Error inequalities for an optimal 3-point quadrature formula of closed type

Nenad Ujević

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Abstract

An optimal 3-point quadrature formula of closed type is derived. Various error inequalities are established. Applications in numerical integration are also given.

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1 Introduction

In recent years a number of authors have considered an error analysis for quadrature rules of Newton-Cotes type. In particular, the mid-point, trapezoid and Simpson rules have been investigated more recently ([2], [4], [5], [6], [11]) with the view of obtaining bounds on the quadrature rule in terms of a variety of norms involving, at most, the first derivative. In the mentioned papers explicit error bounds for the quadrature rules are given. These results are obtained from an inequalities point of view. The authors use Peano type kernels for obtaining a specific quadrature rule.

Quadrature formulas can be formed in many different ways. For example, we can integrate a Lagrange interpolating polynomial of a function $f$ to obtain a corresponding quadrature formula (Newton-Cotes formulas). We can also seek a quadrature formula such that it is exact for polynomials of maximal degree (Gauss formulas). Gauss-like quadrature formulas are considered in [12].

Here we present a new approach to this topic. Namely, we give a type of quadrature formula. We also give a way of estimation of its error and all parameters which appear in the estimation. Then we seek a quadrature formula of the given type such that the estimation of its error is best possible. Let us consider the above described procedure with more details.

If we define

$$K_2(\alpha, \beta, \gamma, \delta, t) = \begin{cases} \frac{1}{2}(t - \alpha)(t - \beta), & t \in \left[\alpha, \frac{\alpha + \beta}{2}\right] \\ \frac{1}{2}(t - \gamma)(t - \delta), & t \in \left(\frac{\alpha + \beta}{2}, \beta\right] \end{cases}$$
then, integrating by parts, we obtain

\[
\int_a^b K_2(\alpha, \beta, \gamma, \delta, t) f''(t) \, dt
\]

\[
= \frac{1}{2} \left\{ f'(b) (b - \gamma) (b - \delta) + f' \left( \frac{a + b}{2} \right) \times \left[ \left( \frac{a + b}{2} - \alpha \right) \left( \frac{a + b}{2} - \beta \right) - \left( \frac{a + b}{2} - \gamma \right) \left( \frac{a + b}{2} - \delta \right) \right] \right. \\
- f'(a) (a - \alpha) (a - \beta) \right. \\
+ \left. \left( a - \frac{\alpha + \beta}{2} \right) f(a) - \left( \frac{\gamma + \delta}{2} \cdot \frac{\alpha + \beta}{2} \right) f \left( \frac{a + b}{2} \right) - \left( b - \frac{\gamma + \delta}{2} \right) f(b) \right. \\
+ \left. \int_a^b f(t) \, dt. \right\}
\]

If we choose \( \alpha = \beta = a \) and \( \gamma = \delta = b \) then we get the mid-point quadrature rule. If we choose \( \alpha = \gamma = a \) and \( \beta = \delta = b \) then we get the trapezoid rule. If we choose \( \alpha = 0, \beta = \frac{a + 2b}{3} \) and \( \gamma = \frac{2a + b}{3}, \delta = 1 \) then we get Simpson’s rule.

If we require that

\[
\left( \frac{a + b}{2} - \alpha \right) \left( \frac{a + b}{2} - \beta \right) - \left( \frac{a + b}{2} - \gamma \right) \left( \frac{a + b}{2} - \delta \right) = 0 \\
(a - \alpha) (a - \beta) = 0
\]

then we get a classical quadrature formula of the form

\[
\int_a^b K_2(\alpha, \beta, \gamma, \delta, t) f''(t) \, dt
\]

\[
= \left( a - \frac{\alpha + \beta}{2} \right) f(a) - \left( \frac{\gamma + \delta}{2} \cdot \frac{\alpha + \beta}{2} \right) f \left( \frac{a + b}{2} \right) - \left( b - \frac{\gamma + \delta}{2} \right) f(b) \\
+ \int_a^b f(t) \, dt.
\]

In practice we cannot find an exact value of the remainder term (error)

\[
\int_a^b K_2(\alpha, \beta, \gamma, \delta, t) f''(t) \, dt. \quad \text{All we can do is to estimate the error. It can be done in different ways. For example,}
\]

\[
\left| \int_a^b K_2(\alpha, \beta, \gamma, \delta, t) f''(t) \, dt \right| \leq \max_{t \in [a, b]} |f''(t)| \int_a^b |K_2(\alpha, \beta, \gamma, \delta, t)| \, dt. \quad (2)
\]
It is a natural question which formula of the type \(1\) is optimal, with respect to a given way of estimation of the error. The main aim of this paper is to give an answer to this question and to consider the formula from an inequalities point of view. In fact, we seek a quadrature formula of the given type such that its error bound is minimal. Note that we can minimize only the factor \(\int_a^b |K_2(\alpha, \beta, \gamma, \delta, t)| dt\) in \(2\). A general approach is: we first consider the minimization problem and then we formulate final results. Various error inequalities for the obtained optimal formula are established. Applications in numerical integration are also given. Finally, let us mention that the obtained optimal quadrature formula has better estimations of error than the Simpson’s formula (see Remark \(2\)).

