Accurate integration rules for functions with singularities

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Abstract

This work is devoted to the construction and analysis of a new nonlinear technique that allows to improve the accuracy of classical numerical integration formulas of any order when dealing with data that contains discontinuities. The novelty of the technique consists in the inclusion of correction terms with a closed expression that depends on the size of the jumps of the function and its derivatives at the discontinuities. The addition of these terms allows to recover the accuracy of classical numerical integration formulas even close to the discontinuities, as these correction terms account for the error that the classical integration formulas commit up to their accuracy at smooth zones. Thus, the correction terms can be added during the integration or as a post-processing, which is useful if the main calculation of the integral has been already done using classical formulas. The numerical experiments performed allow to confirm the theoretical conclusions reached in this paper.

Keywords: Accurate numerical integration formulas, adaption to singularities, definite integration, adapted interpolation, 65D05, 65D17, 65M06, 65N06.

1. Introduction

Classical integration formulas, such as the trapezoidal rule, the Simpson’s rule or the Newton-Cotes formulas, are based on the integration of interpolatory polynomials over an interval. The classical problem that arises from using such interpolatory polynomials is the losing of the accuracy whenever the original data does not present enough regularity. In this article we introduce a new method inspired by the Immersed Interface Method (IIM) \textsuperscript{1}, originally created as a high resolution technique for the discretization of elliptic partial differential equations with interfaces. The strategy followed by the IIM has been proved to be useful in other contexts such as the adaption of interpolatory Newton polynomials \textsuperscript{2} and can be somehow related to other interpolation techniques for discontinuous functions \textsuperscript{3}. In this article we pretend to use the adapted Newton polynomials
introduced in [2] for the obtention of adapted integration formulas that manage to take into account the presence of discontinuities through the addition of correction terms with closed explicit expressions. In order to find these correction terms we need to know the position of the singularities plus the jumps in the function and its derivatives at the singularities. This information might be available from the beginning if the function that we want to integrate is given explicitly as a piecewise continuous function. It can also happen that we start from discretized data that we want to use in order to recover an approximation of the integral of the original function. In this case, the new technique can be used as a post-processing that needs to detect and locate [4] the position of the singularity and approximate the jumps in the function and its derivatives at the singularity with certain precision. Only with this information we are able to compute the correction terms that allow to increase the accuracy close to the discontinuity. Logically, if we start from a discretization in the point values, we will only be able to obtain accurate correction terms for functions with discontinuities in the derivatives, but not in the function as, in this case, the position of the discontinuity is lost during the discretization process [4]. Our aim is to show that, through this new technique, it is possible to reach the maximum theoretical accuracy in terms of the length of the stencil.

The present work is organized as follows: Section 2 describes how to obtain correction terms for the trapezoid rule and the Simpson’s rule. Section 3 presents a generalization for Newton-Cotes formulas. Section 3.1 presents expressions of the correction terms for commonly used Newton-Cotes Formulas. Section 4 presents some numerical experiments that endorse the theoretical results. Finally, Section 5 presents some conclusions.

2. Obtainment of adapted numerical integration formulas

We consider the space of finite sequences $V$ and a uniform partition $X$ of the interval $[a,b]$ in $J$ subintervals,

$$X = \{x_i\}_{i=0}^{J}, \quad x_0 = a, \quad h = x_i - x_{i-1}, \quad x_J = b.$$  

We will consider a piecewise smooth function $f$ discretized through the point values,

$$f_i = f(x_i), \quad f = \{f_i\}_{i=0}^{J},$$

that, therefore, conserves the information of $f$ only at the $x_i$ nodes. We also assume that discontinuities are placed far enough from each other and that their position is known exactly or can be approximated with enough accuracy. Figure 1 presents the kind of singularities that we will be dealing with in this work. We will refer to these figures along the article. From these considerations we can directly proceed to obtain the correction terms and error formulas for these cases. Let’s start with the trapezoidal rule.

2.1. Error formula for the corrected trapezoid rule

We can consider the situation presented in Figure 1. Let’s denote by $E(f)$ the error committed by the classical trapezoidal rule and by $E^{\ast}(f)$ the error by the corrected rule. The classical trapezoid rule for a uniform grid of mesh-size $h$ and its error at smooth zones reads,

$$I(f) = \frac{h}{2} (f_j + f_{j+1}),$$

$$E(f) = -\frac{h^3}{12} f''(\eta), \quad \eta \in [x_j, x_{j+1}].$$
Lemma 1. Let be a real number, different from the nodes \( x_0, x_1, \ldots, x_n \). Being \( n \) the degree, the polynomial interpolation error to \( f(x) \) at \( t \) is \( f(t) - p_n(t) = (t - x_0) \cdots (t - x_n)f[x_0, \ldots, x_n, t] \), where \( f[x_0, \ldots, x_n, t] \) denotes the \((n+1)\)-th order divided difference.
If we denote by $E_{[a,b]}(f)$ the error of integration in the interval $[a,b]$, now we can state the following theorem:

**Theorem 1.** Let $f$ be a function with a discontinuity in the function or the first derivative and maybe in higher order derivatives at $x^*$. The addition of the correction term,

$$C = - \left( \frac{(-h + 2\alpha)}{2} [f] + \frac{(h\alpha - \alpha^2)}{2} [f'] \right),$$

(6)

to the trapezoid numerical integration formula in the interval $[x_j, x_{j+1}]$ that contains the singularity assures that the error is equal to,

$$E^*(f) = E_{[x_j,x^*]}(f) + E_{[x^*,x_{j+1}]}(f) + C + O(h^3),$$

(7)

with

$$E_{[x_j,x^*]}(f) = -\frac{1}{12} \left( \alpha^3 f_{xx}^-(\eta^-) \right) + O(h^3),$$

and

$$E_{[x^*,x_{j+1}]}(f) = -\frac{1}{12} \left( (h - \alpha)^3 f_{xx}^+(\eta^+) \right) + O(h^3),$$

and $\eta^- \in [x_j, x^*]$, $\eta^+ \in [x^*, x_{j+1}]$.

**Proof.** At the − part of the interval we will denote

$$E(f)_{[x_j, x^*]} = \int_{x_j}^{x_{j+\alpha}} f^-(x) - p(x) dx.$$  

Let’s write this error using the Lagrange’s form of the polynomial and take into account that there is a singularity at $x^* = x_j + \alpha$, so we can use the expressions in (4),

$$p(x) = \frac{x - x_{j+1}}{x_j - x_{j+1}} f_j^- + \frac{x - x_j}{x_{j+1} - x_j} f_{j+1}^- = \frac{x - x_{j+1}}{x_j - x_{j+1}} f_j^- + \frac{x - x_j}{x_{j+1} - x_j} f_{j+1}^- + \frac{x - x_j}{x_{j+1} - x_j} \left( (f) + [f'] (h - \alpha) + O(h^2) \right)$$

(8)

Then, using (8) and denoting by $p^-(x)$ to the piecewise polynomial to the left of the discontinuity, the error can be expressed as,

$$E^{*-}(f) = \int_{x_j}^{x_{j+\alpha}} f^-(x) - p^-(x) dx = -\frac{1}{12} \alpha^3 f_{xx}^-(\eta^-)$$

$$= \int_{x_j}^{x_{j+\alpha}} f^-(x) - p(x) dx + \int_{x_j}^{x_{j+\alpha}} \frac{x - x_j}{x_{j+1} - x_j} \left( (f) + [f'] (h - \alpha) \right) dx + O(h^3)$$

(9)

$$= \int_{x_j}^{x_{j+\alpha}} f^-(x) - p(x) dx + \frac{1}{2h} \left( \alpha^2 (f) + \alpha^2 (h - \alpha) [f'] \right) + O(h^3)$$

$$= E(f)_{[x_j, x^*]} + C^- + O(h^3),$$

4
with \( \eta^- \in [x_j, x^*] \), where we have used the error for the classical trapezoid rule. So we have that in the interval \([x_j, x^*]\) the error is,

\[
E'^-(f) = E(f)_{[x_j,x^*]} + C^- = -\frac{1}{12} \alpha^3 f_x^-(\eta^-) + O(h^3), \quad \text{with } \eta^- \in [x_j, x^*],
\]

\[
C^- = -\left( \frac{\alpha^2}{2h} f_x^-(\eta^-) - \frac{\alpha^2(h-\alpha)}{2h} f_x' \right).
\]

