

## SOME MODIFICATIONS OF THE TRAPEZOIDAL RULE

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ABSTRACT. By using the quadratic interpolating spline a new class of the quadrature rules was obtained. Those formulas are modifications of the well known trapezoidal rule. The basic characteristic of those formulas is a free parameter. With appropriate choice of that parameter, accuracy of the trapezoidal rule can be improved up to  $O(h^4)$ . Besides this, by using this nonstandard techniques some well known quadrature rules were also obtained.

### 1. INTRODUCTION AND PRELIMINARIES

**1.1. Classical quadrature rules.** Classical quadrature rules are studied at basic courses in numerical analysis and they are here just used to provide an system of notation.

Let  $a = x_0 < x_1 < \dots < x_{2m} = b$ , where  $x_k = x_0 + kh$  and let  $f_k = f(x_k)$ ,  $0 \leq k \leq 2m$ . Then

$$\int_a^b f(x)dx = Q_R[f, a, b, 2m] + E_R[f, a, b, 2m],$$

or

$$\int_a^b f(x)dx = Q_S[f, a, b, 2m] + E_S[f, a, b, 2m],$$

where

$$Q_R[f, a, b, 2m] = 2h \sum_{k=1}^m f_{2k-1} \quad (1)$$

is a generalized rule for the central rectangles, while

$$Q_S[f, a, b, n] = \frac{h}{3} \left( f_0 + 2 \sum_{k=1}^{m-1} f_{2k} + 4 \sum_{k=1}^m f_{2k-1} + f_{2m} \right) \quad (2)$$

is a generalized Simpsons rule. Errors of those formulas are respectively:

$$E_R[f, a, b, 2m] = \frac{(b-a)f''(\bar{\xi}_R)}{6} h^2, \quad (3)$$

for some  $\bar{\xi}_R \in [a, b]$ , supposing  $f \in C^2[a, b]$  and

$$E_S[f, a, b, 2m] = -\frac{(b-a)f^{iv}(\bar{\xi}_S)}{180} h^4, \quad (4)$$

for some  $\bar{\xi}_S \in [a, b]$ , supposing  $f \in C^4[a, b]$ . Furthermore, if  $a = x_0 < x_1 < \dots < x_n = b$ , then

$$\int_a^b f(x)dx = Q_T[f, a, b, n] + E_T[f, a, b, n],$$

where

$$Q_T[f, a, b, n] = \frac{h}{2} \left( f_0 + 2 \sum_{k=1}^{n-1} f_k + f_n \right)$$

is the generalized trapezoidal rule and

$$E_T[f, a, b, n] = -\frac{(b-a)f''(\bar{\xi}_T)}{12} h^2,$$

for some  $\bar{\xi}_T \in [a, b]$ , supposing  $f \in C^2[a, b]$ , is error for this rule.

**1.2. Quadratic interpolating spline.** Since that quadratic interpolating spline is usually avoided in the literature, basic details about its construction are presented here (the cubic spline is most often considered, see [1, 3]).

**Definition 1.** Let  $\Delta = \{a = x_0 < x_1 < \dots < x_n = b\}$  be partition of the interval  $[a, b]$ . The function  $S_\Delta : [a, b] \rightarrow \mathbb{R}$ , with the following properties:

1.  $S_\Delta$  is a polynomial of the second degree in every subinterval  $[x_k, x_{k+1}]$ ,  $0 \leq k \leq n-1$  and
2.  $S_\Delta \in C^1[a, b]$

is called the quadratic spline in relation to the partition  $\Delta$ . If the interpolating properties

$$\bullet S_\Delta(x_k) = f(x_k), 0 \leq k \leq n$$

are added to the previous definition, the quadratic interpolating spline of the function  $f$  will be obtained, usually denoted by  $S_{\Delta, f}$ .