2 An optimal quadrature formula

We consider the problem, described in Section 1, on the interval \([0, 1]\). Let \(\alpha, \beta, \gamma, \delta \in \mathbb{R}\). We define the mapping

\[
K_2(\alpha, \beta, \gamma, \delta, t) = \begin{cases} 
\frac{1}{2}(t - \alpha)(t - \beta), & t \in \left[0, \frac{1}{2}\right] \\
\frac{1}{2}(t - \gamma)(t - \delta), & t \in \left(\frac{1}{2}, 1\right] 
\end{cases}
\]

Let \(I \subset \mathbb{R}\) be an open interval such that \([0, 1] \subset I\) and let \(f : I \rightarrow \mathbb{R}\) be a twice differentiable function such that \(f''\) is bounded and integrable. We denote

\[
\|f\|_\infty = \sup_{t \in [0,1]} |f(t)|.
\]

Integrating by parts, we obtain

\[
\int_0^1 K_2(\alpha, \beta, \gamma, \delta, t)f''(t)dt
\]

\[
= \frac{1}{2} \int_0^{1/2} (t - \alpha)(t - \beta)f''(t) + \int_{1/2}^1 (t - \gamma)(t - \delta)f''(t)dt
\]

\[
= -\frac{1}{2} \alpha \beta f'(0) + \frac{1}{2} (1 - \gamma)(1 - \delta) f'(1)
\]

\[
+ \frac{1}{2} \left[ \left(\frac{1}{2} - \alpha\right) \left(\frac{1}{2} - \beta\right) - \left(\frac{1}{2} - \gamma\right) \left(\frac{1}{2} - \delta\right) \right] f'(1/2)
\]

\[- \int_0^1 K_1(\alpha, \beta, \gamma, \delta, t)f'(t)dt,
\]

where
\[ K_1(\alpha, \beta, \gamma, \delta, t) = \begin{cases} t - \frac{\alpha + \beta}{2}, & t \in [0, \frac{1}{2}] \\ t - \frac{\gamma + \delta}{2}, & t \in (\frac{1}{2}, 1] \end{cases}. \]

We require that the coefficients \(-\frac{1}{2} \alpha \beta, \frac{1}{2} \left[ (\frac{1}{2} - \alpha) (\frac{1}{2} - \beta) - (\frac{1}{2} - \gamma) (\frac{1}{2} - \delta) \right]\) and \(\frac{1}{2} (1 - \gamma) (1 - \delta)\) be equal to zero. Hence, we require that \(\alpha = 0\) or \(\beta = 0\) and \(\gamma = 1\) or \(\delta = 1\). If we choose \(\alpha = 0\) and \(\delta = 1\) then we get \(\beta + \gamma = 1\). If we now substitute \(\alpha = 0\), \(\gamma = 1\), and \(\delta = 1\) in (5) then we have

\[
\int_0^1 K_2(0, \beta, 1 - \beta, 1, t) f''(t) \, dt \tag{6}
\]

\[
= - \int_0^1 K_1(0, \beta, 1 - \beta, 1, t) f'(t) \, dt
\]

\[
= - \int_0^{\frac{1}{2}} (t - \frac{\beta}{2}) f'(t) \, dt - \int_{\frac{1}{2}}^1 (t - \frac{2 - \beta}{2}) f'(t) \, dt
\]

\[
= -\frac{\beta}{2} f(0) - (1 - \beta) f\left(\frac{1}{2}\right) - \frac{\beta}{2} f(1) + \int_0^1 f(t) \, dt.
\]

We also have

\[
\left| \int_0^1 K_2(0, \beta, 1 - \beta, 1, t) f''(t) \, dt \right| \leq \| f'' \|_{\infty} \int_0^1 |K_2(0, \beta, 1 - \beta, 1, t)| \, dt \tag{7}
\]

and

\[
\int_0^1 |K_2(0, \beta, 1 - \beta, 1, t)| \, dt = \frac{1}{2} \int_0^{\frac{1}{2}} t |t - \beta| \, dt + \frac{1}{2} \int_{\frac{1}{2}}^1 |t - 1 + \beta| (1 - t) \, dt. \tag{8}
\]

We now define

\[
g(\beta) = \frac{1}{2} \int_0^{\frac{1}{2}} t |t - \beta| \, dt + \frac{1}{2} \int_{\frac{1}{2}}^1 |t - 1 + \beta| (1 - t) \, dt \tag{9}
\]

and consider the problem

\[
\text{minimize } g(\beta), \quad \beta \in \mathbb{R}. \tag{10}
\]

Hence, we should like to find a global minimizer of \(g\). Recall, a global minimizer is a point \(\beta^*\) that satisfies

\[
g(\beta^*) \leq g(\beta), \text{ for all } \beta \in \mathbb{R}. \tag{11}
\]
We consider the following cases:
(i) \( \beta \leq 0 \),
(ii) \( 0 \leq \beta \leq \frac{1}{2} \),
(iii) \( \beta \geq \frac{1}{2} \).

**The case (i).** If \( \beta \leq 0 \) then \( t|t - \beta| = t(t - \beta) \), for \( t \in [0, \frac{1}{2}] \) and \( |t - 1| |t - 1| = (t - 1 + \beta)(t - 1) \), for \( t \in \left( \frac{1}{2}, 1 \right] \). Thus,

\[
g(\beta) = \frac{1}{2} \int_0^{\frac{1}{2}} t(t - \beta)dt + \frac{1}{2} \int_{\frac{1}{2}}^1 (t - 1 + \beta)(t - 1)dt
\]

\[
= \frac{1}{24} - \beta \geq \frac{1}{24}.
\]

**The case (iii).** If \( \beta \geq \frac{1}{2} \) then \( t|t - \beta| = t(\beta - t) \), for \( t \in [0, \frac{1}{2}] \) and \( |t - 1| |t - 1| = (t - 1 + \beta)(1 - t) \), for \( t \in \left( \frac{1}{2}, 1 \right] \). Thus,

\[
g(\beta) = \frac{1}{2} \int_0^{\frac{1}{2}} t(\beta - t)dt + \frac{1}{2} \int_{\frac{1}{2}}^1 (t - 1 + \beta)(1 - t)dt
\]

\[
= \frac{\beta}{8} - \frac{1}{24} \geq \frac{1}{48}.
\]

