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OPTIMIZED FIRST-ORDER TAYLOR-LIKE FORMULAS AND GAUSS QUADRATURE ERRORS

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Abstract. In this article, we derive an optimal first-order Taylor-like formula. In a seminal paper [15], we introduced a new first-order Taylor-like formula that yields a reduced remainder compared to the classical Taylor's formula. In this work, we relax the assumption of equally spaced points in our formula. Instead, we consider a sequence of unknown points and a sequence of unknown weights. We then solve an optimization problem to determine the optimal distribution of points and weights that minimizes the corresponding remainder. Numerical results are provided to illustrate our findings.

Key words. Taylor's theorem, Taylor-like formula, error estimate, interpolation error, approximation error, finite elements.

1. Introduction

Even today, improving the accuracy of approximations remains a challenging problem in numerical analysis. In this context, Taylor's formula plays a crucial role in various domains, especially when one considers error estimates to assess the accuracy of a numerical approximation method (for example, see [25], [2], [28] for finite element methods). This challenge becomes even more crucial when comparing the relative accuracy between two given numerical methods. All error estimates share a common structure, whether applied to the finite elements method [6], [21], numerical approximations of ordinary differential equations [16], or to quadrature formulas used for approximating integrals [16].

Let us specify these ideas in this context of numerical integration. Consider, for instance, a composite quadrature rule of order k. For a given interval $[a,b]$, let f be a function in $C^{k+1}([a,b])$. The corresponding error of the composite quadrature rule can be expressed as (refer to, e.g., [4], [7] or [16]), for a non-zero integer N:

$$\left|\int_a^b f(x)dx - \sum_{i=0}^{N}\lambda_i f(x_i)\right| \leq C_k\, h^{k+1}\,. \tag{1}$$

In this formula, h denotes the size of the $N+1$ equally spaced panels $[x_i, x_{i+1}]$, $0 \leq i \leq N$, that discretize the interval $[a,b]$, and λ_i are $N+1$ real numbers. Moreover, C_k is an unknown constant, independent of h, but dependent on f and k. The fact that C_k is unknown arises from the presence of an unknown point in the remainder term of Taylor's expansion, as an heritage of Rolle's theorem. This prevents the precise determination of the approximation error of a given numerical method, leading to a kind of "uncertainty". In this way, this constant is directly linked to the uncertainty associated with the remainder of Taylor's formula [3].

To better understand the importance of Taylor's formula in assessing the accuracy of a numerical approximation method, we can also consider the case of the finite element method. We refer the reader to [13], Section 4, for a detailed explanation of how this formula is directly related to finite element error approximation.

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Indeed, in this context, with the help of Céa's lemma [21], since the approximation error is bounded by the interpolation error, using the corrected interpolation polynomial derived from the new Taylor-like formula enables us to obtain a tighter upper bound for the interpolation error compared to the usual one.

Usually, to overcome the lack of information regarding the unknown value of the left-hand side of (1) which lies within the interval $[0, C_k h^{k+1}]$, only the asymptotic convergence rate comparison is considered. This comparison allows us to assess the relative accuracy between two numerical quadratures of order k_1 and $k_2, (k_1 < k_2)$, as h tends to zero. However, when comparing two composite quadrature rules for a fixed value of h, as is common in many applications, the asymptotic convergence rate is no longer a meaningful criterion (since h is fixed). Therefore, we focus on minimizing the constants C_k by refining the estimation of the remainder in Taylor's formula. More precisely, assuming that the remainder lies within an interval $[L, U]$, $(L < U)$, our goal is to minimize it by reducing the width of the interval, i.e., minimizing $U - L$.

From another point of view, several approaches have been proposed to determine a way to enhance the accuracy of approximation. For example, within the framework of numerical integration, we refer the reader to [5], [8] or [20], and references therein, where the authors propose an improved quadrature formula that refines the trapezoid inequalities. To achieve this, they consider functions with varying levels of regularity, and based on Grüss's inequality, they derive the corresponding trapezoid quadrature errors. In contrast, our approach primarily focuses on minimizing the remainder in Taylor's expansion. Alternatively, due to the lack of information, heuristic methods were considered, basically based on a probabilistic approach, see for instance [1], [3], [22], [23] or [9], [10] and [11]. This allows to compare different numerical methods, and more precisely finite element, for a given fixed mesh size, [12].

In this context, we recently developed a first-order Taylor-like formula in [15] and a second-order Taylor-like formula in [14]. The goal was to minimize, in the sense defined above, the corresponding remainder by transferring part of the numerical weight of this remainder to the polynomial involved in the Taylor expansion. In both of these cases, we *a priori* introduced a linear combination of f' (and f'' in [14]) computed at equally spaced points in $[a, b]$, and we determined the corresponding weights in order to minimize the remainder. We proved that the associated upper bound in the error estimate is $2n$ times smaller than the classical one for the first-order Taylor's theorem, and $3/16n^2$ times smaller than the corresponding one in the classical second-order Taylors's formula.

In this paper, we relax the assumption of equally spaced points and consider a sequence of unknown points in the interval $[a, b]$, where a given function f needs to be evaluated. Simultaneously, we introduce a sequence of unknown weights to be determined with the goal of minimizing the remainder. Then, we will prove that the remainder of the corresponding first-order expansion is minimized when the points between a and b are equally spaced, with two different configurations depending on whether the endpoints a and b of the interval are included or excluded.

The paper is organized as follows. In Section 2, we present a new first-order Taylor-like formula built on a sequence of given points $x_k, (k = 0, \dots, n)$, in $[a, b]$, and given weights $\omega_k, (k = 0, \dots, n)$. In Section 3 we derive the two main results of this paper, focusing on the optimal choice of points x_k and weights ω_k that allow us to minimize the remainder of the first-order Taylor-like formula. Section 4 aims to numerically evaluate the results of these theorems and proposes numerical simulations that illustrate the optimality of the derived formula. Concluding remarks follow.

