QUADRATURE FORMULAS AND TAYLOR SERIES OF SECANT AND TANGENT

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Abstract. Second-order quadrature formulas and their fourth-order expansions are derived from the Taylor series of the secant and tangent functions. The errors of the approximations are compared to the error of the midpoint approximation. Third and fourth order quadrature formulas are constructed as linear combinations of the second-order approximations and the trapezoidal approximation.

Key words: Quadrature formula, Fourier transform, generating function, Euler-McLaurin formula.

1. Introduction

Numerical quadrature is a term used for numerical integration in one dimension. Numerical integration in more than one dimension is usually called cubature. There is a broad class of computational algorithms for numerical integration. The Newton-Cotes quadrature formulas (1.1) are a group of formulas for numerical integration where the integrand is evaluated at equally spaced points. Let \( h = (b - a)/n \).

\[
\int_{a}^{b} f(x) \, dx \approx h \sum_{k=0}^{n} w_k f(b - kh) \quad (1.1)
\]

The two most popular approximations for the definite integral are the trapezoidal approximation (1.2) and the midpoint approximation (1.3).

\[
A_h f(x) = \frac{h}{2} \left( f(a) + 2 \sum_{k=1}^{n-1} f(a + kh) + f(b) \right) = \int_{a}^{b} f(x) \, dx + O(h^2), \quad (1.2)
\]
\[ A_M^h f(x) = h \sum_{k=1}^{n-1} f(a + (k + 1/2)h) = \int_a^b f(x) \, dx + O(h^2). \] (1.3)

The midpoint approximation and the trapezoidal approximation for the definite integral are Newton-Cotes quadrature formulas with accuracy \(O(h^2)\). The trapezoidal and the midpoint approximations are constructed by dividing the interval \([a, b]\) to subintervals of length \(h\) and interpolating the integrand function by Lagrange polynomials of degree zero and one. Another important Newton-Cotes quadrature formula is the Simpson’s approximation. The Simpson’s approximation has fourth-order accuracy and is obtained by interpolating the function by a second degree Lagrange polynomial. Denote by \(E_T^h f(x)\) and \(E_M^h f(x)\) the errors of the trapezoidal and the midpoint approximations.

\[ E_T^h f(x) = A_T^h f(x) - \int_a^b f(x) \, dx + O(h^2), \quad E_M^h f(x) = A_M^h f(x) - \int_a^b f(x) \, dx + O(h^2). \]

From the Euler-McLaurin formula the error of the trapezoidal approximation on the interval \([a, b]\) is expressed as

\[ E_T^h f(x) = \sum_{k=1}^{m} \frac{B_{2k}}{(2k)!} \left( f^{(2k-1)}(b) - f^{(2k-1)}(a) \right) h^{2k} + R_{2m}^T(h) h^{2m}, \] (1.4)

where \(\bar{B}_n(x) = B_n(\{x\}) = B_n(x - \lfloor x \rfloor)\) is the Bernoulli 1-periodic function and \(B_n(x) = \sum_{k=0}^{n} \binom{n}{k} B_{n-k} x^k\) is the Bernoulli polynomial of degree \(n\). The error of the midpoint approximation satisfies (Kouba 2013)

\[ E_M^h f(x) = \sum_{k=1}^{m} \frac{(2^{1-2k} - 1) B_{2k}}{(2k)!} \left( f^{(2k-1)}(b) - f^{(2k-1)}(a) \right) h^{2k} + R_{2m}^M(h) h^{2m}, \] (1.5)

\[ R_{2m}^T(h) = \frac{1}{(2m)!} \int_a^b \bar{B}_{2m} \left( a - \frac{t}{h} \right) f^{(2m)}(t) \, dt, \]

\[ R_{2m}^M(h) = \frac{1}{(2m)!} \int_a^b \bar{B}_{2m} \left( \frac{a + b}{2} - \frac{t}{h} \right) f^{(2m)}(t) \, dt. \]

The terms \(R_{2m}^T(h)\) and \(R_{2m}^M(h)\) satisfy \(\lim_{h \to 0} R_{2m}^T(h) = \lim_{h \to 0} R_{2m}^M(h) = 0\), when the function \(f(x) \in C^{2m}[a, b]\). From (4), (5) and \(m = 2\) we obtain the fourth-order expansion formulas (2.1), (2.14) of the trapezoidal and midpoint rules. The midpoint approximation is around two times more accurate than the trapezoidal approximation. The Simpson’s approximation is constructed as a linear combination of the midpoint approximation and the trapezoidal approximation with weights 1/3 and 2/3. With this choice of the weights the second-order terms of expansion formulas (1.4) and (1.5) are cancelled and the Simpson’s approximation has an accuracy \(O(h^4)\).

The Gaussian quadrature formulas \(\sum_{k=1}^{n} w_k f(x_k)\) are approximations for the definite integral where the integrand is evaluated at unequally spaced points (Gil et al. 2007). The Gaussian quadrature formulas are constructed to yield an exact result for the polynomials of degree \(2n - 1\) by using suitable values of the nodes \(x_k\) and weights \(w_k\). The accuracy of the Newton-Cotes and the Gaussian quadrature formulas is lower when the function \(\widetilde{f}(x)\) has singularities.
The Monte Carlo methods for numerical integration are computational algorithms where the nodes are chosen as pseudo-random or quasi-random numbers in the area of integration, the unit hypercube (Dimov 2008). The Monte-Carlo and quasi-Monte Carlo methods are suitable for approximation of multidimensional integrals, since the convergence of the methods is independent of the dimension (Atanassov & Dimov 1999; Georgieva 2009; Todorov & Dimov 2016). The generating function of quadrature formula (1.1) is defined as