**The case (ii).** If \( 0 \leq \beta \leq \frac{1}{2} \) then

\[
t|t - \beta| = \begin{cases} 
  t(\beta - t), & t \in [0, \beta] \\
  t(t - \beta), & t \in (\beta, \frac{1}{2}] 
\end{cases}
\]

and

\[
|t - 1 + \beta| |t - 1| = \begin{cases} 
  (t - 1 + \beta)(t - 1), & t \in \left[ \frac{1}{2}, 1 - \beta \right] \\
  (t - 1 + \beta)(1 - t), & t \in \left( 1 - \beta, 1 \right]
\end{cases}.
\]

Thus,

\[
g(\beta) = \frac{1}{2} \int_0^\beta t(\beta - t)dt + \frac{1}{2} \int_{\beta}^{\frac{1}{2}} t(t - \beta)dt
\]

\[
+ \frac{1}{2} \int_{\frac{1}{2}}^{1-\beta} (t - 1 + \beta)(t - 1)dt + \frac{1}{2} \int_{1-\beta}^1 (t - 1 + \beta)(1 - t)dt
\]

\[
= \frac{\beta^3}{3} - \beta \frac{1}{8} + \frac{1}{24}.
\]

We have

\[
g'(\beta) = \beta^2 - \frac{1}{8} \quad \text{and} \quad g''(\beta) = 2\beta.
\]
From the equation \( g'(\beta) = 0 \) we find that \( \beta_{1,2} = \pm \frac{\sqrt{2}}{4} \). Since \( g''(\frac{\sqrt{2}}{4}) > 0 \) we conclude that \( \beta = \frac{\sqrt{2}}{4} \) is, at least, a local minimizer. We have

\[
g(\frac{\sqrt{2}}{4}) = \frac{2 - \sqrt{2}}{48}.
\]

From (12), (13) and (16) we conclude that \( \beta = \frac{\sqrt{2}}{4} \) is the global minimizer. If we now substitute \( \beta = \frac{\sqrt{2}}{4} \) in (6) then we get

\[
\int_0^1 K_2(0, \frac{\sqrt{2}}{4}, 1 - \frac{\sqrt{2}}{4}, 1, t)f''(t)dt
\]

\[
= \int_0^1 f(t)dt - \frac{\sqrt{2}}{8}f(0) - \left(1 - \frac{\sqrt{2}}{4}\right)f(1) - \frac{\sqrt{2}}{8}f(1).
\]

The above quadrature formula is optimal in the sense described in Section 1.

From the previous considerations we can formulate the following result.

**Theorem 1** Let \( I \subset R \) be an open interval such that \([0, 1] \subset I \) and let \( f : I \rightarrow R \) be a twice differentiable function such that \( f'' \) is bounded and integrable.

Then we have

\[
\left| \int_0^1 f(t)dt - \frac{\sqrt{2}}{8}f(0) - \left(1 - \frac{\sqrt{2}}{4}\right)f(\frac{1}{2}) - \frac{\sqrt{2}}{8}f(1) \right| \leq \frac{2 - \sqrt{2}}{48} \|f''\|_{\infty}. \] (18)

**Remark 2** If we set \( \beta = \frac{1}{3} \) in (6) then we get the well-known Simpson’s rule:

\[
\int_0^1 f(t)dt - \frac{1}{6} \left[f(0) + 4f(\frac{1}{2}) + f(1)\right] = \int_0^1 K_2(0, \frac{1}{3}, 1, 1, t)f''(t)dt.
\]

We have

\[
\left| \int_0^1 f(t)dt - \frac{1}{6}f(0) - \frac{2}{3}f(\frac{1}{2}) - \frac{1}{6}f(1) \right| \leq \frac{\|f''\|_{\infty}}{81}. \] (20)

It is obvious that (18) is a better estimate than (20). Note that (17) and (19) are 3-point quadrature rules of the same (closed) type.

If we consider the above problem on the interval \([a, b] \) then we get the following result.
Theorem 3 Let $I \subset \mathbb{R}$ be an open interval such that $[a, b] \subset I$ and let $f : I \to \mathbb{R}$ be a twice differentiable function such that $f''$ is bounded and integrable. Then we have

$$\left| \int_{a}^{b} f(t) dt - \left[ \frac{\sqrt{2}}{8} f(a) + \left(1 - \frac{\sqrt{2}}{4}\right) f\left(\frac{a+b}{2}\right) + \frac{\sqrt{2}}{8} f(b) \right] (b-a) \right| \leq \frac{2 - \sqrt{2}}{48} \|f''\|_{\infty} (b-a)^{3},$$

where $\|f''\|_{\infty} = \sup_{t \in [a,b]} |f''(t)|$.

3 Error inequalities

First we consider some basic properties of the spaces $L_{p}(a, b)$, for $p = 1, 2, \infty$. As we know, $X = (L_2(a, b), \langle \cdot, \cdot \rangle)$ is a Hilbert space with the inner product

$$\langle f, g \rangle = \int_{a}^{b} f(t)g(t) dt. \quad (22)$$

In the space $X$ the norm $\|\cdot\|_2$ is defined in the usual way,

$$\|f\|_2 = \left( \int_{a}^{b} f(t)^2 dt \right)^{1/2}. \quad (23)$$

We also consider the space $Y = (L_{2}(a, b), \langle \cdot, \cdot \rangle)$ where the inner product $\langle \cdot, \cdot \rangle$ is defined by

$$\langle f, g \rangle = \frac{1}{b-a} \int_{a}^{b} f(t)g(t) dt. \quad (24)$$

It is not difficult to see that $Y$ is a Hilbert space, too. In the space $Y$ the norm $\|\cdot\|$ is defined by

$$\|f\| = \sqrt{\langle f, f \rangle}. \quad (25)$$

We also define the Chebyshev functional

$$T(f, g) = \langle f, g \rangle - \langle f, e \rangle \langle g, e \rangle,$$

where $f, g \in L_{2}(a, b)$ and $e = 1$. This functional satisfies the pre-Gr"{u}ss inequality ([9, p. 296]),

$$T(f, g)^2 \leq T(f, f)T(g, g). \quad (27)$$

Specially, we define

$$\sigma(f) = \sigma(f; a, b) = \sqrt{(b-a)T(f, f)}.$$

The space $L_{1}(a, b)$ is a Banach space with the norm

$$\|f\|_{1} = \int_{a}^{b} |f(t)| dt \quad (29)$$
and the space $L_\infty(a, b)$ is also a Banach space with the norm

$$\|f\|_\infty = \text{ess sup}_{t \in [a, b]} |f(t)|.$$  

(30)