2. First-order Taylor-like expansion

Let us begin by recalling the well-known first-order Taylor formula [26]. For two real numbers a and b, where $a < b$, consider a function $f \in \mathcal{C}^2([a,b])$. Then, there exist $(m_2, M_2) \in \mathbb{R}^2$ such that, for all $x \in [a,b]$,

$$m_2 \leqslant f''(x) \leqslant M_2,$$

and we have

$$f(b) = f(a) + (b-a)f'(a) + (b-a)\epsilon_{a,1}(b), \tag{2}$$

with

$$\lim_{b \to a} \epsilon_{a,1}(b) = 0,$$

and

$$\frac{(b-a)}{2} m_2 \leqslant \epsilon_{a,1}(b) \leqslant \frac{(b-a)}{2} M_2.$$

In a previous paper [15], we derived a first-order Taylor-like formula aimed at minimizing its remainder $\epsilon_{a,n+1}(b)$, in the sense that, if $L \leq \epsilon_{a,n+1}(b) \leq U$ then $U - L$ is minimum.

More precisely, to minimize the difference between the upper and lower bounds $U - L$, we first express these bounds as functions of t_k and ω_k, which represent the points locations and the weights used in the Taylor-like formula, (see Formula (6)), which leads to a parameterized interval $[L, U]$. Finally, the width of this interval is minimized over the parameter set.

Hence, we proved the following result:

Theorem 2.1. *Let f be a real mapping defined on $[a,b]$ which belongs to $\mathcal{C}^2([a,b])$, such that: $\forall x \in [a,b], -\infty < m_2 \leqslant f''(x) \leqslant M_2 < +\infty$.*

Then, for a given non-zero integer n, we have the following first-order expansion:

$$f(b) = f(a) + (b-a)\left(\frac{f'(a)+f'(b)}{2n} + \frac{1}{n}\sum_{k=1}^{n-1} f'\left(a + k\frac{(b-a)}{n}\right)\right) + (b-a)\epsilon_{a,n+1}(b), \tag{3}$$

where

$$|\epsilon_{a,n+1}(b)| \leqslant \frac{(b-a)}{8n}(M_2 - m_2).$$

Moreover, for an a priori *choice of regularly spaced points $a + k\dfrac{(b-a)}{n}$, $\epsilon_{a,n+1}(b)$ is minimum.*

In the sequel of the paper, our goal is to relax the assumption of *a priori* equidistant points in order to determine the optimal set of points $\{x_k\}_{k=0,n} \in [a,b]$, along with the associated weights $\{\omega_k\}_{k=0,n}$. This determination will enable us to minimize the quantity $\epsilon_{a,n+1}(b)$ in (3), in the sense defined above.

To derive the main result below, we first introduce the function ϕ defined by

$$\begin{aligned} \phi : \quad [0,1] &\longrightarrow \mathbb{R} \\ t &\longmapsto f'(a + t(b-a)), \end{aligned} \tag{4}$$

that satisfies $\phi(0) = f'(a)$ and $\phi(1) = f'(b)$. Moreover, we proved in [15] that $\epsilon_{a,1}(b)$ introduced in (2) satisfies the following result:

Proposition 2.2. *The quantity $\epsilon_{a,1}(b)$ in formula (2) can be expressed as*

$$\epsilon_{a,1}(b) = \int_0^1 (1-t)\phi'(t)dt\,. \tag{5}$$

For a given integer $n \in \mathbb{N}^*$, we consider a set of points $\{x_k\}_{k=0,n}$ in the interval $[a,b]$, and a set of real weights $\{\omega_k\}_{k=0,n}$.

Next, we define the quantity $\epsilon_n^*(a,b)$ by the formula

$$f(b) = f(a) + (b-a)\left(\sum_{k=0}^{n} \omega_k f'(x_k)\right) + (b-a)\epsilon_n^*(a,b), \tag{6}$$

where the two sequences $\{x_k\}_{k=0,n}$ and $\{\omega_k\}_{k=0,n}$ are to be determined in order to minimize the quantity $\epsilon_n^*(a,b)$.

For the upcoming result, we need to introduce some notations. Let $t_k, (k = 0,\dots,n)$, be a sequence of real numbers in $[0,1]$ that allows us to represent the points x_k in $[a,b]$ as a barycentric combination of a and b, that is:

$$x_k = a + t_k(b-a),\ (0 \le t_k \le 1). \tag{7}$$

For each integer k in $[\![0,n]\!]$, we introduce the quantity S_k defined as the partial sum of the weights ω_j, $(\forall j \in [\![0,k]\!])$, defined by:

$$S_k = \sum_{j=0}^{k} \omega_j\,. \tag{8}$$

Consequently, S_n represents the sum of all the $n+1$ weights ω_k from $k=0$ to n. Therefore, we can prove the following result:

Theorem 2.3. *Let f be a real mapping defined on $[a,b]$ which belongs to $\mathcal{C}^2([a,b])$ and assume that $S_n = 1$. Then, the quantity $\epsilon_n^*(a,b)$ defined by (6) is bounded as follows:*

$$\begin{aligned} \epsilon_n^*(a,b) \ &\geq\ \frac{(b-a)}{2}\Bigg[\sum_{k=0}^{n-1}\Big(m_2(S_k-t_k)^2 - M_2(S_k-t_{k+1})^2\Big) \\ &\qquad + m_2(1-t_n)^2 - M_2 t_0^2\Bigg], \end{aligned} \tag{9}$$

$$\begin{aligned} \epsilon_n^*(a,b) \ &\leq\ \frac{(b-a)}{2}\Bigg[\sum_{k=0}^{n-1}\Big(M_2(S_k-t_k)^2 - m_2(S_k-t_{k+1})^2\Big) \\ &\qquad + M_2(1-t_n)^2 - m_2 t_0^2\Bigg]. \end{aligned} \tag{10}$$