Replicating the process for the interval \([x^*, x_{j+1}]\), but this time expressing the quantities from the \(-\) side in terms of the \(+\) side (or just by symmetry), we obtain that,

\[
E'^+(f) = E(f)_{[x^*,x_{j+1}]} + C^+ = -\frac{1}{12} (h-\alpha)^3 f_x^+(\eta^+) + O(h^3), \quad \text{with } \eta^+ \in [x^*, x_{j+1}],
\]

\[
C^+ = -\left( \frac{(h-\alpha)^2}{2h} f_x^+(\eta^+) - \frac{(h-\alpha)^2 \alpha}{2h} f_x' \right).
\]

Adding the errors obtained in both intervals, as expressed in (10) and (11), we get

\[
E^*(f) = E'^-(f) + E'^+(f) = E(f)_{[x^*,x_{j+1}]} + C^- + E(f)_{[x_j,x^*]} + C^+ = E(f)_{[x^*,x_{j+1}]} + E(f)_{[x_j,x^*]} + C,
\]

and we finish the proof.

\[
\square
\]

2.2. Correction terms and error formula for the corrected Simpson’s \( \frac{1}{3} \) rule

![Diagram](image)

Figure 2: Two examples of functions with singularities (solid line) placed in different intervals at a position \( x^* \). We have labeled the domain to the left of the singularity as \(-\) and the one to the right as \(+\). We have also represented with a dashed line the prolongation of the functions through Taylor expansions at both sides of the discontinuity.

In this section we will proceed to analyze how to adapt Simpson’s rule following the same process that we used to adapt the trapezoidal rule in the previous Subsection. Simpson’s rule is obtained by integrating a parabola in the corresponding interval. In this case we need to enlarge the stencil and we will need to use the three data values \((f_{j-1}, f_j, f_{j+1})\), placed at the positions \((x_{j-1}, x_j, x_{j+1})\) in order to build the parabola. In this occasion we must consider two cases: when the discontinuity is in the interval \([x_{j-1}, x_j]\) or in the interval \([x_j, x_{j+1}]\), as shown in the plots of Figure 2. The classical Simpson’s \( \frac{1}{3} \) rule for a uniform grid of mesh-size \( h \) and its error \( [3] \) at smooth zones reads,

\[
I(f) = \frac{h}{3} (f_{j-1} + 4f_j + f_{j+1}),
\]

\[
E(f) = -\frac{h^5}{90} f^{(4)}(\eta), \quad \eta \in [x_j, x_{j+2}].
\]
Theorem 2. Let’s suppose that the function \( f \) has singularities at \( x^* \) up to the third derivative at least. The addition of the correction term,

\[
C = - \left( \gamma \left( \alpha - \frac{h}{3} \right) \alpha + \frac{\alpha^2}{6} (3\alpha - 2h) [f'] + \frac{\alpha^2}{6} (\alpha - h) [f''] + \frac{\alpha^2}{36} (3\alpha^2 + 6h - 8\alpha) [f'''] \right),
\]

(13)
to the Simpson’s numerical integration formula, with \( \gamma = -1 \), if the singularity is placed at an odd interval, and \( \gamma = 1 \), if the singularity is placed at an even interval, ensures that the error is equal to,

\[
E(f) + C = \frac{f_{x_{max}}(\eta_1)}{24} (\frac{3h^2\alpha^2}{2} - h\alpha^3 - \frac{h^3}{4}) + \frac{f_{x_{max}}(\eta_2)}{6} (\frac{\alpha^4}{4} + \frac{h^2\alpha^2}{2}) + \frac{f_{x_{max}}(\eta_3)}{24} (\frac{\alpha^4}{4} - h\alpha^3 + h^2\alpha^2) + O(h^5),
\]

(14)
with \( \eta_1 \in [x_{j-1} + \alpha, x_{j+1} - \alpha] \). If the discontinuity falls at an odd interval, then \( \eta_2 \in [x_{j+1} - \alpha, x_{j+1}], \eta_3 \in [x_{j-1}, x_{j+1} + \alpha] \). If the discontinuity falls at an even interval, the case is symmetric and \( \eta_2 \in [x_{j-1}, x_{j+1} + \alpha], \eta_3 \in [x_{j+1} - \alpha, x_{j+1}] \).

Proof. Let’s start by the case when the discontinuity is placed in the interval \([x_{j-1}, x_j]\),

1. As in the trapezoidal rule, we know that for the + part of the integral,

\[
E^{s+}(f) = \int_{x_{j-1} + \alpha}^{x_{j+1}} f^+(x) - p^+(x)dx.
\]

The interpolating polynomial \( p(x) \) in the Lagrange form is,

\[
p(x) = \frac{(x - x_j)(x - x_{j+1})}{(x_{j-1} - x_j)(x_{j-1} - x_{j+1})} f^-_{j-1} + \frac{(x - x_{j-1})(x - x_{j+1})}{(x_j - x_{j-1})(x_j - x_{j+1})} f^+_j + \frac{(x - x_{j-1})(x - x_j)}{(x_{j+1} - x_{j-1})(x_{j+1} - x_j)} f^+_{j+1}.
\]

(15)
Proceeding in the same way as we did in (8) for the trapezoid rule, we can use the expression of \( f^-_{j-1} \) in terms of the quantities from the + side to write,

\[
f^-_{j-1} = f^+_j - [f] + [f']\alpha - [f'']\frac{\alpha^2}{2} + [f''']\frac{\alpha^3}{6} + O(h^4).
\]

(16)
Now we can write,

\[
p(x) = \frac{(x - x_j)(x - x_{j+1})}{(x_{j-1} - x_j)(x_{j-1} - x_{j+1})} \left( f^-_{j-1} - [f] + [f']\alpha - [f'']\frac{\alpha^2}{2} + [f''']\frac{\alpha^3}{6} \right) + \frac{(x - x_{j-1})(x - x_{j+1})}{(x_j - x_{j-1})(x_j - x_{j+1})} f^+_j + \frac{(x - x_{j-1})(x - x_{j})}{(x_{j+1} - x_{j-1})(x_{j+1} - x_{j})} f^+_{j+1}
\]

\[= p^+(x) + \frac{(x - x_{j-1})(x - x_{j+1})}{(x_{j-1} - x_j)(x_{j-1} - x_{j+1})} \left( -[f] + [f']\alpha - [f'']\frac{\alpha^2}{2} + [f''']\frac{\alpha^3}{6} \right) + O(h^4).\]

(17)
Then, the error for the integral at the + side in the interval \([x^*, x_{j+1}]\), as shown in Figure
Integrating by parts the first integral, we have

\[
E^+ (f) = \int_{x_{j-1} + \alpha}^{x_{j+1}} f^+(x) - p^+(x) \, dx = \int_{x_{j-1} + \alpha}^{x_{j+1}} f^+(x) - p(x) \, dx
\]

\[
+ \int_{x_{j-1} + \alpha}^{x_{j+1}} \frac{(x - x_j)(x - x_{j+1})}{(x_{j-1} - x_j)(x_{j-1} - x_{j+1})} \left( - [f] + [f'] \alpha - [f''] \frac{\alpha^2}{2} + [f'''] \frac{\alpha^3}{6} \right) \, dx + O(h^5)
\]

\[
= E(f)_{[x^*, x_{j+1}]}
\]

\[
- \frac{1}{72} \left( -6 [f] - 6 \alpha [f'] + 3 \alpha^2 [f''] - \alpha^3 [f'''] \right) \left( -4 h^3 + 2 \alpha^3 - 9 h \alpha^2 + 12 h^2 \alpha \right) + O(h^5)
\]

\[
= E(f)_{[x^*, x_{j+1}]} + C^+ + O(h^5),
\]

and we also have that,

\[
E^+ (f) = \int_{x_{j-1} + \alpha}^{x_{j+1}} (x - x_{j-1})(x - x_j)(x - x_{j+1}) f^+[x_{j-1}, x_j, x_{j+1}, x] \, dx.
\]

(19)