If $f \in L_1(a, b)$ and $g \in L_\infty(a, b)$ then we have

$$|(f, g)| \leq \|f\|_1 \|g\|_\infty.$$  

(31)

More about the above mentioned spaces can be found, for example, in [1].

Finally, we define the functional

$$Q(f) = Q(f; a, b) = \int_a^b f(t) dt - \left[ \frac{\sqrt{2}}{8} f(a) + \left(1 - \frac{\sqrt{2}}{4}\right) f\left(\frac{a + b}{2}\right) + \frac{\sqrt{2}}{8} f(b) \right] (b - a).$$  

(32)

We also need the following lemma.

**Lemma 4** Let $f(t) = \begin{cases} f_1(t), & t \in [a, x_0] \\ f_2(t), & t \in (x_0, b) \end{cases}$, where $x_0 \in [a, b]$, $f_1 \in C^1(a, x_0)$, $f_2 \in C^1(x_0, b)$. If $f_1(x_0) = f_2(x_0)$ then $f$ is an absolutely continuous function.

A proof of this lemma can be found in [13].

**Theorem 5** Let $f : [0, 1] \to \mathbb{R}$ be an absolutely continuous function such that $f' \in L_1(0, 1)$ and there exist real numbers $\gamma_1, \Gamma_1$ such that $\gamma_1 \leq f'(t) \leq \Gamma_1$, $t \in [0, 1]$. Then

$$|Q(f; 0, 1)| \leq \frac{\Gamma_1 - \gamma_1}{32}(5 - 2\sqrt{2}),$$  

(34)

$$|Q(f; 0, 1)| \leq \left(\frac{1}{2} - \frac{\sqrt{2}}{8}\right) (S - \gamma_1),$$  

(35)

$$|Q(f; 0, 1)| \leq \left(\frac{1}{2} - \frac{\sqrt{2}}{8}\right) (\Gamma_1 - S),$$  

(36)

where $Q(f; 0, 1)$ is defined by (32) and $S = f(1) - f(0)$.

**Proof.** We define the function

$$p_1(t) = \begin{cases} t - \frac{\sqrt{2}}{8}, & t \in [0, \frac{1}{2}] \\ t - 1 + \frac{\sqrt{2}}{8}, & t \in (\frac{1}{2}, 1) \end{cases}.$$  

(37)

It is easy to verify that

$$(p_1, f') = -Q(f; 0, 1).$$  

(38)
On the other hand, we have
\[
\left( f' - \frac{\Gamma_1 + \gamma_1}{2}, p_1 \right) = (f', p_1), \tag{39}
\]
since \((p_1, e) = 0\). From (31) we get
\[
\left| f' - \frac{\Gamma_1 + \gamma_1}{2}, p_1 \right| \leq \left\| f' - \frac{\Gamma_1 + \gamma_1}{2} \right\|_\infty \left\| p_1 \right\|_1 \leq \frac{\Gamma_1 - \gamma_1}{32} (5 - 2\sqrt{2}), \tag{40}
\]
since
\[
\left\| f' - \frac{\Gamma_1 + \gamma_1}{2} \right\|_\infty \leq \frac{\Gamma_1 - \gamma_1}{2}
\]
and
\[
\left\| p_1 \right\|_1 = \frac{5}{16} - \frac{\sqrt{2}}{8}.
\]
From (38)-(40) we see that (34) holds. We now prove that (35) holds. We have
\[
\left| (f' - \gamma_1, p_1) \right| \leq \left\| p_1 \right\|_\infty \| f' - \gamma_1 \|_1 = \left( \frac{1}{2} - \frac{\sqrt{2}}{8} \right) (S - \gamma_1),
\]
since
\[
\left\| p_1 \right\|_\infty = \frac{1}{2} - \frac{\sqrt{2}}{8}
\]
and
\[
\| f' - \gamma_1 \|_1 = \int_0^1 (f'(t) - \gamma_1) dt = f(1) - f(0) - \gamma_1.
\]
In a similar way we can prove that (36) holds. ■

**Remark 6** Note that we can apply the estimate (34) only if the first derivative
\(f'\) is bounded. It means that we cannot use (34) to estimate directly the error
when approximating the integral of such a well-behaved function as \(f(t) = \sqrt{t}\)
on \([0, 1]\), (since \(f'(t) = 1/(2\sqrt{t})\) is unbounded on \([0, 1]\)). On the other hand, we
can use the estimation (35), (since \(\gamma = 1/2\) on \([0, 1]\) for the given function).