Proof : Rewriting formula (2) and (6) using the function ϕ defined in (4), we derive the quantity $\frac{f(b)-f(a)}{b-a}$ and obtain:

$$\frac{f(b)-f(a)}{b-a} = \phi(0) + \epsilon_{a,1}(b) = \sum_{k=0}^{n} \omega_k \phi(t_k) + \epsilon_n^*(a,b),$$

which can be re-written as:

$$\begin{aligned}\epsilon_n^*(a,b) &= \phi(0)+\epsilon_{a,1}(b)-\sum_{k=0}^{n}\omega_k\phi(t_k),\\ &= \phi(0)+\int_0^1(1-t)\phi'(t)dt-\sum_{k=0}^{n}\omega_k\phi(t_k),\\ &= \phi(1)-\int_0^1 t\phi'(t)dt-\sum_{k=0}^{n}\omega_k\phi(t_k),\\ &= \phi(1)-\int_0^1 t\phi'(t)dt+\sum_{k=0}^{n}\omega_k\left(\phi(1)-\phi(t_k)\right)-\sum_{k=0}^{n}\omega_k\phi(1),\\ &= \left(1-\sum_{k=0}^{n}\omega_k\right)\phi(1)-\int_0^1 t\phi'(t)dt+\sum_{k=0}^{n}\omega_k\left(\phi(1)-\phi(t_k)\right). \qquad (11)\end{aligned}$$

Using the definition (8) of S_n introduced above, equation (11) can be expressed as

$$\begin{aligned}&\epsilon_n^*(a,b)-(1-S_n)\phi(1)\\ &= -\int_0^1 t\phi'(t)dt+\sum_{k=0}^{n}\omega_k\left(\phi(1)-\phi(t_k)\right),\\ &= -\int_0^1 t\phi'(t)dt+\sum_{k=0}^{n}\omega_k\int_{t_k}^1\phi'(t)dt,\\ &= -\int_0^{t_0} t\phi'(t)dt-\int_{t_n}^1 t\phi'(t)dt-\sum_{k=0}^{n-1}\int_{t_k}^{t_{k+1}} t\phi'(t)dt+\sum_{k=0}^{n}\omega_k\int_{t_k}^1\phi'(t)dt. \qquad (12)\end{aligned}$$

Considering the last term of (12), it can be transformed as follows:

$$\begin{aligned}&\sum_{k=0}^{n}\omega_k\int_{t_k}^1\phi'(t)dt\\ &= \int_{t_0}^1\omega_0\phi'(t)dt+\int_{t_1}^1\omega_1\phi'(t)dt+\cdots+\int_{t_n}^1\omega_n\phi'(t)dt,\\ &= \int_{t_0}^{t_1}\omega_0\phi'(t)dt+\int_{t_1}^{t_2}(\omega_0+\omega_1)\phi'(t)dt+\cdots+\int_{t_n}^1(\omega_0+\cdots+\omega_n)\phi'(t)dt.\\ &= \sum_{k=0}^{n-1}\int_{t_k}^{t_{k+1}} S_k\,\phi'(t)dt+\int_{t_n}^1 S_n\,\phi'(t)dt, \qquad (13)\end{aligned}$$

where S_k is defined by (8).

Then, using (13) in (12) enables to write $\epsilon_n^*(a,b)$ as

$$\epsilon_n^*(a,b)=(1-S_n)\phi(1)+\sum_{k=0}^{n-1}\int_{t_k}^{t_{k+1}}(S_k-t)\phi'(t)dt-\int_0^{t_0} t\phi'(t)dt+\int_{t_n}^1(S_n-t)\phi'(t)dt. \qquad (14)$$

Moreover, to ensure that $(b-a)\epsilon_n^*(a,b)=o(b-a)$, (where $o(b-a)$ denotes the classical Landau notation), we impose the condition $(1-S_n)\phi(1)$=0, which implies that $S_n=1$.

Then, (14) leads to

$$\epsilon_n^*(a,b) = \sum_{k=0}^{n-1} \int_{t_k}^{t_{k+1}} (S_k - t)\phi'(t)dt - \int_0^{t_0} t\phi'(t)dt + \int_{t_n}^{1} (1-t)\phi'(t)dt. \tag{15}$$

In the estimations below, we will use that

$$\forall\, t \in [0,1], \phi'(t) = (b-a)f''(a+t(b-a)), \quad \text{and } \forall\, x \in [a,b], m_2 \leqslant f''(x) \leqslant M_2.$$

Then, the second and third term of (15) are bounded as follows:

$$\begin{aligned} \frac{(b-a)}{2}\Big[m_2(1-t_n)^2 - M_2 t_0^2\Big] &\leq -\int_0^{t_0} t\phi'(t)dt + \int_{t_n}^{1}(1-t)\phi'(t)dt \\ &\leq \frac{(b-a)}{2}\Big[M_2(1-t_n)^2 - m_2 t_0^2\Big]. \end{aligned} \tag{16}$$

Next, to derive a double inequality of the first term of (15), we consider the three following cases, depending on the location of S_k related to the interval $[t_k, t_{k+1}]$.

(1) If $t_k \leq S_k \leq t_{k+1}$, the first integral in (15) can be decomposed as follows:

$$\int_{t_k}^{t_{k+1}} (S_k - t)\phi'(t)dt = \int_{t_k}^{S_k} (S_k - t)\phi'(t)dt + \int_{S_k}^{t_{k+1}} (S_k - t)\phi'(t)dt. \tag{17}$$

Now, using that $(S_k - t)$ is positive on $[t_k, S_k]$, and negative on $[S_k, t_{k+1}]$, we can write

$$\begin{cases} (b-a)m_2 \displaystyle\int_{t_k}^{S_k} (S_k - t)dt \leq \int_{t_k}^{S_k} (S_k - t)\phi'(t)dt \\ \qquad\qquad\qquad\qquad \leq (b-a)M_2 \displaystyle\int_{t_k}^{S_k} (S_k - t)dt, \\ (b-a)M_2 \displaystyle\int_{S_k}^{t_{k+1}} (S_k - t)dt \leq \int_{S_k}^{t_{k+1}} (S_k - t)\phi'(t)dt \\ \qquad\qquad\qquad\qquad \leq (b-a)m_2 \displaystyle\int_{S_k}^{t_{k+1}} (S_k - t)dt. \end{cases}$$

Summing up these two relations, we obtain first that

$$\begin{aligned} &\int_{t_k}^{t_{k+1}} (S_k - t)\phi'(t)dt \\ \leq\; & (b-a)M_2 \int_{t_k}^{S_k} (S_k - t)dt + (b-a)m_2 \int_{S_k}^{t_{k+1}} (S_k - t)dt, \end{aligned}$$

and also

$$\begin{aligned} &\int_{t_k}^{t_{k+1}} (S_k - t)\phi'(t)dt \\ \geq\; & (b-a)m_2 \int_{t_k}^{S_k} (S_k - t)dt + (b-a)M_2 \int_{S_k}^{t_{k+1}} (S_k - t)dt\,. \end{aligned}$$