$$G(x) = \sum_{k=0}^{\infty} w_k x^k.$$  

The Riemann sum approximation for the definite integral is related to the trapezoidal approximation and has a generating function $1/(1 - x)$. The Riemann sum approximation for the fractional integral of order $\alpha$ has a generating function $Li_{1-\alpha}(x)$, where $Li_{1-\alpha}(x)$ is the polylogarithm function of order $1 - \alpha$. The midpoint approximation is a shifted approximation with shift parameter $h/2$. The midpoint approximation has a generating function $\sqrt{x}/(1 - x)$. Methods for approximation of fractional integrals and derivatives based on the Fourier transform and the generating function of the approximation have been studied by (Chen & Deng 2016; Ding & Li 2016; Lubich 1986; Tuan & Gorenflo 1995). In (Dimitrov 2016) we use the series expansion formula of the polylogarithm function $Li_{1-\alpha}(e^x)$, to derive the expansion formula of the trapezoidal approximation for the fractional integral of order $\alpha$. In the present paper we construct second, third and fourth order approximations for the definite integral with generating functions $G_1(x) = \pi \sec(\pi \sqrt{x}/2)/4$ and $G_2(x) = \pi \tan(\pi \sqrt{x}/2)/(4\sqrt{x})$. The two generating functions $G_1(x)$ and $G_2(x)$ are positive, increasing functions and have a vertical asymptote at the point $x = 1$. The graphs of the functions $G_1(x)$, $G_2(x)$ and $1/(1 - x)$ are given in Figure 1.

![Figure 1. Graphs of the generating functions $G_1(x) = \pi \sec(\pi \sqrt{x}/2)/4$ (left, blue) and $G_2(x) = \pi \tan(\pi \sqrt{x}/2)/(4\sqrt{x})$ (right, blue) and the function $1/(1 - x)$ (red).](image)

The tangent and secant functions have Maclaurin series expansions

$$\sec x = \sum_{k=0}^{\infty} \frac{(-1)^k E_{2k}}{(2k)!} x^{2k}, \quad (1.6)$$

$$\tan x = \sum_{k=0}^{\infty} \frac{(-4)^{k+1} (1 - 4^{k+1}) B_{2k+2}}{(2k + 2)!} x^{2k+1}. \quad (1.7)$$
The radius of convergence of power series (1.6) and (1.7) is $|x| < \pi/2$. The first eight elements of the sequences of Euler and Bernoulli numbers are $1, 0, -1, 1/6, 0, -1/30, 0, 1/42, 0, \ldots$. The Euler and Bernoulli numbers with an odd index are equal to zero. The sequence of Euler numbers $\{E_{2n}\}$ is an alternating sequence of integers, and $\{B_{2n}\}$ is an alternating sequence of rational numbers. The Bernoulli and Euler numbers satisfy the asymptotic relation $4^n (1 - 4^n) B_{2n} / E_{2n} \sim \pi/2$. Efficient methods for computation of the Euler numbers, Bernoulli numbers and the series expansions of the secant and tangent functions are discussed by (Atkinson 1986; Brent & Harvey 2013; Knuth & Buckholtz 1967). The values of the Euler numbers, Bernoulli numbers and the zeta function are included in the modern software packages for scientific computing. Denote by $\bar{E}_k$ and $\bar{B}_k$ the coefficients of the Maclaurin series expansions of the generating functions $G_1(x)$ and $G_2(x)$.

$$\bar{E}_k = \frac{|E_{2k}|}{(2k)!} \left( \frac{\pi}{2} \right)^{2k+1}, \quad \bar{B}_k = \frac{(4^{k+1} - 1) \pi^{2k+2} |B_{2k+2}|}{(2k + 2)!}.$$

In section 2 and section 3 we obtain the fourth-order expansion formulas of the approximations with generating functions $G_1(x)$ and $G_2(x)$ and the second-order quadrature formulas

$$\frac{h}{2} \left( \frac{\pi - 1}{2} f(a) + \sum_{k=1}^{n-1} \bar{E}_k f(a + kh) + f(b) \right) = \int_a^b f(x) \, dx + O(h^2),$$

$$\frac{h}{2} \left( \frac{\pi^2 - 6}{4} f(a) + \sum_{k=1}^{n-1} \bar{B}_k f(a + kh) + f(b) \right) = \int_a^b f(x) \, dx + O(h^2).$$

The substitution $\bar{f}(x) = f(a + b - x)$ yields the second-order quadrature formulas (2.12) and (3.6). In Theorem 2 and Theorem 4 we derive the conditions for the integrand function, such that the errors of second-order approximations are smaller than the error of the midpoint approximation. In section 4 we obtain third and fourth order approximations for the definite integral as linear combinations of approximations (2.12), (2.12), (3.6) and (3.7) and the trapezoidal approximation.

2. Second-order quadrature formulas with generating function $G_1(x)$

In this section we derive the fourth-order expansion formula (2.9) of the approximation for the definite integral with generating function $G_1(x) = \pi \sec(\pi \sqrt{x}/2)/4$, and the second-order quadrature formulas (2.12) and (2.13). The generating function of an approximation is directly related to the result of the Fourier transform of the approximation. The Fourier transform of the function $f(x)$ is defined as

$$\mathcal{F}[f(x)](\omega) = \hat{f}(\omega) = \int_{-\infty}^{\infty} e^{i \omega t} f(t) \, dt.$$
and by \( f^{(-n)}(x) \) the \( n \)-fold integral on the interval \((-\infty, x]\). When the function \( f(x) \) is defined on the interval \([a, b]\) we extend the function to \((-\infty, b]\) by setting \( f(x) = 0 \) on \((-\infty, a]\). The Fourier transform has properties

\[
\mathcal{F}[f(x-a)](\omega) = e^{i\omega a} \hat{f}(\omega), \quad \mathcal{F}[f^{(n)}(x)](\omega) = (-i\omega)^n \hat{f}(\omega).
\]

The trapezoidal approximation has a fourth-order expansion formula (1.4)

\[
A^b_a f(x) = \int_a^b y(t) \, dt + \frac{1}{12} (f''(b) - f''(a)) h^2 + O(h^4). \tag{2.1}
\]