**Theorem 7** Let \(f: [a, b] \to \mathbb{R}\) be an absolutely continuous function such that
\(f' \in L_1(a, b)\) and there exist real numbers \(\gamma_1, \Gamma_1\) such that \(\gamma_1 \leq f'(t) \leq \Gamma_1, \)
t \(t \in [a, b].\) Then
\[
|Q(f; a, b)| \leq \frac{\Gamma_1 - \gamma_1}{32} (5 - 2\sqrt{2})(b - a)^2, \tag{41}
\]
\[
|Q(f; a, b)| \leq \left( \frac{1}{2} - \frac{\sqrt{2}}{8} \right) (S - \gamma_1) (b - a)^2, \tag{42}
\]
\[
|Q(f; a, b)| \leq \left( \frac{1}{2} - \frac{\sqrt{2}}{8} \right) (\Gamma_1 - S) (b - a)^2, \tag{43}
\]
where \(Q(f; a, b)\) is defined by (32) and \(S = (f(b) - f(a))/(b - a).\)
Theorem 8 Let \( f : [0, 1] \to \mathbb{R} \) be an absolutely continuous function such that \( f' \in L_2(0, 1) \). Then

\[
|Q(f; 0, 1)| \leq \sqrt{\frac{11}{96} - \frac{\sqrt{2}}{16}} \sigma(f'; 0, 1),
\]

(44)

where \( \sigma(f; 0, 1) \) is defined by (28). The inequality (44) is sharp in the sense that the constant \( \sqrt{\frac{11}{96} - \frac{\sqrt{2}}{16}} \) cannot be replaced by a smaller one.

Proof. Let \( p_1 \) be defined by (37). We have

\[
\langle p_1, f' \rangle = -Q(f; 0, 1),
\]

since (38) holds and \( \langle f, g \rangle = (f, g) \) if \( a, b = [0, 1] \). On the other hand, we have

\[
\langle p_1, f' \rangle = T(f', p_1),
\]

since \( \langle p_1, e \rangle = 0 \). From (27) it follows

\[
|T(f', p_1)| \leq \sqrt{T(p_1, p_1)} \sqrt{T(f', f')} = \|p_1\| \sigma(f'; 0, 1)
\]

\[= \sqrt{\frac{11}{96} - \frac{\sqrt{2}}{16}} \sigma(f'; 0, 1),
\]

since

\[
\|p_1\| = \sqrt{\frac{11}{96} - \frac{\sqrt{2}}{16}}.
\]

Hence, the inequality (44) is proved. We have to prove that this inequality is sharp. For that purpose, we define the function

\[
f(t) = \begin{cases} 
\frac{1}{2}t^2 - \frac{\sqrt{2}}{8}t, & t \in [0, \frac{1}{2}] \\
\frac{1}{2}t^2 - (1 - \frac{\sqrt{2}}{8})t + \frac{1}{2} - \frac{\sqrt{2}}{8}, & t \in \left(\frac{1}{2}, 1\right)
\end{cases}
\]

(45)

such that \( f'(t) = p_1(t) \). From Lemma 4 we see that the function \( f \), defined by (45), is an absolutely continuous function. For this function the left-hand side of (44) becomes

\[
L.H.S. (44) = \left| - \frac{11}{96} + \frac{\sqrt{2}}{16} \right|.
\]

The right-hand side of (44) becomes

\[
R.H.S. (44) = \frac{11}{96} - \frac{\sqrt{2}}{16}.
\]

We see that \( L.H.S. (44) = R.H.S. (44) \). Thus, (44) is sharp. \( \blacksquare \)
Remark 9 The estimate (34) is better than the estimate (44). However, note that the estimate (34) can be applied only if \( f' \) is bounded. On the other hand, the estimate (22) can be applied for an absolutely continuous function if \( f' \in L_2(a, b) \).

There are many examples where we cannot apply the estimate (34) but we can apply (44).

Example 10 Let us consider the integral \( \int_0^1 \sqrt{\sin t^2} \, dt \). We have

\[
 f(t) = \sqrt{\sin t^2} \quad \text{and} \quad f'(t) = \frac{2t \cos^2 t}{3\sqrt{\sin t^2}}
\]

such that \( f'(t) \to \infty \), \( t \to 0 \) and we cannot apply the estimate (34). On the other hand, we have

\[
\int_0^1 [f'(t)]^2 \, dt \leq \frac{4}{9} \max_{t \in [0,1]} t^2 \cos^2 t \leq \frac{16}{9},
\]

i.e. \( \|f'\|_2 \leq \frac{4}{3} \) and we can apply the estimate (44).

Theorem 11 Let \( f : [a, b] \to \mathbb{R} \) be an absolutely continuous function such that \( f' \in L_2(a, b) \). Then

\[
|Q(f; a, b)| \leq \sqrt{\frac{11}{96} - \frac{\sqrt{2}}{16}} \sigma(f'; a, b)(b - a)^{3/2},
\]

where \( \sigma(f; a, b) \) is defined by (28). The inequality (46) is sharp in the sense that the constant \( \sqrt{\frac{11}{96} - \frac{\sqrt{2}}{16}} \) cannot be replaced by a smaller one.

We define

\[
P(f; a, b) = \frac{(b - a)^2}{96} \left(4 - 3\sqrt{2}\right) [f'(b) - f'(a)].
\]

Theorem 12 Let \( f' : [0, 1] \to \mathbb{R} \) be an absolutely continuous function such that \( f'' \in L_1(0, 1) \) and there exist real numbers \( \gamma_2, \Gamma_2 \) such that \( \gamma_2 \leq f''(t) \leq \Gamma_2, \ t \in [0, 1] \). Then

\[
|Q(f; 0, 1) - P(f; 0, 1)| \leq \frac{\Gamma_2 - \gamma_2}{2} \left(\frac{5}{96} \sqrt{6} - \frac{29}{432} \sqrt{3}\right),
\]

\[
|Q(f; 0, 1) - P(f; 0, 1)| \leq \frac{1}{12} - \frac{\sqrt{2}}{32} (S_1 - \gamma_2),
\]

\[
|Q(f; 0, 1) - P(f; 0, 1)| \leq \frac{1}{12} - \frac{\sqrt{2}}{32} (\Gamma_2 - S_1),
\]

where \( Q(f; 0, 1) \) and \( P(f; 0, 1) \) are defined by (32) and (47), respectively and \( S_1 = f'(1) - f'(0) \).
Proof. We define the function
\[
\tilde{p}_2(t) = \begin{cases} 
\frac{1}{2} t (t - \sqrt{2}/4) + \frac{\sqrt{2}}{32} - \frac{1}{24}, & t \in [0, 1/2] \\
\frac{1}{2} (t - 1) (t - 1 + \sqrt{2}/2) + \frac{\sqrt{2}}{32} - \frac{1}{24}, & t \in (1/2, 1].
\end{cases}
\] (51)

Let \( p_1 \) be defined by (37). Then we have
\[
(\tilde{p}_2, f'') = -(p_1, f') - P(f; 0, 1) = Q(f; 0, 1) - P(f; 0, 1) \tag{52}
\]
since (38) holds.