The polynomial in the integrand of (19) changes the sign in the interval \((x_{j-1} + \alpha, x_{j+1})\). Thus, we can not use the integral mean value theorem. Instead, we can define the function

\[
w(x) = \int_{x_{j-1} + \alpha}^{x} (x - x_{j-1})(x - x_j)(x - x_{j+1}) \, dx,
\]

that satisfies, \(w(x_{j-1} + \alpha) = 0\), and \(w(x) > 0\) for \(x \in (x_{j-1} + \alpha, x_{j+1} - \alpha)\) and \(w(x) < 0\) for \(x \in (x_{j+1} - \alpha, x_{j+1})\). Then, we can divide the integral in two parts,

\[
E^+ (f) = \int_{x_{j-1} + \alpha}^{x_{j+1}} w(x) f^+[x_{j-1}, x_j, x_{j+1}, x] \, dx = \int_{x_{j-1} + \alpha}^{x_{j+1}} w(x) f^+[x_{j-1}, x_j, x_{j+1}, x] \, dx
\]

\[
+ \int_{x_{j-1} + \alpha}^{x_{j+1}} w'(x) f^+[x_{j-1}, x_j, x_{j+1}, x] \, dx.
\]

Integrating by parts the first integral,

\[
\int_{x_{j-1} + \alpha}^{x_{j+1} - \alpha} w'(x) f^+[x_{j-1}, x_j, x_{j+1}, x] \, dx = \left[ w(x) f^+[x_{j-1}, x_j, x_{j+1}, x] \right]_{x_{j-1} + \alpha}^{x_{j+1} - \alpha}
\]

\[
- \int_{x_{j-1} + \alpha}^{x_{j+1} - \alpha} w(x) \frac{d}{dx} f^+[x_{j-1}, x_j, x_{j+1}, x] \, dx.
\]

Using now that \(w(x_{j+1} - \alpha) = 0\), due to the symmetry of the polynomial that appears in the integrand of \(w(x)\) in a uniform grid, that (see 3.2.17 page 147 of Atkinson)

\[
\frac{d}{dx} f^+[x_{j-1}, x_j, x_{j+1}, x] = f^+[x_{j-1}, x_j, x_{j+1}, x, x],
\]

(21)
and the integral mean value theorem, we get,

\[- \int_{x_{j-1} + \alpha}^{x_{j+1} - \alpha} w(x)f^+[x_{j-1}, x_j, x_{j+1}, x, x]dx = -f^+[x_{j-1}, x_j, x_{j+1}, \xi_1, \xi_1] \int_{x_{j-1} + \alpha}^{x_{j+1} - \alpha} w(x)dx = \]

\[- f^+[x_{j-1}, x_j, x_{j+1}, \xi_1, \xi_1] \left( -\frac{3h^2\alpha^2}{2} + h\alpha^3 + \frac{h^4}{4} \right) = f^+_{xxx}(\eta_1) \left( \frac{3h^2\alpha^2}{2} - h\alpha^3 - \frac{h^4}{4} \right), \]

for some \( \xi_1, \eta_1 \in [x_{j-1} + \alpha, x_{j+1} - \alpha] \). For the second integral in (20), \( w'(x) \) does not change the sign in \([x_{j-1} + 1 - \alpha, x_{j+1} - 1]\) so we can apply the integral mean value theorem,

\[ \int_{x_{j+1} - \alpha}^{x_{j+1}} w'(x)f^+[x_{j-1}, x_j, x_{j+1}, x]dx = f^+[x_{j-1}, x_j, x_{j+1}, \xi_2] \int_{x_{j+1} - \alpha}^{x_{j+1}} w'(x)dx = \]

\[ f^+_{xxx}(\eta_2) \left( -\frac{\alpha^4}{4} + \frac{h^2\alpha^2}{2} \right), \]

for some \( \xi_2, \eta_2 \in [x_{j+1} - \alpha, x_{j+1}] \). Thus,

\[ \int_{x_{j-1} + \alpha}^{x_{j+1}} w'(x)f^+[x_{j-1}, x_j, x_{j+1}, x]dx = f^+_{xxx}(\eta_1) \left( \frac{3h^2\alpha^2}{2} - h\alpha^3 - \frac{h^4}{4} \right) \]

\[ + f^+_{xxx}(\eta_2) \left( -\frac{\alpha^4}{4} + \frac{h^2\alpha^2}{2} \right). \]

So, from (18) we get that the corrected error for the integral in the + side of the left plot of Figure 2 is,

\[ E^+(f)[x^*, x_{j+1}] + C^+ + O(h^5) = E^{**}(f) = \]

\[ \frac{f^+_{xxx}(\eta_1)}{24} \left( \frac{3h^2\alpha^2}{2} - h\alpha^3 - \frac{h^4}{4} \right) \]

\[ + \frac{f^+_{xxx}(\eta_2)}{6} \left( -\frac{\alpha^4}{4} + \frac{h^2\alpha^2}{2} \right), \]

(23)

with \( \xi_2, \eta_2 \in [x_{j+1} - \alpha, x_{j+1}] \) and \( \xi_1, \eta_1 \in [x_{j-1} + \alpha, x_{j+1} - \alpha] \).

2. For the integral in the - side of the left plot of Figure 2, we want to obtain the error

\[ E^-(f) = \int_{x_{j-1}}^{x_{j-1} + \alpha} f^-(x) - p^-(x)dx. \]

From (16) we can express the quantities from the + side in terms of the - side using the
jump conditions in (3), as we did before,

\[
p(x) = \frac{(x - x_j)(x - x_{j+1})}{(x_{j-1} - x_j)(x_{j-1} - x_{j+1})} f_j^{-1} + \frac{(x - x_j)(x - x_{j+1})}{(x_j - x_{j-1})(x_j - x_{j+1})} \left( f_j^{-} + [f] + [f'](h - \alpha) + \frac{[f']^2(h - \alpha)}{2} + \frac{[f'']^3(h - \alpha)^3}{6} \right) + O(h^4)
\]

\[
+ \frac{(x - x_j)(x - x_{j+1})}{(x_{j-1} - x_j)(x_{j-1} - x_{j+1})} \left( f_j^{-1} + [f] + [f'](h + \alpha) + \frac{[f']^2(h + \alpha)}{2} + \frac{[f'']^3(h + \alpha)^3}{6} \right) + O(h^4)
\]

\[
= p^{-}(x) + \frac{(x - x_j)(x - x_{j+1})}{(x_j - x_{j-1})(x_j - x_{j+1})} \left( [f] + [f'](h - \alpha) + \frac{[f']^2(h - \alpha)}{2} + \frac{[f'']^3(h - \alpha)^3}{6} \right) + O(h^4).
\]

Now, the error for the integral on the \(-\) side, as shown in Figure 2 to the left, can be expressed as,

\[
E^{-}(f) = \int_{x_{j-1}}^{x_{j-1}+\alpha} f^{-}(x) - p^{-}(x)dx = \int_{x_{j-1}}^{x_{j-1}+\alpha} f^{-}(x) - p(x)dx
\]

\[
+ \int_{x_{j-1}}^{x_{j-1}+\alpha} \frac{(x - x_j)(x - x_{j+1})}{(x_j - x_{j-1})(x_j - x_{j+1})} \left( [f] + [f'](h - \alpha) + \frac{[f']^2(h - \alpha)}{2} + \frac{[f'']^3(h - \alpha)^3}{6} \right) dx
\]

\[
+ \int_{x_{j-1}}^{x_{j-1}+\alpha} \frac{(x - x_j)(x - x_{j+1})}{(x_j - x_{j-1})(x_j - x_{j+1})} \left( [f] + [f'](2h - \alpha) + \frac{[f']^2(2h - \alpha)^2}{2} + \frac{[f'']^3(2h - \alpha)^3}{6} \right) dx + O(h^5)
\]

\[
= E(f) - \frac{1}{72} \left( \frac{1}{h^2} \left[ f + 3 \alpha^2 (-54h + 12\alpha) \right] + \frac{\alpha^2 (54h^2 - 12\alpha^2 - 12h^3\alpha) + 24h^2\alpha^2 + 27h \alpha^2)}{h^2} \right) + O(h^5)
\]

\[
= E(f)_{(x_{j-1}, x^*)} + C^{-} + O(h^5) = \int_{x_{j-1}}^{x_{j-1}+\alpha} (x - x_j)(x - x_{j+1})f^{-}[x_{j-1}, x_j, x_{j+1}, x]dx.
\]