In (Dimitrov 2016) we use Fourier transform to prove the Euler-Mclaurin formula and we derive the asymptotic expansion formula of the trapezoidal approximation for the fractional integral. In Lemma 1 and Theorem 1 we derive the fourth-order expansion formula of the approximation for the definite integral with generating function \( G_1(x) \). From the Mclaurin series of secant (1.6) we obtain

\[
G_1(x) = \frac{\pi}{4} \sec \left( \frac{\pi x}{2} \right) = \frac{1}{2} \sum_{n=0}^{\infty} \frac{(-1)^n E_{2n}}{(2n)!} \left( \frac{\pi}{2} \right)^{2n+1} x^n. \tag{2.2}
\]

Denote by \( H_1(x) \) the function

\[
H_1(x) = xG_1(e^{-x}) = \frac{\pi}{4} x \sec \left( \frac{\pi e^{-x/2}}{2} \right).
\]

The function \( H_1(x) \) has a first derivative

\[
H'_1(x) = \frac{\pi}{4} x \sec \left( \frac{\pi e^{-x/2}}{2} \right) - \frac{\pi^2}{16} x e^{-x/2} \sec \left( \frac{\pi e^{-x/2}}{2} \right) \tan \left( \frac{\pi e^{-x/2}}{2} \right). \tag{2.3}
\]

Now we use L’Hospital’s rule to compute the values of the functions \( H_1(x) \) and \( H'_1(x) \) at \( x = 0 \). Substitute

\[
y = \frac{\pi}{2} e^{-x/2}, \quad x = -2 \ln \left( \frac{2y}{\pi} \right). \tag{2.4}
\]

Then

\[
H_1(0) = \lim_{x \to 0^+} \frac{\pi x}{4} \sec \left( \frac{\pi e^{-x/2}}{2} \right) = \frac{\pi}{4} \lim_{y \to 0^+} \frac{-2 \ln \left( \frac{2y}{\pi} \right)}{\cos y} = \frac{\pi}{2} \lim_{y \to 0^+} \frac{1}{y \sin y} = 1.
\]

From (2.3) and (2.4)

\[
H'_1(x) = \frac{\pi}{4} \left( \sec y + y \ln(2y/\pi) \tan y \right) = \frac{\pi}{4} \left( \frac{\cos y + y \ln(2y/\pi) \sin y}{\cos^2 y} \right),
\]

\[
H'_1(0) = \lim_{y \to 0^+} \frac{\cos y + y \ln(2y/\pi) \sin y}{\cos^2 y} = \lim_{y \to 0^+} \frac{1 - \sin 2y}{2 \cos 2y} = 1.
\]

Similarly, we obtain the values of the second and third derivatives of the function \( H_1(x) \) at the point \( x = 0 \).
The function $H_1(x)$ has a fourth-order Mclaurin series expansion
\begin{equation}
H_1(x) = \frac{\pi x}{4} \sec \left( \frac{\pi e^{-x^2/2}}{2} \right) = 1 + \frac{1}{4} x + \frac{2 + \pi^2}{96} x^2 - \frac{\pi^2}{384} x^3 + O(x^4).
\end{equation}
(2.5)

Denote by $A_h^k f(x)$ the quadrature formula with generating function $G_1(x)$.
\begin{equation}
A_h^k f(x) = \frac{h}{2} \sum_{k=0}^{n-1} \tilde{E}_k f(b - kh) = \frac{h}{2} \sum_{k=0}^{n-1} (-1)^k E_{2k} \left( \frac{\pi}{2} \right)^{2k+1} f(b - kh).
\end{equation}
(2.6)

Approximation (2.6) has weights $\tilde{E}_k/2$ which are the coefficients of the Mclaurin series of the generating function $G_1(x)$. In Theorem 1 we use Fourier transform to show that the coefficients of the fourth-order expansion formula of (2.6) at the endpoint $x = b$ are the coefficients of the Mclaurin series of the function $H_1(x)$. The method is used in (Chen & Deng 2016; Dimitrov 2016; Ding & Li 2016; Lubich 1986; Tadjeran et al. 2006; Tuan & Gorenflo 1995) for construction of approximations of fractional integrals and derivatives. In (Dimitrov 2014) we discuss the conditions for the function $f(x)$ at the point $x = a$ for the Grünwald approximation of the Caputo derivative. The $n$-th order approximation for the definite integral at the point $x = b$ requires that the value of the integrand function and its derivatives of order $1, 2, \ldots, n - 1$ at the point $x = a$ are equal to zero.

**Lemma 1** Let $f \in C^4[a, b]$ and $f^{(n)}(0) = 0$ for $n = 1, 2, 3, \ldots$. Then
\begin{equation}
A_h^k f(x) = \int_a^b f(x) dx + \frac{1}{4} h f(b) h + \frac{2 + \pi^2}{96} f'(b) h^2 - \frac{\pi^2}{384} f''(b) h^3 + O(h^4).
\end{equation}
(2.7)

**Proof.** By applying Fourier transform to $A_h^k f(x)$ we obtain
\begin{equation}
\mathcal{F}[A_h^k f(x)](\omega) = \frac{\pi h}{4} \sum_{k=0}^{n-1} \tilde{E}_k e^{i\omega k h} \hat{f}(\omega) = \pi \frac{h}{4} \sum_{k=0}^{n-1} \tilde{E}_k (e^{i\omega h/2})^k \hat{f}(\omega).
\end{equation}

From (2.2) and $n \to \infty$ we obtain
\begin{equation}
\mathcal{F}[A_h^k f(x)](\omega) = \frac{\pi h}{4} \sec \left( \frac{\pi}{2} e^{i\omega h/2} \right) \hat{f}(\omega) = -\frac{\pi}{4i\omega} \sec \left( \frac{\pi}{2} e^{i\omega/2} \right) \hat{f}(\omega).
\end{equation}

Substitute $x = -i\omega h$ in (2.5)
\begin{equation}
\mathcal{F}[A_h^k f(x)](\omega) = \left( (-i\omega)^{-1} + \frac{1}{4} h + \frac{2 + \pi^2}{96} (i\omega)^2 h^2 - \frac{\pi^2}{384} (i\omega)^2 h^3 \right) \hat{f}(\omega) + O(h^4).
\end{equation}

By applying inverse Fourier transform we obtain
\begin{equation}
\mathcal{F}[A_h^k f(x)](\omega) = \int_a^b f(x) dx + \frac{1}{4} h f(b) h + \frac{2 + \pi^2}{96} f'(b) h^2 - \frac{\pi^2}{384} f''(b) h^3 + O(h^4).
\end{equation}

In Theorem 1 we show that the fourth-order expansion formula of quadrature formula $A_h^k f(x)$ at the left endpoint $x = a$ is given by the Euler-Mclaurin formula.