Let the values  $f_k = f(x_k)$ ,  $0 \leq k \leq n$ , of the function  $f$ , be given. From the property 1. of the Definition 1, it follows that

$$x \in [x_k, x_{k+1}] \Rightarrow S_{\Delta, f}(x) = a_k x^2 + b_k x + c_k = s_k(x), 0 \leq k \leq n-1,$$

which means that there are  $3n$  unknown coefficients. To determine those coefficients  $2n$  equations will be obtained from the interpolating properties, while  $n-1$  equations will be obtained from property 2. of the same definition.

So, there is one parameter which can be chosen freely. The mentioned equations are:

$$a_k x_k^2 + b_k x_k + c_k = f_k, \quad 0 \leq k \leq n-1, \quad (5)$$

$$a_k x_{k+1}^2 + b_k x_{k+1} + c_k = f_{k+1}, \quad 0 \leq k \leq n-1, \quad (6)$$

$$2a_k x_{k+1} + b_k = 2a_{k+1} x_{k+1} + b_{k+1}, \quad 0 \leq k \leq n-2. \quad (7)$$

After subtracting equation (5) from equation (6) we obtain:

$$b_k = \frac{f_{k+1} - f_k}{x_{k+1} - x_k} - a_k(x_{k+1} + x_k).$$

The last equation, together with equation (7), after elementary calculation gives the recurrence formulas for calculating the coefficients  $a_k$ ,  $1 \leq k \leq n-1$ . Hence, the coefficients of the quadratic interpolating spline can be calculated in the following way:

$$\begin{aligned} a_0 & - \text{arbitrary,} \\ a_{k+1} & = \frac{f_{k+2} - f_{k+1}}{(x_{k+2} - x_{k+1})^2} - \frac{f_{k+1} - f_k}{(x_{k+2} - x_{k+1})(x_{k+1} - x_k)} \\ & \quad - a_k \frac{x_{k+1} - x_k}{x_{k+2} - x_{k+1}}, \quad 0 \leq k \leq n-2, \\ b_k & = \frac{f_{k+1} - f_k}{x_{k+1} - x_k} - a_k(x_{k+1} + x_k), \quad 0 \leq k \leq n-1, \\ c_k & = f_k - a_k x_k^2 - b_k x_k, \quad 0 \leq k \leq n-1. \end{aligned} \quad (8)$$

By using the formulas (8), again after elementary calculations, the basic modification of the trapezoidal rule will be obtained:

$$\begin{aligned} \int_{x_k}^{x_{k+1}} f(x) dx & = \int_{x_k}^{x_{k+1}} s_k(x) dx + E[f, x_k, x_{k+1}] \\ & = (x_{k+1} - x_k) \left[ \frac{1}{2}(f_{k+1} + f_k) \right. \\ & \quad \left. - \frac{a_k}{6}(x_{k+1} - x_k)^2 \right] + E[f, x_k, x_{k+1}]. \end{aligned}$$

If the partition of the interval  $[a, b]$  is uniform, i.e. if  $x_k = x_0 + kh$ ,  $0 \leq k \leq n$ , where  $x_0 = a$  and  $h = \frac{b-a}{n}$ , then the first relation in (8) and the previous relation becomes much more simple:

$$\begin{aligned} a_k & = \frac{f_{k+1} - 2f_k + f_{k-1}}{h^2} - a_{k-1} \\ & = \sum_{i=1}^k (-1)^{k-i} \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} + (-1)^k a_0, \quad 1 \leq k \leq n-1 \end{aligned} \quad (9)$$

and

$$\int_{x_k}^{x_{k+1}} f(x)dx = \frac{h}{2}(f_k + f_{k+1}) - \frac{h^3}{6}a_k + E[f, x_k, x_{k+1}], \quad 0 \leq k \leq n-1. \quad (10)$$

Generalized formula (10) is

$$\int_a^b f(x)dx = Q_T[f, a, b, n] - \frac{h^3}{6} \sum_{k=0}^{n-1} a_k + E[f, a, b, n]. \quad (11)$$