It is not difficult to see that the polynomial in the integrand does not change the sign in the interval \((x_{j-1}, x_{j-1} + \alpha)\). Thus, using the integral mean value theorem

\[
E^{-}(f) = \int_{x_{j-1}}^{x_{j-1}+\alpha} (x - x_j)(x - x_{j+1})f^{-}[x_{j-1}, x_j, x_{j+1}, x]dx
\]

\[
= f^{-}[x_{j-1}, x_j, x_{j+1}, \xi_3] \int_{x_{j-1}}^{x_{j-1}+\alpha} (x - x_j)(x - x_{j+1})dx
\]

\[
= \frac{f^{-}_{xx}(\eta_3)}{24} \left( \frac{\alpha^4}{4} - 3h^2\alpha^2 \right),
\]

for some \(\xi_3, \eta_3 \in [x_{j-1}, x_{j-1} + \alpha]\). So, from (25) we get that the corrected error for the left part of the integral is,

\[
E(f)_{(x_{j-1}, x^*)} + C^{-} + O(h^5) = E^{-}(f) = \frac{f^{-}_{xx}(\eta_3)}{24} \left( \frac{\alpha^4}{4} - 3h^2\alpha^2 \right),
\]

for some \(\xi_3, \eta_3 \in [x_{j-1} + \alpha, x_{j+1}]\).
Adding the correction terms $C^+$ and $C^-$ obtained in (18) and (24), we obtain

$$C = C^+ + C^- = - \left( \alpha - \frac{h}{3} \right) [f] + \frac{\alpha^2}{6} (3\alpha - 2h) [f'] - \frac{\alpha^2}{6} (\alpha - h) [f''] + \frac{\alpha^2}{36} (\alpha^2 + 6h^2 - 8\alpha) [f'''] .$$

Adding now the errors in the intervals $[x^*, x_{j+1}]$ and $[x_{j-1}, x^*]$ as expressed respectively in (23) and (27), and denoting again

$$E(f) = E(x_{j-1}, x^*) + E[x^*, x_{j+1}] ,$$

we obtain,

$$E^*(f) = E^{++}(f) + E^{--}(f) = E(f) + C + O(h^5) = \frac{f_{xxx}^+(\eta_1)}{24} \left( \frac{3h^2\alpha^2}{2} - h\alpha^3 - \frac{h^4}{4} \right) + \frac{f_{xxx}^-(\eta_2)}{6} \left( \frac{\alpha^4}{4} + \frac{h^2\alpha^2}{2} \right) + \frac{f_{xxx}^-(\eta_3)}{24} \left( \frac{\alpha^4}{4} - h\alpha^3 + h^2\alpha^2 \right) ,$$

with $\eta_1 \in [x_{j-1} + \alpha, x_{j+1} - \alpha], \eta_2 \in [x_{j+1} - \alpha, x_{j+1}], \eta_3 \in [x_{j-1}, x_{j-1} + \alpha]$.

- If the singularity is placed in the interval $(x_j, x_{j+1})$ at a distance $\alpha$ from $x_{j+1}$, that is the case presented in Figure 2, the case is symmetrical and the correction term is:

$$C = - \left( \alpha - \frac{h}{3} \right) [f] + \frac{\alpha^2}{6} (3\alpha - 2h) [f'] - \frac{\alpha^2}{6} (\alpha - h) [f''] + \frac{\alpha^2}{36} (\alpha^2 + 6h^2 - 8\alpha) [f'''] .$$

In this case the error reads,

$$E^*(f) = E(f) + C + O(h^5) = \frac{f_{xxx}^+(\eta_1)}{24} \left( \frac{3h^2\alpha^2}{2} - h\alpha^3 - \frac{h^4}{4} \right) + \frac{f_{xxx}^-(\eta_2)}{6} \left( \frac{\alpha^4}{4} + \frac{h^2\alpha^2}{2} \right) + \frac{f_{xxx}^-(\eta_3)}{24} \left( \frac{\alpha^4}{4} - h\alpha^3 + h^2\alpha^2 \right) ,$$

with $\eta_1 \in [x_{j-1} + \alpha, x_{j+1} - \alpha], \eta_2 \in [x_{j-1}, x_{j-1} + \alpha], \eta_3 \in [x_{j+1} - \alpha, x_{j+1}]$.

$\square$

**Remark 1.** Theorems 1 and 2 imply that we can use the classical composed trapezoidal rule or the composed Simpson’s rule to obtain the integral over a large interval and, then, add the corresponding correction terms (6) or (13) to obtain $O(h^2)$ or $O(h^4)$ global accuracy respectively, if singularities are present in the data. Mind that the correction terms are typically added to take into account the effect of the set of singularities, which cardinal is usually small (one dimension lower) comparing with the number of points in the data. Thus, it is enough if the correction terms provide the order of the global error of the classical composed integration rule. The existence of singularities can be known a priory or can be checked through a pre or post-processing of the data.

**Remark 2.** Let’s assume now that there is an error in the location of the singularity. For simplicity we can assume that it is located to the right of the true singularity at a distance $\beta$ (that is the error
of location) and let’s represent its position by \( x_\beta \), then using Taylor’s expansion on the jump in the function or the first derivative we get

\[
[f(x_\beta)] = [f] + \beta [f'] + \frac{\beta^2}{2} [f''] + \cdots,
\]

\[
[f'(x_\beta)] = [f'] + \beta [f''] + \frac{\beta^2}{2} [f'''] + \cdots.
\]

So, replacing these expressions in the correction terms in (3) for the trapezoidal rule or the correction terms in (13) for the Simpson’s rule, it is clear that, in order to keep order of accuracy \( O(h^s) \) in the integral, we just need the error of location \( \beta \) to be of order \( O(h^{s-1}) \), being \( s = 2 \) for the trapezoidal rule and \( s = 4 \) for the Simpson’s rule. Mind that, if there is a false detection of the singularity at a smooth zone, the jumps should be zero (if known a priory) or close enough to zero (if approximated).

3. Corrected Newton-Cotes integration formulas

The Trapezoidal rule and the Simpson’s \( \frac{1}{3} \) formula, that we have analysed in previous sections, are the first two cases of Newton-Cotes integration formulas. In what follows, we will try to obtain expressions for the errors of corrected integration formulas of any order. In order to do so, let’s present some previous lemmas that we will use afterwards in the proofs.

**Lemma 2.** Let \( f(x) \) be \( n + 1 \) times continuously differentiable in \([a, b]\) except at a point \( x^* \in (a, b) \). Let’s denote the function to the left of \( x^* \) by \( f^-(x) \) and to the right of \( x^* \) as \( f^+(x) \). If we know the jumps in the function and its derivatives at \( x^* \) and they are finite, denoted by \([f] = f^+(x^*) - f^-(x^*), [f'] = f'^+(x^*) - f'^-(x^*), \ldots, [f^{(n)}] = f^{(n)+}(x^*) - f^{(n)-}(x^*)\), then at any node \( x_i \) we can express any value of \( f^+(x_i) \) in terms of the jumps and the continuous extension of the function from the other side of the discontinuity (see for example, Figures 14 and 9), that is:

\[
f_i^+ = f_i^- + [f] + [f'](x_i - x^*) + \frac{1}{2} [f''](x_i - x^*)^2 + \cdots + \frac{1}{n!} [f^{(n)}](x_i - x^*)^n + O(h^{n+1}).
\]

Isolating, we can obtain \( f_i^- \) in terms of \( f_i^+ \).

**Proof.** The proof is direct using Taylor expansions.

Let’s denote by \( \lfloor x \rfloor \) greatest integer less than or equal to \( x \) and \( \lceil x \rceil \) the least integer greater than or equal to \( x \).