**Claim 1** Let $n \geq 10$. Then
\begin{equation}
3^{n+1} > n^5.
\end{equation}
(2.8)
**Proof.** Let $F(n) = (n + 1) \ln 3 - 5 \ln n$. The first derivative $F'(n) = \ln 3 - 5/n$ is positive for $n > 5/\ln 3$. We have that $F(10) > 0$. When $n \geq 10$ we obtain 
$(n + 1) \ln 3 - 5 \ln n > 0, \quad 3^{n+1} > n^5.$

**Theorem 1** Let $f \in C^4[a, b]$. Then

$$
\frac{h}{2} \sum_{k=0}^{n-1} \frac{(-1)^k E_{2k}}{(2k)!} \left( \frac{\pi}{2} \right)^{2k+1} f(b - kh) = \int_a^b f(x)dx + \left( \frac{1}{4} f(b) - \frac{1}{2} f(a) \right) h + \left( \frac{2 + \pi^2}{96} f'(b) - \frac{1}{12} f'(a) \right) h^2 - \frac{\pi^2}{384} f''(b) h^3 + O(h^4). \tag{2.9}
$$

**Proof.** The Euler numbers satisfy (Borwein et al. 1989)

$$
\sum_{l=0}^{\infty} \frac{(-1)^l}{(2l + 1)^{2k+1}} = \frac{(-1)^k E_{2k} \pi^{2k+1}}{2^{2k+2} (2k)!}. \tag{2.10}
$$

Then

$$1 - \frac{1}{3^{k+1}} < \sum_{k=m}^{n-1} \frac{E_k}{2} < 1 - \frac{1}{3^{k+1}} + \frac{1}{5^{k+1}},$$

$$0 < \frac{1}{3^{k+1}} - \frac{1}{5^{k+1}} < 1 - \frac{2}{3^{k+1}} < \frac{1}{3^{k+1}}.$$

Let $m = [n/2]$ and $A_h f(x)$ be the Riemann sum approximation for the definite integral on the interval $[a, b/2]$.

$$A_h f(x) = h \sum_{k=m}^{n-1} f(b - kh).$$

From the Euler-Mcclaurin formula, the fourth-order expansion formula of $A_h f(x)$ at the left endpoint is

$$L_4(A_h f(x)) = -\frac{f(a)}{2} h - \frac{f'(a)}{12} h^2 + O(h^4).$$

Denote by $A_h^* f(x)$ the approximation for the definite integral on the interval $[a, b/2]$, obtained from (2.6) with coefficients $E_k/2$, where $m \leq k \leq n - 1$.

$$A_h^* f(x) = \frac{h}{2} \sum_{k=m}^{n-1} E_k f(b - kh) = \frac{h}{2} \sum_{k=m}^{n-1} \frac{(-1)^k E_{2k}}{(2k)!} \left( \frac{\pi}{2} \right)^{2k+1} f(b - kh).$$

Let $M = \max_{x \in [a,b]} |f(x)|$. Now we estimate $|A_h f(x) - A_h^* f(x)|$.

$$|A_h f(x) - A_h^* f(x)| = h \sum_{k=m}^{n-1} \left( 1 - \frac{E_k}{2} \right) |f(b - kh)| < M h \sum_{k=m}^{n-1} \left( 1 - \frac{E_k}{2} \right).$$

From (2.11)
In Table 1 we compute the error and the order of approximations (2.12) and (2.13) for the definite integral of the functions and . In Theorem 2 we derive the condition for the integrand function such that the errors of second-order approximations (2.12) and (2.13) are smaller than the error of the midpoint approximation. The midpoint approximation has a fourth-order expansion (1.5)

The first and second derivatives of the function satisfy

From (2.9) and (2.15) we obtain the third-order expansions of (2.12) and (2.13)

Theorem 2 Let \( f \in C^2[a, b] \). Then

(i) The error of approximation (2.12) is smaller than the error of the midpoint approximation when the integrand function \( f(x) \) satisfies
The error of approximation (2.13) is smaller than the error of the midpoint approximation when the integrand function \( f(x) \) satisfies

\[
\frac{f'(b)}{f'(a)} \in \left( \frac{4}{\pi^2 - 2}, \frac{12}{\pi^2 + 6} \right) = (0.5683, 0.7562). \tag{2.18}
\]

(ii) The error of approximation (2.13) is smaller than the error of the midpoint approximation when the integrand function \( f(x) \) satisfies

\[
\frac{f'(b)}{f'(a)} \in \left( \frac{\pi^2 + 6}{12}, \frac{\pi^2 - 2}{4} \right) = (1.3225, 1.9674). \tag{2.19}
\]

**Proof.** From (2.14) and (2.16) the error of approximation (2.12) is smaller than the error of the midpoint approximation when

\[
\left| \frac{2 + \pi^2}{96} f'(b) - \frac{1}{12} f'(a) \right| < \frac{1}{24} |f''(b) - f'(a)|. \tag{2.20}
\]

Denote \( R = \frac{f'(b)}{f'(a)} \).

\[
\left| \frac{2 + \pi^2}{4} R - 2 \right| < |R - 1|.
\]

The two equations \( R - 1 = \pm \left( (2 + \pi^2) R / 4 - 2 \right) \) have solutions \( R' = 4/(\pi^2 - 2) \) and \( R'' = 12/(\pi^2 + 6) \). Therefore the error of approximation \( A_h^2 f(x) \) is smaller than the error of the midpoint approximation when the function \( f(x) \) satisfies the condition

\[
\frac{f''(b)}{f'(a)} \in \left( \frac{4}{\pi^2 - 2}, \frac{12}{\pi^2 + 6} \right).
\]

The error terms of (2.16) and (2.17) contain third-order terms \( (h^3) \). Inequality (2.20) is satisfied when the step size \( h \) is a small positive number. Similarly we show that, the error of approximation \( A_h^2 f(x) \) is smaller than the error of the midpoint approximation when the function \( f(x) \) satisfies (2.19).

