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ERROR BOUNDS FOR NUMERICAL INTEGRATION OF FUNCTIONS OF LOWER SMOOTHNESS AND GAUSS-LEGENDRE QUADRATURE RULE

SAMUEL A. SURULERE AND ABIOLA O. OLADEJI

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TSHWANE UNIVERSITY OF TECHNOLOGY, DEPARTMENT OF MATHEMATICS AND STATISTICS, 175, NELSON MANDELA DRIVE, ARCADIA, PRETORIA, SOUTH AFRICA.
samuel.abayomi.sas@gmail.com

ABSTRACT. The error bounds of the rectangular, trapezoidal and Simpson's rules which are commonly used in approximating the integral of a function $f(x)$ over an interval $[a, b]$ were estimated. The error bounds of the second, and third generating functions of the Gauss-Legendre quadrature rules were also estimated in this paper. It was shown that for an $f(t)$ whose smoothness is increasing, the accuracy of the fourth, sixth and eighth error bound of the second, and third generating functions of the Gauss-Legendre quadrature rule does not increase. It was also shown that the accuracy of the fourth error bound of the Simpson's $1/3$ and $3/8$ rules does not increase.

Key words and phrases: Generating functions; Newton-Cotes formulas; Quadrature rules; Numerical integration.

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1. INTRODUCTION

This paper deals with quadrature rules for functions having lower order of derivatives than is usually required. We aim to establish some new error estimates that are sometimes exact and convenient for the evaluation of the quadrature error using another approach to the numerical integration. The formula

$$\int_a^b u_n(x,t)df(t) = \int_a^b f(t)dt - \sum_{k=0}^{n} f(x_k)s_{nk}, \tag{1.1}$$

was obtained in [7] and considered in further details in [4]. Formula 1.1 appeared in connection with the trapezoidal rule presented in [2]. Several works has been presented in the literature (see [6, 5, 3]). We can write the right-hand-side of 1.1 as the error functional $E_n(f) = I(f) - I_n(f)$. It follows that

$$E_n(f) = \int_a^b u_n(x,t)df(t). \tag{1.2}$$

The error of the quadrature rule is

$$|E_n(f)| \leq \max|f'(t)| \int_a^b u_n(x,t)dt. \tag{1.3}$$

The theorem containing formula 1.3 as well as its proof was detailed in [7]. Formulas 1.2 and 1.3 are the main notations used in this paper. The method of generating functions was introduced in [7]. For example, the generating functions

$$u_n(t) = \chi(a,b)\left[a - t + \sum_{k=0}^{n} s_{nk}(t)\theta^+(t-x_k)\right], \tag{1.4}$$

where $a = x_0 < x_1 < \ldots < x_{n-1} < x_n = b$, were integrated until we obtain nonzero values at the endpoints. In what follows, we are omitting $\chi(a,b)$, implying that everywhere in the definition of $\mathbb{R}$, this factor is present. The generating functions describes the complete rule for numerical integration, including the numerical integration formula and the error estimate for the integrand with arbitrary smoothness. The estimation of error bounds using generating functions and geometry was introduced in [4]. Both methods will also be applied in this paper to estimate the error bounds for functions of lower smoothness.

2. ERROR BOUNDS FOR RECTANGULAR RULE

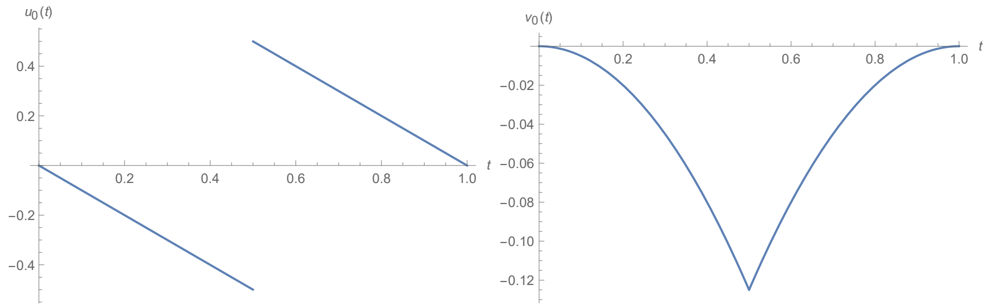
To estimate the error bounds of the rectangular rule, we define the following: $x_0 = a$, $x_1 = \frac{b-a}{2}$, $x_2 = b$. Now we write $I_0(f) = (b-a)f(x_1) = s_{00}f(x_1)$ and we calculate the integral

$$U_{01}(t,a,b) = \int_a^t u_0(\tau)d\tau. \tag{2.1}$$

We define the functions

$$u_0(t,a,b) = \begin{cases} 0 & \text{if} \quad t < a, \\ a - t & \text{if} \quad t < \dfrac{a+b}{2}, \\ b - t & \text{if} \quad \dfrac{a+b}{2} \leq t, \\ 0 & \text{if} \quad b < t, \end{cases} \quad U_{01}(t,a,b) = \begin{cases} 0 & \text{if} \quad t < a, \\ -\frac{1}{2}(a-t)^2 & \text{if} \quad t < \dfrac{a+b}{2}, \\ -\frac{1}{2}(b-t)^2 & \text{if} \quad \dfrac{a+b}{2} \leq t, \\ 0 & \text{if} \quad b < t. \end{cases}$$

$u_0(t,0,1)$ and $U_{01}(t,0,1)$ are illustrated in Figure 1



(a) (b)

Figure 1: (a) Graph of $u_0(t,0,1)$ (b) Graph of $U_{01}(t,0,1)$

Figure 1 was obtained by replacing $[a,b]$ with $[0,1]$. This was also the case for all the figures in this paper. We now write the error functional for $u_0(t)$ and $U_{01}(t)$ as

$$E_0(f) = \int_a^b u_0(t)df(t), \text{ and} \tag{2.2}$$

$$E_1(f) = \int_a^b u_0(\tau)df(\tau). \tag{2.3}$$

The error bound for $f(t) \in C^{(1)}[a,b]$ is defined as

$$|E_0(f)| \leq \left| \int_a^b u_0(t)df(t) \right| = \left| \int_a^b f'(t)u_0(t)dt \right| \leq \max|f'(t)| \int_a^b |u_0(t)|dt,$$

$$\max|f'(t)| \int_a^b \left| \left(-t + \frac{a+b}{2}\right) \right| dt = \frac{1}{4}(b-a)^2 \max|f'(t)|. \tag{2.4}$$

Therefore

$$|E_0(f)| \leq \frac{1}{4}(b-a)^2 \max|f'(t)|. \tag{2.5}$$

The value $\frac{1}{4}(b-a)^2$ can also be verified by geometry, using Figure 1(a). For the error bound of $f(t) \in C^{(2)}[a,b]$, we simplify formula 2.3 as follows

$$E_1(f) = \int_a^b u_0(\tau)df(\tau) = \int_a^b f'(\tau)dU_{01}(\tau), \tag{2.6}$$

and apply integration by parts to obtain

$$E_1(f) = -\int_a^b U_{01}(\tau)f''(\tau)d\tau. \tag{2.7}$$

The error bound for $f(t) \in C^{(2)}[a,b]$ is calculated using the definition below

$$|E_1(f)| \leq \left| -\int_a^b U_{01}(\tau)f''(\tau)d\tau \right| \leq \max|f''(t)| \int_a^b \frac{1}{2}|U_{01}(\tau)|d\tau.$$

We know that $\int_a^b |U_{01}(\tau)|d\tau = \int_a^{\frac{a+b}{2}} \left|-\frac{1}{2}(a-\tau)^2\right| d\tau + \int_{\frac{a+b}{2}}^b \left|-\frac{1}{2}(b-\tau)^2\right| d\tau$. Therefore

$$|E_1(f)| \leq \frac{(b-a)^3}{24} \max|f''(t)|. \tag{2.8}$$

3. Error bound for Trapezoidal rule

In what follows, we define: $x_0 = a, x_1 = b, s_{10} = s_{11} = \dfrac{b+a}{2}$. Then

$$I_1(f) = s_{10}f(x_0) + s_{11}f(x_1),$$

and $u_1(t) = -t + s_{10}\theta^+(t-x_0) + s_{11}\theta^+(t-x_1)$. The integral

$$U_1(t,a,b) = \int_a^t u_1(\tau)d\tau, \tag{3.1}$$

will be calculated to obtain the function, $U_1(t,a,b)$. We now define the functions

$$u_1(t,a,b) = \begin{cases} 0 & \text{if} \quad t < a, \\ -t + \dfrac{a+b}{2} & \text{if} \quad a < t < b, \\ 0 & \text{if} \quad b < t, \end{cases} \quad U_{11}(t,a,b) = \begin{cases} 0 & \text{if} \quad t < a, \\ -\frac{1}{2}(a-t)(b-t) & \text{if} \quad a < t < b, \\ 0 & \text{if} \quad b < t. \end{cases}$$

