# A new second order Taylor-like theorem with an optimized reduced remainder

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Joël Chaskalovic [*] Franck Assous [†] Hessam Jamshidipour [‡]

**Abstract**

In this paper, we derive a variant of the Taylor theorem to obtain a new minimized remainder. For a given function $f$ defined on the interval $[a, b]$, this formula is derived by introducing a linear combination of $f'$ computed at $n + 1$ equally spaced points in $[a, b]$, together with $f''(a)$ and $f''(b)$. We then consider two classical applications of this Taylor-like expansion: the interpolation error and the numerical quadrature formula. We show that using this approach improves both the Lagrange $P_2$- interpolation error estimate and the error bound of the Simpson rule in numerical integration.

*keywords*: Taylor's theorem, Lagrange interpolation, interpolation error, Simpson rule, quadrature error.

## 1 Introduction

Even today, improving the accuracy of approximation remains a challenging problem in numerical analysis. Here, we are concerned with the difficulty of accurately determining the error estimate in numerical methods. This article is part of a series of articles in which this topic is addressed. More precisely, we derive here a variant of Taylor's theorem to obtain a new minimized remainder that we apply to interpolation error and numerical quadrature formula.

From a mathematical point of view, the origin of such problems already appears in Rolle's theorem and in Lagrange and Taylor's theorems, see for instance [3]. Indeed, there exists an unknown point involved in the remainder of Taylor's expansion, that leads to some "uncertainty".

Consequently, most error estimates focus generally on the *asymptotic behavior* of the error. For instance in finite element approximation, *a priori* error estimates consider the asymptotic behavior of the difference between the exact and the approximate solution, as the mesh size h tends to zero.

In this context, several approaches have been proposed to determine a way to improve the accuracy of approximation. For example, within the framework of numerical integration, we refer the reader to [4], [6] or [17], and references therein. From another point of view, due to the lack of information, heuristic methods were considered, basically based on a probabilistic approach, see for instance [1], [2], [19], [22] or [7], [9] and [10]. This allows to compare different numerical

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methods, and more precisely finite element, for a given fixed mesh size, see [11].

Nevertheless, Taylor's theorem introducing an unknown point in its remainder, this makes it very difficult (often impossible) to compute the interpolation error, and consequently the approximation error of a given numerical method. Therefore, the possibility to accurately estimate the upper bounds of the error remains an important issue. In this article, we study the values of the numerical constants involved in such estimates, trying to reduce them as small as possible.

In this framework, we proposed in [12] a refined first-order expansion formula in $\mathbb{R}^n$, to get an reduced remainder, compared to the one obtained by usual Taylor's formula. Then, we investigate the related properties in the interpolation error estimates and in Lagrange finite element error estimates. In the context of quadrature rules applications, such a problem was considered in the past years, and is often referred as the perturbed (or corrected) quadrature rules, see for instance [6] or [17]. In other examples, the authors obtained in [14], [18] or [21], the trapezoid inequality by the difference of sup and inf bound of the first derivative.

In this paper, we are concerned by a second order Taylor-like theorem, leading to an optimized reduced remainder. Applications we have in mind are the interpolation error based on a second-order polynomial and the Simpson quadrature rule (see for instance [5]). Concerning the Simpson inequality, we also refer the reader to [20].

The paper is organized as follows. In Section 2, we present the main result, which treats on the improved second order Taylor-like formula. In Section 3, we consider two classical applications of the Taylor expansion: the interpolation error is investigated in subsection 3.1, whereas the Simpson's quadrature rule is studied subsection 3.2. In both cases, we derive new results on error estimate. Concluding remarks follow.

## 2 A new second order expansion formula

To begin with, let us recall the well known second order Taylor's formula [23]. We consider $(a,b) \in \mathbb{R}^2$, $a < b$, and a function $f \in \mathcal{C}^3([a,b])$. Then, following Taylor's theorem in one real variable, there exist two real constants $m_3$ and $M_3$ such that, for all $x \in [a,b]$,

$$-\infty < m_3 = \inf_{a \leq x \leq b} f'''(x) \text{ and } M_3 = \sup_{a \leq x \leq b} f'''(x) < +\infty\,, \tag{1}$$

and we have

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

where

$$\lim_{b \to a} \epsilon_{a,2}(b) = 0,$$

and

$$\frac{(b-a)}{6} m_3 \leqslant \epsilon_{a,2}(b) \leqslant \frac{(b-a)}{6} M_3. \tag{3}$$

In the same spirit we proposed in [13] for the first order case, our aim is now to derive a new second order Taylor-like formula that gives us a minimized remainder. To that aim, let us first recall the main result obtained in [13] for the first order case. Given two reals $a, b \in \mathbb{R}$, $a < b$ and an integer $n \in \mathbb{N}^*$, we proved the following result

**Theorem 2.1** *Let $f$ be a real mapping define 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 we have the following first order expansion:*

$$f(b) = f(a) + (b-a)\left(\frac{f'(b)+f'(a)}{2n} + \frac{1}{n}\sum_{k=1}^{n-1} f'\left(a + k\frac{(b-a)}{n}\right)\right) + (b-a)\epsilon_{a,n+1}^{(1)}(b), \qquad (4)$$

*where :*

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

Moreover, this result is optimal in the sense that the weights in (4) involved in the linear combination of $f'$ at the equally spaced points $a + k\dfrac{(b-a)}{n}$ guarantee the remainder $\epsilon_{a,n+1}^{(1)}(b)$ to be minimum.

In order to prove the main theorem for the second order case considered in this paper, we will need the following lemma proved in [13]:

**Lemma 2.2** *Let $u$ be a continuous function on $[a,b]$, and, for $n \in \mathbb{N}^*$, let $(a_k)_{0\leqslant k\leqslant n}$ be a finite sequence of real numbers. We have the following formula:*

$$\sum_{k=0}^{n-1} \int_k^n a_k u(t)dt = \sum_{k=0}^{n-1} \int_k^{k+1} S_k u(t)dt, \quad \text{with } S_k = \sum_{j=0}^{k} a_j.$$

From now on, we assume that $n \in \mathbb{N}^*$. To obtain a second order Taylor-like formula, we first consider the following generalization of (4) involving the "reminder" $\epsilon_{a,n+1}^{(2)}(b)$:

$$\begin{aligned} f(b) = f(a) + (b-a)\left(\frac{f'(b)+f'(a)}{2n} + \frac{1}{n}\sum_{k=1}^{n-1} f'\left(a + k\frac{(b-a)}{n}\right)\right) \\ +(b-a)^2 \sum_{k=0}^{n} \omega_k(n) f''\left(a + k\frac{(b-a)}{n}\right) + (b-a)^2\epsilon_{a,n+1}^{(2)}(b), \end{aligned} \qquad (5)$$

that we rewrite for simplicity as

$$f(b) = f(a) + (b-a)\Lambda_n^{(1)}(a,b) + (b-a)^2\Lambda_n^{(2)}(a,b) + (b-a)^2\epsilon_{a,n+1}^{(2)}(b),$$

with

$$\Lambda_n^{(1)}(a,b) = \frac{f'(b)+f'(a)}{2n} + \frac{1}{n}\sum_{k=1}^{n-1} f'\left(a + k\frac{(b-a)}{n}\right), \qquad (6)$$

and $\Lambda_n^{(2)}(a,b)$ defined by determining

$$\Lambda_n^{(2)}(a,b) = \sum_{k=0}^{n} \omega_k(n) f''\left(a + k\frac{(b-a)}{n}\right), \qquad (7)$$

such that (5) holds, and so, $\epsilon_{a,n+1}^{(2)}(b)$ goes to 0 when $b \to a$. Our aim is now to determine the sequence of real weights $(\omega_k(n))_{0\leq k\leq n}$ that minimizes the remainder $\epsilon_{a,n+1}^{(2)}(b)$. this result is stated in the following theorem:

**Theorem 2.3** *Let $f$ be a real mapping defined on $[a,b]$ which belongs to $\mathcal{C}^3([a,b])$, such that: $\forall x \in [a,b], -\infty < m_3 \leqslant f'''(x) \leqslant M_3 < +\infty$. If the weights $(\omega_k(n))_{0\leq k\leq n}$ satisfy $\sum_{k=0}^{n} \omega_k(n) = 0$, then we have:*

$$\omega_0(n) = -\omega_n(n) = \frac{3}{32n^2} \quad \textit{and} \quad \omega_k(n) = 0, \ \forall 0 < k < n, \tag{8}$$

*and the following second order expansion hold:*

$$f(b) = f(a) + (b-a)\Lambda_n^{(1)}(a,b) + (b-a)^2\Lambda_n^{(2)}(a,b) + (b-a)^2\epsilon_{a,n+1}^{(2)}(b), \tag{9}$$

*where $\Lambda_n^{(1)}(a,b)$ is given by (6) and $\Lambda_n^{(2)}(a,b)$ is expressed as*

$$\Lambda_n^{(2)}(a,b) \ = \ -\frac{3}{32n^2}\Big(f''(b) - f''(a)\Big). \tag{10}$$

*Moreover, this result is optimal since the weights introduced in (8) guarantee that the remainder $\epsilon_{a,n+1}^{(2)}(b)$ is minimum, and satisfies:*

$$\frac{(b-a)}{96n^2}(2m_3 - M_3) \leq \epsilon_{a,n+1}^{(2)}(b) \leq \frac{(b-a)}{96n^2}(2M_3 - m_3). \tag{11}$$

*Consequently,* $\lim_{b\to a} \epsilon_{a,n+1}^{(2)}(b) = 0$.