Let \( f_1(x) = e^{-x/3} \) and \( f_2(x) = e^{x/2} \) on the interval \([0,1]\). The functions \( f_1(x) \) and \( f_2(x) \) satisfy conditions (2.18) and (2.19), because

\[
f_1'(1) = e^{-1/3} = 0.7165, \quad f_2'(1) = e^{1/2} = 1.6487.
\]

In Table 1 and Table 2 we compare the error and the order of approximations (2.12) and (2.13) with the error and the order of the midpoint approximation of the definite integral of the functions \( e^{-x/3} \) and \( e^{x/2} \) on the interval \([0,1]\).

### Table 1.

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<th>( \ln(x + 1) )</th>
<th>( \arctan x )</th>
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<td></td>
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Source: Own calculations
Table 2.

Error and order of approximation (2.12)[left] and the midpoint approximation (1.3)[right]
for the definite integral of $f(x) = e^{-x^3}$ on $[0, 1]$.

<table>
<thead>
<tr>
<th>$h$</th>
<th>Error</th>
<th>Order</th>
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<tr>
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</tbody>
</table>

Source: Own calculations

Table 3.

Error and order of approximation (2.13)[left] and the midpoint approximation (1.3)[right]
for the definite integral of $f(x) = e^{x^2}$ on $[0, 1]$.

<table>
<thead>
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<tbody>
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</tbody>
</table>

<table>
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<th>Order</th>
</tr>
</thead>
<tbody>
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<td>1.9999</td>
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<td>0.0125</td>
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<td>0.00625</td>
<td>5.28×10^{-7}</td>
<td>2.0000</td>
</tr>
<tr>
<td>0.003125</td>
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<td>2.0000</td>
</tr>
</tbody>
</table>

Source: Own calculations

3. Second-order quadrature formulas with generating function $G_2(x)$

In this section we use the McLaurin series expansion of tangent to derive the fourth-order expansion formula (3.3) of the approximation for the definite integral with generating function $G_2(x) = \pi \tan(\pi \sqrt{x}/2)/(4 \sqrt{x})$ and the second-order quadrature formulas (3.6) and (3.7). From (1.7)

$$\tan\left(\frac{\pi \sqrt{x}}{2}\right) = \sum_{k=1}^{\infty} \frac{(-4)^k(1 - 4^k)B_{2k}}{(2k)!} \left(\frac{\pi}{2}\right)^{2k-1} x^{(2k-1)/2}, \quad (|x| < 1).$$

The function $G_2(x)$ has a McLaurin series expansion

$$G_2(x) = \frac{\pi}{4 \sqrt{x}} \tan\left(\frac{\pi \sqrt{x}}{2}\right) = \frac{1}{2} \sum_{k=0}^{\infty} \frac{(-4)^k(1 - 4^k+1)B_{2k+2}}{(2k+2)!} \left(\frac{\pi}{2}\right)^{2k+2} x^k,$$

$$G_2(x) = \frac{1}{2} \sum_{k=0}^{\infty} \frac{(-1)^k(4^{k+1} - 1)\pi^{2k+2}2^{2k+2}B_{2k+2}}{(2k+2)!} x^k. \quad (3.1)$$

Let

$$H_2(x) = xG_2(e^{-x}) = \frac{\pi}{4} x e^{x/2} \tan\left(\frac{\pi e^{-x/2}}{2}\right).$$

Similarly to section 2, we determine the values of the derivatives of the function $H_2(x)$ at $x = 0$.

$$H_2(0) = 1, \quad H'_2(0) = \frac{3}{4}, \quad H''_2(0) = \frac{13 - \pi^2}{24}, \quad H'''_2(0) = \frac{12 - \pi^2}{32}.$$

The function $H_2(x)$ has a fourth-order McLaurin series
Denote by

\[ A^T_h f(x) = \frac{h}{2} \sum_{k=0}^{\infty} B_k f(b - kh), \]

the approximation for the definite integral with a generating function \( G_2(x) \). In Lemma 2 and Theorem 3 we obtain the fourth-order expansion formula of approximation \( A^T_h f(x) \).

**Lemma 2** Let \( f \in C^4[a, b] \) and \( f^{(n)}(0) = 0 \) for \( n = 0, 1, 2, 3 \). Then

\[
A^T_h f(x) = \frac{h}{2} \sum_{k=0}^{n-1} (-1)^k (4k+1 - 1) \pi^{2k+2} B_{2k+2} f(b - kh) = \int_a^b f(x) \, dx + \frac{3}{4} f(b) h + \frac{13 - \pi^2}{48} f''(b) h^2 + \frac{12 - \pi^2}{192} f''(b) h^3 + O(h^4). \tag{3.2}
\]

**Theorem 3** Let \( f \in C^4[a, b] \). Then

\[
A^T_h f(x) = \frac{h}{2} \sum_{k=0}^{n-1} B_k f(b - kh) = \int_a^b f(x) \, dx + \left( \frac{3}{4} f(b) - \frac{1}{2} f(a) \right) h + \frac{13 - \pi^2}{48} f'(b) h^2 + \frac{12 - \pi^2}{192} f'(b) h^3 + O(h^4). \tag{3.3}
\]

The Bernoulli numbers are expressed with values of the zeta function as

\[
B_{2k+2} = 2(-1)^k \zeta(2k + 2) \frac{(2k + 2)!}{(2\pi)^{2k+2}}. \tag{3.4}
\]

Then

\[
B_k = \frac{(-1)^k (4k+1 - 1) \pi^{2k+2} B_{2k+2} (2k + 2)!}{4k+1 - 1} = 2 \frac{4k+1}{4k+1} \frac{\zeta(2k + 2)}{\zeta(2k + 1)}, \tag{3.5}
\]