$u_1(t,0,1)$ and $U_{11}(t,0,1)$ are both illustrated in Figure 2

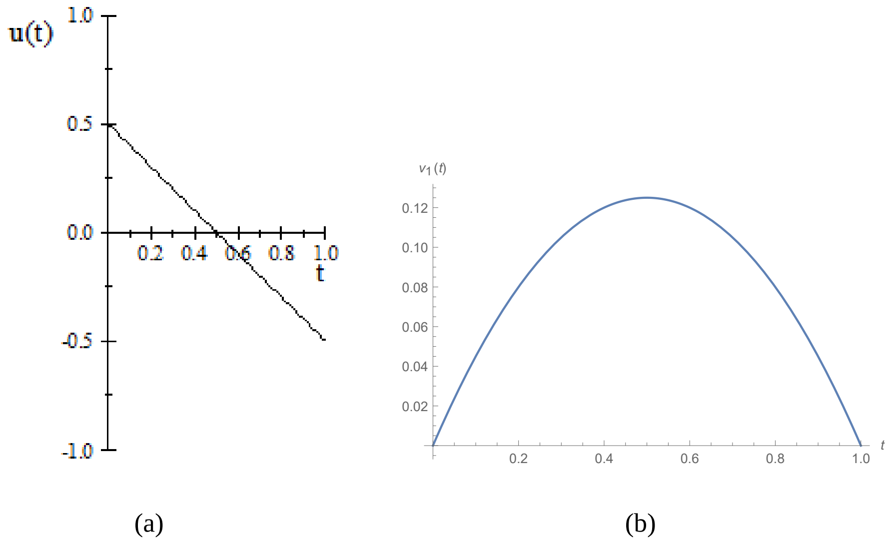


Figure 2: (a) Graph of $u_1(t,0,1)$ (b) Graph of $U_{11}(t,0,1)$

The error bound for $f(t) \in C^{(1)}[a,b]$ is

$$|E_1(f)| \leq \left|\int_a^b u_1(t)df(t)\right| = \left|\int_a^b f'(t)u_1(t)dt\right| \leq \max|f'(t)| \int_a^b |u_1(t)|dt,$$

$$\max|f'(t)| \int_a^b \left|\frac{a+b}{2} - t\right| dt = \frac{(b-a)}{4} \max|f'(t)|,$$

The same result can also be obtained from Figure 2(a). Therefore

$$|E_1(f)| \leq \frac{1}{4}(b-a)\max|f'(t)|. \tag{3.2}$$

Let us write the error functional for $U_{11}(t)$ as

$$E_2(f) = \int_a^b u_1(\tau)df(\tau). \tag{3.3}$$

We simplify formula 3.3 as follows

$$E_2(f) = \int_a^b u_1(\tau)df(\tau) = \int_a^b f'(\tau)dU_{11}(\tau), \tag{3.4}$$

and apply integration by parts to obtain

$$E_2(f) = -\int_a^b U_{11}(\tau)f''(\tau)d\tau. \tag{3.5}$$

Therefore

$$|E_2(f)| \leq \left| -\int_a^b U_{11}(\tau)f''(\tau)d\tau \right| \leq \max|f''(t)| \int_a^b \left| -\frac{1}{2}\tau[\tau-(a+b)] \right| d\tau.$$

We know that $\int_a^b |U_{11}(\tau)|d\tau = \int_a^b \left| -\frac{1}{2}\tau[\tau-(a+b)] \right| d\tau = \frac{(b-a)^3}{12}$. Therefore, the error bound for $f(t) \in C^{(2)}[a,b]$ is

$$|E_2(f)| \leq \frac{(b-a)^3}{12}\max|f''(t)|. \tag{3.6}$$

4. ESTIMATION OF ERROR BOUNDS FOR SIMPSON'S $1/3$ RULE

We now estimate the error bounds for the Simpson's $1/3$ rule (which is a quadratic parabola). We define the following: $x_0 = a, x_1 = \frac{a+b}{2}, x_2 = b$. The three nodes are defined as:

$$s_{20} = \frac{1}{6}(b-a), s_{21} = \frac{4}{6}(b-a), s_{22} = \frac{1}{6}(b-a).$$

Then

$$I_2(f) = s_{20}f(x_0) + s_{21}f(x_1) + s_{22}f(x_2),$$

and the generating function is $u_2(t) = -t + s_{20}\theta^+(t-x_0) + s_{21}\theta^+(t-x_1) + s_{22}\theta^+(t-x_2)$. The integrals

$$U_{21}(t,a,b) = \int_a^t u_2(\tau)d\tau, U_{22}(t,a,b) = \int_a^t U_{21}(\tau)d\tau, U_{23}(t,a,b) = \int_a^t U_{22}(\tau)d\tau, \tag{4.1}$$

are used to obtain functions $U_{21}(t,a,b), U_{22}(t,a,b)$ and $U_{23}(t,a,b)$.

$$u_2(t,a,b) = \begin{cases} 0 & \text{if} \quad t < a, \\ -t + \frac{5a+b}{6} & \text{if} \quad t < \frac{a+b}{2}, \\ -t + \frac{a+5b}{6} & \text{if} \quad \frac{a+b}{2} \leq t, \\ 0 & \text{if} \quad b < t, \end{cases}$$

$$U_{21}(t,a,b) = \begin{cases} 0 & \text{if} \quad t < a, \\ -\dfrac{1}{6}(a-t)(2a+b-3t) & \text{if} \quad t < \dfrac{a+b}{2}, \\ -\dfrac{1}{6}(b-t)(a+2b-3t) & \text{if} \quad \dfrac{a+b}{2} \leq t, \\ 0 & \text{if} \quad b < t. \end{cases}$$

$$U_{22}(t,a,b) = \begin{cases} 0 & \text{if} \quad t < a, \\ \dfrac{1}{12}(a-t)^2(a+b-2t) & \text{if} \quad t < \dfrac{a+b}{2}, \\ \dfrac{1}{12}(b-t)^2(a+b-2t) & \text{if} \quad \dfrac{a+b}{2} \leq t, \\ 0 & \text{if} \quad b < t. \end{cases}$$

$$U_{23}(t,a,b) = \begin{cases} 0 & \text{if} \quad t < a, \\ -\dfrac{1}{72}(a-t)^3(a+2b-3t) & \text{if} \quad t < \dfrac{a+b}{2}, \\ -\dfrac{1}{72}(b-t)^3(2a+b-3t) & \text{if} \quad \dfrac{a+b}{2} \leq t, \\ 0 & \text{if} \quad b < t. \end{cases}$$

The functions are graphically represented in Figure 3.