**Lemma 3.** Let’s consider an interpolating polynomial of degree \( n \) in the Lagrange form in the interval \([a, b]\), constructed using \( n + 1 \) points belonging to a piecewise continuous function that contains a singularity at \( x^* \in (a, b) \) and that is \( n \) times piecewise continuously differentiable. Let’s follow the same notation as before and denote the information to the left of the singularity with the \( - \) symbol and to the right with the \( + \) symbol. Then in the interval of interest \([a, b]\):

- We can express this polynomial as a continuous extension in the \( - \) region of the polynomial at the \( + \) region, plus additional terms as,

\[
p_n(x) = \sum_{i=0}^{n+1} f^+(x_i) \prod_{j=0, j \neq i}^{j=n+1} \frac{x - x_j}{x_i - x_j} + Q^-(x) = p_n^+(x) + Q^-(x).
\]

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If we denote by,
\[ \hat{f}_i = [f] + [f'](x_i - x^*) + \frac{1}{2}[f''](x_i - x^*)^2 + \cdots + \frac{1}{n!}[f^{(n)}](x_i - x^*)^n + O(h^{n+1}), \]
then \( Q^-(x) \) contains all the information of the singularity and takes the expression,
\[ Q^-(x) = \sum_{i=0}^{n} \sum_{j=0, j \neq i}^{n+1} \hat{f}_i \prod_{j=0}^{n+1} \frac{x - x_j}{x_i - x_j}, \]
\[ (33) \]

- We can express this polynomial as a continuous extension in the + region of the polynomial at the − region, plus additional terms as,
\[ p_n(x) = \sum_{i=0}^{n+1} f^-(x_i) \prod_{j=0, j \neq i}^{n+1} \frac{x - x_j}{x_i - x_j} + Q^+(x) = p_n^+(x) + Q^+(x). \]

In this case \( Q^+(x) \) takes the expression,
\[ Q^+(x) = \sum_{i=\lceil \frac{x - x^*}{h} \rceil}^{n+1} \hat{f}_i \prod_{j=0, j \neq i}^{n+1} \frac{x - x_j}{x_i - x_j}, \]
\[ (34) \]

**Proof.** The proof is direct using Lemma 2 and replacing \( f_i \) in the Lagrange form of the polynomial
\[ p_n(x) = \sum_{i=0}^{n+1} f_i \prod_{j=0, j \neq i}^{n+1} \frac{x - x_j}{x_i - x_j}, \]
by the values \( f_i^+ \) or \( f_i^- \) provided in (33), depending of \( f_i \) belonging to the + or − side. \( \square \)

**Lemma 4.** Let’s consider the integral of the polynomial interpolation error from Lemma 1 in the smooth interval \([x_0, x^*] \),
\[ E_n = \int_{x_0}^{x^*} f(x) - p_n(x)dx = \int_{x_0}^{x^*} (x - x_0) \cdots (x - x_n)f[x_0, \cdots, x_n, x]dx. \]

- If there is not a change of sign in the polynomial of the integrand in the interval \([x_0, x^*] \), the error can be written as,
\[ E_n = \frac{f^{(n+1)}(\xi)}{(n + 1)!} h^{n+2} \int_{0}^{\frac{x^* - x_0}{h}} \mu(\mu - 1) \cdots (\mu - n + 1)(\mu - n)d\mu \]
\[ (35) \]
for some \( \xi \in [x_0, x_n] \).
• If there is a change of sign in the polynomial of the integrand in the interval \([x_0, x^*]\), the error can be written as,

\[
E_n = \int_{x_0}^{x^*} f(x) - p_n(x)dx = \frac{f^{(n+1)}(\xi)}{(n+1)!} \int_0^{\frac{x^*-x_0}{h}} \mu(\mu - 1) \cdots (\mu - n)(\mu - n) d\mu + \frac{f^{(n+2)}(\xi_2)}{(n+2)!} \int_0^{\frac{x^*-x_0}{h}} \mu(\mu - 1) \cdots (\mu - n)(\mu - n - \frac{x^*-x_0}{h}) d\mu.
\]

(36)

for some \(\xi_1, \xi_2 \in [x_0, x_n]\).

Proof.  
• If there is not a change of sign in the polynomial of the integrand in the smooth interval \([x_0, x^*]\), we can directly use the integral mean value theorem and the fact that,

\[
f[x_0, \cdots, x_n] = \frac{f^{(n)}(\xi)}{n!} \text{ for some } \xi \in [x_0, \cdots, x_n],
\]

(37)

to write,

\[
E_n = \int_{x_0}^{x^*} f(x) - p_n(x)dx = \int_{x_0}^{x^*} (x - x_0) \cdots (x - x_n)f[x_0, \cdots, x_n, x]dx = \frac{f^{(n+1)}(\xi)}{(n+1)!} \int_{x_0}^{x^*} (x - x_0) \cdots (x - x_n)dx.
\]

for some \(\xi \in [x_0, x_n]\). Applying the change of variables \(x = x_0 + \mu h, 0 \leq \mu \leq n\), we can write,

\[
E_n = \frac{f^{(n+1)}(\xi)}{(n+1)!} \int_{x_0}^{x^*} (x - x_0) \cdots (x - x_n)dt = \frac{f^{(n+1)}(\xi)}{(n+1)!} h^{n+2} \int_0^{\frac{x^*-x_0}{h}} \mu(\mu - 1) \cdots (\mu - n)(\mu - n - \frac{x^*-x_0}{h}) d\mu.
\]

• If there is a change of sign in the polynomial of the integrand in the smooth interval \([x_0, x^*]\), we can define

\[
w(y, x) = \int_y^x (t - x_0) \cdots (t - x_n)dt,
\]

(38)

that satisfies that, at smooth zones,

\[
w(x_0, x_0) = w(x_0, x_n) = 0, \quad w(x_0, x) > 0 \quad \text{for } x_0 < x < x_n,
\]

when \(n\) is even, and

\[
w(x_0, x_0) = 0, \quad w(x_0, x) < 0 \quad \text{for } x_0 < x < x_n,
\]

when \(n\) is odd. In [6] (page 309) there is a complete proof of these facts.

Now, we can write,

\[
E_n = \int_{x_0}^{x^*} w'(x_0, x)f[x_0, \cdots, x_n, x]dx.
\]

(39)
Integrating by parts and using that $w(x_0, x_0) = 0$,

$$
\int_{x_0}^{x^*} w'(x_0, x)f[x_0, \cdots, x, x]dx = [w(x_0, x)f[x_0, \cdots, x, x]]^x_{x_0} - \int_{x_0}^{x^*} w(x_0, x)\frac{d}{dx}f[x_0, \cdots, x, x]dx
$$

$$= w(x_0, x^*)f[x_0, \cdots, x, x^*] - \int_{x_0}^{x^*} w(x_0, x)\frac{d}{dx}f[x_0, \cdots, x, x]dx. \quad \text{(40)}
$$

Using now (37), we can write,

$$w(x_0, x^*)f[x_0, \cdots, x, x^*] = \frac{f(n+1)(\xi_1)}{(n+1)!} w(x_0, x^*) = \frac{f(n+1)(\xi_1)}{(n+1)!} \int_{x_0}^{x^*} (t - x_0)\cdots(t - x_n)dt,$$

for some $\xi_1 \in [x_0, x^*]$. Applying again the change of variables $t = x_0 + \mu h, 0 \leq \mu \leq n$, we can write,

$$\int_{x_0}^{x^*} (t - x_0)\cdots(t - x_n)dt = h^{n+2} \int_0^{\frac{x^*-x_0}{h}} \mu(\mu - 1)\cdots(\mu - n+1)(\mu - n)d\mu.$$

Thus, we have that,

$$w(x_0, x^*)f[x_0, \cdots, x, x^*] = \frac{f(n+1)(\xi_1)}{(n+1)!} h^{n+2} \int_0^{\frac{x^*-x_0}{h}} \mu(\mu - 1)\cdots(\mu - n+1)(\mu - n)d\mu, \quad \text{(41)}$$

for some $\xi_1 \in [x_0, x_n].$

For the last integral in (41), we can use the fact that (see 3.2.17 page 147 of Atkinson)

$$\frac{d}{dx}f[x_0, \cdots, x, x] = f[x_0, \cdots, x, x, x], \quad \text{(42)}$$

the integral mean value theorem, and (37) to write

$$-\int_{x_0}^{x^*} w(x_0, x)\frac{d}{dx}f[x_0, \cdots, x, x]dx = -\int_{x_0}^{x^*} w(x_0, x)f[x_0, \cdots, x, x, x]dx$$

$$= -f[x_0, \cdots, x, x, \eta_2, \eta_2] \int_{x_0}^{x^*} w(x_0, x)dx$$

$$= -\frac{f(n+2)(\xi_2)}{(n+2)!} \int_{x_0}^{x^*} \int_{x_0}^{x} (t - x_0)\cdots(t - x_n)dtdx,$$

for some $\eta_2, \xi_2 \in [x_0, x_n]$. Now we can change the order of integration and apply the change of variables $t = x_0 + \mu h, 0 \leq \mu \leq n$:

$$\int_{x_0}^{x^*} \int_{x_0}^{x} (t - x_0)\cdots(t - x_n)dtdx = \int_{x_0}^{x^*} \int_{x_0}^{x} (t - x_0)\cdots(t - x_n)dtdx$$

$$= \int_{x_0}^{x^*} (t - x_0)\cdots(t - x_n)(d - t)dt \quad \text{(43)}$$

$$= -h^{n+3} \int_0^{\frac{x^*-x_0}{h}} \mu(\mu - 1)\cdots(\mu - n+1)(\mu - n)(\mu - \frac{x^*-x_0}{h})d\mu.$$
Thus, we can write that
\[
- \int_{x_0}^{x^*} w(x_0, x) \frac{d}{dx} f[x_0, \cdots, x_n, x] \, dx
= \frac{f^{(n+2)}(\xi_2)}{(n+2)!} h^{n+3} \int_0^{\frac{x^*-x_0}{h}} \mu (\mu - 1) \cdots (\mu - n + 1)(\mu - n)(\mu - \frac{x^*-x_0}{h}) \, d\mu.
\]