By simply computing the integrals involved in these inequalities, we obtain, in that case, the following estimate

$$\begin{aligned} & \frac{(b-a)}{2}\Big(m_2(S_k-t_k)^2 - M_2(S_k-t_{k+1})^2\Big) \\ \leq & \int_{t_k}^{t_{k+1}} (S_k-t)\phi'(t)dt \\ \leq & \frac{(b-a)}{2}\Big(M_2(S_k-t_k)^2 - m_2(S_k-t_{k+1})^2\Big). \end{aligned} \tag{18}$$

(2) If $S_k \geq t_{k+1}$ then $S_k - t \geq 0$ for all $t \in [t_k, t_{k+1}]$, and we have:

$$\begin{aligned} (b-a)m_2\int_{t_k}^{t_{k+1}}(S_k-t)dt & \leq \int_{t_k}^{t_{k+1}}(S_k-t)\phi'(t)dt \\ & \leq (b-a)M_2\int_{t_k}^{t_{k+1}}(S_k-t)dt\,. \end{aligned}$$

This yields

$$\begin{aligned} & \frac{(b-a)m_2}{2}\Big((S_k-t_k)^2 - (S_k-t_{k+1})^2\Big) \\ \leq & \int_{t_k}^{t_{k+1}} (S_k-t)\phi'(t)dt \\ \leq & \frac{(b-a)M_2}{2}\Big((S_k-t_k)^2 - (S_k-t_{k+1})^2\Big), \end{aligned}$$

which also leads to (18), by simply using that $m_2 \leq M_2$.

(3) If $S_k \leq t_k$ then $S_k - t \leq 0$ for all $t \in [t_k, t_{k+1}]$, and in the same way as above, we get

$$\begin{aligned} & \frac{(b-a)M_2}{2}\Big((S_k-t_k)^2 - (S_k-t_{k+1})^2\Big) \\ \leq & \int_{t_k}^{t_{k+1}} (S_k-t)\phi'(t)dt \\ \leq & \frac{(b-a)m_2}{2}\Big((S_k-t_k)^2 - (S_k-t_{k+1})^2\Big), \end{aligned}$$

that also gives estimates (18).

Hence, in all cases, we arrive at the same estimate (18). Finally, by summing (18) over all values of k from 0 to $n-1$, and by the help of (16), we get inequalities (9)-(10) for $\epsilon_n^*(a,b)$. ■

With the aim of minimizing $\epsilon_n^*(a,b)$, we introduce the function χ defined by

$$\chi = \frac{(b-a)(M_2-m_2)}{2}\left\{\sum_{k=0}^{n-1}\left[\left(\sum_{j=0}^{k}\omega_j - t_k\right)^2 + \left(\sum_{j=0}^{k}\omega_j - t_{k+1}\right)^2\right] + t_0^2 + (1-t_n)^2\right\}, \tag{19}$$

which represents the difference between the upper bound (10) and the lower bound (9) of $\epsilon_n^*(a,b)$.

As a consequence, in the next section, we will minimize the function χ which depends on $2n+2$ variables, namely $(t_0, \dots, t_n, \omega_0, \dots, \omega_n)$, under the constraint $S_n = 1$.

3. Optimal first order Taylor-like formulas

In this section we will prove the two main theorems of this paper. In the first theorem, we will fix $x_0 = a$ and $x_n = b$ *a priori*, while the points $\{x_k\}_{k=1,n-1}$ can be arbitrarily distributed in $[a, b]$. In the second theorem, we will consider the case where the points $\{x_k\}_{k=0,n}$ can be arbitrarily distributed in the interval $[a, b]$.

Theorem 3.1. *For a given integer $n \in \mathbb{N}^*$, let f be a real function defined on $[a, b]$ that belongs to $\mathcal{C}^2([a, b])$. We set $x_0 = a$ and $x_n = b$. Then, the optimal unknown weights $\{\omega_k\}_{k=0,n}$ together with the optimal set of points $\{x_k\}_{k=1,n-1}$, that minimize the quantity $\epsilon_n^*(a, b)$ defined by (6), are given by:*

$$\omega_0 = \omega_n = \frac{1}{2n} \text{ and } \omega_k = \frac{1}{n}, \forall k = 1, \dots, n-1, \tag{20}$$

$$x_k = a + k\frac{(b-a)}{n}, \ \forall k = 1, \dots, n-1. \tag{21}$$

As a result, the corresponding optimal first-order Taylor-like formula is given by the following expression:

$$f(b) = f(a) + (b-a)\left(\frac{f'(a) + f'(b)}{2n} + \frac{1}{n}\sum_{k=1}^{n-1} f'(x_k)\right) + (b-a)\epsilon_n^*(a, b), \tag{22}$$

with

$$|\epsilon_n^*(a, b)| \leqslant \frac{(b-a)}{8n}(M_2 - m_2). \tag{23}$$

Theorem 3.2. *For a given integer $n \in \mathbb{N}$, let f be a real function defined on $[a, b]$ that belongs to $\mathcal{C}^2([a, b])$. Then, the optimal unknown weights $\{\omega_k\}_{k=0,n}$ together with the optimal set of points $\{x_k\}_{k=0,n}$, that minimize the quantity $\epsilon_n^*(a, b)$ defined by (6), are given by:*

$$\omega_k = \frac{1}{n+1}, \forall k = 0, \dots, n, \tag{24}$$

$$x_k = a + \left(k + \frac{1}{2}\right)\frac{b-a}{n+1}, \ \forall k = 0, \dots, n. \tag{25}$$

As a result, the corresponding optimal first-order Taylor-like formula is given by the following expression:

$$f(b) = f(a) + (b-a)\frac{1}{n+1}\sum_{k=0}^{n} f'(x_k) + (b-a)\epsilon_n^*(a, b), \tag{26}$$

with

$$|\epsilon_n^*(a, b)| \leqslant \frac{(b-a)}{8(n+1)}(M_2 - m_2). \tag{27}$$

We remark that the points x_k in (26) are the midpoints of the intervals involved in Theorem 3.1.