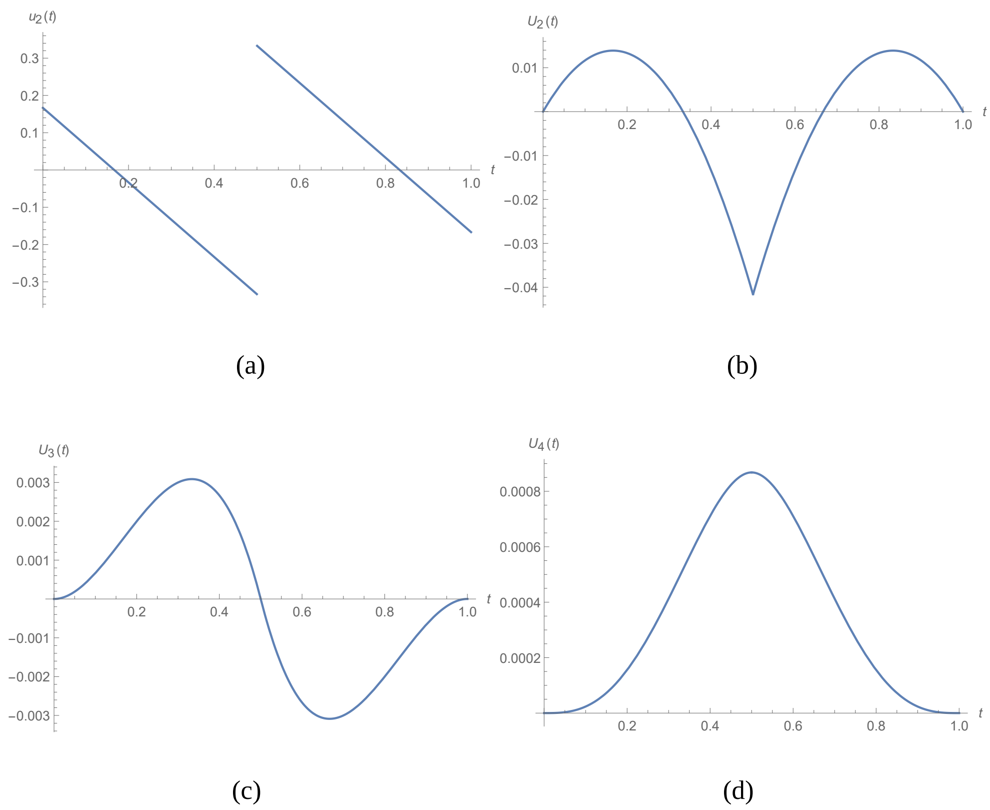


Figure 3: (a) Graph of $u_2(t,0,1)$ *(b) Graph of* $U_{21}(t,0,1)$ *(c) Graph of* $U_{22}(t,0,1)$ *(d) Graph of* $U_{23}(t,0,1)$

The error functional for $f(t) \in C^{(1)}[a,b]$ is

$$E_1(f) = \int_a^b u_2(t) df(t) = \int_a^b f'(t) u_2(t) dt,$$

and the error bound is calculated using

$$|E_1(f)| \leq \Big| \int_a^b f'(t) u_2(t) dt \Big| \leq \max|f'(t)| \int_a^b |u_2(t)| dt.$$

Since $2\displaystyle\int_a^{\frac{a+b}{2}} \Big| -t + \frac{5a+b}{6} \Big| dt = \frac{5(b-a)^2}{36}$, therefore

$$|E_1(f)| \leq \frac{5(b-a)^2}{36} \max|f'(t)|.$$

Integral $\int_a^b |u_2(t)| dt$ can also be evaluated geometrically, by computing the area of triangles in Figure 3(a).
The error functional for $f(t) \in C^{(2)}[a,b]$ is

$$E_2(f) = \int_a^b u_2(\tau) df(\tau) = \int_a^b f'(\tau) u_2(\tau) d\tau, \tag{4.2}$$

where $u_2(\tau) d\tau = dU_{21}(\tau)$. Integrating $E_2(f)$ by parts returns $E_2(f) = -\displaystyle\int_a^b f''(\tau) U_{21}(\tau) d\tau$.
Hence

$$|E_2(f)| \leq \Big| -\int_a^b f''(t) U_{21}(t) dt \Big| \leq \max|f''(t)| \int_a^b |U_{21}(t)| dt,$$

$$\int_a^b |U_{21}(t)| dt = 2 \int_a^{\frac{a+b}{2}} \Big| -\frac{1}{6}(a-t)(2a+b-3t) \Big| dt = \frac{(b-a)^3}{81}.$$

Finally, the error bound is

$$|E_2(f)| \leq \frac{(b-a)^3}{81} \max|f''(t)|. \tag{4.3}$$

We obtain the Simpson's third error bound using the definition

$$E_3(f) = \int_a^b u_2(\tau) df(\tau) = -\int_a^b f''(\tau) U_{21}(\tau) d\tau = \int_a^b f'(\tau) dU_{22}(\tau). \tag{4.4}$$

After integration by parts, we obtain the error functional as

$$E_3(f) = \int_a^b f'''(\tau) U_{22}(\tau) d\tau, \tag{4.5}$$

and

$$\int_a^b |U_{22}(\tau)| d\tau = 2 \int_a^{\frac{a+b}{2}} \frac{1}{12}(a-t)^2(a+b-2t) = \frac{(b-a)^4}{576}. \tag{4.6}$$

Hence

$$|E_3(f)| \leq \Big| \int_a^b f'''(t) U_{22}(t) dt \Big| \leq \max|f'''(t)| \int_a^b |U_{22}(t)| dt,$$

$$|E_3(f)| \leq \frac{(b-a)^4}{576} \max|f'''(t)|. \tag{4.7}$$

We know that

$$E_4(f) = \int_a^b f'''(\tau)U_{22}(\tau)d\tau = \int_a^b f'''(\tau)dU_{23}(\tau). \tag{4.8}$$

After integration by parts

$$E_4(f) = -\int_a^b f^{(4)}(\tau)U_{23}(\tau)d\tau, \tag{4.9}$$

The Simpson's fourth error bound is

$$|E_4(f)| \leq \Big| -\int_a^b f^{(4)}(t)U_{23}(t)dt\Big| \leq \max|f^{(4)}(t)| \int_a^b |U_{23}(t)|dt, \tag{4.10}$$

while $\int_a^b |U_{23}(t)|dt = \frac{(b-a)^5}{2880}$. Hence

$$|E_4(f)| \leq \frac{(b-a)^5}{2880} \max|f^{(4)}(t)|. \tag{4.11}$$

We define $E_5(f)$ as

$$E_5(f) = -\int_a^b f^{(4)}(\tau)U_{23}(\tau)d\tau = -\int_a^b f^{(4)}(\tau)dU_{24}(\tau), \tag{4.12}$$

where $U_{24}(t,a,b) = \int_a^t U_{23}(\tau)d\tau$. The graph of $U_{24}(t,a,b)$ is presented in Figure 4.

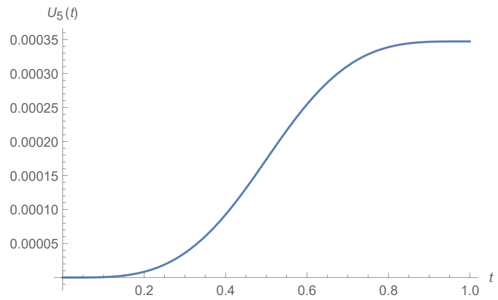


Figure 4: Simpson's rule graph of $U_{24}(t,a,b)$

It is true that

$$E_5(f) = [-f^{(5)}(\tau)U_{24}(\tau)]_a^b + \int_a^b f^{(5)}(\tau)U_{24}(\tau)d\tau. \tag{4.13}$$

Clearly $[-f^{(5)}(\tau)U_{24}(\tau)]_a^b \neq 0$ (from Figure 4). Hence, the accuracy of evaluation of $E_4(f)$ with increasing smoothness does not increase.

5. ESTIMATION OF ERROR BOUNDS FOR SIMPSON'S $3/8$ RULE

The errors of the Simpson's $3/8$ rule (which is a cubic parabola) will be evaluated. The following definitions are true: $x_0 = a, x_1 = \frac{2a+b}{3}, x_2 = \frac{a+2b}{3}, x_3 = b$. The nodes are

$$s_{30} = \frac{1}{8}(b-a), s_{31} = \frac{3}{8}(b-a), s_{32} = \frac{3}{8}(b-a), s_{33} = \frac{1}{8}(b-a).$$

And

$$I_3(f) = s_{30}f(x_0) + s_{31}f(x_1) + s_{32}f(x_2) + s_{33}f(x_3),$$

the generating function is

$$u_3(t) = -t + s_{30}\theta^+(t - x_0) + s_{31}\theta^+(t - x_1) + s_{32}\theta^+(t - x_2) + s_{33}\theta^+(t - x_3).$$

The integrals

$$U_{31}(t, a, b) = \int_a^t u_3(\tau)d\tau, U_{32}(t, a, b) = \int_a^t U_{31}(\tau)d\tau, U_{33}(t, a, b) = \int_a^t U_{32}(\tau)d\tau, \tag{5.1}$$

will be used to obtain $U_{31}(t, a, b), U_{32}(t, a, b)$ and $U_{33}(t, a, b)$.