## 2. BASIC RESULTS

### 2.1. The case $n = 2m$ .

2.1.1. *Simpsons rule.* From the relations (9) and (11) it follows

$$\int_a^b f(x)dx = Q[f, a, b, 2m] + E[f, a, b, 2m],$$

where

$$\begin{aligned} Q[f, a, b, 2m] &= \frac{h}{2} \left( f_0 + 2 \sum_{k=1}^{2m-1} f_k + f_{2m} \right) - \frac{h^3}{6} \sum_{k=0}^{2m-1} a_k \\ &= \frac{h}{2} \left( f_0 + 2 \sum_{k=1}^{2m-1} f_k + f_{2m} \right) \\ &\quad - \frac{h^3}{6} \sum_{k=1}^m \frac{f_{2k} - 2f_{2k-1} + f_{2k-2}}{h^2} \\ &= Q_S[f, a, b, 2m]. \end{aligned} \quad (12)$$

Now from (4) it follows that

$$E[f, a, b, 2m] = E_S[f, a, b, 2m] = -\frac{(b-a)f^{iv}(\bar{\xi}_S)}{180} h^4,$$

for some  $\bar{\xi}_S \in [a, b]$ , assuming  $f \in C^4[a, b]$ .

2.1.2. *The first modification.* If the equation

$$\frac{f_{2k} - 2f_{2k-1} + f_{2k-2}}{h^2} = f''_{2k-1} + \frac{f^{iv}(\tau_k)}{12} h^2,$$

(for some  $\tau_k \in [x_{2k-2}, x_{2k}]$ , assuming  $f \in C^4[a, b]$ ) is put in (12), the first modification of the trapezoidal rule will be obtained

$$\int_a^b f(x)dx = Q_1[f, a, b, 2m] + E_1[f, a, b, 2m],$$

where

$$Q_1[f, a, b, 2m] = \frac{h}{2} \left( f_0 + 2 \sum_{k=1}^{2m-1} f_k + f_{2m} \right) - \frac{h^3}{6} \sum_{k=1}^m f''_{2k-1} \quad (13)$$

and

$$\begin{aligned} E_1[f, a, b, 2m] &= -\frac{(b-a)f^{iv}(\bar{\xi}_S)}{180} h^4 - \frac{h^3}{6} \sum_{k=1}^m \frac{h^2}{12} f^{iv}(\tau_k) \\ &= -\frac{(b-a)f^{iv}(\bar{\xi}_S)}{180} h^4 - \frac{(b-a)f^{iv}(\bar{\tau})}{144} h^4 \\ &= -\frac{(b-a)f^{iv}(\bar{\tau}_1)}{80} h^4, \end{aligned}$$

for some  $\bar{\tau}_1 \in [a, b]$ .

2.1.3. *The second modification.* Formulas (1) and (3) together give:

$$f'_{2m} - f'_0 = \int_{x_0}^{x_{2m}} f''(x) dx = 2h \sum_{k=1}^m f''_{2k-1} + \frac{(b-a)f^{iv}(\bar{\xi}_R)}{6} h^2,$$

and from this relation follows the second modification of the trapezoidal rule (well known Hermits quadrature rule, for example see [2, 3]). Hence:

$$\int_a^b f(x) dx = Q_2[f, a, b, 2m] + E_2[f, a, b, 2m],$$

where

$$Q_2[f, a, b, 2m] = \frac{h}{2} \left( f_0 + 2 \sum_{k=1}^{2m-1} f_k + f_{2m} \right) - \frac{h^2}{12} (f'_{2m} - f'_0) \quad (14)$$

and

$$\begin{aligned} E_2[f, a, b, 2m] &= \frac{(b-a)f^{iv}(\bar{\xi}_R)}{72} h^4 - \frac{(b-a)f^{iv}(\bar{\tau}_1)}{80} h^4 \\ &= \frac{b-a}{720} (10f^{iv}(\bar{\xi}_R) - 9f^{iv}(\bar{\tau}_1)) h^4, \end{aligned} \quad (15)$$

for some  $\bar{\xi}_R, \bar{\tau}_1 \in [a, b]$ .

