 2\frac{\epsilon^{n+1}}{n+1} + \mathcal{O}(t^2) & \text{for even } n \\ 2\frac{\epsilon^{n+2}}{n+2}t + \mathcal{O}(t^3) & \text{for odd } n \end{cases} \tag{2.44}$$

It is worth noting that in the limit $t \rightarrow 0$ the algorithm converges identically to the definite integral. It is also interesting to mention that the precision of the technique depends on the parity of the function. On the other hand, although the explicit form of the function $h(t)$ did not play any role in the demonstration of prop. (2.6), it could exist, however, some situations where the knowledge of $h(t)$ turns out to be convenient, e.g, if we need to compute the indefinite integral (2.40). Then, let us determine its value for completeness purposes. For the sake of simplicity, we assume that $f(x)$ is analytic and admits a MacLaurin expansion around $x = 0$. Then, we can substitute in Eq. (2.40) $f(x)$ by

$$\int f(x)dx = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} \int x^n dx = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{(n+1)!} x^{n+1} \tag{2.45}$$

On the other hand, developing the right hand side of (2.40) we find

$$\begin{aligned} \lim_{t \rightarrow 0} \left(f\left(\frac{d}{dt}\right)\frac{e^{tx}}{t} + h(t) \right) &= \lim_{t \rightarrow 0} \left(\sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} \frac{d^n}{dt^n} \left(\frac{1}{t} + x + \frac{x^2 t}{2} + \frac{x^3 t^2}{3!} + \dots \right) + h(t) \right) \\ &= \lim_{t \rightarrow 0} \left(\sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} \frac{d^n}{dt^n} \left(\frac{1}{t} \right) + h(t) \right) + \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{(n+1)!} x^{n+1} \end{aligned} \tag{2.46}$$

Then, comparing (2.45) with (2.46), we obtain

$$\lim_{t \rightarrow 0} \left(\sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} \frac{d^n}{dt^n} \left(\frac{1}{t} \right) + h(t) \right) = 0 \quad (2.47)$$

Or equivalently

$$h(t) = - \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} \frac{d^n}{dt^n} \left(\frac{1}{t} \right) = -f \left(\frac{d}{dt} \right) \frac{1}{t} \quad (2.48)$$

Therefore, the indefinite integral (2.40) will acquire the final expression

$$\int f(x) dx = \lim_{t \rightarrow 0} f \left(\frac{d}{dt} \right) \left(\frac{e^{tx} - 1}{t} \right) \quad (2.49)$$

An arbitrary constant C may be added to the last equation. It is interesting to note again that the right hand side involves a differential operator that depends on the form of $f(x)$. Shortly after completing this work, we discovered that in two recent papers (see Ref.[19, 20]), another mechanism was introduced for integration by differentiation, including interesting applications to Fourier and Laplace transforms. Nevertheless, after comparing their results with ours, we conclude that both approaches are equivalent¹, including our picture an explicit discussion on the role of the function $h(t)$, and other important aspects concerning the accuracy or precision of the technique. It is also worth mentioning that (2.49), allows to find automatically the general (non-symmetric) definite integral

$$\int_x^{x'} f(x) dx = \lim_{t \rightarrow 0} f \left(\frac{d}{dt} \right) \left(\frac{e^{tx} - 1}{t} \right) \Big|_x^{x'} = \lim_{t \rightarrow 0} f \left(\frac{d}{dt} \right) \left(\frac{e^{tx'} - e^{tx}}{t} \right) \quad (2.50)$$

This formula, which can also be deduced by virtue of (2.40) (recall that explicit form of $h(t)$ is irrelevant for the computation of the definite integral, the subtraction involved removes the function), agrees with the result that Kempf et al.[20] obtained by another approach. With this outcome, it is straightforward to generalize the method for improper integrals by taking the corresponding limits directly from the previous expression. Having reached this point, it would be interesting to analyze the accuracy of the algorithm for the indefinite case as well. For this purpose, we can test the method for the function $f(x) = x^n$, because if a given function is analytic and admits a MacLaurin or a Taylor expansion, it is sufficient to verify the behavior of the n -esime term of the series. Then we have

$$f \left(\frac{d}{dt} \right) \left(\frac{e^{tx} - 1}{t} \right) = \frac{d^n}{dx^n} \left(\frac{e^{tx} - 1}{t} \right) = \frac{d^n}{dx^n} \sum_{m=1}^{\infty} \frac{x^m t^{m-1}}{m!} = \frac{x^{n+1}}{n+1} + \frac{x^{n+2}}{n+2} t + \dots \quad (2.51)$$

Hence, in this case the accuracy is $\mathcal{O}(t)$ and does not depend on the parity of the function. Investigations to extend these methods to more general situations are currently underway.

3 Final Remarks

In this work, we have shown that the Lanczos Derivative $f'_L(x)$ is not a mathematical oddity, rather, it only represents the first ($k = 1$) of a broad class of integrals $D_k f(x)$, $k \in 2\mathbb{Z}^+ + 1$, that converge to the derivative of a function in the limit $\epsilon \rightarrow 0$ (differentiation by integration). As we have proved, any member of this family can be used to compute derivatives of functions at points where the standard derivative does not exist. The properties of the class were also investigated in detail. In particular, we have demonstrated that for some special cases of continuous but not differentiable functions (and even at points of discontinuity) the family of operators D_k are well-behaved, such as the higher-order derivatives, that maintain under control the level of accuracy always at $\mathcal{O}(\epsilon^2)$. In addition, we have presented other examples of generalized LD where the structure of the integrand is extended to include more generic odd functions (periodic or hyperbolic) yielding similar results. This allowed us to realize that the Lanczos mechanism may be

¹I thank Achim Kempf for pointing out to me the equivalence of both approximations

generalized by an arbitrary odd function $g(t)$ of their integrand. In the last part of the work, we discussed a mechanism for the opposite process, namely, integration by differentiation. We have shown that the accuracy of the method may depend on the parity of the function (at least for some definite integrals). Nevertheless, this does not seem a shortcoming of the mechanism, rather, it seems inherent to the integration process itself, although further investigations are required to better understand this point.

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