$$u_3(t,a,b) = \begin{cases} 0 & \text{if} \quad t < a, \\ -t + \frac{7a+b}{8} & \text{if} \quad a < t < \frac{2a+b}{3}, \\ -t + \frac{a+b}{2} & \text{if} \quad \frac{2a+b}{3} < t < \frac{a+2b}{3}, \\ -t + \frac{a+7b}{8} & \text{if} \quad \frac{a+2b}{3} < t < b, \\ 0 & \text{if} \quad b < t, \end{cases} \quad U_{31}(t,a,b) = \begin{cases} 0 & \text{if} \quad t < a, \\ -\frac{1}{8}(a-t)(3a+b-4t) & \text{if} \quad a < t < \frac{2a+b}{3}, \\ -\frac{1}{8}(a+b-2t)^2 & \text{if} \quad \frac{2a+b}{3} < t < \frac{a+2b}{3}, \\ -\frac{1}{8}(b-t)(a+3b-4t) & \text{if} \quad \frac{a+2b}{3} < t < b, \\ 0 & \text{if} \quad b < t. \end{cases}$$

$$U_{32}(t,a,b) = \begin{cases} 0 & \text{if} \quad t < a, \\ \frac{1}{48}(a-t)^2(5a+3b-8t) & \text{if} \quad a < t < \frac{2a+b}{3}, \\ \frac{1}{48}(a+b-2t)^3 & \text{if} \quad \frac{2a+b}{3} < t < \frac{a+2b}{3}, \\ \frac{1}{48}(b-t)^2(3a+5b-8t) & \text{if} \quad \frac{a+2b}{3} < t < b, \\ 0 & \text{if} \quad b < t. \end{cases} \quad U_{33}(t,a,b) = \begin{cases} 0 & \text{if} \quad t < a, \\ -\frac{1}{48}(a-t)^3(a+b-2t) & \text{if} \quad a < t < \frac{2a+b}{3}, \\ -\frac{1}{3456}(a-b)^4 - \frac{1}{384}(a+b-2t)^4 & \text{if} \quad \frac{2a+b}{3} < t < \frac{a+2b}{3}, \\ -\frac{1}{48}(b-t)^3(a+b-2t) & \text{if} \quad \frac{a+2b}{3} < t < b, \\ 0 & \text{if} \quad b < t. \end{cases}$$

The functions are graphically represented in Figure 5.

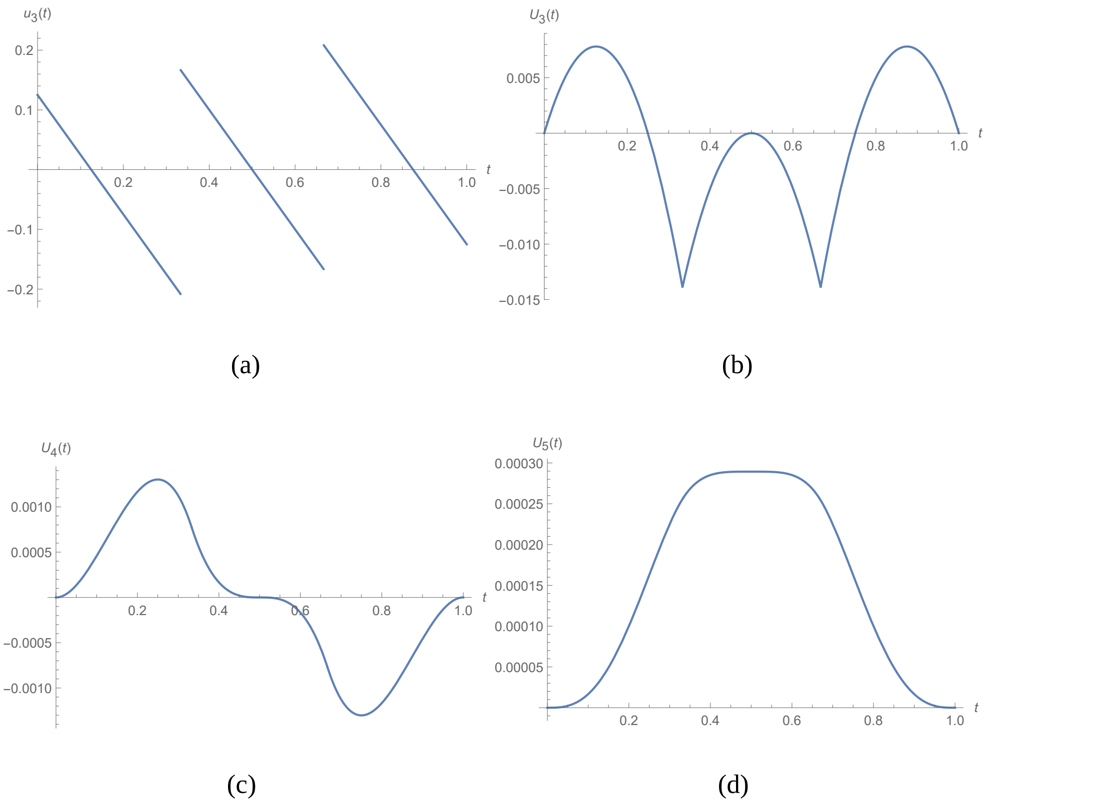


Figure 5: (a) Graph of $u_3(t, 0, 1)$ (b) Graph of $U_{31}(t, 0, 1)$ (c) Graph of $U_{32}(t, 0, 1)$ (d) Graph of $U_{33}(t, 0, 1)$

The error functional for $f(t) \in C^{(1)}[a,b]$ is defined

$$E_1(f) = \int_a^b u_3(t)df(t) = \int_a^b f'(t)u_3(t)dt,$$

and the error bound is

$$|E_1(f)| \leq \Big| \int_a^b f'(t)u_3(t)dt \Big| \leq \max|f'(t)| \int_a^b |u_3(t)|dt.$$

It is true that $\int_a^b |u_3(t)|dt = \frac{25(b-a)^2}{288}$, hence

$$|E_1(f)| \leq \frac{25(b-a)^2}{288} \max|f'(t)|.$$

The error functional for $f(t) \in C^{(2)}[a,b]$ is

$$E_2(f) = \int_a^b u_3(\tau)df(\tau) = \int_a^b f'(\tau)dU_{31}(\tau), \tag{5.2}$$

We integrate $E_2(f)$ by parts and write the second error bound

$$|E_2(f)| \leq \max|f''(t)| \int_a^b |U_{31}(t)|dt,$$

$$\int_a^b |U_{31}|dt = \frac{(b-a)^3}{192}.$$

Finally

$$|E_2(f)| \leq \frac{(b-a)^3}{192} \max|f''(t)|. \tag{5.3}$$

The third error bound for Simpson's $3/8$ rule is calculated as follows

$$E_3(f) = \int_a^b u_3(\tau)df(\tau) = -\int_a^b f''(\tau)U_{31}(\tau)d\tau = \int_a^b f''(\tau)dU_{32}(\tau). \tag{5.4}$$

Integrating by parts, we obtain

$$E_3(f) = \int_a^b f'''(\tau)U_{32}(\tau)d\tau, \tag{5.5}$$

and

$$\int_a^b |U_{32}(\tau)|d\tau = \frac{(b-a)^4}{1728}. \tag{5.6}$$

Therefore

$$|E_3(f)| \leq \Big| \int_a^b f'''(t)U_{32}(t)dt \Big| \leq \max|f'''(t)| \int_a^b |U_{32}(t)|dt,$$

$$|E_3(f)| \leq \frac{(b-a)^4}{1728} \max|f'''(t)|. \tag{5.7}$$

The same approach is used to calculate the fourth error bound

$$E_4(f) = \int_a^b f'''(\tau)U_{32}(\tau)d\tau = \int_a^b f'''(\tau)dU_{33}(\tau). \tag{5.8}$$

Integration by parts returns

$$E_4(f) = -\int_a^b f^{(4)}(\tau)U_{33}(\tau)d\tau, \tag{5.9}$$

The Simpson's $3/8$ fourth error bound is

$$|E_4(f)| \leq \Big| -\int_a^b f^{(4)}(t)U_{33}(t)dt\Big| \leq \max|f^{(4)}(t)| \int_a^b |U_{33}(t)|dt, \tag{5.10}$$

and $\int_a^b |U_{33}(t)|dt = \frac{(b-a)^5}{6480}$. Hence

$$|E_4(f)| \leq \frac{(b-a)^5}{6480} \max|f^{(4)}(t)|. \tag{5.11}$$

$E_5(f)$ is defined below

$$E_5(f) = -\int_a^b f^{(4)}(\tau)U_{33}(\tau)d\tau = -\int_a^b f^{(4)}(\tau)dU_{34}(\tau), \tag{5.12}$$

where $U_{34}(t,a,b) = \int_a^t U_{33}(\tau)d\tau$. $U_{34}(t,a,b)$ is presented in Figure 6.