The estimation of the error (15) is much less exact then the estimation which can be found in [2], but these estimations becomes equal if we assume that  $10f^{iv}(\bar{\xi}_R) - 9f^{iv}(\bar{\tau}_1) \in [m_4, M_4]$ , where  $m_4 = \min_{x \in [a, b]} f^{iv}(x)$  and  $M_4 = \max_{x \in [a, b]} f^{iv}(x)$ .

One can check that both of formulas (13) and (14) are exact for all polynomials of the third degree.

2.2. **The case  $n = 2m + 1$ .** Combining the formulas (2) and (10) gives

$$\begin{aligned} \int_a^b f(x)dx &= \int_{x_0}^{x_1} f(x)dx + \int_{x_1}^{x_{2m+1}} f(x)dx \\ &= Q_T[f, x_0, x_1] - \frac{h^3}{6}a_0 + Q_S[f, x_1, b, 2m] \\ &\quad + E[f, a, b, 2m + 1], \end{aligned} \quad (16)$$

where  $Q_T[f, x_0, x_1] = \frac{h}{2}(f_0 + f_1)$ , and parameter  $a_0$  can be chosen arbitrarily. In general, accuracy of the previous rule is  $O(h^3)$ , but it can be improved up to  $O(h^4)$  with an appropriate choice of the parameter  $a_0$ . One of the possibilities is to choose the parameter  $a_0$  to be equal to the main part of the reminder  $E_T[f, x_0, x_1] = -\frac{f''(\xi_T)}{12}h^3$ ,  $\xi_T \in [x_0, x_1]$ .

2.2.1. *The first modification.* For every  $\lambda \in [0, 1]$ , there exists (at least one)  $X \in [x_0, x_1]$  such that  $f''(X) = \lambda f''_0 + (1 - \lambda)f''_1$ . Then

$$f''(\xi_T) = f''(X) + f'''(\theta)(\xi_T - X), \theta \in [\xi_T, X],$$

so that with the choice  $a_0 = \frac{f''(X)}{2}$  we get:

$$\int_a^b f(x)dx = Q_1[f, a, b, 2m + 1] + E_1[f, a, b, 2m + 1],$$

where

$$Q_1[f, a, b, 2m + 1] = \frac{h}{2}(f_0 + f_1) - \frac{h^3 f''(X)}{12} + Q_S[f, x_1, b, 2m] \quad (17)$$

and

$$E_1[f, a, b, 2m + 1] = -\frac{f'''(\theta)}{12}(\xi_T - X)h^3 - \frac{(b - x_1)f^{iv}(\bar{\xi}_S)}{180}h^4,$$

for some  $\xi_T, X \in [x_0, x_1]$ ,  $\theta \in [\xi_T, X]$ ,  $\bar{\xi}_S \in [x_1, b]$ .

The combination of the formulas (13) and (17) gives

$$\int_a^b f(x)dx = \tilde{Q}_1[f, a, b, 2m + 1] + \tilde{E}_1[f, a, b, 2m + 1],$$

where

$$\tilde{Q}_1[f, a, b, 2m + 1] = \frac{h}{2} \left( f_0 + 2 \sum_{k=1}^{2m} f_k + f_{2m+1} \right) - \frac{h^3}{6} \left( \frac{f''(X)}{2} + \sum_{k=1}^m f''_{2k} \right)$$

and

$$\tilde{E}_1[f, a, b, 2m + 1] = -\frac{f'''(\theta)}{12}(\xi_T - X)h^3 - \frac{(b - x_1)f^{iv}(\bar{\tau}_1)}{80}h^4$$

for some  $\xi_T, X \in [x_0, x_1], \theta \in [\xi_T, X], \bar{\tau}_1 \in [x_1, b]$ .