When \( k \geq 1 \), the zeta function satisfies (Kouba 2013)

\[
\zeta(2k) < 1 + \frac{1}{2^{2k}} + \frac{1}{2k - 1 2^{2k}} < 1 + \frac{3}{4k}. \]

Hence

\[
\frac{B_k}{2} = \left( 1 - \frac{1}{4k+1} \right) \zeta(2k + 2) < \left( 1 - \frac{1}{4k+1} \right) \left( 1 + \frac{3}{4k+1} \right) < 1 + \frac{2}{4k+1}. \]

The proofs of Lemma 2 and Theorem 3 are similar to the proofs of Lemma 1 and Theorem 1. The value of \( B_0 \) is \( B_0 = \pi^2/6 \). From (3.3) we obtain the second-order quadrature formula

\[
A^T_h f(x) = \frac{h}{2} \left( f(a) + \sum_{k=0}^{n-1} B_k f(b - kh) + \frac{\pi^2 - 6}{4} f(b) \right) = \int_a^b f(x) \, dx + O(h^2). \tag{3.6}
\]
From (3.5), we can express the formula for approximation $A_h^f(x)$ as
\[
h \left( \frac{f(a) + \sum_{k=0}^{n-1} \left(1 - \frac{1}{4^{k+1}}\right) \zeta(2k + 2)f(b - kh) - \frac{3f(b)}{4}}{2} \right) = \int_a^b f(x)dx + O(h^2).
\]

The substitution $\tilde{f}(x) = f(a + b - x)$ yields the second-order quadrature formula
\[
\tilde{A}_h^f(x) = \frac{h}{2} \left( \frac{\pi^2 - 6}{4} f(a) + \sum_{k=0}^{n-1} \tilde{B}_k f(a + kh) + f(b) \right) = \int_a^b f(x)dx + O(h^2) . \tag{3.7}
\]

In Table 4 we compute the error and the order of approximations (3.6) and (3.7) for the definite integral of the functions $\cos x, \ln(x + 1)$ and $\arctan x$. In Theorem 4 we determine the conditions for the function $f(x)$ which ensure that the error of quadrature formulas (3.6) and (3.7) is smaller than the error of the midpoint approximation. From (3.3) approximations $A_h^f(x)$ and $\tilde{A}_h^f(x)$ have third-order expansion formulas
\[
A_h^f(x) = \int_a^b f(x)dx + \left( \frac{13 - \pi^2}{48} f'(b) - \frac{1}{12} f'(a) \right) h^2 + O(h^2), \tag{3.8}
\]
\[
\tilde{A}_h^f(x) = \int_a^b f(x)dx + \left( \frac{1}{12} f'(b) - \frac{13 - \pi^2}{48} f'(a) \right) h^2 + O(h^2). \tag{3.9}
\]

**Theorem 4** Let $f \in C^2[a, b]$. Then

(i) The error of approximation (3.6) is smaller than the error of the midpoint approximation when the integrand function $f(x)$ satisfies
\[
\frac{f'(b)}{f'(a)} \in \left( \frac{6}{15 - \pi^2}, \frac{2}{11 - \pi^2} \right) = (1.1695, 1.7693). \tag{3.10}
\]

(ii) The error of approximation (3.7) is smaller than the error of the midpoint approximation when the integrand function $f(x)$ satisfies
\[
\frac{f'(b)}{f'(a)} \in \left( \frac{11 - \pi^2}{2}, \frac{15 - \pi^2}{6} \right) = (0.5652, 0.855). \tag{3.11}
\]

**Proof.** From (2.14) and (3.9) the error of approximation $A_h^f(x)$ is smaller than the error of the midpoint approximation when
\[
\left| \frac{1}{12} f'(b) - \frac{13 - \pi^2}{48} f'(a) \right| < \frac{1}{24} |f'(b) - f'(a)|.
\]

Denote $R = f'(b)/f'(a)$. Then $2|R + (\pi^2 - 13)/4| < |R - 1|$. The equations $1 - R = \pm(R + (\pi^2 - 13)/4)$ have solutions: $R' = (11 - \pi^2)/2$ and $R'' = (15 - \pi^2)/6$. The error of approximation (3.7) is smaller than the error of the midpoint approximation when the function $f(x)$ satisfies the condition
\[
\frac{f'(b)}{f'(a)} \in \left( \frac{11 - \pi^2}{2}, \frac{15 - \pi^2}{6} \right).
\]

Similarly, the error of approximation (3.6) is smaller than the error of the midpoint approximation when the function $f(x)$ satisfies (3.11).

The functions $f(x) = e^{x/2}$ and $f(x) = e^{-x/3}$ satisfy conditions (3.10) and (3.11) on the interval $[0, 1]$. In Table 3.2 and Table 3.3 we compare approximations (3.6) and (3.7) with the midpoint approximation of the functions $e^{-x/3}$ and $e^{x/2}$ on the interval $[0, 1]$. 

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Table 4.

Error and order of second-order approximation (3.6) for the definite integral of the functions $f(x) = \cos x$ on the interval [1,3], $f(x) = \ln(x + 1)$ on [0,2] and approximation (2.13) for $f(x) = \arctan x$ on [0,3].

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<td>4.11×10^{-7}</td>
</tr>
</tbody>
</table>

Source: Own calculations

Table 5.

Error and order of approximation (3.6)[left] and the midpoint approximation (1.3)[right] for the definite integral of $f(x) = e^{x/2}$ on [0,1].

<table>
<thead>
<tr>
<th>$h$</th>
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</tbody>
</table>

Source: Own calculations

Table 6.

Error and order of approximation (3.7)[left] and the midpoint approximation (1.3)[right] for the definite integral of $f(x) = e^{-x/3}$ on [0,1].