*Proof :* Let us observe first that, using (4), $\epsilon_{a,n+1}^{(2)}(b)$ can be written as

$$\epsilon_{a,n+1}^{(2)}(b) = \frac{\epsilon_{a,n+1}^{(1)}(b)}{b-a} - \Lambda_n^{(2)}(a,b)\,. \tag{12}$$

In [13], it is proved (see expression (16) together with (28)) that the remainder $\epsilon_{a,n+1}^{(1)}(b)$ of the expansion (4) can be expressed by

$$\epsilon_{a,n+1}^{(1)}(b) = \sum_{k=0}^{n-1} \int_{\frac{k}{n}}^{\frac{k+1}{n}} \left(\frac{1}{2n} + \frac{k}{n} - t\right)\phi'(t)dt, \tag{13}$$

where $\phi'$ is the derivative of the function $\phi$ defined by:

$$\begin{array}{rccl} \phi & : & [0,1] & \longrightarrow & \mathbb{R} \\ & & t & \longmapsto & f'(a+t(b-a)). \end{array}$$

Now, we perform an integration by parts of the integral involved in (13) and we get

$$\begin{aligned} \int_{\frac{k}{n}}^{\frac{k+1}{n}} \left(\frac{1}{2n} + \frac{k}{n} - t\right)\phi'(t)dt \ &= \ \frac{k(k+1)}{2n^2}\left[\phi'\left(\frac{k+1}{n}\right) - \phi'\left(\frac{k}{n}\right)\right] - \int_{\frac{k}{n}}^{\frac{k+1}{n}} \left[\left(\frac{1}{2n} + \frac{k}{n}\right)t - \frac{t^2}{2}\right]\phi''(t)dt, \\ &= \ \int_{\frac{k}{n}}^{\frac{k+1}{n}} \left[\frac{k(k+1)}{2n^2} - \left(\frac{1}{2n} + \frac{k}{n}\right)t + \frac{t^2}{2}\right]\phi''(t)dt. \end{aligned}$$

Using this expression, $\epsilon_{a,n+1}^{(1)}(b)$ can be rewritten as:

$$\epsilon_{a,n+1}^{(1)}(b) = \sum_{k=0}^{n-1} \int_{\frac{k}{n}}^{\frac{k+1}{n}} \left[\frac{t^2}{2} - \left(\frac{1}{2n} + \frac{k}{n}\right)t + \frac{k(k+1)}{2n^2}\right]\phi''(t)dt.$$

Consequently, from (12), $\epsilon^{(2)}_{a,n+1}(b)$ can be written

$$\epsilon^{(2)}_{a,n+1}(b) = \frac{1}{b-a}\sum_{k=0}^{n-1}\int_{\frac{k}{n}}^{\frac{k+1}{n}}\left[\frac{t^2}{2} - \left(\frac{1}{2n}+\frac{k}{n}\right)t + \frac{k(k+1)}{2n^2}\right]\phi''(t)dt - \frac{1}{b-a}\sum_{k=0}^{n}\omega_k(n)\phi'\left(\frac{k}{n}\right). \tag{14}$$

Now, using that $\phi'\left(\frac{k}{n}\right) = \phi'(1) - \int_{\frac{k}{n}}^{1}\phi''(t)dt$ together with Lemma 2.2, and a change of variable $t' = nt$, the last sum in (14) can be expressed as:

$$\sum_{k=0}^{n}\omega_k(n)\phi'\left(\frac{k}{n}\right) = \sum_{k=0}^{n}\omega_k(n)\phi'(1) - \sum_{k=0}^{n-1}\int_{\frac{k}{n}}^{\frac{k+1}{n}} S_k(n)\phi''(t)dt,$$

where $S_k(n) = \sum_{j=0}^{k}\omega_j(n)$, for all $0 \le k \le n-1$.

Consequently, expression (14) becomes:

$$\epsilon^{(2)}_{a,n+1}(b) = \frac{1}{b-a}\sum_{k=0}^{n-1}\int_{\frac{k}{n}}^{\frac{k+1}{n}}\left[\frac{t^2}{2} - \left(\frac{1}{2n}+\frac{k}{n}\right)t + \frac{k(k+1)}{2n^2} + S_k(n)\right]\phi''(t)dt - \frac{1}{b-a}\phi'(1)\sum_{k=0}^{n}\omega_k(n). \tag{15}$$

Let us assume for simplicity (see Remark 1 below) that:

$$\sum_{k=0}^{n}\omega_k(n) = 0. \tag{16}$$

Then, setting

$$\lambda = S_k(n) + \frac{k(k+1)}{2n^2},$$

the expression (15) of $\epsilon^{(2)}_{a,n+1}(b)$ becomes:

$$\epsilon^{(2)}_{a,n+1}(b) = \frac{1}{b-a}\sum_{k=0}^{n-1}\int_{\frac{k}{n}}^{\frac{k+1}{n}}\left[\frac{t^2}{2} - \left(\frac{1}{2n}+\frac{k}{n}\right)t + \lambda\right]\phi''(t)dt.$$

Substituting $t = \dfrac{k+s}{n}$ in this integral, and setting $P_{\bar\lambda}(s) = s^2 - s + \bar\lambda$ with

$$\bar\lambda \equiv 2n^2\lambda - k(k+1) = 2n^2 S_k(n)\,, \tag{17}$$

we get:

$$\epsilon^{(2)}_{a,n+1}(b) = \frac{1}{2(b-a)n^3}\sum_{k=0}^{n-1}\int_0^1 P_{\bar\lambda}(s)\phi''\left(\frac{s+k}{n}\right)ds. \tag{18}$$

Now, assuming that the discriminant $\Delta = 1 - 4\bar\lambda$ of $P_{\bar\lambda}$ is strictly positive, it exists $(t_1, t_2) \in \mathbb{R}^2, t_1 < t_2$, such that: $P_{\bar\lambda}(t_1) = P_{\bar\lambda}(t_2) = 0$.

In the following, our aim is to derive an estimate of $\epsilon^{(2)}_{a,n+1}(b)$. For this purpose, we split the integral above depending on the roots of $P_{\bar\lambda}$. We get:

$$\int_0^1 P_{\bar\lambda}(t)\phi''\left(\frac{t+k}{n}\right)dt = \int_0^{t_1} P_{\bar\lambda}(t)\phi''\left(\frac{t+k}{n}\right)dt + \int_{t_1}^{t_2} P_{\bar\lambda}(t)\phi''\left(\frac{t+k}{n}\right)dt + \int_{t_2}^1 P_{\bar\lambda}(t)\phi''\left(\frac{t+k}{n}\right)dt.$$