In the following, we will present the proof of Theorem 3.1. Since the proof of Theorem 3.2 is similar, afterwards, we will only highlight the differences.

Proof : Recalling that in Theorem 3.1, we assume that $x_0 = a$ and $x_n = b$, that corresponds to assume that $t_0 = 0$ and $t_n = 1$. In these conditions, function χ defined in (19) is expressed as:

$$\chi = \frac{(b-a)(M_2-m_2)}{2}\sum_{k=0}^{n-1}\left[\left(\sum_{j=0}^{k}\omega_j - t_k\right)^2 + \left(\sum_{j=0}^{k}\omega_j - t_{k+1}\right)^2\right]. \tag{28}$$

We then begin by deriving a lemma that provides a necessary condition for function χ to have an extremum at the point $(t_1,\ldots,t_{n-1},\omega_0,\ldots,\omega_{n-1})$.

Lemma 3.3. *Let $(t_1,\ldots,t_{n-1},\omega_0,\ldots,\omega_{n-1})$ be an extremum of function χ.*

Then, we have:

$$\begin{cases} S_k = \dfrac{1}{2}(t_k + t_{k+1}),\ (k=0,\ldots,n-1), & (29)\\[2ex] t_k = S_{k-1} + \dfrac{\omega_k}{2}, \quad (k=1,\ldots,n-1). & (30)\end{cases}$$

Proof : The necessary conditions that guarantee that $(t_1,\ldots,t_{n-1},\omega_0,\ldots,\omega_{n-1})$ is an extremum is written as (see for instance [24])

$$\forall k = 0,\ldots,n-1 : \frac{\partial\chi}{\partial\omega_k} = 0 \ \text{ and } \ \forall k=1,\ldots,n-1 : \frac{\partial\chi}{\partial t_k} = 0.$$

Regarding first the dependence of the function χ on the variables ω_k, $(k=0,\ldots,n-1)$, the conditions $\dfrac{\partial\chi}{\partial\omega_k} = 0$ are expressed as

$$\sum_{m=k}^{n-1}\left[2S_m - t_m - t_{m+1}\right] = 0\,,$$

or equivalently

$$\sum_{m=k}^{n-1} S_m = \frac{1}{2}\sum_{m=k}^{n-1}(t_m + t_{m+1})\,. \tag{31}$$

Since this system of equations is triangular, it can be easily solved. Writing two consecutive equations for a given $k\in\{0,\ldots,n-2\}$ leads to

$$\begin{aligned} S_k \quad + \quad S_{k+1}+\cdots+S_{n-1} &= \frac{1}{2}\big[(t_k+t_{k+1}) + (t_{k+1}+t_{k+2}) + \cdots + (t_{n-1}+t_n)\big],\\ S_{k+1}+\cdots+S_{n-1} &= \frac{1}{2}\big[(t_{k+1}+t_{k+2}) + \cdots + (t_{n-1}+t_n)\big]\,,\end{aligned}$$

which readily gives, by difference,

$$S_k = \frac{1}{2}(t_k + t_{k+1})\,,$$

and the case $k = n-1$ corresponds directly to the last equation of the system (31).

Now, to study the dependence of the function χ on the variables t_k, $\forall k = 1, \dots, n-1$, we expand formula (28), using that $t_0 = 0$ and $t_n = 1$. We obtain that

$$\begin{aligned}
\frac{2}{(b-a)(M_2-m_2)}\chi &= \sum_{k=0}^{n-1}\left[\Big(\omega_0+\cdots+\omega_k-t_k\Big)^2+\Big(\omega_0+\cdots+\omega_k-t_{k+1}\Big)^2\right] \\
&= (\omega_0-0)^2+(\omega_0-t_1)^2 \\
&\quad +(\omega_0+\omega_1-t_1)^2+(\omega_0+\omega_1-t_2)^2 \\
&\quad +\dots \\
&\quad +(\omega_0+\cdots+\omega_k-t_k)^2+(\omega_0+\cdots+\omega_k-t_{k+1})^2 \\
&\quad +\dots \\
&\quad +(\omega_0+\cdots+\omega_{n-1}-t_{n-1})^2+(\omega_0+\cdots+\omega_{n-1}-1)^2 .
\end{aligned}$$

So, by taking the derivative of the function χ with respect to t_k, we obtain, for each $k = 1, \dots, n-1$:

$$\frac{\partial\chi}{\partial t_k}=0 \quad\Leftrightarrow\quad 2(\omega_0+\cdots+\omega_{k-1}-t_k)+2(\omega_0+\cdots+\omega_k-t_k)=0\,.$$

This can be expressed as

$$S_{k-1}+S_k-2t_k=0,$$

that is, using the definition (8) of S_k

$$2t_k=2S_{k-1}+\omega_k\,,$$

which corresponds to (30). ■

From Lemma 3.3, we can now prove Theorem 3.1 as follows:

- We begin by proving that ω_k is constant for all values of k belonging to $\{1, \dots, n-1\}$.

  From (29) and (30), we have

  $$2S_k=t_k+t_{k+1}=S_{k-1}+\frac{\omega_k}{2}+S_k+\frac{\omega_{k+1}}{2},\ \forall k=1,\dots,n-2,$$

  that yields, using again (8),

  $$S_k-S_{k-1}:=\omega_k=\frac{\omega_k+\omega_{k+1}}{2}.$$

  Then,

  $$\omega_{k+1}=\omega_k,\ \forall k=1,\dots,n-2, \tag{32}$$

  that corresponds to

  $$\omega_1=\cdots=\omega_{n-1}.$$

- We will now establish the relation between ω_0 and ω_k, for $k = 1, \dots, n-1$.

  Firstly, let us write (29) for $k = 0$ and (30) for $k = 1$. Using that $t_0 = 0$, we obtain that

  $$\begin{aligned}
  2S_0 &= t_0+t_1=t_1, \\
  t_1 &= S_0+\frac{\omega_1}{2}=\omega_0+\frac{\omega_1}{2},
  \end{aligned}$$

from which we get

$$\omega_1 = 2\omega_0 \,.$$

This allows us to conclude, using (32), that

(33) $$\omega_1 = \omega_2 = \cdots = \omega_{n-1} = 2\omega_0.$$

- Let us compute now the value of ω_0.