(44)

Joining the partial results in (44) and (41), we finish the proof,
\[
E_n = \int_{x_n}^{x^*} f(x) - p_n(x) \, dx = \int_{x_0}^{x^*} (x - x_0) \cdots (x - x_0) f[x_0, \cdots, x_n, x] \, dx
= \frac{f^{(n+1)}(\xi_1)}{(n+1)!} h^{n+2} \int_0^{\frac{x^*-x_0}{h}} \mu (\mu - 1) \cdots (\mu - n + 1)(\mu - n) \, d\mu
+ \frac{f^{(n+2)}(\xi_2)}{(n+2)!} h^{n+3} \int_0^{\frac{x^*-x_0}{h}} \mu (\mu - 1) \cdots (\mu - n + 1)(\mu - n)(\mu - \frac{x^*-x_0}{h}) \, d\mu,
\]
for some \(\xi_1, \xi_2 \in [x_0, x_n]\).

From Lemma 4 we can get the following corollary.

Corollary 1. If the smooth interval is \([x^*, x_n]\):

- If there is not a change of sign in the polynomial of the integrand in the interval \([x^*, x_n]\), the error can be written as,
\[
E_n = \int_{x_n}^{x^*} f(x) - p_n(x) \, dx = (-1)^{n+2} \frac{f^{(n+1)}(\xi)}{(n+1)!} h^{n+2} \int_0^{\frac{x^*-x_0}{h}} \mu (\mu - 1) \cdots (\mu - n + 1)(\mu - n) \, d\mu
\]
for some \(\xi \in [x_0, x_n]\).

- If there is a change of sign in the polynomial of the integrand in the interval \([x^*, x_n]\), the error can be written as,
\[
E_n = \int_{x_n}^{x^*} f(x) - p_n(x) \, dx = -\frac{f^{(n+1)}(\xi_1)}{(n+1)!} h^{n+2} \int_0^{\frac{x^*-x_0}{h}} \mu (\mu - 1) \cdots (\mu - n + 1)(\mu - n) \, d\mu
+ \frac{f^{(n+2)}(\xi_2)}{(n+2)!} h^{n+3} \int_0^{\frac{x^*-x_0}{h}} \mu (\mu - 1) \cdots (\mu - n + 1)(\mu - n)(\mu - \frac{x^*-x_0}{h}) \, d\mu.
\]

(46)

for some \(\xi_1, \xi_2 \in [x_0, x_n]\).

Proof. If there is not a change of sign in the polynomial of the integrand in the interval \([x^*, x_n]\), we just need to do the change of variables \(y = x_n - x\) and proceed as in Lemma 4.
If there is a change of sign in the polynomial of the integrand in the smooth interval \([x^n, x_n]\), we obtain

$$E_n = \int_{x^n}^{x_n} f(x) - p_n(x) \, dx = \int_{x^n}^{x_n} (x - x_0) \cdots (x - x_n) f[x_0, \ldots, x_n, x] \, dx$$

$$= (-1)^{n+2} \int_0^{x_n-x^*} (y - (x_n - x_0)) \cdots (y - (x_n - x_{n-1})) y f[x_0, \ldots, x_n, x_n - y] \, dy$$

$$= (-1)^{n+2} \frac{f^{(n+1)}(\xi)}{(n+1)!} \int_0^{x_n-x^*} (y - nh) \cdots (y - h) y \, dy,$$

for some \(\xi \in [x_0, x_n]\). Applying the change of variables \(y = \mu h, 0 \leq \mu \leq n\), we can write,

$$E_n = (-1)^{n+2} \frac{f^{(n+1)}(\xi)}{(n+1)!} h^{n+2} \int_0^{x_n-x^*} \mu(\mu - 1) \cdots (\mu - n + 1)(\mu - n) \, d\mu.$$  

**If there is a change of sign in the polynomial of the integrand in the smooth interval \([x^n, x_n]\), we can define**

$$w(x_n, x) = \int_{x_n}^{x} (t - x_0) \cdots (t - x_n) \, dt.$$  

(47)

that satisfies, by the symmetry of the polynomials used, that at smooth zones,

$$w(x_n, x_n) = w(x_n, x_0) = 0, \quad w(x_n, x) < 0 \quad \text{for} \quad x_0 < x < x_n,$$

when \(n\) is even, and

$$w(x_n, x_n) = 0, \quad w(x_n, x) < 0 \quad \text{for} \quad x_0 < x < x_n,$$

when \(n\) is odd.

Following similar arguments to those in [6] (page 309), or just using symmetry arguments, the proof of these facts can be easily obtained.

Now, we can write the error as in Lemma 3

$$E_n = \int_{x^n}^{x_n} w'(x_n, x) f[x_0, \ldots, x_n, x] \, dx.$$  

and integrate by parts,

$$\int_{x^n}^{x_n} w'(x_n, x) f[x_0, \ldots, x_n, x] \, dx = [w(x_n, x) f[x_0, \ldots, x_n, x]]_{x^n}^{x_n} - \int_{x^n}^{x_n} w(x_n, x) \frac{d}{dx} f[x_0, \ldots, x_n, x] \, dx$$

$$= -w(x_n, x^*) f[x_0, \ldots, x_n, x^*] - \int_{x^n}^{x_n} w(x_n, x) \frac{d}{dx} f[x_0, \ldots, x_n, x] \, dx.$$  

(48)

Proceeding exactly as in Lemma 3 and observing that,

$$w(x_n, x^*) = -w(x^*, x_n),$$

we obtain

$$w(x_n, x^*) f[x_0, \ldots, x_n, x^*] = -\frac{f^{(n+1)}(\xi)}{(n+1)!} h^{n+2} \int_{x^*}^{x_n-x_0} \mu(\mu - 1) \cdots (\mu - n + 1)(\mu - n) \, d\mu,$$

(49)
for some \( \xi_1 \in [x_0, x_n] \).

For the last integral in (48) we can proceed again as in Lemma 4 to write

\[
- \int_{x^*}^{x_n} w(x_n, x) \frac{d}{dx} f[x_0, \ldots, x_n, x] dx = - \int_{x^*}^{x_n} w(x_n, x) f[x_0, \ldots, x_n, x, x] dx \\
= - f[x_0, \ldots, x_n, \eta_2, \eta_2] \int_{x^*}^{x_n} w(x_n, x) dx \\
= - f(n+2)(\xi_2) (n+2)! \int_{x^*}^{x_n} \int_{x_n}^{x} (t-x_0) \cdots (t-x_n) dt dx,
\]

for some \( \eta_2, \xi_2 \in [x_0, x_n] \). Now we can change the order of integration and apply the change of variables \( t = x_0 + \mu h, 0 \leq \mu \leq n \):

\[
- \int_{x^*}^{x_n} \int_{x_n}^{x} (t-x_0) \cdots (t-x_n) dt dx = - \int_{x^*}^{x_n} \int_{t}^{x_n} (t-x_0) \cdots (t-x_n) dx dt \\
= - \int_{x^*}^{x_n} (t-x_0) \cdots (t-x_n) (x_n-t) dt \\
= h^{n+3} \int_{x^*}^{x_n} \int_{x_n}^{x} \mu(\mu-1) \cdots (\mu-n+1)(\mu-n)(\mu-\frac{x_n-x_0}{h}) d\mu.
\]

Thus, we can write that

\[
- \int_{x^*}^{x_n} w(x_n, x) \frac{d}{dx} f[x_0, \ldots, x_n, x] dx \\
= \frac{f(n+2)(\xi_2)}{(n+2)!} h^{n+3} \int_{x^*}^{x_n} \int_{x_n}^{x} \mu(\mu-1) \cdots (\mu-n+1)(\mu-n)(\mu-\frac{x_n-x_0}{h}) d\mu.
\]

(51)

Joining the partial results in (49) and (51), we finish the proof.

\[
E_n = \int_{x^*}^{x_n} f(x) - p_n(x) dx = \int_{x^*}^{x_n} (x-x_0) \cdots (x-x_n) f[x_0, \ldots, x_n, x] dx \\
= - \frac{f(n+1)(\xi_1)}{(n+1)!} h^{n+2} \int_{x^*}^{x_n} \int_{x_n}^{x} \mu(\mu-1) \cdots (\mu-n+1)(\mu-n) d\mu \\
+ \frac{f(n+2)(\xi_2)}{(n+2)!} h^{n+3} \int_{x^*}^{x_n} \int_{x_n}^{x} \mu(\mu-1) \cdots (\mu-n+1)(\mu-n)(\mu-\frac{x_n-x_0}{h}) d\mu,
\]

for some \( \xi_1, \xi_2 \in [x^*, x_n] \).