Keeping in mind that, for all $x \in [0,1]$ and for all $t \in [a,b]$,

$$\phi''(x) = (b-a)^2 f'''(a+x(b-a)) \text{ and } m_3 \leqslant f'''(t) \leqslant M_3,$$

then, $P_{\bar{\lambda}}(t)$ keeps a constant sign on each of the three above integrals and we have:

$$\begin{aligned}
m_3(b-a)^2 \int_0^{t_1} P_{\bar{\lambda}}(t)dt &\leq \int_0^{t_1} P_{\bar{\lambda}}(t)\phi''\left(\frac{t+k}{n}\right)dt \leq M_3(b-a)^2 \int_0^{t_1} P_{\bar{\lambda}}(t)dt,\\
M_3(b-a)^2 \int_{t_1}^{t_2} P_{\bar{\lambda}}(t)dt &\leq \int_{t_1}^{t_2} P_{\bar{\lambda}}(t)\phi''\left(\frac{t+k}{n}\right)dt \leq m_3(b-a)^2 \int_{t_1}^{t_2} P_{\bar{\lambda}}(t)dt,\\
m_3(b-a)^2 \int_{t_2}^{1} P_{\bar{\lambda}}(t)dt &\leq \int_{t_2}^{1} P_{\bar{\lambda}}(t)\phi''\left(\frac{t+k}{n}\right)dt \leq M_3(b-a)^2 \int_{t_2}^{1} P_{\bar{\lambda}}(t)dt,
\end{aligned}$$

that yields the two following inequalities

$$\int_0^1 P_{\bar{\lambda}}(t)\phi''\left(\frac{t+k}{n}\right)dt \leq m_3(b-a)^2 \int_{t_1}^{t_2} P_{\bar{\lambda}}(t)dt + M_3(b-a)^2\left[\int_0^{t_1} P_{\bar{\lambda}}(t)dt + \int_{t_2}^1 P_{\bar{\lambda}}(t)dt\right], \quad (19)$$

$$\int_0^1 P_{\bar{\lambda}}(t)\phi''\left(\frac{t+k}{n}\right)dt \geq M_3(b-a)^2 \int_{t_1}^{t_2} P_{\bar{\lambda}}(t)dt + m_3(b-a)^2\left[\int_0^{t_1} P_{\bar{\lambda}}(t)dt + \int_{t_2}^1 P_{\bar{\lambda}}(t)dt\right]. \quad (20)$$

We have now to deal with these inequalities. Since they have the same structure, we will consider only the first one, the second one can be treated in the same way.

Dividing by $(b-a)^2$ and computing the integrals, $P_{\bar{\lambda}}(t)$ being a second-degree polynomial function, we easily get:

$$\frac{\int_0^1 P_{\bar{\lambda}}(t)\phi''\left(\frac{t+k}{n}\right)dt}{(b-a)^2} \leq (M_3-m_3)(t_1-t_2)\left[\frac{t_1^2+t_1t_2+t_2^2}{3} - \frac{t_1+t_2}{2} + \bar{\lambda}\right] + M_3\left(\bar{\lambda} - \frac{1}{6}\right).$$

Using that $t_i, (i=1,2)$, are the roots of the polynomial $P_{\bar{\lambda}}(.)$, we have, for $i=1,2$, $t_i^2 = t_i - \bar{\lambda}$ and this inequality becomes:

$$\frac{\int_0^1 P_{\bar{\lambda}}(t)\phi''\left(\frac{t+k}{n}\right)dt}{(b-a)^2} \leq (M_3-m_3)(t_1-t_2)\left[\frac{t_1+t_2+t_1t_2-2\bar{\lambda}}{3} - \frac{t_1+t_2}{2} + \bar{\lambda}\right] + M_3\left(\bar{\lambda} - \frac{1}{6}\right).$$

Since $t_1, t_2$ are the roots of the second-degree polynomial $P_{\bar{\lambda}}(.)$,

$$t_1+t_2 = 1,\ t_1t_2 = \bar{\lambda} \text{ and } t_1 - t_2 = -\sqrt{1-4\bar{\lambda}},$$

that leads to:

$$\frac{\int_0^1 P_{\bar{\lambda}}(t)\phi''\left(\frac{t+k}{n}\right)dt}{(b-a)^2} \leq \frac{(M_3-m_3)}{6}(1-4\bar{\lambda})^{3/2} + M_3\left(\bar{\lambda} - \frac{1}{6}\right).$$

Finally, due to the symmetry between $m_3$ and $M_3$ in the right-hand sides of (19) and (20), we can write

$$\varphi_1(\bar{\lambda}) \leq \frac{\int_0^1 P_{\bar{\lambda}}(t)\phi''\left(\frac{t+k}{n}\right)dt}{(b-a)^2} \leq \varphi_2(\bar{\lambda}), \quad (21)$$

where $\varphi_i(\bar{\lambda}), (i = 1, 2)$ are defined by:

$$\begin{aligned}\varphi_1(\bar{\lambda}) &= \frac{(m_3 - M_3)}{6}(1 - 4\bar{\lambda})^{3/2} + m_3\left(\bar{\lambda} - \frac{1}{6}\right),\\ \varphi_2(\bar{\lambda}) &= \frac{(M_3 - m_3)}{6}(1 - 4\bar{\lambda})^{3/2} + M_3\left(\bar{\lambda} - \frac{1}{6}\right).\end{aligned}$$

We conclude the proof by determining the $\bar{\lambda}$ that minimizes the distance between $\varphi_1(\bar{\lambda})$ and $\varphi_2(\bar{\lambda})$. Let us define

$$\varphi(\bar{\lambda}) = \varphi_2(\bar{\lambda}) - \varphi_1(\bar{\lambda}) = (M_3 - m_3)\left[\frac{(1 - 4\bar{\lambda})^{3/2}}{3} + \bar{\lambda} - \frac{1}{6}\right],$$

which satisfies $\varphi'(\bar{\lambda}) = 0$ for $\bar{\lambda} = \dfrac{3}{16}$, that is, the minimum of $\varphi(\bar{\lambda})$. This also shows *a posteriori* that $1 - 4\bar{\lambda} > 0$, i.e. the discriminant of $P_{\bar{\lambda}}(t)$ is positive. For this value of $\bar{\lambda}$, the inequalities (21) are written as:

$$\frac{2m_3 - M_3}{48} \leq \frac{\displaystyle\int_0^1 P_{\bar{\lambda}}(t)\phi''\left(\frac{t+k}{n}\right)dt}{(b-a)^2} \leq \frac{2M_3 - m_3}{48},$$

and summing then over $k$, we obtain for $\epsilon^{(2)}_{a,n+1}(b)$ in (18):

$$\frac{(b-a)}{96n^2}(2m_3 - M_3) \leq \epsilon^{(2)}_{a,n+1}(b) \leq \frac{(b-a)}{96n^2}(2M_3 - m_3).$$

Moreover, we can also get the weights $\omega_k(n), (k = 0, n)$, involved in $\Lambda^{(2)}_n(a, b)$ (cf. (7)). Indeed, substituting $\bar{\lambda} = \dfrac{3}{16}$ in the expression $\bar{\lambda} = 2n^2 S_k(n)$, from (17), we get

$$S_k(n) = \sum_{j=0}^{k} \omega_j(n) = \frac{3}{32n^2}, \forall k = 0, \ldots, n-1.$$

Hence, for $k = 0$, $\omega_0(n) = \dfrac{3}{32n^2}$ whereas $\omega_k(n) = 0$ for all $0 \leq k \leq n-1$. Finally, we determine the last weight $w_n(n)$ by using the assumption (16), that leads to

$$\omega_n(n) = -\omega_0(n) = -\frac{3}{32n^2}.$$

and $\Lambda^{(2)}_n(a, b)$ introduced in (7) satisfies (10). ■

*Remark 1 Condition (16) on the weights $\omega_k(n)$ in Theorem 2.3 is a kind of* closure condition *but is not a restrictive one. Indeed, without (16), we will replace in (18) $\epsilon^{(2)}_{a,n+1}(b)$ by*

$$\epsilon^{(2)}_{a,n+1}(b) = \frac{1}{2(b-a)n^3}\sum_{k=0}^{n-1}\int_0^1 P_{\bar{\lambda}}(t)\phi''\left(\frac{t+k}{n}\right)dt - \frac{1}{b-a}\phi'(1)\sum_{k=0}^{n-1}\omega_k(n)\,,$$

*and consequently, the corresponding weights $\omega_k(n)$ would be written as:*

$$\omega_0(n) = \frac{3}{32n^2} \quad \textit{and} \quad \omega_k(n) = 0,\ \forall\, 1 \leq k \leq n.$$

*Then, following the same steps, we will get the following estimates for* $\epsilon^{(2)}_{a,n+1}(b)$*:*

$$\frac{(2m_3 - M_3)(b-a)}{96n^2} - \frac{3}{32n^2}\frac{\phi'(1)}{(b-a)} \leq \epsilon^{(2)}_{a,n+1}(b) \leq \frac{(2M_3 - m_3)(b-a)}{96n^2} - \frac{3}{32n^2}\frac{\phi'(1)}{(b-a)},$$