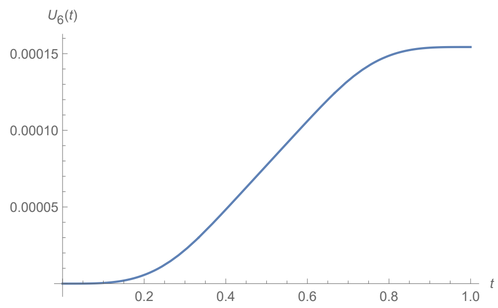


Figure 6: Simpson's rule graph of $U_{34}(t,a,b)$

Clearly

$$E_5(f) = [-f^{(5)}(\tau)U_{34}(\tau)]_a^b + \int_a^b f^{(5)}(\tau)U_{34}(\tau)d\tau. \tag{5.13}$$

$[-f^{(5)}(\tau)U_{34}(\tau)]_a^b \neq 0$ from Figure 6. As was the case for Simpson's $1/3$ rule, the evaluation of $E_4(f)$ with increasing smoothness does not increase for the Simpson's $3/8$ rule.

5.1. **Remark about Simpson's rule for $n = 4$ and $n = 8$.** The generating functions for $u_4(t,a,b)$ and $u_8(t,a,b)$ are presented on page 842 in [4]. Using the approach explained in this paper, the estimation of the error bounds for $n = 4$ can be conveniently calculated. However, it was observed that for $n = 8$, the right-hand-side of the first integral was not equal to zero (i.e. $U_{81}(b) \neq 0$). It was necessary to consider this particular Simpson's rule because it is the first case where the generating function has both positive and negative jumps (see Figure 4(c) on page 842 in [4]).

6. GAUSSIAN QUADRATURE

This is an opened quadrature rule

$$\int_{-1}^{1} f(x)dx \approx \sum_{j=1}^{n} s_j f(x_j), \tag{6.1}$$

where s_j, x_j are unknown. To find $2n$ unknowns we need at least $2n$ equations. These equations can be obtained if we require the exactness of the rule 6.1 on all polynomials of degree $\leq 2n-1$. In particular, Equation 6.1 must be true for $f(t) = 1, t, t^2, \ldots, t^{2n-1}$. Let us write these equations using a tabular system

Table 6.1: Error for different n values

$f(t)$		Eq
1	$\int_{-1}^{1} 1dt = \sum_{j=1}^{n} s_j$	$\sum_{j=1}^{n} s_j = 2$
t	$\int_{-1}^{1} tdt = \sum_{j=1}^{n} s_j x_j$	$\sum_{j=1}^{n} s_j x_j = 0$
t^2	$\int_{-1}^{1} t^2 dt = \sum_{j=1}^{n} s_j x_j^2$	$\sum_{j=1}^{n} s_j x_j^2 = \frac{2}{3}$
$\vdots$	$\vdots$	$\vdots$
t^{2n-1}		$\sum_{j=1}^{n} s_j 2_j^{2n-1} = \int_{-1}^{1} t^{2n-1} dt$

Carl Gauss has shown that the exactness for polynomials of degree not exceeding $2n-1$ can be attained if and only if the values $x_1, x_2, \ldots, x_n$ are the n-zeros of the Legendre polynomials, $P_n(x)$. The Legendre polynomials can be computed through the formulae

$$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n}[(x^2-1)^n]. \tag{6.2}$$

It is known that Legendre polynomials can be obtained as solutions of the Legendre equation

$$(1-x^2)y'' - 2xy' + n(n+1)y = 0. \tag{6.3}$$

Thus, the nodal points of the Gauss method are the roots of the Legendre polynomials $P_n(x)$. The weights s_j can be found from the following formula

$$s_j = \frac{2}{(1-x_j^2)(P_n'(x_j))^2}. \tag{6.4}$$

Example 1: The roots of $P_3(x)$ are $x_1 = 0.775; x_2 = 0; x_3 = 0.775$, using the formula presented in Equation 6.4, we obtain

$$s_1 = \frac{2}{(1-(0.775)^2)(\frac{15}{2} \times (0.775)^2 - \frac{3}{2})^2} = 0.556$$

$$s_2 = \frac{2}{(-\frac{3}{2})^2} = 0.889; s_3 = 0.556.$$

For the comprehensive table of roots and weights, see [1]. It is possible to prove that for the smooth enough function, $f(x)$, the Gaussian quadrature formula can be written as

$$\int_{-1}^{1} f(x)dx = \sum_{j=1}^{n} s_j f(x_j) + R_n,$$

where

$$R_n \leq \frac{2}{(2n+1)!}\left[\frac{2^n(n!)^2}{(2n)!}\right]^2 \max|f^{2n}(\varsigma)|.$$

We can compute that the factor in the error $C_n = \frac{2}{(2n+1)!}\left[\frac{2^n(n!)^2}{(2n)!}\right]^2$ for different n

Table 6.2: Error for different n values

n	C_n
1	0.333
2	7.41×10^{-3}
3	6.35×10^{-5}
4	2.88×10^{-7}
5	8.08×10^{-10}

7. ESTIMATION OF ERROR BOUNDS FOR SECOND GENERATING FUNCTION OF GAUSS-LEGENDRE QUADRATURE RULE

The two nodal generating function for Gauss-Legendre rule is given as the function

$$\bar{\bar{u}}_2(t) = -t - 1 + \theta^+\left(t + \frac{1}{\sqrt{3}}\right) + \theta^+\left(t - \frac{1}{\sqrt{3}}\right). \tag{7.1}$$

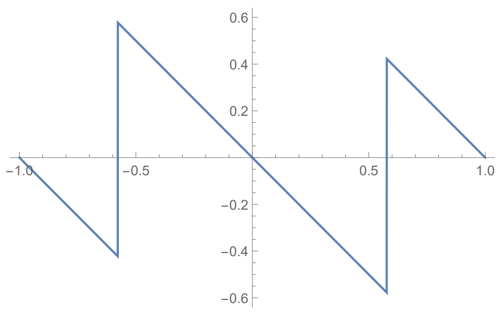


Figure 7: Second generating function for Gauss-Legendre rule

The error functional for the Gauss-Legendre quadrature rules are the same as previously defined in Equation 1.2, we only replace $[a, b]$ by $[-1, 1]$

$$E_n(f) = \int_{-1}^{1} u_n(t)df(t). \tag{7.2}$$

7.1. **Error bound for Gauss-Legendre rule, second generating function** $f(t) \in C^{(1)}[-1,1]$**.** The first error bound for the second generating function $u_2(t)$ is defined as

$$E_{21}(f) = \int_{-1}^{1} u_2(t) df(t) = \int_{-1}^{1} f'(\tau) u_2(\tau) d\tau. \tag{7.3}$$

The first subscript "2" in $E_{21}(f)$ indicates that we are dealing with 2 nodal points, the 2nd subscript indicates that the integrand belongs to the space $C^{(1)}$. This applies throughout the paper. Then

$$|E_{21}(f)| \leq \Big| \int_{-1}^{1} f'(\tau) u_2(\tau) d\tau \Big| \leq \int_{-1}^{1} \Big| f'(\tau) u_2(\tau) \Big| d\tau \leq \max|f'(t)| \int_{-1}^{1} |u_2(\tau)| d\tau. \tag{7.4}$$

$\int_{-1}^{1} |u_2(\tau)| d\tau = 0.512$ was calculated from Equation 7.1. Finally

$$|E_{21}(f)| \leq 0.512 \max_{[-1,1]} |f'(t)| \leq 0.512 \, \|f\| \,. \tag{7.5}$$

7.2. **Gauss-Legendre quadrature rule in case of two nodal points for** $f(t) \in C^{(2)}[-1,1]$**.** As before

$$E_{22}(f) = \int_{-1}^{1} u_2(\tau) df(\tau) = \int_{-1}^{1} f'(\tau) u_2(\tau) d\tau. \tag{7.6}$$