2.2.2. *The second modification.* Since we have

$$f''(\xi_T) = \frac{f'_1 - f'_0}{h} - \frac{(x_1 - \xi_T)^2 f'''(\theta_1) - (x_0 - \xi_T)^2 f'''(\theta_0)}{2h},$$

for some  $\theta_0 \in [x_0, \xi_T], \theta_1 \in [\xi_T, x_1]$ , the choice  $a_0 = \frac{f'_1 - f'_0}{2h}$  gives

$$\int_a^b f(x)dx = Q_2[f, a, b, 2m+1] + E_2[f, a, b, 2m+1],$$

where

$$Q_2[f, a, b, 2m+1] = \frac{h}{2}(f_0 + f_1) - \frac{h^2}{12}(f'_1 - f'_0) + Q_S[f, x_1, b, 2m] \quad (18)$$

and

$$E_2[f, a, b, 2m+1] = \frac{(x_1 - \xi_T)^2 f'''(\theta_1) - (x_0 - \xi_T)^2 f'''(\theta_0)}{24} h^2 - \frac{(b - x_1) f^{iv}(\bar{\xi}_S)}{180} h^4,$$

for some  $\theta_0 \in [x_0, \xi_T], \theta_1 \in [\xi_T, x_1], \bar{\xi}_S \in [x_1, b]$ . Similarly as in the previous case, the formulas (14) and (18) together give

$$\int_a^b f(x)dx = \tilde{Q}_2[f, a, b, 2m+1] + \tilde{E}_2[f, a, b, 2m+1],$$

where

$$\tilde{Q}_2[f, a, b, 2m+1] = \frac{h}{2} \left( f_0 + 2 \sum_{k=1}^{2m} f_k + f_{2m+1} \right) - \frac{h^3}{12} (f'_{2m+1} - f'_0)$$

(again Hermits quadrature rule) and

$$\tilde{E}_2[f, a, b, 2m+1] = \frac{(x_1 - \xi_T)^2 f'''(\theta_1) - (x_0 - \xi_T)^2 f'''(\theta_0)}{24} h^2 - \frac{(b - x_1) h^4}{720} (10 f^{iv}(\bar{\xi}_R) - 9 f^{iv}(\bar{\tau}_1)),$$

for some  $\theta_0 \in [x_0, \xi_T], \theta_1 \in [\xi_T, x_1], \bar{\xi}_R, \bar{\tau}_1 \in [x_1, b]$ .

**2.3. Another possibility for the choice of the parameter  $a_0$ .** One can check that the parameter  $a_0$  can not be chosen in a such way that formula (16) (without the last term) integrates exactly all polynomials with degree not greater than three. But, if  $P(x) = Ax^3 + Bx^2 + Cx + D$ , with the choice

$$a_0 = B + 3A(x_0 + \frac{h}{2}), \quad (19)$$

the formula (16) will be true for the polynomial  $P$ .

Furthermore, for every  $X \in [x_0, x_1]$  one has

$$f(x) \approx f(X) + f'(X)(x - X) + \frac{1}{2}f''(X)(x - X)^2 + \frac{1}{6}f'''(X)(x - X)^3,$$

and in accordance with (19), with the choice

$$a_0 = \frac{1}{2}[f''(X) + f'''(X)(x_0 + \frac{h}{2} - X)],$$

the formula (16) (again without the last term) becomes exact for the “main part” of the function  $f$ . Hence,

$$\int_a^b f(x)dx = \bar{Q}_2[f, a, b, 2m + 1] + \bar{E}_2[f, a, b, 2m + 1].$$

In the last formula one has

$$\begin{aligned} \bar{Q}_2[f, a, b, 2m + 1] = Q_T[f, x_0, x_1] - \frac{h^3}{12}[f''(X) + f'''(X)(x_0 + \frac{h}{2} - X)] \\ + Q_S[f, x_1, b, 2m], \end{aligned}$$

while the order of accuracy is still  $O(h^4)$ , since

$$f''(\xi_T) = f''(X) + f'''(X)(\xi_T - X) + \frac{1}{2}f^{iv}(\theta)(\xi_T - X)^2,$$

and finally

$$\bar{E}_2 = -\frac{(\xi_T - x_0 - \frac{h}{2})f'''(X) + \frac{1}{2}(\xi_T - X)^2 f^{iv}(\theta)}{12}h^3 - \frac{(b - x_1)f^{iv}(\bar{\xi}_S)}{180}h^4.$$

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