  To this end, we write (29) and (30) for $k = n-1$. Given that $t_n = 1$ and using (33), this yields

$$\begin{aligned} 2S_{n-1} &= t_{n-1} + t_n = t_{n-1} + 1, \\ &= S_{n-2} + \frac{\omega_{n-1}}{2} + 1. \end{aligned}$$

  Then, substituting the expressions of S_{n-1} and S_{n-2}, we get with (33) that

$$2\omega_0 + 4(n-1)\omega_0 = \omega_0 + 2(n-2)\omega_0 + \frac{\omega_{n-1}}{2} + 1,$$

  that leads to

$$2(2n+1)\omega_0 - 2 = \omega_{n-1} = 2\omega_0$$

  that is

(34) $$\omega_0 = \frac{1}{2n}.$$

- It remains now to compute the value of ω_n. Using (33) and (34) gives directly that

(35) $$\omega_1 = \omega_2 = \cdots = \omega_{n-1} = \frac{1}{n}.$$

  Finally, the value of ω_n is obtained from relation (8), that is

$$\omega_n = 1 - \omega_0 - \sum_{k=1}^{n-1} \omega_k = 1 - \frac{1}{2n} - \frac{n-1}{n} = \frac{1}{2n}.$$

- Let us now consider the values of the t_k, for $k = 1 \ldots, n-1$.

  Using the expressions (30) of the t_k, together with the expressions (34) and (35) of the weights ω_k, we obtain that

$$\begin{aligned} t_k &= \omega_0 + \sum_{j=1}^{k-1} \omega_j + \frac{\omega_k}{2}, (k = 1, \ldots, n-1), \\ &= \frac{1}{2n} + \frac{k-1}{n} + \frac{1}{2n} = \frac{k}{n}, \end{aligned}$$

  that yields with (7), the following expressions of the optimal points x_k:

(36) $$x_k = a + \frac{k}{n}(b-a), (k = 1, \ldots, n-1).$$

- We conclude the proof of this theorem by determining the optimal lower and upper bounds of $\epsilon_n^*(a,b)$ given in (9)-(10). We first evaluate the quantity $\displaystyle\sum_{k=0}^{n-1}(S_k - t_k)^2$:

Using the expression (20) of the ω_j, we obtain that

$$S_k = \sum_{j=0}^{k} \omega_j = \omega_0 + \sum_{j=1}^{k} \omega_j = \frac{1}{2n} + \frac{k}{n} = \frac{2k+1}{2n}, (k = 0, \dots, n-1)\,,$$

so that, together with the expression (21) of the t_k, we have

$$\sum_{k=0}^{n-1} (S_k - t_k)^2 = \sum_{k=0}^{n-1} \left(\frac{2k+1}{2n} - \frac{k}{n} \right)^2 = \frac{1}{4n}. \tag{37}$$

Similarly, we evaluate the quantity $\sum_{k=0}^{n-1} (S_k - t_{k+1})^2$. The same arguments yield

$$\begin{aligned} \sum_{k=0}^{n-1} (S_k - t_{k+1})^2 &= \sum_{k=0}^{n-2} (S_k - t_{k+1})^2 + (S_{n-1} - t_n)^2 \\ &= \sum_{k=0}^{n-2} \left(\frac{2k+1}{2n} - \frac{k+1}{n} \right)^2 + \left(\frac{2n-1}{2n} - 1 \right)^2 \\ &= \sum_{k=0}^{n-2} \left(\frac{-1}{2n} \right)^2 + \frac{1}{4n^2} = \frac{1}{4n}. \end{aligned} \tag{38}$$

Therefore, combining (37) and (38), we obtain optimal lower bound and upper bounds in (9)-(10) for the quantity $\epsilon_n^*(a,b)$ as follows:

$$\frac{(b-a)}{8n}(m_2 - M_2) \leq \epsilon_n^*(a,b) \leq \frac{(b-a)}{8n}(M_2 - m_2)\,.$$

This exactly corresponds to the result we derived in [15], where we minimized $\epsilon_n^*(a,b)$ by only deriving the values of the weights $\omega_k, (k \in [\![0,n]\!])$, having fixed *a priori* the points $x_k, (k \in [\![1,n-1]\!])$, as equidistant.

■

Let us now detail the main differences which have to be taken into account in the proof of Theorem 3.2:

Proof : The proof follows the same principle of the proof of Theorem 3.1. The only difference being in the additional term in the function χ introduced in (19), which depends on t_0 and t_n, i.e., $t_0^2 + (1-t_n)^2$.

- For this reason, when sketching the proof of Theorem 3.1, from the condition $\dfrac{\partial \chi}{\partial \omega_k} = 0$, we find again that

$$S_k = \frac{1}{2}(t_k + t_{k+1}). \tag{39}$$

Similarly, for $k = 1, \dots, n-1$, the relation $\dfrac{\partial \chi}{\partial t_k} = 0$ also gives:

$$t_k = S_{k-1} + \frac{\omega_k}{2}\,. \tag{40}$$

The only two additional equations we need to solve are $\dfrac{\partial \chi}{\partial t_0} = 0$ and $\dfrac{\partial \chi}{\partial t_n} = 0$.

- For the first one, we find that:

$$t_0 = \frac{\omega_0}{2}\,, \tag{41}$$

while the second leads to, using that $S_n = 1$,

$$2t_n + \omega_n = 2\,.$$

Now, using the relations (39) and (40), we get:

$$\omega_0 = \omega_1 = \cdots = \omega_{n-1} \text{ and } \omega_0 + \omega_1 + \cdots + \omega_n = 1\,.$$

- It remains to address the case $k = n - 1$.

From (39) and (40), after some algebra, we obtain that

$$\omega_0 = \frac{1}{n+1}, \text{ and consequently, } \omega_n = \frac{1}{n+1},$$

that proves (24).