*or also*

$$\frac{(2m_3 - M_3)(b-a)}{96n^2} - \frac{3M_2}{32n^2} \leq \epsilon^{(2)}_{a,n+1}(b) \leq \frac{(2M_3 - m_3)(b-a)}{96n^2} - \frac{3m_2}{32n^2}.$$

*Furthermore, still without the condition (16) on the weights, the second order Taylor's-like formula (9) would be expressed as*

$$f(b) = f(a) + (b-a)\Lambda^{(1)}_n(a,b) + \frac{3}{32n^2}(b-a)^2 f''(a) + (b-a)^2\epsilon^{(2)}_{a,n+1}(b), \tag{22}$$

*the coefficient before* $f''(b)$ *vanishes.*

Let us compare now the remainder (11) of the new formula (9)-(10) with the reminder (3) of the classical formula (2). As one can see, the former remainder is significantly smaller than the latter one: indeed, we have to compare $1/6$ with $1/32n^2$ whose ratio is equal $3/16n^2$. The worst case of this ratio corresponds to $n = 1$ where the new remainder is approximatively 5 times smaller than the one obtained by the classical formula.

# 3 Applications to the approximation error

In this section, we consider two classical applications of the Taylor expansion: the Lagrange polynomial interpolation and the numerical quadrature. In both cases, we will derive new formula of interpolation and quadrature, obtained by using the refined second-order expansion formula (9)-(10). Then, we will compare the errors obtained when using the standard Taylor expansion and our generalized approach. We begin with the interpolation error.

## 3.1 The interpolation error

Consider first the generalized Taylor-like expansion (9)-(10) for $n = 2$ In this case, for any function $f$ which belongs to $C^3([a,b])$, this formula is expressed as

$$f(b) = f(a) + (b-a)\frac{f'(b) + 2f'(\frac{a+b}{2}) + f'(a)}{4} - \frac{3(b-a)^2}{128}\left(f''(b) - f''(a)\right) + (b-a)^2\epsilon^{(2)}_{a,3}(b), \tag{23}$$

where the remainder $\epsilon_{a,3}(b)$ satisfies

$$\frac{(b-a)}{384}(2m_3 - M_3) \leq \epsilon^{(2)}_{a,3}(b) \leq \frac{(b-a)}{384}(2M_3 - m_3). \tag{24}$$

In order to derive a first application of this formula, let us consider the case of the $P_2$-Lagrange interpolation (see for instance [5], [3]), where a given function $f$ is interpolated on $[a,b]$ by a polynomial $\Pi_{[a,b]}(f)$ of degree less than or equal to two. Hence, we can write:

$$\forall x \in [a,b] : \Pi_{[a,b]}(f)(x) = \frac{(x-c)(x-b)}{(a-c)(a-b)}\, f(a) + \frac{(x-a)(x-c)}{(b-a)(b-c)}\, f(b) + \frac{(x-a)(x-b)}{(c-a)(c-b)}\, f(c)\,, \tag{25}$$

where $c = \dfrac{a+b}{2}$ denotes the midpoint of $[a,b]$.

As it is well known, one has by construction $\Pi_{[a,b]}(f)(a) = f(a)$, $\Pi_{[a,b]}(f)(b) = f(b)$ and $\Pi_{[a,b]}(f)(c) = f(c)$.

Let us investigate the consequences of formula (23) when it is used to evaluate the interpolation error $e(.)$ defined by

$$\forall x \in [a,b] : e(x) = \Pi_{[a,b]}(f)(x) - f(x)\,,$$

and compare it with the one obtained when using the classical first order Taylor's formula.

The classical result [15] concerning the $P_2-$Lagrange interpolation error claims that, for any function $f$ that belongs to $C^3([a,b])$, we have:

$$|e(x)| \leq \frac{(x-a)(b-x)|x-c|}{6} \sup_{a\leq x\leq b} |f'''(x)|\,,$$

and using that $\sup\limits_{a\leq x\leq b} (x-a)(b-x)|x-c| = \dfrac{(b-a)^3}{12\sqrt{3}}$, we get

$$|e(x)| \leq \frac{(x-a)(b-x)|x-c|}{6} \sup_{a\leq x\leq b} |f'''(x)| \leq \frac{(b-a)^3}{72\sqrt{3}} \sup_{a\leq x\leq b} |f'''(x)|. \tag{26}$$

This result is usually derived by considering, for $x \in [a,b]$, $x$ different from $a, b$ and $c$, the function $g(t)$ defined by

$$g(t) = f(t) - \Pi_{[a,b]}(f)(t) - \Big(f(x) - \Pi_{[a,b]}(f)(x)\Big)\frac{(t-a)(t-c)(t-b)}{(x-a)(x-c)(x-b)}\,.$$

By construction, $g(t)$ vanishes on $a, c, b$ and on the point $t = x$. Then, by applying three times Rolle's theorem, we obtain that there exists a point $\xi_x \in ]a,b[\backslash\{c,x\}$ such that $g'''(\xi_x) = 0$.

Moreover, the third-order derivative of $\Pi_{[a,b]}(f)(t)$, which is a polynomial of degree 2, vanishes, and the third-order derivative of the function $t \longrightarrow (t-a)(t-c)(t-b)$ is a constant equal to 6. Therefore, we obtain that there exists $\xi_x \in ]a,b[\backslash\{c,x\}$ such that

$$g'''(\xi_x) = f'''(\xi_x) - \Big(f(x) - \Pi_{[a,b]}(f)(x)\Big)\frac{6}{(x-a)(x-c)(x-b)} = 0\,,$$

that leads to (26).

Now, to evaluate the difference between the classical Taylor's formula and the formula we derived in (23), we consider the two constants $m_3$ and $M_3$ introduced in (1), and we reformulate estimate (26) by using the classical Taylor formula (1). We get the following result:

**Lemma 3.1** *Let $f$ be a function $C^3([a,b])$ satisfying (1). Then the second order Taylor's theorem leads to the following interpolation error estimate:*

$$|e(x)| \leq \frac{(b-a)^3}{72\sqrt{3}}(2M_3 - m_3)\,. \tag{27}$$

*Proof :* We begin by writing the Lagrange $P_2-$polynomial $\Pi_{[a,b]}(f)$ given by (25) by using the classical second order Taylor's formula (2).

For this purpose, we substitute in (25), $f(a)$, $f(b)$ and $f(c)$ expressed in the following form:

$$\begin{aligned} f(a) &= f(x) + (a-x)f'(x) + \frac{(a-x)^2}{2}f''(x) + (a-x)^2\epsilon_{x,2}(a), \\ f(b) &= f(x) + (b-x)f'(x) + \frac{(b-x)^2}{2}f''(x) + (b-x)^2\epsilon_{x,2}(b), \\ f(c) &= f(x) + (c-x)f'(x) + \frac{(c-x)^2}{2}f''(x) + (c-x)^2\epsilon_{x,2}(c), \end{aligned}$$

where, by the help of (3) and (1), the remainders $\epsilon_{x,2}(a)$, $\epsilon_{x,2}(b)$ and $\epsilon_{x,1}(c)$ satisfy the inequations, with $M = \max\{|m_3|, |M_3|\}$,

$$|\epsilon_{x,2}(a)| \leq \frac{(x-a)}{6}M,\ |\epsilon_{x,2}(b)| \leq \frac{(b-x)}{6}M \ \text{ and } \ |\epsilon_{x,2}(c)| \leq \frac{|c-x|}{6}M.$$

Then, (25) gives:

$$\begin{aligned} \Pi_{[a,b]}(f)(x) &= \frac{(x-c)(x-b)}{(a-c)(a-b)}\left(f(x) + (a-x)f'(x) + \frac{(a-x)^2}{2}f''(x) + (a-x)^2\epsilon_{x,2}(a)\right) \\ &+ \frac{(x-a)(x-c)}{(b-a)(b-c)}\left(f(x) + (b-x)f'(x) + \frac{(b-x)^2}{2}f''(x) + (b-x)^2\epsilon_{x,2}(b)\right) \\ &+ \frac{(x-a)(x-b)}{(c-a)(c-b)}\left(f(x) + (c-x)f'(x) + \frac{(c-x)^2}{2}f''(x) + (c-x)^2\epsilon_{x,2}(c)\right). \end{aligned}$$