On the other hand, we have
\[
(\tilde{p}_2, f'') = (\tilde{p}_2, e), \tag{53}
\]
since \((\tilde{p}_2, e) = 0\). From (27) we get
\[
\begin{aligned}
\left\| f'' - \frac{\Gamma_2 + \gamma_2}{2}, \tilde{p}_2 \right\| & \leq \left\| f'' - \frac{\Gamma_2 + \gamma_2}{2} \right\| \left\| \tilde{p}_2 \right\|_1 \\
& \leq \left( \frac{5}{96} \sqrt{6} - \frac{29}{432} \sqrt{3} \right) \frac{\Gamma_2 - \gamma_2}{2},
\end{aligned}
\]
(54)
since
\[
\left\| f'' - \frac{\Gamma_2 + \gamma_2}{2} \right\| \leq \frac{\Gamma_2 - \gamma_2}{2}
\]
and
\[
\left\| \tilde{p}_2 \right\|_1 = \frac{5}{96} \sqrt{6} - \frac{29}{432} \sqrt{3}.
\]
From (52)-(54) we see that (48) holds.

We now prove that (49) holds. We have
\[
\left| (f'' - \gamma_2, \tilde{p}_2) \right| \leq \left\| f'' - \gamma_2 \right\|_1 \left\| \tilde{p}_2 \right\|_\infty = \left( \frac{1}{12} - \frac{\sqrt{2}}{32} \right) (S_1 - \gamma_2),
\]
since
\[
\left\| f'' - \gamma_2 \right\|_1 = \int_0^1 (f''(t) - \gamma_2) dt = f'(1) - f'(0) - \gamma_2
\]
and
\[
\left\| \tilde{p}_2 \right\|_\infty = \frac{1}{12} - \frac{\sqrt{2}}{32}.
\]
In a similar way we can prove that (50) holds.

Remark 13 Note that we can apply the estimate (48) only if the second derivative \( f'' \) is bounded. It means that we cannot use (48) to estimate directly the error when approximating the integral of such a well-behaved function as \( f(t) = \sqrt{t^3} \) on \([0, 1]\), (since \( f''(t) = 3/(4\sqrt{t}) \) is unbounded on \([0, 1]\)). On the other hand, we can use the estimation (49), (since \( \gamma = 3/4 \) on \([0, 1]\) for the given function).
Theorem 14 Let \( f' : [a, b] \rightarrow \mathbb{R} \) be an absolutely continuous function such that \( f'' \in L_1(a, b) \) and there exist real numbers \( \gamma_2, \Gamma_2 \) such that \( \gamma_2 \leq f''(t) \leq \Gamma_2, \) \( t \in [a, b] \). Then

\[
|Q(f; a, b) - P(f; a, b)| \leq \frac{\Gamma_2 - \gamma_2}{2} \left( \frac{5}{96} \sqrt{6} - \frac{29}{432} \sqrt{3} \right) (b - a)^3, \tag{55}
\]

\[
|Q(f; a, b) - P(f; a, b)| \leq \left( \frac{1}{12} - \frac{\sqrt{2}}{32} \right) (S_1 - \gamma_2)(b - a)^3, \tag{56}
\]

\[
|Q(f; a, b) - P(f; a, b)| \leq \left( \frac{1}{12} - \frac{\sqrt{2}}{32} \right) (\Gamma_2 - S_1)(b - a)^3, \tag{57}
\]

where \( Q(f; a, b) \) and \( P(f; a, b) \) are defined by (32) and (47), respectively and 
\( S_1 = (f'(b) - f'(a))/(b - a) \).

Theorem 15 Let \( f' : [0, 1] \rightarrow \mathbb{R} \) be an absolutely continuous function such that \( f'' \in L_2(0, 1) \). Then

\[
|Q(f; 0, 1) - P(f; 0, 1)| \leq \sqrt{\frac{47}{23040} - \frac{2^{1/3} \sqrt{2}}{768} \sigma(f''; 0, 1)} \tag{58}
\]

where \( \sigma(f; 0, 1) \) is defined by (28). The inequality (58) is sharp in the sense that the constant \( \sqrt{\frac{47}{23040} - \frac{2^{1/3} \sqrt{2}}{768}} \) cannot be replaced by a smaller one.

Proof. We define the function

\[
p_2(t) = \begin{cases} 
\frac{1}{2} t(t - \frac{\sqrt{3}}{4}), & t \in [0, \frac{1}{2}] \\
\frac{1}{2} (t - 1)(t - 1 + \frac{\sqrt{3}}{4}), & t \in (\frac{1}{2}, 1] 
\end{cases}
\]

Then we have

\[
\langle \tilde{p}_2, f'' \rangle = \langle p_2, f'' \rangle - \langle p_2, e \rangle \langle f'', e \rangle \tag{60}
\]

since \( \tilde{p}_2 = p_2 - \langle p_2, e \rangle \). From (52) and (60) it follows

\[
T(p_2, f'') = Q(f; 0, 1) - P(f; 0, 1), \tag{61}
\]

since \( \langle \tilde{p}_2, f'' \rangle = (\tilde{p}_2, f'') \) if \( [a, b] = [0, 1] \). From (29) we get

\[
|T(p_2, f'')| \leq \sqrt{T(p_2, p_2)} \sqrt{T(f'', f'')} = \sqrt{\frac{47}{23040} - \frac{2^{1/3} \sqrt{2}}{768} \sigma(f''; 0, 1)}, \tag{62}
\]

since

\[
T(p_2, p_2) = \frac{47}{23040} - \frac{2^{1/3} \sqrt{2}}{768}.
\]