Finally, for the t_k's, using relation (41), we readily get that

$$t_0 = \frac{1}{2n+1} \text{ and } t_n = \frac{2n+1}{2(n+1)},$$

yielding relation (25), for all $k = 0, \ldots, n$.

■

4. Application to Gaussian quadrature error estimates

To evaluate the results of Theorems 3.1 and 3.2, we propose numerical simulations that illustrates formula (6) in different cases. To establish the optimality of the formula, we consider several sequences of points $\{x_k\}_{k=0,n}$ and weights $\{\omega_k\}_{k=0,n}$, comparing them with those obtained in the two previous theorems.

4.1. Comparison with random points and weights. In the sequel of this section, we will focus our analysis on comparing the accuracy of the estimation of a given exact value of a function f at a point x_0 using statistical tools. Specifically, we will compare the results obtained from formula (3), which corresponds to equidistant points and the associated optimal weights, with those obtained from other distributions of points and weights. To this end, let us consider the particular case of the function f defined by $f(x) = \ln(1 + x)$, and set $a = 0$ and $b = 1$ that is, $[a, b] = [0, 1]$. Using formula (6), an approximation of $\ln(2)$ is given by:

$$\ln(2) \simeq \sum_{k=0}^{n} \frac{\omega_k}{1 + x_k}. \tag{42}$$

Next, for different values of n, we generated several sets of random points $\{x_k\}_{k=1,n-1}$ and weights $\{\omega_k\}_{k=0,n}$, implementing Excel's random function.

We then considered 3, 6, 12, and 26 points, respectively, to approximate $\ln(2)$ using formula (42). In each case, we computed samples of different sizes, consisting of 100, 200 and 500 individuals, each individual being defined by a set of random points and weights used to approximate $\ln(2)$. For each number of points, the random points and weights were computed along with the approximation of $\ln(2)$ using formula (42).

Remark 1. *The number of points was chosen as 3, 6, 12, or 26, as an example. Similarly, we could have selected 4, 8, 16, or 32 points. The main idea is to consider a small, medium, and large number of points to test the method. Additional tests were conducted with similar but slightly different numbers of points (such as 4, 8, 16, or 32) and demonstrated statistically stable behavior.*

Finally, once the sample of approximations was constructed, we performed several statistical analysis, including a Student's test applied to the corresponding one-sample, to assess how the random points and weights produced accurate estimates of ln(2). The results are presented in Table 1, which shows the average of the relative error between each approximation and ln(2), for each number of points used in Taylor-formula (6), and for each sample. As one can see, this average lies between

TABLE 1. Average relative error of ln(2) approximation for random points and weights.

Number of points \ Sample size	100	200	500
3	10.7%	10.9%	11.4%
6	8.7%	7.9%	8.2%
12	5.9%	6.3%	5.8%
26	4.1%	4.4%	3.6%

3.6% and 11.4%. As expected, the fewer the number of points, the greater the average relative error, and this trend remains consistent regardless of the sample size.

We also compared the average relative errors of the approximations of ln(2) with the relative error obtained by Taylor-like formula (3), using equidistant points and optimal weights. The results are summarized in Table 2. Once again, the more

TABLE 2. Approximations of ln(2) using the Taylor-like formula (3) with equidistant points and optimal weights.

Number of equidistant points	3	6	12	26
Approximation of ln(2)	0.7083	0.6956	0.6937	0.6932
Relative error	2.2%	0.4%	0.1%	0.01%

points considered in the Taylor-like formula, the more accurate the approximation of ln(2) becomes. However, as clearly shown in Table 2, the order of magnitude of the relative error is significantly smaller than those presented in Table 1. This illustrates that equidistant points and their associated weights lead to a much more accurate approximation than the random ones used in this study.

To further this analysis, we now examine stronger statistical characteristics of the results provided by random points and weights in approximating the value of ln(2), specifically using Student's test. The goal is to determine whether the random approximations exhibit a significant systematic bias in estimating ln(2). The results are summarized in Table 3.

TABLE 3. Student's test $p-$value for different numbers of points in Taylor-like formula (3), computed in several samples.

Number of points \ Sample size	100	200	500
3	$1{,}49.10^{-7}$	$1{,}09.10^{-9}$	$4{,}17.10^{-16}$
6	$1{,}94.10^{-3}$	$2{,}58.10^{-7}$	$3{,}63.10^{-13}$
12	$9{,}33.10^{-6}$	$5{,}86.10^{-10}$	$7{,}77.10^{-7}$
26	$2{,}11.10^{-3}$	$5{,}53.10^{-9}$	$6{,}05.10^{-17}$

According to Student's test theory [27], a low $p-$value in this test indicates strong evidence against the null hypothesis - which assumes that the sample mean value is equal to a known target value - suggesting a significant difference between the sample mean and the target value. Conversely, a high $p-$ value indicates that the results are consistent with the null hypothesis. To determine whether the $p-$value is low or high, it is compared to a predefined threshold called the significance level, which is typically set at 0.05.

In our case, the very small p-value indicates strong evidence against the null hypothesis, which assumes that our sample mean is equal to $\ln(2)$. As a result, we reject the null hypothesis. This suggests that the sample data does not provide a reliable approximation for $\ln(2)$ and the observed differences are statistically significant. In other words, the very low p-value indicates that the approximated values (corresponding to a given sample of 100, 200, or 500 individuals) are highly unlikely to match the exact value of $\ln(2)$. This provides strong evidence against the null hypothesis, suggesting that $\ln(2)$ is unlikely to be the true population mean. Therefore, we conclude that there is a significant difference between the approximations computed for each random sample, across all sets of points and weights considered, and the exact value of $\ln(2)$.

In summary, using the random function available in Excel to generate random samples, we conclude that no random set of points and associated random weights can approximate $\ln(2)$ with satisfactory accuracy. By contrast, the approximations derived from equidistant points and their corresponding optimal weights are highly accurate.

4.2. Taylor-like expansion and Gauss quadratures. In the previous subsection, we considered random points and weights to compare the accuracy of corresponding $\ln(2)$ approximation with those obtained by equidistant points and the associated optimal weights we derived in Theorem 3.2.