From this expression, we can compute the coefficients of $f(x)$, $f'(x)$ and $f''(x)$. We get that the first one is equal to 1, whereas the two others are equal to 0. Consequently, we obtain for $\Pi_{[a,b]}(f)(x)$:

$$\begin{aligned} \Pi_{[a,b]}(f)(x) &= f(x) + \frac{(x-c)(x-b)}{(a-c)(a-b)}(a-x)^2\epsilon_{x,2}(a) + \frac{(x-a)(x-c)}{(b-a)(b-c)}(b-x)^2\epsilon_{x,2}(b) \\ &\quad + \frac{(x-a)(x-b)}{(c-a)(c-b)}(c-x)^2\epsilon_{x,2}(c)\,. \quad (28) \end{aligned}$$

In order to determine the error $e(x)$ introduced above, we have to compute the three last terms involved in (28), namely

$$\frac{(x-c)(x-b)}{(a-c)(a-b)}(a-x)^2\epsilon_{x,2}(a) + \frac{(x-a)(x-c)}{(b-a)(b-c)}(b-x)^2\epsilon_{x,2}(b) + \frac{(x-a)(x-b)}{(c-a)(c-b)}(c-x)^2\epsilon_{x,2}(c)\,.$$

Now recall that, from the classical Taylor formula, $\epsilon_{x,2}(a) = \dfrac{a-x}{6}f'''(\xi(a,x))$ (the same for $\epsilon_{x,2}(b)$ and $\epsilon_{x,2}(c)$). Using that $c$ is the midpoint of $[a,b]$, we have $c - a = \dfrac{b-a}{2}$, and the expression above is equal to

$$\frac{(a-x)(b-x)(c-x)}{3(b-a)^2}\left[(x-a)^2f'''(\xi(a,x)) + (b-x)^2f'''(\xi(b,x)) - 2(c-x)^2f'''(\xi(c,x))\right]. \quad (29)$$

To get an estimation of (29), we will bound separately the two terms involved. For the first one, by studying the function $f(x) = (a-x)(b-x)(c-x)$, we easily obtain that

$$-\frac{(b-a)}{36\sqrt{3}} \leq \frac{(a-x)(b-x)(c-x)}{3(b-a)^2} \leq \frac{(b-a)}{36\sqrt{3}}\,.$$

or equivalently that

$$\frac{|(a-x)(b-x)(c-x)|}{3(b-a)^2} \leq \frac{(b-a)}{36\sqrt{3}}\,.$$

For the second term of (29), using (1), we obtain that

$$g_{min}(x) \leq (x-a)^2 f'''(\xi(a)) + (b-x)^2 f'''(\xi(b)) - 2(c-x)^2 f'''(\xi(c)) \leq g_{max}(x)\,,$$

where

$$\begin{aligned} g_{min}(x) &= m_3(x-a)^2 + m_3(b-x)^2 - 2M_3(c-x)^2\,, \\ g_{max}(x) &= M_3(x-a)^2 + M_3(b-x)^2 - 2m_3(c-x)^2\,. \end{aligned}$$

To continue, we have to determine the extremum values of the functions $g_{min}(x)$ and $g_{max}(x)$. We will consider only $g_{max}(x)$, the case of $g_{min}(x)$ being analogous. A simple computation gives that the maximum of $g_{max}$ is reached at the boundaries $x = a, x = b$ , with

$$g_{max}(a) = g_{max}(b) = (b-a)^2\left(M_3 - \frac{m_3}{2}\right).$$

Similarly, we obtain the minimum of $g_{min}(x)$ is equal to

$$g_{min}(a) = g_{min}(b) = (b-a)^2\left(m_3 - \frac{M_3}{2}\right),$$

so that the second term of (29) can be bounded as follows:

$$(2m_3 - M_3)\frac{(b-a)^2}{2} \leq (x-a)^2 f'''(\xi(a)) + (b-x)^2 f'''(\xi(b)) - 2(c-x)^2 f'''(\xi(c)) \leq (2M_3 - m_3)\frac{(b-a)^2}{2}\,.$$

Now, putting these results together, we finally get that

$$|e(x)| \leq \frac{(b-a)^3}{72\sqrt{3}}(2M_3 - m_3)$$

■

*Remark 2 This result can be compared with the more classical one recalled in (26). In fact the only difference comes from the term* $\sup_{a\leq x\leq b}|f'''(x)|$ *that is replaced here by* $2M_3 - m_3$*, that takes care of the difference between the* sup *and the* inf *of the function* $f'''(x)$*, rather than considering their maximum.*

Let us now derive the corresponding result when we use the new first order Taylor-like formula (23) in the expression of the interpolation polynomial $\Pi_{[a,b]}(f)$ defined by (25). This is the purpose of the following lemma.

**Lemma 3.2** *Let* $f \in C^3([a,b])$*, then we have the following interpolation error estimate:*

$$\forall x \in [a,b] : \left| f(x) - \Pi^*_{[a,b]}(f)(x) \right| \leq \frac{(b-a)^3}{1536\sqrt{3}}(2M_3 - m_3)\,, \tag{30}$$

*where* $\Pi^*_{[a,b]}(f)(x)$ *is defined by*

$$\begin{aligned} \Pi^*_{[a,b]}(f)(x) &= \Pi_{[a,b]}(f)(x) \\ &- \frac{(x-a)(b-x)(c-x)}{(b-a)^3}\left[\frac{f'(a) - 2f'(c) + f'(b)}{2} + f'\left(\frac{x+a}{2}\right) - 2f'\left(\frac{x+c}{2}\right) + f'\left(\frac{x+b}{2}\right)\right] \\ &- \frac{3(x-a)(b-x)(c-x)}{64(b-a)^2}\left(f''(a)(a-x) + 2f''(c)(x-c) + f''(b)(b-x)\right) \end{aligned} \tag{31}$$

*Proof :* We begin to write $f(a)$, $f(b)$ and $f(c)$ by the help of (23):

$$f(a) = f(x) + (a-x)\frac{f'(a) + 2f'(\frac{x+a}{2}) + f'(x)}{4} - \frac{3(a-x)^2}{128}\left(f''(a) - f''(x)\right) + (a-x)^2\epsilon^{(2)}_{x,3}(a),$$

$$f(b) = f(x) + (b-x)\frac{f'(b) + 2f'(\frac{x+b}{2}) + f'(x)}{4} - \frac{3(b-x)^2}{128}\left(f''(b) - f''(x)\right) + (b-x)^2\epsilon^{(2)}_{x,3}(b),$$

$$f(c) = f(x) + (c-x)\frac{f'(c) + 2f'(\frac{x+c}{2}) + f'(x)}{4} - \frac{3(c-x)^2}{128}\left(f''(c) - f''(x)\right) + (c-x)^2\epsilon^{(2)}_{x,3}(c),$$

where $\epsilon_{x,3}$ satisfies (24) with obvious changes of notations. More precisely, we have

$$|\epsilon^{(2)}_{x,3}(a)| \leq \frac{(x-a)}{384}(2M_3 - m_3)\,, \quad |\epsilon^{(2)}_{x,3}(b)| \leq \frac{(b-x)}{384}(2M_3 - m_3)\,, \quad |\epsilon^{(2)}_{x,3}(c)| \leq \frac{|c-x|}{384}(2M_3 - m_3)\,. \tag{32}$$

Then, by substituting $f(a)$, $f(b)$ and $f(c)$ in the interpolation polynomial (25), we obtain

$$\begin{aligned}
\Pi_{[a,b]}(f)(x) = &\\
&\frac{(x-c)(x-b)}{(a-c)(a-b)}\left(f(x) + (a-x)\frac{f'(a) + 2f'\left(\frac{x+a}{2}\right) + f'(x)}{4} - \frac{3(a-x)^2}{128}\left(f''(a) - f''(x)\right) + (a-x)^2\epsilon^{(2)}_{x,3}(a)\right)\\
&+\frac{(x-a)(x-c)}{(b-a)(b-c)}\left(f(x) + (b-x)\frac{f'(b) + 2f'\left(\frac{x+b}{2}\right) + f'(x)}{4} - \frac{3(b-x)^2}{128}\left(f''(b) - f''(x)\right) + (b-x)^2\epsilon^{(2)}_{x,3}(b)\right)\\
&+\frac{(x-a)(x-b)}{(c-a)(c-b)}\left(f(x) + (c-x)\frac{f'(c) + 2f'\left(\frac{x+c}{2}\right) + f'(x)}{4} - \frac{3(c-x)^2}{128}\left(f''(c) - f''(x)\right) + (c-x)^2\epsilon^{(2)}_{x,3}(c)\right)
\end{aligned}$$

From this expression, we obtain that the coefficients of $f(x)$ is equal to 1, whereas the one before $f'(x)$ is equal to 0.