<table>
<thead>
<tr>
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Source: Own calculations

4. Higher-order quadrature formulas

In section 2 and section 3 we obtained second–order quadrature formulas (2.12), (2.13), (3.6) and (3.7). The trapezoidal approximation has a fourth–order expansion formula (2.14). From Theorem 1, Theorem 3 and (2.15), approximations (2.13) and (3.7) have fourth–order expansion formulas:

$$
\begin{align*}
\tilde{A}_h^3 f(x) &= \frac{h}{2} \left( \frac{\pi}{2} f(a) + \sum_{k=1}^{n-1} \tilde{e}_k f(a + kh) + f(b) \right) - \frac{2 + \pi^2}{96} f'(a)h^2 - \frac{\pi^2}{384} f''(a)h^3 + \frac{1}{12} f'''(b)h^4 + O(h^5),
\end{align*}
$$

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By substituting in (2.12) and (3.6) we obtain

$$A_h^T f(x) = \frac{h}{2} \left( f(a) + \sum_{k=1}^{n-1} B_k f(a + kh) + f(b) \right) = \int_a^b f(x) dx - \frac{13 - \pi^2}{48} f''(a) h^2 + \frac{12 - \pi^2}{192} f''(a) h^3 + \frac{1}{12} f'(b) h^2 + O(h^4).$$

By substituting $K = n - k$ in (2.12) and (3.6) we obtain

$$A_h^K f(x) = \frac{h}{2} \left( f(a) + \sum_{k=1}^{n-1} E_k f(a + Kh) + \frac{\pi - 1}{2} f(b) \right) = \int_a^b f(x) dx - \frac{1}{12} f'(a) h^2 + \frac{2 + \pi^2}{96} f'(b) h^2 - \frac{\pi^2}{384} f''(b) h^3 + O(h^4),$$

$$A_h^T f(x) = \frac{h}{2} \left( f(a) + \sum_{k=1}^{n-1} B_k f(a + Kh) + \frac{\pi - 1}{2} f(b) \right) = \int_a^b f(x) dx - \frac{1}{12} f'(a) h^2 + \frac{13 - \pi^2}{48} f'(b) h^2 + \frac{12 - \pi^2}{192} f''(b) h^3 + O(h^4).$$

### 4.1 Third-order quadrature formulas

Similarly to the construction of the Simpson’s approximation we construct third and fourth order approximations (4.2), (4.3) and (4.4) for the definite integral as linear combinations of the trapezoidal approximation (1.2) and approximations (2.12), (2.13), (3.6) and (3.7). Let

$$B_h^K f(x) = c_0 A_h^K f(x) + c_1 A_h^K f(x) + c_2 A_h^K f(x),$$

where, the numbers $c_i$ satisfy the system of equations

$$\begin{align*}
c_0 + c_1 + c_2 &= 1, \\
8c_0 + (2 + \pi^2)c_1 + 8c_2 &= 0, \\
8c_0 + 8c_1 + (2 + \pi^2)c_2 &= 0.
\end{align*}$$

(4.1)

The condition $c_0 + c_1 + c_2 = 1$ for the coefficients $c_i$ ensures that $B_h^K f(x)$ is an approximation for the definite integral. The second and third equations of (4.1) are chosen such that the second order terms of $B_h^K f(x)$ at the endpoints $x = a$ and $x = b$ are equal to zero. The system of equations (4.1) has the solution

$$c_0 = \frac{10 + \pi^2}{\pi^2 - 6}, \quad c_1 = c_2 = \frac{8}{6 - \pi^2}.$$  

With this choice of the coefficients $c_i$, approximation $B_h^K f(x)$ for the definite integral has third-order accuracy

$$B_h^K f(x) = \frac{h}{\pi^2 - 6} \left( w_0(f(a) + f(b)) + \sum_{k=1}^{n-1} w_k f(a + kh) \right) = \int_a^b f(x) dx + O(h^3).$$

(4.2)

The weights of approximation $B_h^K f(x)$ satisfy

$$w_0 = \frac{1}{2} (\pi^2 - 4\pi + 6), \quad w_k = \pi^2 + 10 - 4(\bar{E}_k + \bar{E}_{n-k}), \quad (1 \leq k \leq n - k).$$

Similarly, we construct a third-order approximation $\bar{B}_h^K f(x)$ for the definite integral as a linear combination of the trapezoidal approximation and approximations (3.6) and (3.7). Let
where, the numbers $c_i$ satisfy
\[
\begin{align*}
c_0 + c_1 + c_2 &= 1, \\
4c_0 + (13 - \pi^2)c_1 + 4c_2 &= 0, \\
4c_0 + 4c_1 + (13 - \pi^2)c_2 &= 0.
\end{align*}
\]

The system of equations has the solution
\[
\begin{align*}
c_0 &= \frac{\pi^2 - 17}{\pi^2 - 9}, \\
c_1 &= c_2 = \frac{4}{\pi^2 - 9}.
\end{align*}
\]

We obtain the third-order approximation $\tilde{B}_3^h f(x)$ for the definite integral
\[
\begin{align*}
\tilde{B}_3^h f(x) &= \frac{h}{\pi^2 - 9} \left( w_0(f(a) + f(b)) + \sum_{k=1}^{n-1} w_k f(a + kh) \right) = \int_a^b f(x) \, dx + O(h^3). \quad (4.3)
\end{align*}
\]

where $w_0 = \frac{1}{2}(2\pi^2 - 19)$, $w_k = \pi^2 - 17 + 2(\vec{B}_k + \vec{B}_{n-k})$, $(1 \leq k \leq n - k)$.

In Table 7 and Table 8 we compute the error and the order of approximations (4.2) and (4.3) for the definite integral of the functions $\cos x, \ln(x + 1)$ and $\arctan x$.

