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MAXIMAL GENERALIZATION OF LANCZOS' DERIVATIVE USING ONE-DIMENSIONAL INTEGRALS

Andrej Liptaj

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Abstract. The derivative of a function can be expressed in terms of integration over a small neighborhood of the point of differentiation, so-called *differentiation by integration* method. In this text a maximal generalization of existing results which use one-dimensional integrals is presented together with some interesting non-analytic weight functions.

1 Introduction

Cornelius Lanczos in his work [1] published a method of differentiation by integration[1], where the derivative of a function is approximated by an integral. The integral is performed over a small interval around the point of differentiation with the approximation becoming exact in the limit of the interval length approaching zero. For differentiable functions one has

$$f'(x_0) \equiv f'(x)\,|_{x=x_0} = \lim_{h\to 0} \frac{3}{2h^3} \int_{-h}^{h} t f(x_0+t)\, dt.$$

The expression is interesting from several aspects: it generalizes the ordinary derivative[2] and, also, its modifications might be useful for numerical differentiation (see e.g. [3, 4]).

Since, the topic was addressed by several authors with noticeable growth of interest in the last decade [3, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17]. The millennial work [7] is probably the most interesting of them: the authors actually provide a very broad generalization of the Lanczos' formula for the first derivative and their approach can be further and straightforwardly generalized to higher orders (as done in this article). Their text is, surprisingly, widely overlook by later works with exception of [4, 9, 12], which, however, do not exploit the potential of it.

In what follows, the second section will be dedicated to the generalization of the Lanczos' approach for the first derivative. The next section will cover the generalization to higher-order derivatives and, in the fourth section, a short discussion will follow. A summary and conclusion will constitute the last section.

Let us remark that generalizations based on multidimensional integrals can be found in literature (e.g. formula 2.31 in [17]). Unlike other approaches, they, presumably, do not represent a special case of the generalization presented here and remain an independent way of generalizing the Lanczos' derivative.

2 First derivative

Let us restate the findings from [7]. The key observation which allows for large generalizations is, that the approximation of the derivative can be seen as averaging the derivative over some

[1]The first person to publish such a method was Cioranescu [2]. The name of the method is however usually associated with Lanczos.

[2]Converges in situations, where the ordinary derivative is not defined.

small interval $[x_0 - h, x_0 + h]$ around the point of differentiation x_0. This average might be understood as weighted average with a weight function w_h

$$f'(x_0) \approx \int_{x_0-h}^{x_0+h} w_h(t) f'(t)\, dt, \tag{2.1}$$
$$\text{where } \int_{x-h}^{x+h} w_h(t)\, dt = 1.$$

Negative weights cannot be excluded, yet the condition $0 \le w_h(t)$ might be adopted if desired. Because the weight functions are of the most interest here, a modified version of (2.1) will be used throughout this text

$$f'(x_0) \approx \int_{-1}^{1} w(t) f'(x_0 + ht)\, dt,$$
$$\int_{-1}^{1} w(t)\, dt = 1,$$

so that the weight functions are defined on a "standard" interval $[-1, 1]$. One has

$$w(t) = h w_h(x_0 + ht).$$

Using the integration by partes one arrives to

$$f'(x_0) \approx \frac{1}{h}\left[w(t) f(x_0 + ht)\right]_{t=-1}^{t=1} - \frac{1}{h}\int_{-1}^{1} w'(t) f(x_0 + ht)\, dt.$$

Two interesting observations can be done:

- If w is constant $w(t) = 0.5$ then the standard definition of the derivative is recovered

$$f'(x_0) \approx \frac{f(x_0 + h) - f(x_0 - h)}{2h}.$$

- If $w(-1) = w(+1) = 0$ then a *differentiation by integration* method is constructed

$$f'(x_0) \approx -\frac{1}{h}\int_{-1}^{1} w'(t) f(x_0 + ht)\, dt.$$

The usual Lanczos' expression is obtained for

$$w(t) = \frac{3}{4}\left(1 - t^2\right).$$

Indeed

$$w'(t) = -\frac{3}{2}t \quad \longrightarrow \quad f'(x_0) \approx \frac{3}{2h}\int_{-1}^{1} t f(x_0 + ht)\, dt = \frac{3}{2h^3}\int_{-h}^{h} z f(x_0 + z)\, dz.$$