From (61) and (62) we see that (58) holds.
We now prove that (58) is sharp. For that purpose we define the function
\[ f(t) = \begin{cases} 
\frac{t^4}{24} - \frac{\sqrt{2}}{48}t^3, & t \in [0, \frac{1}{2}] \\
\frac{t^4}{24} - (\frac{1}{6} - \frac{\sqrt{2}}{48})t^3 + (\frac{1}{4} - \frac{\sqrt{2}}{16})t^2 - (\frac{1}{8} - \frac{\sqrt{2}}{32})t + \frac{1}{16} - \frac{\sqrt{2}}{192}, & t \in (\frac{1}{2}, 1]
\end{cases} \]
(63)
such that
\[ f'(t) = \begin{cases} 
\frac{t^3}{6} - \frac{\sqrt{2}}{16}t^2, & t \in [0, \frac{1}{2}] \\
\frac{t^3}{6} - \left(\frac{1}{2} - \frac{\sqrt{2}}{8}\right)t^2 + \left(\frac{1}{4} - \frac{\sqrt{2}}{8}\right)t - \left(\frac{1}{8} - \frac{\sqrt{2}}{32}\right), & t \in (\frac{1}{2}, 1]
\end{cases} \]
(64)
and \( f''(t) = p_2(t) \). From Lemma 4 we see that the function \( f' \), defined by (64), is an absolutely continuous function. For the function defined by (63) the left-hand side of (58) becomes
\[ \text{L.H.S. (58)} = \frac{47}{23040} - \frac{\sqrt{2}}{768}. \]
The right-hand side of (58) becomes
\[ \text{R.H.S. (58)} = \frac{47}{23040} - \frac{\sqrt{2}}{768}. \]
We see that \( \text{L.H.S. (58)} = \text{R.H.S. (58)} \). Thus, (58) is sharp.

**Remark 16** The estimation (58) is better than the estimation (58). However, note that we can apply the estimate (48) only if the second derivative \( f'' \) is bounded. It means that we cannot use (48) to estimate directly the error when approximating the integral of such a well-behaved function as \( f(t) = \frac{3}{\sqrt[5]{t}} \) on \([0, 1] \), (since \( f''(t) = 10/(9\sqrt[5]{t}) \) is unbounded on \([0, 1] \)). On the other hand, we can use the estimation (58), (since \( \|f''\|^2 = \frac{100}{27} \) for the given function).

**Theorem 17** Let \( f' : [a, b) \to \mathbb{R} \) be an absolutely continuous function such that \( f'' \in L_2(a, b) \). Then
\[ |Q(f; a, b) - P(f; a, b)| \leq \sqrt{\frac{47}{23040} - \frac{\sqrt{2}}{768}} \sigma(f''; a, b)(b - a)^{5/2}, \]
(65)
where \( \sigma(f; a, b) \) is defined by (28). The inequality (65) is sharp in the sense that the constant \( \sqrt{\frac{47}{23040} - \frac{\sqrt{2}}{768}} \) cannot be replaced by a smaller one.

### 4 Applications in numerical integration

Let \( \pi = \{x_0 = a < x_1 < \cdots < x_n = b\} \) be a given subdivision of the interval \([a, b] \) such that \( h_i = x_{i+1} - x_i = h = (b - a)/n \). From (52) we get
\[
Q(f; x_i, x_{i+1}) = \int_{x_i}^{x_{i+1}} f(t) dt - \left[ \sqrt{2} \frac{8}{f(x_i)} + \left( 1 - \frac{\sqrt{2}}{4} \right) f\left( \frac{x_i + x_{i+1}}{2} \right) + \frac{\sqrt{2}}{8} f(x_{i+1}) \right] h.
\]

If we now sum the above relation over \(i\) from 0 to \(n-1\) then we get

\[
\sum_{i=0}^{n-1} Q(f; x_i, x_{i+1}) = \int_a^b f(t) dt - \frac{\sqrt{2}h}{8} \left[ f(a) + f(b) \right] - \frac{\sqrt{2}h}{4} \sum_{i=1}^{n-1} f(x_i) - \left( 1 - \frac{\sqrt{2}}{4} \right) h \sum_{i=1}^{n-1} f\left( \frac{x_i + x_{i+1}}{2} \right).
\]

We introduce the notation

\[
S(f; a, b) = \sum_{i=0}^{n-1} Q(f; x_i, x_{i+1}). \quad (66)
\]

We also define

\[
P_n(f; a, b) = \frac{(b - a)^2}{96n^2} \left( 4 - 3\sqrt{2} \right) \left[ f'(b) - f'(a) \right], \quad (67)
\]

\[
\sigma_n(f) = \sum_{i=0}^{n-1} \sqrt{\frac{b - a}{n}} \left\| f' \right\|_2^2 - \left[ f(x_{i+1}) - f(x_i) \right]^2 \quad (68)
\]

and

\[
\omega_n(f) = \left[ (b - a) \left\| f' \right\|_2^2 - \frac{1}{n} \left( f(b) - f(a) \right)^2 \right]^{1/2}. \quad (69)
\]

**Theorem 18** Under the assumptions of Theorem \(\Box\) we have

\[
\left| \int_a^b f(t) dt - \sum_{i=0}^{n-1} \left[ \sqrt{2} \frac{8}{f(x_i)} + \left( 1 - \frac{\sqrt{2}}{4} \right) f\left( \frac{x_i + x_{i+1}}{2} \right) + \frac{\sqrt{2}}{8} f(x_{i+1}) \right] h \right| \leq \frac{2 - \sqrt{2}}{48n^2} \left\| f'' \right\|_\infty (b - a)^3,
\]

where \(\{a = x_0 < x_1 < \cdots < x_n = b\}\) is a uniform subdivision of \([a, b]\), i.e. \(x_i = a + ih, h = (b - a)/n, i = 0, 1, \ldots, n\).