Let us denote $u_2(\tau) d\tau = dU_{22}(\tau)$, this means

$$E_{22}(f) = \int_{-1}^{1} f'(\tau) u_2(\tau) d(\tau) = \int_{-1}^{1} f'(\tau) dU_{22}(\tau), \tag{7.7}$$

where $U_{22}(t) = \int_{-1}^{t} u_2(\tau) d\tau$. Therefore

$$U_{22}(t) = \begin{cases} -\frac{1}{2}(t+1)^2, & \text{if } \; -1 \leq t < -\frac{1}{\sqrt{3}}, \\ -\frac{t^2}{2} - \frac{1}{2} + \frac{1}{\sqrt{3}}, & \text{if } \; -\frac{1}{\sqrt{3}} \leq t < \frac{1}{\sqrt{3}}, \\ -\frac{t^2}{2} + t - \frac{1}{2}, & \text{if } \; \frac{1}{\sqrt{3}} < t. \end{cases} \tag{7.8}$$

The graph of Equation 7.8 is shown in Figure 8(a). We know that

$$E_{22}(f) = \int_{-1}^{1} f'(\tau) dU_{22}(\tau) = -\int_{-1}^{1} f''(\tau) U_{22}(\tau) d\tau. \tag{7.9}$$

Then

$$|E_{22}(f)| \leq \Big| -\int_{-1}^{1} f''(\tau) U_{22}(\tau) d\tau \Big| \leq \max|f''(t)| \int_{-1}^{1} |U_{22}(\tau)| d\tau. \tag{7.10}$$

$\int_{-1}^{1} |U_{22}(\tau)| d\tau = 0.0812$, therefore

$$|E_{22}(f)| \leq 0.0812 \max|f''(t)| \leq 0.0812 \, \|f\|_2 \,. \tag{7.11}$$

7.3. **Gauss-Legendre quadrature rule in case of two nodal points for $f(t) \in C^{(3)}[-1,1]$.** The third error functional is

$$E_{23}(f) = \int_{-1}^{1} u_2(\tau) df(\tau). \tag{7.12}$$

$U_{22}(t)$ was obtained in Equation 7.8. The following definitions apply

$$\begin{aligned} E_{23}(f) &= \int_{-1}^{1} u_2(\tau) df(\tau) = \int_{-1}^{1} f'(\tau) u_2(\tau) d\tau = \int_{-1}^{1} f'(\tau) dU_{22}(\tau) \\ &= -\int_{-1}^{1} f''(\tau) U_{22}(\tau) d\tau = -\int_{-1}^{1} f''(\tau) dU_{23}(\tau) = \int_{-1}^{1} f'''(\tau) U_{23}(\tau) d\tau, \end{aligned} \tag{7.13}$$

The graph of $U_{23}(t)$ is illustrated in Figure 8(b).

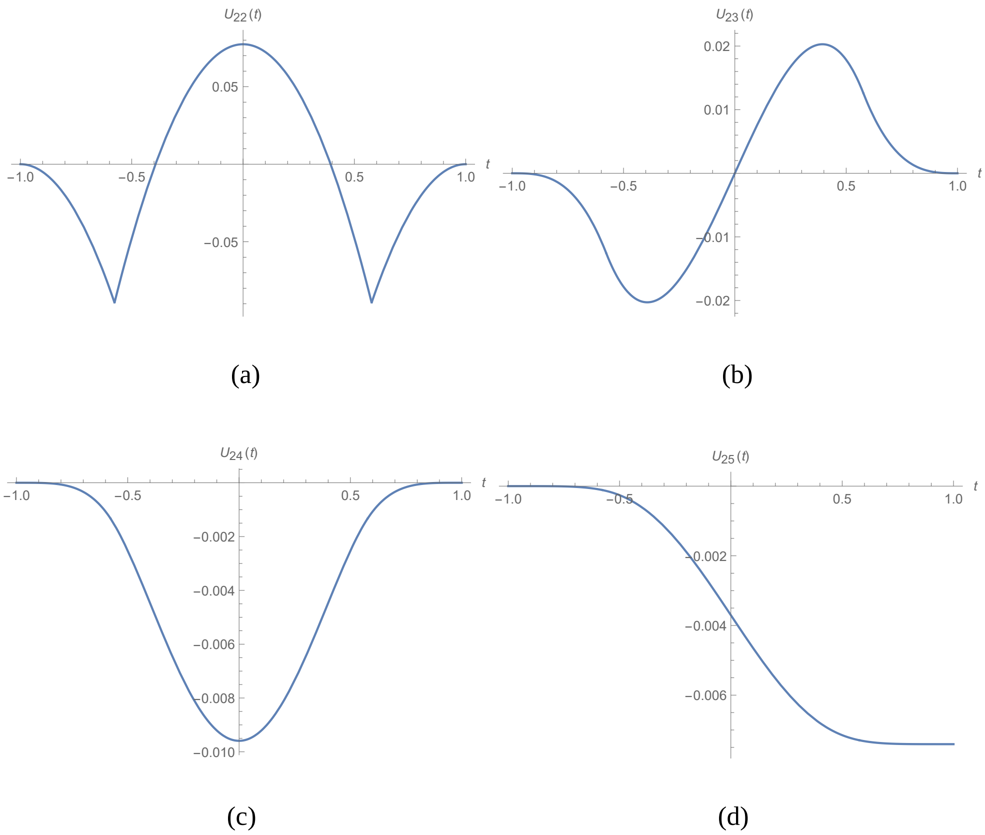


Figure 8: (a) Graph of $U_{22}(t)$ (b) Graph of $U_{23}(t)$ (c) Graph of $U_{24}(t)$ (d) Graph of $U_{25}(t)$

The following is valid

$$|E_{23}(f)| \leq \left| \int_{-1}^{1} f'''(\tau) U_{23}(\tau) d\tau \right| \leq \max|f'''(t)| \int_{-1}^{1} |U_{23}(\tau)| d\tau, \tag{7.14}$$

since $\int_{-1}^{1} |U_{23}(\tau)| d\tau = 0.0192$. If $f(t) \in C^{(3)}[-1,1]$, Equation 7.14 becomes

$$|E_{23}(f)| \leq 0.0192 \max|f'''(t)| \leq 0.0192 \, \|f\|_3 \, . \tag{7.15}$$

7.4. **Gauss-Legendre quadrature rule in case of two nodal points for** $f(t) \in C^{(4)}[-1,1]$**.** We define $E_{24}(f)$

$$E_{24}(f) = \int_{-1}^{1} f'''(\tau)U_{23}(\tau)d\tau = \int_{-1}^{1} f'''(\tau)dU_{24}(\tau) = -\int_{-1}^{1} f^{(4)}(\tau)U_{24}(\tau)d\tau, \tag{7.16}$$

The obtained function, $U_{24}(t)$, is graphically illustrated in Figure 8(c). The relations are valid

$$|E_{24}(f)| \leq \left| \int_{-1}^{1} f^{(4)}(\tau)U_{24}(\tau)d\tau \right| \leq \max|f^{(4)}(t)| \int_{-1}^{1} |U_{24}(\tau)|d\tau. \tag{7.17}$$

$\int_{-1}^{1} |U_{24}(\tau)|d\tau = \frac{1}{135}$. Finally

$$|E_{24}(f)| \leq \frac{1}{135} \max|f^{(4)}(t)| \leq \frac{1}{135} \|f\|_4 . \tag{7.18}$$

Remark: Using the Table 6.2, for $n = 2$ we obtain $c_2 = \frac{2}{5!}\left(\frac{4 \cdot 4}{4!}\right)^2 = \frac{1}{135}$. From the graph of $U_{24}(t)$, the integration of U_{24} from -1 to t will give a point at $t = 1$, whose value is different from zero (see Figure 8(d)). Therefore, if $f(t) \in C^{(5)}[-1,1]$, the substitution for the integration by parts will contain a term $\neq 0$. This means that the formula associated with the error for $f(t) \in C^{(5)}$ cannot be improved. This is the reason why in the literature, a formula related to an error is obtained for $f \in C^{(2n)}[-1,1]$ (in our case $f(t) \in C^{(4)}[-1,1]$) and not for $f(t) \in C^{(5)}$.