**Theorem 3.** Let’s suppose that the piecewise continuous function \( f \) has singularities at \( x^* \) up to the \( n \)-th derivative. The addition of the correction term,

\[
C = \int_{a}^{x^*} Q^+(x) dx + \int_{x^*}^{b} Q^-(x) dx
\]

(52)

to the numerical integration formula, assures that the error is:
• If the discontinuity is placed in the interval \([x_0, x_1]\)

\[
E^*(f) = E(f) + C = C_n^1 \left(\frac{f^-((n+1))(\xi_1)}{(n+1)!}h^{n+2} + C_n^2 \left(\frac{f^+((n+1))(\xi_2)}{(n+1)!}h^{n+2} + C_n^3 \left(\frac{f^+((n+2))(\xi_3)}{(n+2)!}h^{n+3},
\right)\right),
\]

with \(\xi_1, \xi_2, \xi_3 \in [x_0, x_n]\), and

\[
C_n^1 = \int_0^{x^*-x_0} \mu(\mu - 1) \cdots (\mu - n + 1)(\mu - n) d\mu,
C_n^2 = \int_0^{x^*-\frac{x_0}{h}} \mu(\mu - 1) \cdots (\mu - n + 1)(\mu - (\mu - x^* - x_0) d\mu.
C_n^3 = \int_0^{x^*-\frac{x_0}{h}} \mu(\mu - 1) \cdots (\mu - n + 1)(\mu - (\mu - x^* - x_0) d\mu.
\]

• If the discontinuity is placed in the interval \([x_{n-1}, x_n]\),

\[
E(f) - C = C_n^1 \left(\frac{f^-((n+1))(\xi_1)}{(n+1)!}h^{n+2} + C_n^2 \left(\frac{f^+((n+1))(\xi_2)}{(n+1)!}h^{n+2} + C_n^3 \left(\frac{f^+((n+2))(\xi_3)}{(n+2)!}h^{n+3},
\right)\right),
\]

with \(\xi_1, \xi_2, \xi_3 \in [x_0, x_n]\), and

\[
C_n^1 = \int_0^{\frac{x_0}{h}} \mu(\mu - 1) \cdots (\mu - n + 1)(\mu - n) d\mu,
C_n^2 = \int_0^{\frac{x_0}{h}} \mu(\mu - 1) \cdots (\mu - n + 1)(\mu - (\mu - x^* - x_0) d\mu.
C_n^3 = \int_0^{\frac{x_0}{h}} \mu(\mu - 1) \cdots (\mu - n + 1)(\mu - (\mu - x^* - x_0) d\mu.
\]

• In any other case,

\[
E^*(f) = E(f) + C = C_n^1 \left(\frac{f^-((n+1))(\xi_1)}{(n+1)!}h^{n+2} + C_n^2 \left(\frac{f^-((n+2))(\xi_2)}{(n+2)!}h^{n+3} + C_n^3 \left(\frac{f^+((n+1))(\xi_3)}{(n+1)!}h^{n+2} + C_n^4 \left(\frac{f^+((n+2))(\xi_4)}{(n+2)!}h^{n+3},
\right)\right),
\]

with \(\xi_1, \xi_2, \xi_3, \xi_4 \in [x_0, x_n]\), and

\[
C_n^1 = \int_0^{\frac{x_0}{h}} \mu(\mu - 1) \cdots (\mu - n + 1)(\mu - n) d\mu,
C_n^2 = \int_0^{\frac{x_0}{h}} \mu(\mu - 1) \cdots (\mu - n + 1)(\mu - (\mu - x^* - x_0) d\mu.
C_n^3 = \int_0^{\frac{x_0}{h}} \mu(\mu - 1) \cdots (\mu - n + 1)(\mu - (\mu - x^* - x_0) d\mu.
C_n^4 = \int_0^{\frac{x_0}{h}} \mu(\mu - 1) \cdots (\mu - n + 1)(\mu - n) d\mu.
\]

Proof. The proof is straightforward using Lemmas \textit{3, 4} and Corollary \textit{1}.

\[]
3.1. Correction terms for commonly used Newton-Cotes formulas

In Table\ref{table:correction-terms} we present some expressions for the partial correction terms $C_{n,j}$ in \eqref{eq:correction-terms}. In Table\ref{table:correction-terms} we have used the notation $C_{n,j}, j = 1 \cdots n$, being $n$ the degree of the interpolating polynomial used to obtain the integration rule. Thus, for the trapezoidal rule there is only the term $C_{1,1}$. For the Simpson’s 1/3 rule there are two terms: $C_{2,1}$ if the discontinuity falls at an odd interval and $C_{2,2}$ if the discontinuity falls at an odd interval. For the Simpson’s 3/8 rule, there are three terms: $C_{3,1}$ if $\left(\lceil \frac{x}{h} \rceil \mod 3\right) = 1$, $C_{3,2}$ if $\left(\lceil \frac{x}{h} \rceil \mod 3\right) = 2$ and $C_{3,3}$ if $\left(\lceil \frac{x}{h} \rceil \mod 3\right) = 0$. For higher orders, the notation is similar. Just to show an example, in Figure\ref{fig:discontinuities} we should use $C_{3,1}$ in the case presented to the left, $C_{3,2}$ in the case presented at the middle and $C_{3,3}$ in the case to the right.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{discontinuities.png}
\caption{Three examples of functions with singularities (solid line) placed in different intervals at a position $x^*$. We have labeled the domain to the left of the singularity as $-$ and the one to the right as $+$. We have also represented with a dashed line the prolongation of the functions through Taylor expansions at both sides of the discontinuity.}
\end{figure}

4. Numerical experiments

In this section we will apply the classical and corrected composed trapezoid rule and Simpson’s rule to data obtained from the discretisation of the functions presented in \eqref{eq:functions} and plotted in Figure \ref{fig:functions}. We will consider that we start from discretised data and that the location of the discontinuity is known in the case of jump discontinuities in the function. In the case of jump discontinuities in the first derivative, we will numerically obtain an approximation of its location with enough accuracy using the algorithm described in \cite{4}.

\begin{equation}
\begin{aligned}
f(x) &= \begin{cases} 
(x - \frac{a}{h})(x - \frac{a}{h} - 3) + \sin\left(\frac{\pi a}{h}\right) 8 + a, & \text{if } 0 \leq x < \frac{a}{h}, \\
\sin\left(\frac{\pi a}{h}\right) 8, & \text{if } \frac{a}{h} \leq x \leq 1.
\end{cases}
\end{aligned}
\end{equation}

For the experiments using the trapezoidal rule, we have obtained the jump in the function with $O(h^2)$ accuracy and the jump in the first derivative with $O(h)$ accuracy. The reason is that, looking at the correction term in \eqref{eq:correction-term}, that amounts to the local truncation error with a change of sign, we can see that it is enough to obtain the jump in the function with $O(h^2)$ order of accuracy (in the case of kinks, we know that if we detect a singularity, the jump in the function must be zero \cite{4}) and the jump in the first derivative with $O(h)$ accuracy in order to keep the accuracy of the simple trapezoidal rule in \cite{2}. For the composed rule, the requirements are even less strict, and we could just use $O(h)$ accuracy for the jump in the function and $O(1)$ for the jump in the first derivative. Following similar arguments, for the experiments using the Simpson’s $\frac{1}{3}$ rule, we have obtained the jump in the function with $O(h^4)$ accuracy, the jump in the first derivative with $O(h^3)$, the jump in the second derivative with $O(h^2)$ and so on, as the simple Simpson’s rule presents $O(h^3)$ order of accuracy. Again, for the composed rule, the requirements are less strict, and we could just use $O(h^3)$ accuracy for the jump in the function and $O(h^2)$ for the jump in the first derivative, etc.
In Table 2 we present grid refinement experiments in order to show the numerical accuracy obtained using the correction terms presented in Section 2 for the numerical integration of the function in (53) with \(a = 10\), through the composed trapezoidal and Simpson’s rule. It is easy to check that the function in (53) presents jumps in the function and the three first derivatives at \(x = \frac{\pi}{6}\). For this experiment we have supposed that we know the exact position of the discontinuity but that the jumps in the function and derivatives are unknown and calculated through one sided interpolation [2]. For some applications, these jumps could be known a priori. We start from a point value discretization of the data with \(n = 2^i, i = 4, 5, \cdots, 15\) points. The order presents some variability due to the random position of the discontinuity at the interval that contains it.