In the following, we adopt another perspective, interpreting the general Taylor-like formula (6) as a Gauss quadrature formula applied to the integration of a function

f' belonging to $C^1([a,b])$, as follows:

$$\int_a^b f'(x)\,dx = \left(\sum_{k=0}^{n} \Omega_k f'(x_k)\right) + (b-a)\epsilon_n^*(a,b), \tag{43}$$

where $\{x_k\}_{k=0,n}$ are now considered as the nodes of a Gauss quadrature, and $\Omega_k, (k=0,\ldots,n)$, are the corresponding quadrature weights defined by: $\Omega_k := (b-a)\omega_k$. Consequently, the main part of the expansion of formula (26), (respectively (22)) corresponds to the composite midpoint quadrature formula, (respectively, the composite trapezoidal quadrature formula).

From this perspective, Theorems 3.1 and 3.2 demonstrate that, within the family of Gauss quadratures (43), when the function to be integrated belongs to $C^1([a,b])$, the minimal interval for the quadrature error - represented by the term $(b-a)\epsilon_n^*(a,b)$ in Taylor-like formulas - is achieved either by the trapezoidal formula or the midpoint formula. This result complements the work of S.S. Dragomir [19] and X.L. Cheng [17], who considered different classes of functions, included those in C^1. In their studies, they demonstrated that the sharp constant appearing on the right-hand side of the quadrature error cannot be smaller than 1/8, both for the trapezoidal and midpoint formulas.

On the another hand, the estimates (27) and (23) from Theorems 3.1 and 3.2 can also be compared with well-known results found in [18], which address more regular functions. There, it is shown that the Gauss-Legendre formula minimizes the associated quadrature error when f' belongs to C^{2n+2} on the interval of integration.

To simplify our presentation without loss of generality, we now consider the case where $[a,b]=[-1,+1]$. The corresponding quadrature error $E(f')$ defined as:

$$E(f') = \int_{-1}^{1} f'(x)\,dx - \left(\sum_{k=0}^{n} \Omega_k f'(x_k)\right), \tag{44}$$

satisfies the following relation [18]:

$$\exists\, \xi \in]-1,+1[,\ E(f') = \frac{f^{(2n+3)}(\xi)}{(2n+2)!}\int_{-1}^{1} \pi_{n+1}^2(x)\,dx = \frac{f^{(2n+3)}(\xi)}{(2n+2)!}\frac{2}{2n+3}, \tag{45}$$

where π_{n+1} denotes the Legendre polynomial of degree less than or equal to $n+1$. As a result, the corresponding standard estimate for the quadrature is given by:

$$|E(f')| \leq \frac{2}{(2n+3)!}.\|f^{(2n+3)}\|_\infty, \tag{46}$$

where $\|.\|_\infty$ denotes the standard L^∞−norm on the interval of interest.

Our study, however, deals with functions f that are only C^2, while the Gauss-Legendre error estimate (46) applies only if the function belongs at least to $C^3([-1,+1])$, which corresponds to $n=0$. In this case, the quadrature error $E(f')$ given by (46) leads to the following estimate:

$$|E(f')| \leq \frac{\|f'''\|_\infty}{3}. \tag{47}$$

Therefore, it is clear that the first-order Taylor-like formulas of (26) and (22) provide a more accurate result, with the accuracy increasing with the number of points considered within the interval $[a,b]$. More precisely, this is true for any number of points n chosen in the estimate (23) from Theorem 3.1, since for all $n \geq 1$, the constant $\frac{1}{4n}$ is always less than the constant $\frac{1}{3}$ involved in (47). This means that as soon as $n \geq 1$ - which corresponds to having at least 2 points in the interval $[-1, 1]$ - the Taylor-like formula (22) produces a remainder that is upper-bounded by a quantity smaller than that considered in the case of Gauss-Legendre quadrature applied to C^3 functions.

5. Conclusion

In this paper, we derived a new first-order Taylor-like formula constructed as a linear combination of the first derivative of a given function, evaluated at specified points $x_k, (k = 0, \dots, n)$, and weighted by real numbers $\omega_k, (k = 0, \dots, n)$. Unlike the approach in [15], the positions of these points and their corresponding weights were not fixed *a priori*, relaxing the assumption of equally spaced points.

Our aim was to determine the optimal positions of these points and the associated weights for obtaining the "best formula", in the sense that the corresponding remainder is as small as possible. To achieve this, we established an initial result that provides upper and lower bounds for the remainder.

We then proved the existence of an optimal set of points and weights that minimize the remainder in the first-order Taylor-like formula. In a first case, we fixed $x_0 = a$ and $x_n = b$ *a priori*, while the other points are free in $[a, b]$. The result we obtained corresponds to the formula we derived in [15], where we explicitly set *a priori* the values of the points $x_k, (k = 1, \dots, n-1)$, to be uniformly distributed within the interval $[a, b]$. In a second case, the points are arbitrarily distributed in the interval $[a, b]$, leading to a result that involves the midpoints of each interval, all assigned with the same weight.

Consequently, the findings in [15], primarily related to applications in error approximations, can be considered optimal: this includes P_1-interpolation error estimates, the corrected trapezoidal quadrature formula, and finite element error approximations. For instance, using the corrected trapezoidal quadrature formula, we obtained an upper bound that is half the size of the errors produced by the classical trapezoidal quadrature formula. This highlights the significance and impact of the new Taylor-like formula (22)-(23) in assessing the accuracy of a given numerical approximation method.

In the last section, we evaluated the results of Theorems 3.1 and 3.2 and propose numerical simulations that illustrate the optimality of the formula we derived. We also interpret the general Taylor-like formula as a Gauss quadrature formula applied to the integration of a function f' belonging (only) to $C^1([a, b])$. In this context, Theorems 3.1 and 3.2 proved that, within the family of Gauss quadratures, for functions to be integrated belonging to $C^1([a, b])$, the minimal interval where the quadrature error lies corresponds to the cases of the trapezoidal formula or the midpoint formula.

This research can be extended to cases of dimension strictly greater than one. This extension will require a Taylor-like formula that we have already derived in [13]. Additionally, we could expand this work to a second-order Taylor-like formula, as proposed in [14]. Both extensions will be explored to assess their impact on error estimates in the context of numerical analysis applications.

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