7.5. **Gauss-Legendre quadrature rule in case of two nodal points for** $f(t) \in C^{(5)}[-1,1]$**.** In what follows, we validate the preceding remark

$$E_{25}(f) = \int_{-1}^{1} f^{(4)}(\tau)U_{24}(\tau)d\tau = \int_{-1}^{1} f^{(4)}(\tau)dU_{25}(\tau), \tag{7.19}$$

After integration by parts

$$\int_{-1}^{1} f^{(4)}(\tau)dU_{25}(\tau) = \left[f^{(4)}(\tau)U_{25}(\tau)\right]_{-1}^{1} - \int_{-1}^{1} f^{(5)}(\tau)U_{25}(\tau)d\tau. \tag{7.20}$$

From Figure 8(d), $\left[f^{(4)}(\tau)U_{25}(\tau)\right]_{-1}^{1} \neq 0$. Therefore, the remark is validated.

8. THIRD GENERATING FUNCTION OF GAUSS-LEGENDRE RULE

Three nodal generating function for Gauss-Legendre rule is

$$\bar{\bar{u}}_3(t) = -t - 1 + \frac{5}{9}\theta^+\left(t + \sqrt{\frac{3}{5}}\right) + \frac{8}{9}\theta^+ + \frac{5}{9}\theta^+\left(t - \sqrt{\frac{3}{5}}\right). \tag{8.1}$$

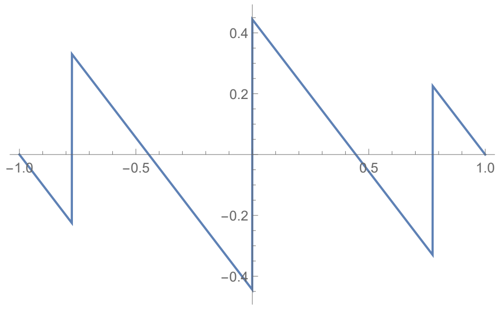


Figure 9: Third generating function for Gauss-Legendre rule

8.1. **Gauss-Legendre quadrature rule in case of three nodal points for** $f(t) \in C^{(1)}[-1,1]$**.** The first error bound $E_{31}(f)$ is

$$E_{31}(f) = \int_{-1}^{1} u_3(t)df(t) = \int_{-1}^{1} f'(\tau)u_3(\tau)d\tau. \tag{8.2}$$

From formula 8.2, we obtain

$$|E_{31}(f)| \leq \left| \int_{-1}^{1} f'(\tau)u_3(\tau)d\tau \right| \leq \int_{-1}^{1} \left| f'(\tau)u_3(\tau) \right| d\tau \leq \max|f'(t)| \int_{-1}^{1} |u_3(\tau)|d\tau. \tag{8.3}$$

$\int_{-1}^{1} |u_3(\tau)|d\tau = 0.357$, finally

$$|E_{31}(f)| \leq 0.357 \max_{[-1,1]} |f'(t)| \leq 0.357 \, \|f\| \, . \tag{8.4}$$

8.2. **Gauss-Legendre quadrature rule in case of three nodal points for** $f(t) \in C^{(2)}[-1,1]$**.**

$$E_{32}(f) = \int_{-1}^{1} f'(\tau)u_3(\tau)d\tau = \int_{-1}^{1} f'(\tau)dU_{32}(\tau), \tag{8.5}$$

Integration by parts is applied

$$\int_{-1}^{1} f'(\tau)dU_{32}(\tau) = [f'(\tau)U_{32}(\tau)]_{-1}^{1} - \int_{-1}^{1} f''(\tau)U_{32}(\tau)d\tau. \tag{8.6}$$

We integrate $u_3(\tau)$ to obtain $U_{32}(\tau)$ i.e. $U_{32}(\tau) = \int_{-1}^{t} u_3(\tau)d\tau$. Hence

$$U_{32}(t) = \begin{cases} -\frac{1}{2}(t+1)^2, & \text{if } \; -1 \leq t < -\sqrt{\frac{3}{5}}, \\ -\frac{t^2}{2} - \frac{4}{9}t - \frac{4}{3\sqrt{15}} + \sqrt{\frac{3}{5}} - \frac{1}{2}, & \text{if } \; -\sqrt{\frac{3}{5}} \leq t < 0, \\ -\frac{t^2}{2} + \frac{4}{9}t - \frac{4}{3\sqrt{15}} + \sqrt{\frac{3}{5}} - \frac{1}{2}, & \text{if } \; 0 \leq t < \sqrt{\frac{3}{5}}, \\ -\frac{t^2}{2} + t - \frac{1}{2}, & \text{if } \; \sqrt{\frac{3}{5}} < t. \end{cases} \tag{8.7}$$

$U_{32}(t)$ is graphically plotted in Figure 10(a).

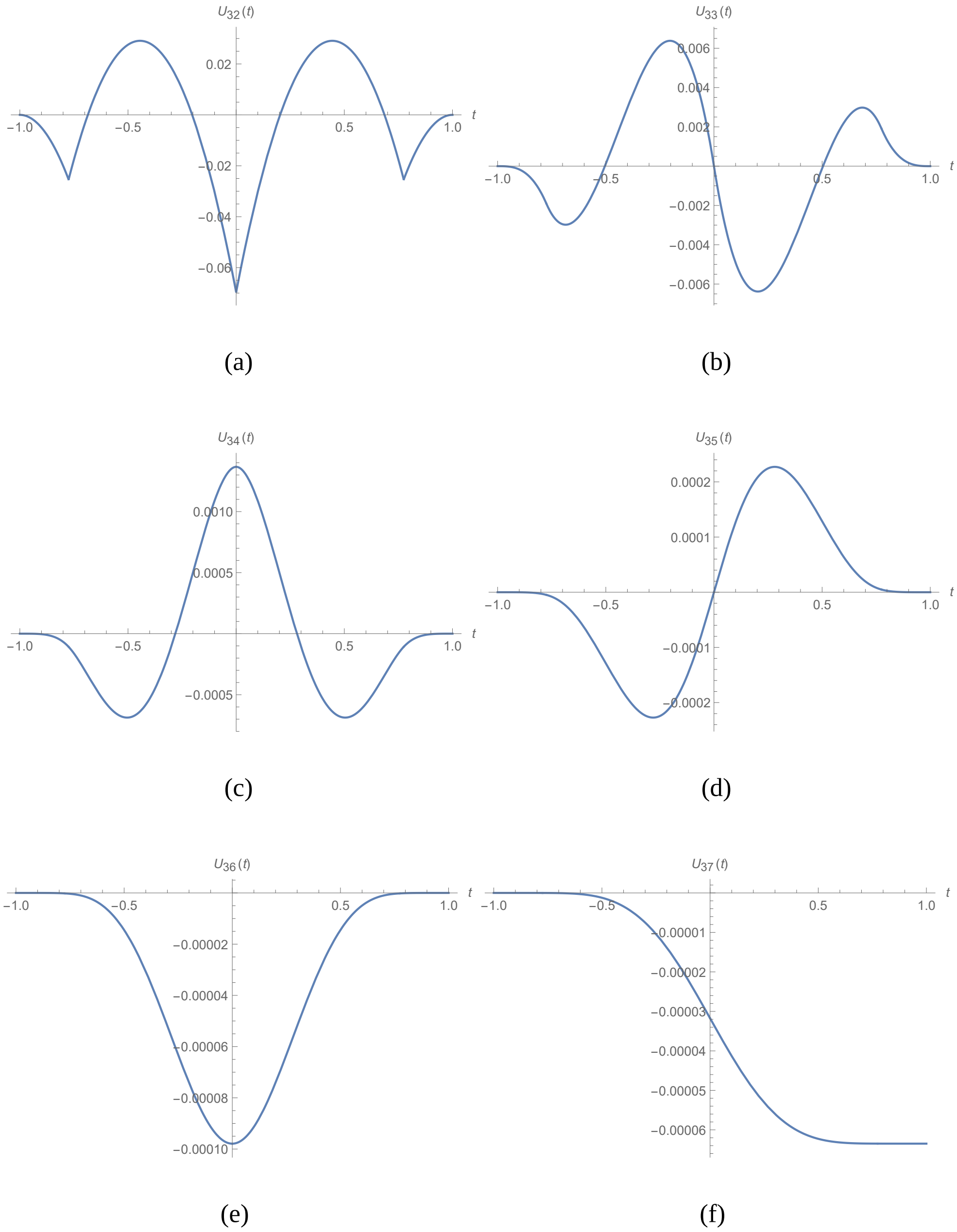


Figure 10: (a) Graph of $U_{32}(t)$ (b) Graph of $U_{33}(t)$ (c) Graph of $U_{34}(t)$ (d) Graph of $U_{35}(t)$ (e) Graph of $U_{36}(t)$ (f) Graph of $U_{37}(t)$