**Proof.** Apply Theorem \(\Box\) to the intervals \([x_i, x_{i+1}]\) and sum. \(\Box\)
Theorem 19  Under the assumptions of Theorem 7 we have
\[ |S(f; a, b)| \leq \frac{\Gamma_1 - \gamma_1}{32n} (b - 2\sqrt{2})(b - a)^2, \]
\[ |S(f; a, b)| \leq \frac{S - \gamma_1}{n} \left( \frac{1}{2} - \frac{\sqrt{2}}{8} \right) (b - a)^2, \]
\[ |S(f; a, b)| \leq \frac{\Gamma_1 - S}{n} \left( \frac{1}{2} - \frac{\sqrt{2}}{8} \right) (b - a)^2, \]
where \( S(f; a, b) \) is defined by (66) and \( \{ a = x_0 < x_1 < \cdots < x_n = b \} \) is a uniform subdivision of \([a, b]\), i.e. \( x_i = a + ih, h = (b - a)/n, i = 0, 1, ..., n \).

Proof.  Apply Theorem 7 to the intervals \([x_i, x_{i+1}]\) and sum. Note that
\[ \sum_{i=0}^{n-1} [f(x_{i+1}) - f(x_i)] = f(b) - f(a). \]

Theorem 20  Under the assumptions of Theorem 11 we have
\[ |S(f; a, b)| \leq \sqrt{\frac{11}{96} - \frac{\sqrt{2} b - a}{16} \sigma_n(f) \leq \sqrt{\frac{11}{96} - \frac{\sqrt{2} b - a}{16} \omega_n(f)}, \quad (70) \]
where \( S(f; a, b), \sigma_n(f) \) and \( \omega_n(f) \) are defined by (62), (68) and (69), respectively and \( \{ a = x_0 < x_1 < \cdots < x_n = b \} \) is a uniform subdivision of \([a, b]\), i.e. \( x_i = a + ih, h = (b - a)/n, i = 0, 1, ..., n \).

Proof.  We apply Theorem 11 to the interval \([x_i, x_{i+1}]\) and sum. Then we have
\[ |S(f; a, b)| \leq \sqrt{\frac{11}{96} - \frac{\sqrt{2} b - a}{16} \sum_{i=0}^{n-1} \left( \frac{\|f''\|}{2} - \frac{1}{h} (f(x_{i+1}) - f(x_i))^2 \right)^{1/2}. \]

From the above relation and the fact \( h = (b-a)/n \) we see that the first inequality in (70) holds.

Using the Cauchy inequality we get
\[ \sum_{i=0}^{n-1} \left[ \frac{\|f''\|}{2} - \frac{1}{h} (f(x_{i+1}) - f(x_i))^2 \right]^{1/2} \]
\[ \leq n \left[ \frac{\|f''\|}{2} - \frac{1}{b - a} \sum_{i=0}^{n-1} (f(x_{i+1}) - f(x_i))^2 \right]^{1/2} \]
\[ \leq n \left[ \frac{\|f''\|}{2} - \frac{1}{b - a} \frac{1}{n} (f(b) - f(a))^2 \right]^{1/2}. \]

Thus the second inequality in (70) holds, too.  \( \blacksquare \)
Theorem 21 Under the assumptions of Theorem 14 we have

\[ |S(f; a, b) - P_n(f; a, b)| \leq \frac{\Gamma_2 - \gamma_2}{2n} \left( \frac{5}{96} \sqrt{6} - \frac{29}{432} \sqrt{2} \right) (b - a)^3, \]

\[ |S(f; a, b) - P_n(f; a, b)| \leq \left( \frac{1}{12} - \frac{\sqrt{2}}{32} \right) \frac{(S_1 - \gamma_2)}{n} (b - a)^3, \]

\[ |S(f; a, b) - P_n(f; a, b)| \leq \left( \frac{1}{12} - \frac{\sqrt{2}}{32} \right) \frac{(\Gamma_2 - S_1)}{n} (b - a)^3, \]

where \( S(f; a, b) \) and \( P_n(f; a, b) \) are defined by (66) and (67), respectively and \( \{a = x_0 < x_1 < \cdots < x_n = b\} \) is a uniform subdivision of \( [a, b] \), i.e. \( x_i = a + ih \), \( h = (b - a)/n \), \( i = 0, 1, \ldots, n \).

Proof. The proof of this theorem is similar to the proof of Theorem 19. Here we apply Theorem 14.

Theorem 22 Under the assumptions of Theorem 14 we have

\[ |S(f; a, b) - P_n(f; a, b)| \leq \sqrt{\frac{47}{23040} \frac{\sqrt{2}}{768} (b - a)^2 \sigma_n(f')} \leq \sqrt{\frac{47}{23040} \frac{\sqrt{2}}{768} (b - a)^2 \omega_n(f'}), \]

where \( S(f; a, b) \) and \( P_n(f; a, b) \) are defined by (66) and (67), respectively and \( \{a = x_0 < x_1 < \cdots < x_n = b\} \) is a uniform subdivision of \( [a, b] \), i.e. \( x_i = a + ih \), \( h = (b - a)/n \), \( i = 0, 1, \ldots, n \).

Proof. The proof of this theorem is similar to the proof of Theorem 20. Here we apply Theorem 17.

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Nenad Ujević
Department of Mathematics
University of Split
Teslina 12/III
21000 Split
CROATIA
E-mail: ujevic@pmfst.hr