Bogusław Bożek, Wiesław Solak, Zbigniew Szydełko

A NOTE ON A FAMILY OF QUADRATURE FORMULAS AND SOME APPLICATIONS

Abstract. In this paper a construction of a one-parameter family of quadrature formulas is presented. This family contains the classical quadrature formulas: trapezoidal rule, midpoint rule and two-point Gauss rule. One can prove that for any continuous function there exists a parameter for which the value of quadrature formula is equal to the integral. Some applications of this family to the construction of cubature formulas, numerical solution of ordinary differential equations and integral equations are presented.

Keywords: quadrature and cubature formulas, numerical integration.

Mathematics Subject Classification: 65D30, 65D32, 65L05, 65L06, 65R20.

1. INTRODUCTION

We will introduce a one-parameter family of quadrature formulas which contains the classical quadrature formulas: trapezoidal rule and midpoint rule.

We consider a family of quadrature formulas

$$Q^{\beta}(f) = \frac{h}{2} \sum_{j=0}^{n-1} \left(f(a+jh+\beta h) + f(a+(j+1)h-\beta h) \right)$$
 (1)

for the integral $I(f)=\int_a^b f(x)\ dx$, where $\beta\in\left[0,\frac{1}{2}\right],\ h=\frac{b-a}{n},\ n\geq 1$ and $f\in C[a,b].$ Let us note that $Q^0=T_{n+1}$ and $Q^{\frac{1}{2}}=M_n$, where

$$T_{n+1}(f) = h\left(\frac{1}{2}(f(a) + f(b)) + \sum_{j=1}^{n-1} f(a+jh)\right)$$

is the trapezoidal rule, while

$$M_n(f) = h \sum_{j=0}^{n-1} f(a + (j + \frac{1}{2})h),$$

is the midpoint rule.

The first part of this paper is devoted to answering the questions on the order of quadrature formula and its error estimate

$$E^{\beta}(f) = I(f) - Q^{\beta}(f), \tag{2}$$

as well as other questions, for example, on whether in a given family there exists a quadrature formula "bringing out" an exact value of integral, or the question of when Q^{β} considered as a function in the variable β (with f fixed) is monotone, or what is the relation between the order of quadrature formula and the parameter β .

In the second part of the paper, some applications of this family to the construction of cubature formulas, numerical solution of one-dimensional Fredholm equation of the second kind and ordinary differential equations are showed.

2. PROPERTIES OF THE FAMILY Q^{β}

Let f be a real-valued function defined on an interval [a, b] and a sequence of points $\{x_j\}$ for $j = 0, 1, \ldots, n$, given as follows

$$x_j = a + jh, \qquad h = \frac{b-a}{n}.$$

We define the following functions F_j and F in the variable $\beta \in [0, 1]$:

$$F_j(\beta) = f(x_j + \beta h) + f(x_{j+1} - \beta h), \qquad j = 0, 1, \dots, n-1,$$

$$F(\beta) = \sum_{j=0}^{n-1} F_j(\beta).$$

Making use of these notations, formula (1) becomes

$$Q^{\beta}(f) = \frac{h}{2}F(\beta).$$

Proposition 1. If the function f is continuous on interval [a,b], then there exists a $\bar{\beta} \in [0,\frac{1}{2}]$ such that

$$\int_{a}^{b} f(x) dx = Q^{\bar{\beta}}(f).$$

Proof. Let us note that making the substitution $x = x_j + \beta h$ in the integral $\int_{x_j}^{x_{j+1}} f(x) dx$ we get $h \int_0^1 f(x_j + \beta h) d\beta$, and by substitution $x = x_{j+1} - \beta h$ we obtain $h \int_0^1 f(x_{j+1} - \beta h) d\beta$, that is

$$2\int_{x_{j}}^{x_{j+1}} f(x) dx = h \int_{0}^{1} F_{j}(\beta) d\beta,$$

and hence

$$\int_{a}^{b} f(x) dx = \sum_{j=0}^{n-1} \int_{x_{j}}^{x_{j+1}} f(x) dx = \sum_{j=0}^{n-1} \frac{h}{2} \int_{0}^{1} F_{j}(\beta) d\beta =$$

$$= \frac{h}{2} \int_{0}^{1} \left(\sum_{j=0}^{n-1} F_{j}(\beta) \right) d\beta = \frac{h}{2} \int_{0}^{1} F(\beta) d\beta = \frac{h}{2} F(\bar{\beta})$$

with a certain $\bar{\beta} \in [0, 1]$. The last passage is correct because the continuity of f(x) on [a, b] implies the continuity of $F(\beta)$ on [0, 1]. We obtain the assertion of this theorem noticing that $F(\beta)$ is symmetric with respect to $\beta = \frac{1}{2}$, that is to say $F(\frac{1}{2} + \beta) = F(\frac{1}{2} - \beta)$.

Under some additional assumptions, the function $F(\beta)$ is monotone. The following assertion is true

Proposition 2. If f is a convex (concave) function on [a,b], then $F(\beta)$ is decreasing (increasing) on the interval $[0,\frac{1}{2}]$.