Let us compute now the terms before the other derivatives of $f(x)$. For the first order derivatives, we have the following expressions

$$\frac{(x-a)(b-x)(c-x)}{(b-a)^3}\left[\frac{f'(a) - 2f'(c) + f'(b)}{2} + f'\left(\frac{x+a}{2}\right) - 2f'\left(\frac{x+c}{2}\right) + f'\left(\frac{x+b}{2}\right)\right],$$

whereas the terms in $f''(x)$ can be expressed as

$$\frac{3(x-a)(b-x)(c-x)}{64(b-a)^2}\left(f''(a)(a-x) + 2f''(c)(x-c) + f''(b)(b-x)\right).$$

Finally, we obtain for $\Pi_{[a,b]}(f)(x)$:

$$\begin{aligned}
\Pi_{[a,b]}(f)(x) = f(x) &+ \frac{(x-a)(b-x)(c-x)}{(b-a)^3}\left[\frac{f'(a) - 2f'(c) + f'(b)}{2} + f'\left(\frac{x+a}{2}\right) - 2f'\left(\frac{x+c}{2}\right) + f'\left(\frac{x+b}{2}\right)\right]\\
&+\frac{3(x-a)(b-x)(c-x)}{64(b-a)^2}\left(f''(a)(a-x) + 2f''(c)(x-c) + f''(b)(b-x)\right)\\
&+\frac{(x-c)(x-b)}{(a-c)(a-b)}(a-x)^2\epsilon^{(2)}_{x,3}(a) + \frac{(x-a)(x-c)}{(b-a)(b-c)}(b-x)^2\epsilon^{(2)}_{x,3}(b) + \frac{(x-a)(x-b)}{(c-a)(c-b)}(c-x)^2\epsilon^{(2)}_{x,3}(c).
\end{aligned} \tag{33}$$

Now, let us consider the new interpolation polynomial $\Pi^*_{[a,b]}(f)$ introduced in (31). With this, the interpolation polynomial $\Pi_{[a,b]}(f)$ of (33) can be expressed as

$$\Pi^*_{[a,b]}(f) = f(x) + E(x,a,b)\,,$$

where the function error $E(x,a,b)$ is defined by

$$E(x,a,b) = \frac{(x-c)(x-b)}{(a-c)(a-b)}(a-x)^2\epsilon^{(2)}_{x,3}(a)+\frac{(x-a)(x-c)}{(b-a)(b-c)}(b-x)^2\epsilon^{(2)}_{x,3}(b)+\frac{(x-a)(x-b)}{(c-a)(c-b)}(c-x)^2\epsilon^{(2)}_{x,3}(c)\,.$$

Using (32), we obtain the following bound

$$|E(x,a,b)| \leq 2\frac{|(a-x)(b-x)(c-x)|}{(b-a)^2}\frac{2M_3-m_3}{384}\left((x-a)^2+(b-x)^2+2(c-x)^2\right)\,. \qquad (34)$$

We already saw before that

$$\frac{|(a-x)(b-x)(c-x)|}{(b-a)^2} \leq \frac{b-a}{12\sqrt{3}}\,,$$

so we only have to bound the second term of (34), that is $(x-a)^2+(b-x)^2+2(c-x)^2$.

Using a method similar to the one used for (29), we obtain that

$$\max_{a\leq x\leq b}\left((x-a)^2+(b-x)^2+2(c-x)^2\right) = \frac{3}{2}(b-a)^2\,.$$

Putting all together, we obtain that

$$|E(x,a,b)| \leq \frac{2M_3-m_3}{1536\sqrt{3}}(b-a)^3\,,$$

which completes the proof of this lemma. ■

Let us compare the interpolation errors of lemma 3.1 and 3.2, namely:

$$\left|f(x)-\Pi_{[a,b]}(f)(x)\right| \leq \frac{(b-a)^3}{72\sqrt{3}}(2M_3-m_3) \text{ and } \left|f(x)-\Pi^*_{[a,b]}(f)(x)\right| \leq \frac{(b-a)^3}{1536\sqrt{3}}(2M_3-m_3)$$

1. By considering the modified interpolation polynomial $\Pi^*_{[a,b]}(f)$ defined by (31), we obtain in (30) a bound almost 22 times smaller than the corresponding one in (27), derived by the classical Taylor formula.

   Now, the price to be paid for this improvement is that $\Pi^*_{[a,b]}(f)$ is a polynomial of degree less than or equal to three which requires the computation of $f'(\cdot)$ in 6 points, together with $f''(a)$, $f''(b)$ and $f''((a+b)/2)$. However, the consequent gain clearly appears in the following application devoted to finite elements: indeed, from Céa's lemma [8], the approximation error is bounded by the interpolation error. In practical applications of finite elements, we want to ensure that the upper bound of the interpolation error will not be greater than a given value $\epsilon$.

   Now, let us denote by $h = b-a$ the local mesh size used for the classical $P_2$-Lagrange interpolation, and by $h^*$ the one used with the interpolation $\Pi^*_{[a,b]}(f)$. Since the convergence is locally in $h^3$ and $h^{*3}$ respectively, we can take a value of $h^*$ almost $\sqrt[3]{22} \simeq 3$ greater

than $h$ for the same given accuracy, which leads to a significative gain of computation.

This improvement will be even more significant for three dimensional applications. Indeed, consider a three-dimensional computational domain discretized by a mesh of size $h$ in each direction. To get the same accuracy with the new approach, we can use a mesh of size $h^*$ in each direction. Hence, the number of nodes of this new mesh can be 22 smaller than in the former one, leading to a significant time reduction in terms of computational time.

2. Let us give an elementary numerical example. Consider the interval $[a, b] = [0, 1]$, and the function $f(x) = \ln(1 + x)$. Formula (23) gives

$$\ln(2) = \ln(1) + \frac{\frac{1}{2} + 2\frac{2}{3} + 1}{4} - \frac{3}{128}(-\frac{1}{4} + 1) + \epsilon^{(2)}_{a,3} = \frac{1061}{1536} + \epsilon^{(2)}_{a,3} \simeq 0.6907 + \epsilon^{(2)}_{a,3}$$

and

$$|\epsilon^{(2)}_{a,3}| \leq \frac{15}{1536} \simeq 1/100\,.$$

With the same data, classical Taylor's formula (2) gives

$$\ln(2) = \ln(1) + 1 + \frac{1}{2}(-1) + \epsilon_{a,2} = -\frac{1}{2} + \epsilon_{a,2}$$

and

$$|\epsilon_{a,2}| \leq \frac{1}{3}\,.$$

Hence, the improved formula leads to a much more accurate approximation of $\ln(2)$.

### 3.2 The quadrature error

We consider now, for any integrable function $f$ defined on $[a, b]$, the Simpson's quadrature rule [15] whose formula is given by

$$\int_a^b f(x)dx \simeq \frac{b-a}{6}\left(f(a) + 4\,f\left(\frac{a+b}{2}\right) + f(b)\right). \tag{35}$$

The reason we consider (35) is that this quadrature formula corresponds to approximate the function $f$ by its Lagrange polynomial interpolation $\Pi_{[a,b]}(f)$, of degree less than or equal to two, which is given by (25).

Thus, in the classical literature of numerical integration (see for example [16], [15] and [6]), we can find the standard *Simpson inequality*

$$\left|\int_a^b f(x)\,dx - \frac{b-a}{6}\left(f(a) + 4\,f\left(\frac{a+b}{2}\right) + f(b)\right)\right| \leq \frac{(b-a)^5}{180}\sup_{a\leq x\leq b}|f^{(4)}(x)|, \tag{36}$$

for any function four times differentiable $f$ on $]a, b[$, whose fourth derivative is accordingly bounded on $]a, b[$.