It is true that

$$|E_{32}(f)| \leq \left| \int_{-1}^{1} f''(\tau)U_{32}(\tau)d\tau \right| \leq \max|f''(t)| \int_{-1}^{1} |U_{32}(\tau)|d\tau. \tag{8.8}$$

$\int_{-1}^{1} |U_{32}(\tau)|d\tau = 0.0374$, thus

$$|E_{32}(f)| \leq 0.0374 \max|f''(t)| \leq 0.0374 \left\| f \right\|_2 . \tag{8.9}$$

8.3. **Gauss-Legendre quadrature rule in case of three nodal points for** $f(t) \in C^{(3)}[-1,1]$**.**

(8.10) $$E_{33}(f) = -\int_{-1}^{1} f''(\tau)U_{32}(\tau)d\tau = -\int_{-1}^{1} f''(\tau)dU_{33}(\tau),$$

We apply integration by parts

(8.11)
$$-\int_{-1}^{1} f''(\tau)dU_{33}(\tau) = -\left[f''(\tau)U_{33}(\tau)\right]_{-1}^{1} + \int_{-1}^{1} f'''(\tau)U_{33}(\tau)d\tau = \int_{-1}^{1} f'''(\tau)U_{33}(\tau)d\tau.$$

$U_{33}(t)$ is plotted in Figure 10(b). The following is valid

(8.12) $$|E_{33}(f)| \leq \left|\int_{-1}^{1} f'''(\tau)U_{33}(\tau)d\tau\right| \leq \max|f'''(t)| \int_{-1}^{1}|U_{33}(\tau)|d\tau.$$

$\int_{-1}^{1}|U_{33}(\tau)|d\tau = 0.00548$, finally

(8.13) $$|E_{33}(f)| \leq 0.00548 \max|f'''(t)| \leq 0.00548 \left\|f\right\|_3 .$$

8.4. **Gauss-Legendre quadrature rule in case of three nodal points for** $f(t) \in C^{(4)}[-1,1]$**.**

(8.14) $$E_{34}(f) = \int_{-1}^{1} f'''(\tau)U_{33}(\tau)d\tau = \int_{-1}^{1} f'''(\tau)dU_{34}(\tau),$$

We integrate as follows

(8.15)
$$\int_{-1}^{1} f'''(\tau)dU_{34}(\tau) = \left[f'''(\tau)U_{34}(\tau)\right]_{-1}^{1} - \int_{-1}^{1} f^{(4)}(\tau)U_{34}(\tau)d\tau = -\int_{-1}^{1} f^{(4)}(\tau)U_{34}(\tau)d\tau.$$

See Figure 10(c) for the graph of U_{34}. The following holds

(8.16) $$|E_{34}(f)| \leq \left|-\int_{-1}^{1} f^{(4)}(\tau)U_{34}(\tau)d\tau\right| \leq \max|f^{(4)}(t)| \int_{-1}^{1}|U_{34}(\tau)|d\tau.$$

$\int_{-1}^{1}|U_{34}(\tau)|d\tau = 0.000909$ and

(8.17) $$|E_{34}(f)| \leq 0.000909 \max|f^{(4)}(t)| \leq 0.000909 \left\|f\right\|_4 .$$

8.5. **Gauss-Legendre quadrature rule in case of three nodal points for** $f(t) \in C^{(5)}[-1,1]$**.**

(8.18) $$E_{35}(f) = -\int_{-1}^{1} f^{(4)}(\tau)U_{34}(\tau)d\tau = -\int_{-1}^{1} f^{(4)}(\tau)dU_{35}(\tau),$$

We integrate Equation 8.18

(8.19)
$$-\int_{-1}^{1} f^{(4)}(\tau)dU_{35}(\tau) = -\left[f^{(4)}(\tau)U_{35}(\tau)\right]_{-1}^{1} + \int_{-1}^{1} f^{(5)}(\tau)U_{35}(\tau)d\tau = \int_{-1}^{1} f^{(5)}(\tau)U_{35}(\tau)d\tau.$$

$U_{35}(\tau)$ is graphically illustrated in Figure 10(d). Now, the following is true

(8.20) $$|E_{35}(f)| \leq \left|\int_{-1}^{1} f^{(5)}(\tau)U_{35}(\tau)d\tau\right| \leq \max|f^{(5)}(t)| \int_{-1}^{1}|U_{35}(\tau)|d\tau.$$

$\int_{-1}^{1}|U_{35}(\tau)|d\tau = 0.000196$ and

(8.21) $$|E_{35}(f)| \leq 0.000196 \max|f^{(5)}(t)| \leq 0.000196 \left\|f\right\|_5 .$$

8.6. **Gauss-Legendre quadrature rule in case of three nodal points for** $f(t) \in C^{(6)}[-1,1]$**.**

$$E_{36}(f) = \int_{-1}^{1} f^{(5)}(\tau)U_{35}(\tau)d\tau = \int_{-1}^{1} f^{(5)}(\tau)dU_{36}(\tau), \tag{8.22}$$

We integrate Equation 8.22
(8.23)

$$\int_{-1}^{1} f^{(5)}(\tau)dU_{36}(\tau) = \left[f^{(5)}(\tau)U_{36}(\tau)\right]_{-1}^{1} - \int_{-1}^{1} f^{(6)}(\tau)U_{36}(\tau)d\tau = -\int_{-1}^{1} f^{(6)}(\tau)U_{36}(\tau)d\tau.$$

$U_{36}(\tau) = \int_{-1}^{t} U_{35}(\tau)$, the result of which is plotted in Figure 10(e). Then

$$|E_{36}(f)| \leq \left| -\int_{-1}^{1} f^{(6)}(\tau)U_{36}(\tau)d\tau \right| \leq \max|f^{(6)}(t)| \int_{-1}^{1} |U_{36}(\tau)|d\tau. \tag{8.24}$$

$\int_{-1}^{1} |U_{36}(\tau)|d\tau = \frac{1}{15750}$ and

$$|E_{36}(f)| \leq \frac{1}{15750} \max|f^{(6)}(t)| \leq \frac{1}{15750} \|f\|_6 \, . \tag{8.25}$$

Remark: Using the Table 6.2, for $n = 3$ we obtain $c_3 = \frac{2}{7!}\left(\frac{8 \cdot 36}{6!}\right)^2 = \frac{1}{15750}$. From the graph of $U_{36}(t)$, it is clear that the integration of U_{36} from -1 to 1, will result in a point $t = 1$, whose value is different from zero (see Figure 10(f)). Therefore, if $f(t) \in C^{(7)}[-1,1]$, the substitution for the integration by parts will contain a term $\neq 0$. This means that the formula associated with the error for $f(t) \in C^{(7)}$ cannot be improved.

8.7. **Gauss-Legendre quadrature rule in case of three nodal points for** $f(t) \in C^{(7)}[-1,1]$**.**

$$E_{37}(f) = -\int_{-1}^{1} f^{(6)}(\tau)U_{36}(\tau)d\tau = -\int_{-1}^{1} f^{(6)}(\tau)dU_{37}(\tau), \tag{8.26}$$

The integration of Equation 8.26 is

$$-\int_{-1}^{1} f^{(6)}(\tau)dU_{37}(\tau) = -\left[f^{(6)}(\tau)U_{37}(\tau)\right]_{-1}^{1} + \int_{-1}^{1} f^{(7)}(\tau)U_{37}(\tau)d\tau. \tag{8.27}$$

From Figure 10(f), $\left[f^{(6)}(\tau)U_{37}(\tau)\right]_{-1}^{1} \neq 0$. Hence, the error bound cannot be improved. The approach applied under Sections 7 and 8 can be used to estimate the error bounds for the fourth and fifth generating functions of the Gauss-Legendre quadrature rules.

9. SUMMARY

The error bounds of selected Newton-Cotes formulas for lower order derivatives were estimated in this paper. We found that the accuracy of the fourth error bound for the Simpson's $1/3$ and $3/8$ rule cannot be improved. The error bounds for the second, and third generating function of the Gauss-Legendre quadrature rules were also evaluated. The findings in this paper agrees with results in the literature and are particularly useful for undergraduate courses on numerical analysis.

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