Proof. Let $0 \le \beta_1 < \beta_2 \le \frac{1}{2}$. Since the function f is convex on [a, b], then, for $j = 0, 1, \ldots, n-1$ with $\mu = (\beta_1 + \beta_2 - 1)(2\beta_1 - 1)^{-1}$ and $\nu = (\beta_1 - \beta_2)(2\beta_1 - 1)^{-1}$, there holds

$$f(x_j + \beta_2 h) \le \mu f(x_j + \beta_1 h) + (1 - \mu) f(x_j + (1 - \beta_1) h) f(x_j + (1 - \beta_2) h) \le \nu f(x_j + \beta_1 h) + (1 - \nu) f(x_j + (1 - \beta_1) h).$$

From these two inequalities and the relation $\mu + \nu = 1$, there follows

$$f(x_j + \beta_2 h) + f(x_j + (1 - \beta_2)h) \le (\mu + \nu)f(x_j + \beta_1 h) + + (2 - (\mu + \nu))f(x_j + (1 - \beta_1)h) = = f(x_j + \beta_1 h) + f(x_j + (1 - \beta_1)h).$$

This means that $F_j(\beta_1) \geq F_j(\beta_2)$ for j = 0, ..., n-1 and, in consequence, $F(\beta_1) \geq F(\beta_2)$.

Let us note that the values of quadrature formulas M_n and T_{n+1} for function f satisfying the assumptions of Theorem 2 determine an interval containing I(f).

Remark 1. If f is a convex function on [a, b], then

$$M_n(f) = Q^{\frac{1}{2}}(f) \le Q^{\beta}(f) \le Q^0(f) = T_{n+1}(f)$$

and if f is a concave function on [a,b], then we have

$$T_{n+1}(f) = Q^0(f) \le Q^{\beta}(f) \le Q^{\frac{1}{2}}(f) = M_n(f)$$

for each $\beta \in (0, \frac{1}{2})$.

2.1. ERROR ESTIMATE

For monomials 1, x, x^2 , x^3 , x^4 , ... the error of quadrature formula (1) is given by:

$$\begin{split} E^{\beta}(1) &= E^{\beta}(x) = 0, \\ E^{\beta}(x^2) &= -\frac{(b-a)h^2}{6} \left(6\beta^2 - 6\beta + 1 \right), \\ E^{\beta}(x^3) &= -\frac{(b^2 - a^2)h^2}{4} \left(6\beta^2 - 6\beta + 1 \right), \\ E^{\beta}(x^4) &= -\frac{h^3}{30n} \bigg(30(b-a)^2\beta^2(\beta-1)^2 + \\ &\qquad \qquad + 10n^2 \big(a^2 + b^2 + ab \big) \big(6\beta^2 - 6\beta + 1 \big) - (b-a)^2 \bigg). \end{split}$$

Thus, the quadrature $Q^{\beta}(f)$ is of the second order for $\beta \neq \bar{\beta} = \frac{3-\sqrt{3}}{6} = \frac{1}{3+\sqrt{3}}$ ($\bar{\beta}$ is a root of the equation $6\beta^2 - 6\beta + 1 = 0$), and for $\beta = \bar{\beta}$, it is of the fourth order, because then

$$E^{\bar{\beta}}(x^i) = 0 \quad \text{for} \quad i = 0, 1, 2, 3, \qquad E^{\bar{\beta}}(x^4) = \frac{(b-a)h^4}{180}.$$
 (3)

In particular, the quadrature formulas T_{n+1} and M_n are of the second order with

$$E^{0}(x^{2}) = -\frac{(b-a)h^{2}}{6}, \qquad E^{\frac{1}{2}}(x^{2}) = \frac{(b-a)h^{2}}{12}.$$
 (4)

Error estimate for quadrature formulas of the second order. Before we give an error estimate for the quadrature formula, let us recall the notation:

$$(t-x)_+^k := \begin{cases} (t-x)^k & \text{for } t > x, \\ 0 & \text{for } t \le x. \end{cases}$$
 (5)

Using the notation, the Peano kernel (see [3]) of second order for the quadrature formula $Q^{\beta}(f)$ ($\beta \neq \bar{\beta}$) takes the form:

$$K_{\beta,2}(x) := \int_{a}^{b} (t-x)_{+} dt - Q^{\beta} ((t-x)_{+}).$$
 (6)

This kernel is a periodic function with h being a period, thus it is sufficient to define it on the interval [a, a + h]. For considered quadrature formula $Q^{\beta}(f)$ of the second order the kernel has the following form

$$K_{\beta,2}(x) = \begin{cases} \frac{h^2}{2} \left(\frac{x-a}{h} \right)^2 & \text{for } x \in [a, a+\beta h], \\ \frac{h^2}{2} \left(\left(\frac{x-a}{h} \right)^2 - \left(\frac{x-a}{h} \right) + \beta \right) & \text{for } x \in (a+\beta h, a+(1-\beta)h), \\ \frac{h^2}{2} \left(\frac{x-a}{h} - 1 \right)^2 & \text{for } x \in [a+(1-\beta)h, a+h]. \end{cases}$$