Now, if the function $f$ is not four times differentiable, or if the fourth derivative $f^{(4)}$ is not bounded on $]a, b[$, we cannot apply the formula above. Therefore, if we consider a function $f$ that is only $\mathcal{C}^3$ on $[a, b]$, we have the following estimation

$$\left|\int_a^b f(x)\,dx - \frac{b-a}{6}\left(f(a) + 4\,f\left(\frac{a+b}{2}\right) + f(b)\right)\right| \leq \frac{(b-a)^4}{192}\sup_{a\leq x\leq b}|f'''(x)|, \tag{37}$$

Let us prove now a result that gives estimate (36) in an alternative display. It will also extend estimation (37) to thrice differentiable functions $f$ which satisfy (1).

**Lemma 3.3** *Let $f \in C^3([a,b])$ which satisfies (1). Then, we have the following estimate:*

$$\left| \int_a^b f(x)\,dx - \frac{b-a}{6}\left( f(a) + 4\,f\left(\frac{a+b}{2}\right) + f(b)\right)\right| \leq \frac{5(b-a)^4}{1152}(M_3 - m_3)\,.$$

*Proof :* To derive this estimate, let us begin with the classical second order Taylor's formula (2), from which we have derived above the expression (28) of polynomial $\Pi_{[a,b]}(f)$. Then, by integrating (28) between $a$ and $b$, we get

$$\begin{aligned}\int_a^b (f(x) - \Pi_{[a,b]}(f)(x))\,dx \;=& \int_a^b \left( \frac{(x-c)(b-x)}{(c-a)(b-a)}\frac{(a-x)^2}{2}\epsilon_{x,2}(a)\right.\\ &\left. + \frac{(x-a)(c-x)}{(b-a)(b-c)}\frac{(b-x)^2}{2}\epsilon_{x,2}(b) + \frac{(x-a)(x-b)}{(c-a)(b-c)}\frac{(c-x)^2}{2}\epsilon_{x,2}(c)\right) dx. \quad (38)\end{aligned}$$

However, it is well known [3] that the $P_2-$Lagrange interpolation polynomial $\Pi_{[a,b]}(f)$ given by (25) also fulfills:

$$\int_a^b \Pi_{[a,b]}(f)(x)\,dx = \frac{b-a}{6}\left(f(a) + 4f(c) + f(b)\right). \quad (39)$$

Now, let us introduce the usual error in the quadrature rule $E(f)$ defined by

$$E(f) \equiv \int_a^b f(x)dx - \frac{b-a}{6}\left(f(a) + 4f(c) + f(b)\right)\,.$$

Using the expressions $\epsilon_{x,2}(a), \epsilon_{x,2}(b)$ and $\epsilon_{x,2}(c)$ (see proof of lemma 3.1), equations (38) and (39) give

$$E(f) \;=\; \int_a^b \frac{(x-a)(b-x)(c-x)}{3(b-a)^2}\left((x-a)^2 f'''(\xi(a)) + (b-x)^2 f'''(\xi(b)) - 2\,(c-x)^2 f'''(\xi(c))\right)dx$$

that we split, for convenience, in three integrals $I(a), I(b)$ and $I(c)$, so that

$$E(f) = I(a) + I(b) - I(c)$$

with

$$\begin{aligned} I(a) &= \frac{1}{3(b-a)^2}\int_a^b (x-a)^3(b-x)(c-x)f'''(\xi(a))dx\,,\\ I(b) &= \frac{1}{3(b-a)^2}\int_a^b (x-a)(b-x)^3(c-x)f'''(\xi(b))dx\,,\\ I(c) &= \frac{2}{3(b-a)^2}\int_a^b (x-a)(b-x)(c-x)^3 f'''(\xi(c))dx\,. \end{aligned}$$

To obtain estimates of $E(f)$, we will consider separately each of these integrals. We detailed here the computations for $I(a)$, the others terms can be treated similarly.

Noting that the term $(x-a)^3(b-x)(c-x)$ is positive for $a \leq x \leq c$ and negative for $c \leq x \leq b$, we split the integral and we get, using the mean value theorem, that there exists a constant $a < C_{1,a} < c$, (respectively $c < C_{2,a} < b$), such that

$$\begin{aligned}\int_a^c (x-a)^3(b-x)(c-x)f'''(\xi(a))dx &= f'''(C_{1,a})\int_a^c (x-a)^3(b-x)(c-x)dx\,,\\ \int_c^b (x-a)^3(b-x)(c-x)f'''(\xi(a))dx &= f'''(C_{2,a})\int_c^b (x-a)^3(b-x)(c-x)dx\,.\end{aligned}$$

It remains now to compute the integral above. Owing to the relation $c = (a+b)/2$, a straightforward computation gives us

$$\int_a^c (x-a)^3(b-x)(c-x)dx = \frac{(b-a)^6}{960}, \quad \text{and} \quad \int_c^b (x-a)^3(b-x)(c-x)dx = -\frac{3(b-a)^6}{320}\,.$$

Using now inequalities (1), we readily get

$$(m_3 - 9M_3)\frac{(b-a)^4}{2880} \le I(a) = \frac{(b-a)^4}{2880}\Big(f'''(C_{1,a}) - 9f'''(C_{2,a})\Big) \le (M_3 - 9m_3)\frac{(b-a)^4}{2880}\,.$$

The same computations for $I(b)$ gives

$$\int_a^c (x-a)(b-x)^3(c-x)dx = \frac{3(b-a)^6}{320}, \quad \text{and} \quad \int_c^b (x-a)(b-x)^3(c-x)dx = -\frac{(b-a)^6}{960}\,,$$

so that

$$(9m_3 - M_3)\frac{(b-a)^4}{2880} \le I(b) = \frac{(b-a)^4}{2880}\Big(9f'''(C_{1,b}) - f'''(C_{2,b})\Big) \le (9M_3 - m_3)\frac{(b-a)^4}{2880}\,.$$

Similarly for $I(c)$, where the polynomial in the integral is odd with respect to $x = c$, we get

$$\int_a^c (x-a)(b-x)(c-x)^3dx = \frac{(b-a)^6}{768}, \quad \text{and} \quad \int_c^b (x-a)(b-x)(c-x)^3dx = -\frac{(b-a)^6}{768}\,,$$

so that

$$(m_3 - M_3)\frac{(b-a)^4}{1152} \le I(c) = \frac{(b-a)^4}{1152}\Big(f'''(C_{1,c}) - f'''(C_{2,c})\Big) \le (M_3 - m_3)\frac{(b-a)^4}{1152}\,.$$

Putting all together, we finally proved that

$$5(m_3 - M_3)\frac{(b-a)^4}{1152} \le E(f) = I(a) + I(b) - I(c) \le 5(M_3 - m_3)\frac{(b-a)^4}{1152}\,.$$

■

Let us consider now the polynomial interpolation $\Pi_{[a,b]}(f)(x)$. Our aim is to compute it by using the generalized Taylor-like expansion (23). We obtain the following result

**Lemma 3.4** *Let $f \in C^3([a,b])$ which satisfies (1). Then, we have the following estimate:*

$$\begin{aligned}\Big|\int_a^b f(x)\,dx - \frac{b-a}{6}\Big(f(a) + 4\,f\big(\frac{a+b}{2}\big) + f(b)\Big) \\ -\frac{1}{(b-a)^3}\int_a^b \Big[(b-x)(c-x) - (x-a)(c-x) - (x-a)(b-x)\Big]F_{a,b,c}(x)dx \\ -\frac{(b-a)^3}{2560}\big(f''(a) + 2f''(c) + f''(b)\big)\Big| \le \frac{1}{32}\frac{5(b-a)^4}{1152}(2M_3 - m_3)\,, \end{aligned} \tag{40}$$

*where* $F_{a,b,c}(x) = 2f\left(\frac{x+a}{2}\right) - 4f\left(\frac{x+c}{2}\right) + 2f\left(\frac{x+b}{2}\right)$.