### 4.2 Fourth-order quadrature formula

We construct a fourth-order quadrature formula as a linear combination of the trapezoidal approximation and approximations (2.12), (2.13), (3.6), (3.7). Let
\[
B_n^h f(x) = c_0 A_1^h f(x) + c_1 A_2^h f(x) + c_2 A_3^h f(x) + c_3 A_4^h f(x) + c_4 A_5^h f(x).
\]

Approximation $B_n^h f(x)$ has a fourth-order accuracy when the coefficients $c_i$ satisfy
\[
\begin{align*}
c_0 + c_1 + c_2 + c_3 + c_4 &= 1, \\
8c_0 + 8c_1 + (2 + \pi^2)c_2 + 8c_3 + 2(13 - \pi^2)c_4 &= 0, \\
8c_0 + (2 + \pi^2)c_1 + 8c_2 + 4(13 - \pi^2)c_3 + 8c_4 &= 0, \\
\pi^2 c_2 + 2(\pi^2 - 12)c_3 &= 0, \\
\pi^2 c_1 + 2(\pi^2 - 12)c_4 &= 0.
\end{align*}
\]

Let $D = 2\pi^4 - 27\pi^2 + 72$. The system of equations has the solution
\[
\begin{align*}
c_0 &= \frac{2\pi^4 - 19\pi^2 - 120}{D}, \\
c_1 &= c_2 = \frac{4(12 - \pi^2)}{D}, \\
&= c_3 = c_4 = \frac{4\pi^2}{D}.
\end{align*}
\]

With this choice of the coefficients $c_i$ we obtain the fourth-order approximation for the definite integral
\[
B_n^h f(x) = \frac{h}{D} \left( w_0(f(a) + f(b)) + \sum_{k=1}^{n-1} w_k f(a + kh) \right) = \int_a^b f(x) \, dx + O(h^4). \quad (4.4)
\]

where $w_0 = (3\pi^4 - 4\pi^3 - 25\pi^2 + 48\pi - 72)/2$ and $w_k = 2\pi^4 - 19\pi^2 - 120 + 4(12 - \pi^2)(\vec{E}_k + \vec{E}_{n-k}) + 2\pi^2(\vec{E}_k + \vec{E}_{n-k})$, for $1 \leq k \leq n - k$. In Table 9 we compute the error and the order of approximation (4.4) for the definite integral of the functions $\cos x, \ln(x + 1)$ and $\arctan x$. 

---

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Table 7.

Error and order of third-order approximation (4.2) for the definite integral of the functions \( f(x) = \cos x, \ln(x + 1), \arctan x \) on the interval [10,30].

<table>
<thead>
<tr>
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<th>( \cos x )</th>
<th>Order</th>
<th>( \ln(x + 1) )</th>
<th>Order</th>
<th>( \arctan x )</th>
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</tr>
</tbody>
</table>

Source: Own calculations

Table 8.

Error and order of third-order approximation (4.3) for the definite integral of the functions \( f(x) = \cos x, \ln(x + 1), \arctan x \) on the interval [10,30].

<table>
<thead>
<tr>
<th>( h )</th>
<th>( \cos x )</th>
<th>Order</th>
<th>( \ln(x + 1) )</th>
<th>Order</th>
<th>( \arctan x )</th>
<th>Order</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.025</td>
<td>0.0058322</td>
<td>3.0509</td>
<td>7.28 \times 10^{-6}</td>
<td>2.9735</td>
<td>1.57 \times 10^{-6}</td>
<td>2.9520</td>
</tr>
<tr>
<td>0.0125</td>
<td>0.0007083</td>
<td>3.0416</td>
<td>9.19 \times 10^{-7}</td>
<td>2.9864</td>
<td>1.99 \times 10^{-7}</td>
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</tr>
<tr>
<td>0.00625</td>
<td>8.70 \times 10^{-6}</td>
<td>3.0251</td>
<td>1.15 \times 10^{-7}</td>
<td>2.9930</td>
<td>2.51 \times 10^{-8}</td>
<td>2.9872</td>
</tr>
<tr>
<td>0.003125</td>
<td>1.08 \times 10^{-6}</td>
<td>3.0137</td>
<td>1.45 \times 10^{-7}</td>
<td>2.9953</td>
<td>3.16 \times 10^{-9}</td>
<td>2.9909</td>
</tr>
</tbody>
</table>

Source: Own calculations

Table 9.

Error and order of third-order approximation (4.4) for the definite integral of the functions \( f(x) = \cos x, \ln(x + 1), \arctan x \) on the interval [0,30].

<table>
<thead>
<tr>
<th>( h )</th>
<th>( \cos x )</th>
<th>Order</th>
<th>( \ln(x + 1) )</th>
<th>Order</th>
<th>( \arctan x )</th>
<th>Order</th>
</tr>
</thead>
<tbody>
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<td>0.00014554</td>
<td>3.3684</td>
<td>0.00017815</td>
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</tr>
<tr>
<td>0.0125</td>
<td>9.20 \times 10^{-6}</td>
<td>4.1317</td>
<td>0.00001189</td>
<td>3.6129</td>
<td>0.00001474</td>
<td>3.5951</td>
</tr>
<tr>
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<td>4.0828</td>
<td>1.64 \times 10^{-7}</td>
<td>3.7781</td>
<td>9.99 \times 10^{-7}</td>
<td>3.8829</td>
</tr>
<tr>
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<td>3.29 \times 10^{-8}</td>
<td>4.0469</td>
<td>4.11 \times 10^{-8}</td>
<td>3.8583</td>
<td>6.33 \times 10^{-8}</td>
<td>3.9805</td>
</tr>
</tbody>
</table>

Source: Own calculations

5. Conclusion

In the present paper we obtained second, third and fourth order quadrature formulas based on the expansion formulas of the approximations for the definite integral with generating functions \( \pi \sec(\pi \sqrt{x}/2)/4 \) and \( \pi \tan(\pi \sqrt{x}/2)/(4\sqrt{x}) \). In Theorem 2 and Theorem 4 we derive the conditions for the integrand function which ensure that the error of second-order quadrature formulas (2.12), (2.13), (3.6) and (3.7) is smaller than the error of the midpoint rule. In future work we are going to extend the results of this paper to multidimensional and fractional integrals.
Acknowledgements
This work was supported by the Bulgarian Academy of Sciences through the Program for Career Development of Young Scientists, Grant DFNP-17-88/2017, Project "Efficient Numerical Methods with an Improved Rate of Convergence for Applied Computational Problems" and by the Bulgarian National Science Fund under Grant DFNI I02-20/2014, Project "Efficient Parallel Algorithms for Large-Scale Computational Problems".

Literature