In Figure 5 we show the errors presented in Table 2 and the theoretical decreasing of the error that each technique should provide. To the left we present the results for the Trapezoid rule in blue and for the corrected trapezoid rule in red. We can see that the non corrected rule shows a decreasing in the error very similar to the dashed line in blue, that shows the division of the error by two each time that the mesh size is divided by two (\(O(h)\) order of accuracy). The corrected trapezoid rule behaves very similarly to the dashed line in red, that divides the error by four when the mesh side is divided by two (\(O(h^2)\) order of accuracy). To the right, the non corrected Simpson \(\frac{1}{3}\) rule behaves very similarly to the dashed line in blue, that represents \(O(h^2)\) order of accuracy. The corrected Simpson’s rule behaves very similarly to the dashed line in red, that represents \(O(h^4)\) order of accuracy. We can see that the orders of accuracy of the corrected composed rules correspond to those of the composed classical rules at smooth zones.

In Table 3 we present a similar experiment, but this time for the function in (53) with \(a = 0\). In this case, the jump in the function is zero but there is a jump in the three first derivatives. Thus, it is possible to locate the singularity using the technique described in [4] and to obtain the jumps in the derivatives as described in [2]. In Figure 6 we can see the errors shown in Table 3. As in the previous experiment, we have also represented the lines that correspond to a decreasing of the error with \(O(h^2)\) accuracy and \(O(h^4)\) accuracy. If we look at the correction term in (6) (remind that this correction term corresponds to minus one times the local truncation error of the integral at the interval that contains the singularity) we can see that a jump in the first derivative will result in a local error of \(O(h^2)\) at the interval that contains the singularity, that corresponds to the global error of the classical composed trapezoidal rule resulting from (2). Thus, for the composed trapezoidal rule, we can not expect to obtain better order of accuracy with the corrected formula than with the classical formula. Even so, the error should be smaller and this fact can be observed in Figure 6 to the left. In Figure 6 to the right, we can observe the result obtained for the Simpson’s \(\frac{1}{3}\) rule. We can see that with the corrected composed formula we obtain the predicted \(O(h^4)\) theoretical accuracy while only \(O(h^2)\) accuracy is recovered through the classical formula.
Figure 4: Function in (53) used in the numerical experiments. To the left with $a = 10$ (left) and $a = 0$ (right), with a singularity at $x = \frac{\pi}{6}$.

Figure 5: Error obtained when numerically integrating the Function in (53) with $a = 10$, that is represented to the left of Figure 4. To the left, using the trapezoid rule, the corrected trapezoid rule. To the right, using the Simpson’s rule, and the corrected Simpson’s rule.
Figure 6: Error obtained when numerically integrating the function in [53] with $a = 0$, that is represented to the right of Figure 4. To the left, using the trapezoid rule and the corrected trapezoid rule. To the right, using the Simpson’s rule and the corrected Simpson’s rule.
\[ C_{1,1} = \frac{1}{2} \int f(x) \, dx - \left( \frac{a + b}{2} \right) f(a) - \left( \frac{a + b}{2} \right) f(b) \]

\[ C_{2,1} = \frac{1}{6} \int f(x) \, dx - \left( \frac{a + b}{2} \right) f(a) - \left( \frac{a + b}{2} \right) f(b) \]

\[ C_{2,2} = \frac{1}{24} \int f(x) \, dx - \left( \frac{a + b}{2} \right) f(a) - \left( \frac{a + b}{2} \right) f(b) \]

\[ C_{3,1} = \frac{1}{120} \int f(x) \, dx - \left( \frac{a + b}{2} \right) f(a) - \left( \frac{a + b}{2} \right) f(b) \]

\[ C_{3,2} = \frac{1}{720} \int f(x) \, dx - \left( \frac{a + b}{2} \right) f(a) - \left( \frac{a + b}{2} \right) f(b) \]

\[ C_{3,3} = \frac{1}{5040} \int f(x) \, dx - \left( \frac{a + b}{2} \right) f(a) - \left( \frac{a + b}{2} \right) f(b) \]

\[ C_{3,4} = \frac{1}{40320} \int f(x) \, dx - \left( \frac{a + b}{2} \right) f(a) - \left( \frac{a + b}{2} \right) f(b) \]

Table 1: Correction terms for the most common integration formulas.

| \( n \) | \( \text{Error T.R. (E)} \) | \( \text{C.S.R.} \) | \( \text{Simpson's Rule (S.R.)} \) | \( \text{Cross-Correlation (C.C.R.)} \) |
|---|---|---|---|---|
| \( 2^1 \) | 1.6050e-09 | 1.4356e-09 | 6.8365e-09 | 3.9676e-09 |
| \( 2^2 \) | 3.4742e-09 | 2.1879e-09 | 1.9876e-09 | 0.9676e-09 |
| \( 2^3 \) | 5.3558e-09 | 2.2859e-09 | 5.9390e-09 | 3.9439e-09 |
| \( 2^4 \) | 1.3438e-08 | 2.1879e-09 | 1.9876e-09 | 0.9676e-09 |

Table 2: Grid refinement analysis for the trapezoidal rule (T.R.), the corrected trapezoidal rule (C.T.R.), the Simpson’s Rule (S.R.) and the corrected Simpson’s rule (C.S.R.) when numerically integrating the Function in (53) with \( a = 10 \), that is represented to the left of Figure 4.

| \( n \) | \( \text{Error T.R. (E)} \) | \( \text{C.S.R.} \) | \( \text{Simpson's Rule (S.R.)} \) | \( \text{Cross-Correlation (C.C.R.)} \) |
|---|---|---|---|---|
| \( 2^1 \) | 2.0604e-02 | 2.4874e-02 | 2.0604e-02 | 2.4874e-02 |
| \( 2^2 \) | 1.1789e-02 | 9.8891e-03 | 1.1789e-02 | 9.8891e-03 |
| \( 2^3 \) | 5.3558e-03 | 2.2859e-03 | 5.3558e-03 | 2.2859e-03 |
| \( 2^4 \) | 2.1879e-03 | 9.8891e-04 | 2.1879e-03 | 9.8891e-04 |

Table 3: Grid refinement analysis for the trapezoidal rule (T.R.), the corrected trapezoidal rule (C.T.R.), the Simpson’s Rule (S.R.) and the corrected Simpson’s rule (C.S.R.) when numerically integrating the Function in (53) with \( a = 0 \), that is represented to the right of Figure 4.
5. Conclusions

In this article we have presented correction terms for the classical trapezoid rule, Simpson’s $\frac{1}{3}$ rule and the most common Newton-Cotes integration formulas. These correction terms have an explicit closed formula that allows to keep, close to the singularities, the global accuracy attained by classical formulas at smooth zones. The correction terms can be used for the simple or composed classical integration formulas and it is possible to compute the integral using these formulas and then, as a post-processing, add the correction terms in order to rise the accuracy. Correction terms for any other integration rule can be found following analogous processes to the ones shown in this work. We have also shown a way of calculating the correction terms for any order of accuracy and we have proved that the use of these correction terms assure the expected theoretical accuracy. The numerical experiments presented confirm the theoretical results obtained.

Conflict of interest

The authors declare that they have no conflict of interest.

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