*Proof :* We consider the polynomial function $\Pi_{[a,b]}(f)(x)$ introduced in (33). By integrating it between $a$ and $b$, we obtain

$$\int_a^b \big(f(x) - \Pi_{[a,b]}(f)(x)\big)\, dx =$$

$$-\int_a^b \frac{(x-a)(b-x)(c-x)}{(b-a)^3}\left(\frac{f'(a)-2f'(c)+f'(b)}{2} + f'(\frac{x+a}{2}) - 2f'(\frac{x+c}{2}) + f'(\frac{x+b}{2})\right) \tag{41}$$

$$-\int_a^b \frac{3(x-a)(b-x)(c-x)}{64(b-a)^2}\left(f''(a)(a-x) + 2f''(c)(x-c) + f''(b)(b-x)\right) dx \tag{42}$$

$$-\int_a^b \frac{(x-c)(x-b)}{(a-c)(a-b)}(a-x)^2\epsilon^{(2)}_{x,3}(a) + \frac{(x-a)(x-c)}{(b-a)(b-c)}(b-x)^2\epsilon^{(2)}_{x,3}(b) + \frac{(x-a)(x-b)}{(c-a)(c-b)}(c-x)^2\epsilon^{(2)}_{x,3}(c)dx \tag{43}$$

In the following of the proof, we will consider one by one, each line of the above formula:

Using that

$$\int_a^b (x-a)(b-x)(c-x)dx = 0\,,$$

the first line (41) can be written as

$$-\frac{1}{(b-a)^3}\int_a^b (x-a)(b-x)(c-x)F'_{a,b,c}(x)dx\,, \tag{44}$$

where we denote $F'_{a,b,c}(x) = f'\left(\frac{x+a}{2}\right) - 2f'\left(\frac{x+c}{2}\right) + f'\left(\frac{x+b}{2}\right)$.

We can also try to rewrite (44). Indeed, using an integration by parts, and because the variation between $a$ and $b$ is equal to 0, (41) is equal to

$$\frac{1}{(b-a)^3}\int_a^b \big((b-x)(c-x) - (x-a)(c-x) - (x-a)(b-x)\big)F_{a,b,c}(x)dx\,,$$

where we introduced the notation $F_{a,b,c}(x) = 2f\left(\frac{x+a}{2}\right) - 4f\left(\frac{x+c}{2}\right) + 2f\left(\frac{x+b}{2}\right)$.

Consider now the second line (42) that can be decomposed into three terms. Let us consider for example the first one, namely

$$-\frac{3f''(a)}{64(b-a)^2}\int_a^b (x-a)(b-x)(c-x)(a-x)dx\,.$$

We can explicitly compute this integral that yields

$$\int_a^b (x-a)(b-x)(c-x)(a-x)dx = -\frac{(b-a)^5}{120}\,.$$

Consequently, the first term of (42) is equal to

$$-\frac{3f''(a)}{64(b-a)^2}\int_a^b (x-a)(b-x)(c-x)(a-x)dx = \frac{(b-a)^3 f''(a)}{40\cdot 64}\,. \tag{45}$$

Similarly, for the second term of (42), we get

$$-\frac{6f''(c)}{64(b-a)^2}\int_a^b (x-a)(b-x)(c-x)(x-c)dx = \frac{(b-a)^3 f''(c)}{20\cdot 64}\,,$$

and, for the last one of (42)

$$-\frac{3f''(b)}{64(b-a)^2}\int_a^b (x-a)(b-x)(c-x)(b-x)dx \;= \frac{(b-a)^3 f''(b)}{40\cdot 64}\,.$$

Summing up, the second line (42) gives the following contribution

$$\frac{(b-a)^3}{40\cdot 64}\big(f''(a)+2f''(c)+f''(b)\big)\,. \tag{46}$$

Let us consider now the last line (43) that can be expressed as, $c$ being the midpoint of $[a,b]$:

$$\frac{2}{(b-a)^2}\int_a^b -(x-a)^2(b-x)(c-x)\epsilon^{(2)}_{x,3}(a)+(x-a)(b-x)^2(c-x)\epsilon^{(2)}_{x,3}(b)-2(x-a)(b-x)(c-x)^2\epsilon^{(2)}_{x,3}(c)dx\,,$$

the absolute value of which being bounded by the sum of three terms $J(a)+J(b)+2J(c)$, where we define

$$\begin{aligned}
J(a) &= \frac{2}{(b-a)^2}\int_a^b (x-a)^2(b-x)|c-x||\epsilon^{(2)}_{x,3}(a)|dx\,,\\
J(b) &= \frac{2}{(b-a)^2}\int_a^b (x-a)(b-x)^2|c-x||\epsilon^{(2)}_{x,3}(b)|dx\,,\\
J(c) &= \frac{2}{(b-a)^2}\int_a^b (x-a)(b-x)(c-x)^2|\epsilon^{(2)}_{x,3}(c)|dx\,.
\end{aligned}$$

Now, we will bound separately each of these 3 terms, using again the estimates (32) to bound $\epsilon^{(2)}_{x,3}(a), \epsilon^{(2)}_{x,3}(c)$ and $\epsilon^{(2)}_{x,3}(b)$. We first have:

$$\begin{aligned}
|J(a)| &\le \frac{2}{(b-a)^2}\frac{2M_3-m_3}{384}\int_a^b (x-a)^3(b-x)|c-x|dx\,,\\
|J(b)| &\le \frac{2}{(b-a)^2}\frac{2M_3-m_3}{384}\int_a^b (x-a)(b-x)^3|c-x|dx\,,\\
|J(c)| &\le \frac{2}{(b-a)^2}\frac{2M_3-m_3}{384}\int_a^b (x-a)(b-x)|c-x|^3dx\,.
\end{aligned}$$

Using similar computations as above (see proof of lemma 3.3), straightforward computations give

$$\int_a^b (x-a)^3(b-x)|c-x|dx = \int_a^b (x-a)(b-x)^3|c-x|dx = \frac{(b-a)^6}{96},$$

and

$$\int_a^b (x-a)(b-x)|c-x|^3dx = \frac{(b-a)^6}{384}\,.$$

Putting all together, we finally obtain that the last line (43) is bounded by the term

$$\frac{1}{32}\frac{5(b-a)^4}{1152}(2M_3-m_3)\,. \tag{47}$$

Combining the estimates (45), (46) and (47), one can get the quadrature error estimate (40). ■

Let us conclude this section by several remarks.

1. Using that $2M_3 - m_3 \leq 3\sup_{a\leq x\leq b}|f'''|$, the quadrature error derived in (40), based on the modified second-order Taylor-like formula is *at least* bounded twenty times less than the one derived in lemma 3.3, using the classical Taylor's formula.
2. Interestingly, this result can also be compared to the optimized result obtained in [16] for a four-times continuously differentiable function on $[a, b]$, for which we have the inequality

$$\left|\int_a^b f(x)\,dx - \frac{b-a}{6}\left(f(a) + 4\,f\left(\frac{a+b}{2}\right) + f(b)\right)\right| \leq \frac{(b-a)^5}{2880}\sup_{a\leq x\leq b}|f^{(4)}(x)|\,. \qquad (48)$$

   Indeed, for a function $f$ smooth enough (at least $C^4([a, b])$),we can (roughly speaking) assume that $|f'''|$ behaves like $(b-a)|f^{(4)}|$.

   With these approximations, comparing the bounds of error estimates (40) and (48), namely, the values $15/36864 \simeq 0.00040$ with $1/2880 \simeq 0.00035$, we observe that the two constants are very comparable, despite the lower regularity required by our result.

# 4 Conclusion

In this paper we proposed a new second-order Taylor-like theorem to obtain some minimized remainders. For a function $f$ defined on the interval $[a, b]$, this formula is derived by introducing a linear combination of the derivative $f'$ computed at $n + 1$ equally spaced points in $[a, b]$, together with the second-order derivatives $f''$ computed at the limit points $a$ and $b$.

We proved that the corresponding remainder can be minimized for an *ad hoc* choice of the weights involved in this linear combination, and can be significantly smaller than the one obtained with the classical second order Taylor's formula.

Then, we considered two usual applications of this Taylor-like expansion: the interpolation error and the numerical quadrature formula. We showed that using this approach improves both the Lagrange $P_2$- interpolation error estimate and the error bound of the Simpson rule in numerical integration.

For the interpolation error applied to finite element approximation, we showed that the upper bound of the errors we obtained is almost twenty two times more precise than the one obtained by the classical Taylor formula. For the numerical integration, the quadrature error based on the new modified formula was found to be bounded twenty times less than the one derived using the classical Taylor's formula.

Other applications could also be concerned by this new second order Taylor-like formula. For instance, we could consider to improve the approximation error involved in ODE's approximation where Taylor's formula is the main tool used to derive numerical schemes.

**Homages:** The authors want to warmly dedicate this research to pay homage to the memory of Professors André Avez and Gérard Tronel who largely promote the passion of research and teaching in mathematics of their students.

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