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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 $x_k, (k = 0, \ldots, n)$, in $[a, b]$, and given weights $\omega_k, (k = 0, \ldots, n)$. 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