At this point one can formulate the generalization: *Any* differentiable function w which satisfies

$$\int_{-1}^{1} w(t)\, dt = 1 \text{ and } w(-1) = w(1) = 0$$

can be used for the *differentiation by integration* in the following manner

$$f'(x_0) \approx -\frac{1}{h}\int_{-1}^{1} w'(t) f(x_0 + ht)\, dt,$$

where its derivative w' appears.

Let us define some useful terms: "kernel function" will from now on refer to the function which is being integrated (together with function values) in the *differentiation by integration* procedure[3] and let us note by a small zero those anti-derivatives of a function k which take value zero at minus one

$$k_0^{(-n)}(t)\,|_{t=-1}=0, \quad \frac{d}{dt}k_0^{(-n)}=k_0^{(-n+1)}.$$

One can now address the question about a proper kernel function (inverse implication). From what was shown one can deduce: k is a valid kernel function iff

$$k_0^{(-1)}(t)\,|_{t=+1}=0 \text{ and } \int_{-1}^{1} k_0^{(-1)}(t)\,dt=1. \tag{2.2}$$

The first of the two conditions is equivalent to

$$\int_{-1}^{1} k(t)\,dt=0.$$

Indeed, proceeding by integration by parts one observes ($\lambda=\Lambda'$)

$$-\frac{1}{h}\int_{-1}^{1}\lambda(t)\,f(x_0+ht)\,dt=-\frac{1}{h}\left[\Lambda(t)\,f(x_0+ht)\right]_{t=-1}^{t=1}+\int_{-1}^{1}\Lambda(t)\,f'(x_0+ht)\,dt.$$

If $\Lambda(\pm1)\neq 0$, one cannot make vanish the first term on the RHS for a general function f. If one takes the limit $h\to 0$ in the second term (using the continuity of f') one arrives to

$$\lim_{h\to 0}\int_{-1}^{1}\Lambda(t)\,f'(x_0+ht)\,dt=\int_{-1}^{1}\Lambda(t)\,f'(x_0)\,dt=f'(x_0)\int_{-1}^{1}\Lambda(t)\,dt.$$

One sees that a function with integral different from one provides a wrong value of the derivative. Formulas (2.2) express sufficient and necessary conditions a kernel function has to fulfill, they represent the largest possible generalization of the Lanczos' approach.

3 Higher order derivatives

3.1 Main result

A repeated integration by parts allows for an immediate generalization

$$\begin{aligned}
&\int_{-1}^{1} w(t)\,f^{(n)}(x_0+ht)\,dt=\\
&=\frac{1}{h}\left[w(t)\,f^{(n-1)}(x_0+ht)\right]_{-1}^{1}-\frac{1}{h}\int_{-1}^{1}w'(t)\,f^{(n-1)}(x_0+ht)\,dt\\
&=\frac{1}{h}\left[w(t)\,f^{(n-1)}(x_0+ht)\right]_{-1}^{1}-\frac{1}{h^2}\left[w'(t)\,f^{(n-2)}(x_0+ht)\right]_{-1}^{1}\\
&\quad+\frac{1}{h^2}\int_{-1}^{1}w''(t)\,f^{(n-2)}(x_0+ht)\,dt\\
&=\left(\frac{-1}{h}\right)^{n}\int_{-1}^{1}w^{(n)}(t)\,f(x_0+ht)\,dt+\sum_{k=0}^{n-1}\frac{(-1)^k}{h^{k+1}}\left[w^{(k)}(t)\,f^{(n-1-k)}(x_0+ht)\right]_{-1}^{1}.
\end{aligned}$$

To make, for a general function f, the second term vanish, one has to require

$$w^{(k)}(-1)=w^{(k)}(1)=0 \text{ for all } k=0,1,\ldots,n-1. \tag{3.1}$$

Having this property, then, with an appropriate weight function

$$\int_{-1}^{1} w(t)\,dt=1, \tag{3.2}$$

[3] In case of the first derivative the kernel function is w'.

and assuming $f^{(n)}$ is continuous, one interprets the first term as an approximation of the n-th derivative

$$\lim_{h\to 0}\left(\frac{-1}{h}\right)^n \int_{-1}^{1} w^{(n)}(t)\, f(x_0+ht)\,dt = \lim_{h\to 0}\int_{-1}^{1} w(t)\, f^{(n)}(x_0+ht)\,dt$$
$$= f^{(n)}(x_0)\int_{-1}^{1} w(t)\,dt$$
$$= f^{(n)}(x_0).$$

Like at the end of the Sec. 2, one can inverse the whole procedure, start with the expression $\int_{-1}^{1} w^{(n)}(t)\, f(x_0+ht)\,dt$ and proceed to n repeated integrations by parts (integrate $w^{(n)}$ and differentiate f). As a result one can immediately conclude: If k is to be a valid kernel for the *differentiation by integration* in the formula

$$f^{(n)}(x_0) \approx \left(\frac{-1}{h}\right)^n \int_{-1}^{1} k(t)\, f(x_0+ht)\,dt \tag{3.3}$$

then

$$k_0^{(-j)}(1) = 0 \text{ for all } j = 1,2,\ldots,n$$

and

$$\int_{-1}^{1} k_0^{(-n)}(t)\,dt = 1.$$

With these statements valid for *any* weight/kernel functions for which appropriate derivatives or integrals exist, one can claim that, for the Lanczos' derivative written in the from (3.3), the generalization is maximal.

3.2 Examples

With the acquired knowledge one can propose some new, potentially interesting kernels and weight functions. The idea of universality might be a compelling one, by which we mean the independence on the order of the derivative (from now on noted n). Kernels have to be n-dependent[4], but one can look for n-independent weight functions. Such a universal weight function has to fulfill the condition (3.1) for all derivatives, yet it cannot be zero so as to respect the condition (3.2). Therefore it must be non-analytic at -1 and 1.

As the first example we propose

$$w_e = \frac{1}{K}\exp\left(\frac{1}{x^2-1}\right) \text{ with } K \approx 0.4439938161680786.$$

With no explicit n-dependence in the weight function, this dependence comes from the differentiation

$$f^{(n)}(x_0) \approx \left(\frac{-1}{h}\right)^n \frac{1}{K}\int_{-1}^{1} dt f(x_0+ht)\,\frac{d^n}{dt^n}\exp\left(\frac{1}{t^2-1}\right).$$

Explicit formulas for the first three derivatives are

$$f^{'}(x_0) \approx \frac{2}{hK}\int_{-1}^{1} dt f(x_0+ht)\,\frac{t}{(t-1)^2(t+1)^2}\exp\left(\frac{1}{t^2-1}\right),$$

$$f^{''}(x_0) \approx \frac{2}{h^2K}\int_{-1}^{1} dt f(x_0+ht)\,\frac{3t^4-1}{(t-1)^4(t+1)^4}\exp\left(\frac{1}{t^2-1}\right),$$

$$f^{'''}(x_0) \approx \frac{4}{h^3K}\int_{-1}^{1} dt f(x_0+ht)\,\frac{t\left(6t^6+3t^4-10t^2+3\right)}{(t-1)^6(t+1)^6}\exp\left(\frac{1}{t^2-1}\right).$$

[4]The LHS of (3.3) is n-dependent, so has to be the RHS. But, with the exception of $\left(\frac{-1}{h}\right)^n$, there are no other explicit n-dependent factors on the RHS, thus the dependence must be hidden in $k(t)$.

Even more interesting example is a one with the shifted Fabius function [18]

$$w_{Fb}(t) = Fb(t+1).$$

The Fabius function (noted Fb) is non-analytic for all $0 \leq x$ and its behavior with respect to the conditions (3.1, 3.2) can be deduced from the differential functional equation

$$Fb'(x) = 2Fb(2x). \tag{3.4}$$

One has

$$\int_0^2 Fb(x)\, dx \overset{x=2z}{=} \int_0^1 2Fb(2z)\, dz = \int_0^1 Fb'(z)\, dz = [Fb(z)]_{z=0}^{z=1} = 1,$$

$$0 = Fb(0) = \frac{1}{2}Fb'(0) = \frac{1}{2}\frac{1}{4}Fb''(0) = \ldots,$$

$$Fb^{(n)}(2) = \frac{1}{2^{n+1}}Fb^{(n+1)}(1) = 0,$$

where the very last equality (all derivatives vanishing at $x = 1$) is the consequence of the symmetry condition $Fb(1-x) = 1 - Fb(x)$ and the behavior of derivatives at $x = 0$. When shifting the Fabius function to the interval $[-1, 1]$ all mentioned properties remain conserved (on the shifted the interval). Equation (3.4) allows us to formulate the corresponding kernel functions in a very elegant way, where the explicit dependence on derivatives is not present[5]

$$f^{(n)}(x_0) \approx \left(\frac{-1}{h}\right)^n 2^{\frac{1}{2}n(n+1)} \int_{-1}^1 Fb\left[2^n(t+1)\right] f(x_0 + ht)\, dt.$$

Value of the Fabius function for $1 < x$ can be very easily related to the value of this function on the interval $[0, 1]$. Using an efficient method[6] for its evaluation on the interval $[0, 1]$, one achieves an effective method for computing kernel function values and thus the whole integral, and this for any order of the derivative.

4 Discussion

One of the most cited results [8] generalizes the Lanczos' derivative by using the Legendre polynomials[7]. It might be interesting to check its behavior from the perspective of the presented results. The authors of [8] propose (among others) the following form of the kernel function[8]

$$k_n(x) = \frac{(-1)^n}{2}(2n+1)!!P_n(x),$$

with $P_n(x)$ being the Legendre polynomials. The latter can be defined by the Rodrigues' formula

$$P_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}\left(x^2-1\right)^n.$$

Observing the inner bracket (going to zero for $x = \pm 1$) being raised to the n-th power, one immediately sees that the condition (3.1) is obeyed. Next, one can study the integral of the weight function

$$\frac{(-1)^n}{2}(2n+1)!!\frac{1}{2^n n!}\int_{-1}^1 \left(x^2-1\right)^n dx.$$

With partial results [22]

$$\int_{-1}^1 \left(x^2-1\right)^n dx = \sqrt{\pi}\,(-1)^n \frac{n!}{\Gamma\left(n+\frac{3}{2}\right)} \text{ and } \Gamma\left(n+\frac{3}{2}\right) = \sqrt{\pi}\frac{(2n+1)!!}{2^{(n+1)}}$$

[5] One can notice that the expression is defined for any real value of n.
[6] Use of tabulated values, or recipes from [19, 20, 21].
[7] A similar result was in the same year published by [9].
[8] The factor $(-1)^n$ is here to cancel the same factor in (3.3) from in front of the integral.

one finds that also the condition (3.2) is respected.

Several other realizations of the *differentiation by integration* can be found in the literature, most of them with a higher technical complexity than the previous one. From what was shown, all of these representations (based on one-dimensional integrals) have to comply with the restrictions (3.1) and (3.2).

This text focuses on the main result of generalizing the Lanczos' derivative and does not address specific issues of precision and rapidity of convergence in case of a numerical implementation and related questions of the kernel function preference. With the kernel function being completely general (possibly non-analytic everywhere) one can hardly rely on standard tools for error estimates (i.e. Taylor series). In any specific context the recipes existing in the literature are to be used.

5 Summary, conclusion

In this text the result published in [7] was generalized to higher-order derivatives and, assuming pattern (3.3), this generalization is maximal. Restrictions (3.1) and (3.2) allow for a very broad family of functions, which might make the search for well performing kernels for numerical purposes more efficient.

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Author information

Andrej Liptaj, Institute of Physics, Slovak academy of Sciences, Dúbravská cesta 9, 845 11 Bratislava, Slovakia.
E-mail: andrej.liptaj@savba.sk

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