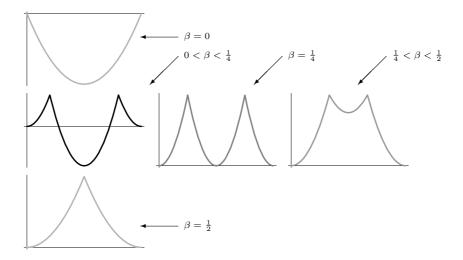


Fig. 1. Graphs of Peano kernels for different values of β



Fig. 2. Overlapping graphs of Peano kernels for different values of β

The Figures 1 and 2 show graphs of Peano kernel depending on the parameter β . A simple calculation leads to the relation

$$\int_{a}^{b} K_{\beta,2}(x) dx = -\frac{(b-a)h^2}{12} (6\beta^2 - 6\beta + 1).$$
 (7)

If $K_{\beta,2}(x)$ is of a constant sign, we can give an error estimate for quadrature formula with a function f of class $C^2([a,b])$:

$$E^{\beta}(f) = I(f) - Q^{\beta}(f) = \int_{a}^{b} f''(x) K_{\beta,2}(x) dx = f''(\xi) \int_{a}^{b} K_{\beta,2}(x) dx =$$

$$= -\frac{(b-a)h^{2}}{12} (6\beta^{2} - 6\beta + 1) f''(\xi), \qquad \xi \in [a,b].$$
(8)

If $\beta \in \{0\} \cup \left[\frac{1}{4}, \frac{1}{2}\right]$ the Peano kernel $K_{\beta,2}(x)$ is of a constant sign. In this case the error of the quadrature Q^{β} can be expressed by (8). For example we can write

$$E^{0}(f) = E_{T_{n+1}}(f) = -\frac{(b-a)h^{2}}{12}f''(\xi), \qquad \xi \in [a,b],$$

$$E^{\frac{1}{4}}(f) = \frac{(b-a)h^{2}}{96}f''(\xi), \qquad \xi \in [a,b],$$

$$E^{\frac{1}{2}}(f) = E_{M_{n}}(f) = \frac{(b-a)h^{2}}{24}f''(\xi), \qquad \xi \in [a,b],$$

The Figure 3 shows the graph of the function $y(\beta) = -\left(6\beta^2 - 6\beta + 1\right), \, \beta \in \left[0, \frac{1}{2}\right]$.

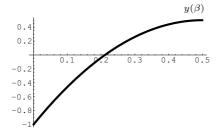


Fig. 3. Graph of the function $y(\beta)$

For a sign-changing kernel $(\beta \in (0, \frac{1}{4}))$ we give the following estimate:

$$E^{\beta}(f) = I(f) - Q^{\beta}(f) = \int_{a}^{b} f''(x)K_{\beta,2}(x) dx = \int_{a}^{b} f''(x) \left(K_{\beta}^{+}(x) + K_{\beta}^{-}(x)\right) dx =$$

$$= \int_{a}^{b} f''(x)K_{\beta}^{+}(x) dx + \int_{a}^{b} f''(x)K_{\beta}^{-}(x) dx =$$

$$= f''(\xi_{1}) \int_{a}^{b} K_{\beta}^{+}(x) dx + f''(\xi_{2}) \int_{a}^{b} K_{\beta}^{-}(x) dx,$$
where
$$K_{\beta}^{+}(x) = \max\{K_{\beta,2}(x), 0\}, \qquad K_{\beta}^{-}(x) = \min\{K_{\beta,2}(x), 0\}.$$

where

Since

$$\int_{a}^{b} K_{\beta}^{-}(x) dx = -\frac{(b-a)h^{2}}{12} \left(\sqrt{1-4\beta}\right)^{3},$$

$$\int_{a}^{b} K_{\beta}^{+}(x) dx = \frac{(b-a)h^{2}}{12} \left(\left(\sqrt{1-4\beta}\right)^{3} - \left(6\beta^{2} - 6\beta + 1\right)\right),$$

it follows that

$$E^{\beta}(f) = \frac{(b-a)h^2}{12} \left\{ \left(\left(\sqrt{1-4\beta} \right)^3 - \left(6\beta^2 - 6\beta + 1 \right) \right) f''(\xi_1) - \left(\sqrt{1-4\beta} \right)^3 f''(\xi_2) \right\}. \tag{9}$$

This estimate is valid for $\beta = \frac{1}{3+\sqrt{3}} = \frac{3-\sqrt{3}}{6}$, thus

$$E^{\frac{1}{3+\sqrt{3}}}(f) = \frac{(b-a)h^2}{12} \left(\sqrt{\frac{2\sqrt{3}-3}{3}}\right)^3 \left(f''(\xi_1) - f''(\xi_2)\right). \tag{10}$$

Error estimate for optimal quadrature formula of the fourth order. The error estimate for the quadrature formula $Q^{\bar{\beta}}$ with $\bar{\beta} = \frac{1}{3+\sqrt{3}}$, which is, obviously of the fourth order, can be found in a more subtle way. In this case the Peano kernel $K_{\frac{1}{3+\sqrt{3}},4}(x)$ has the form:

$$K_{\frac{1}{3+\sqrt{3}},4}(x) = \begin{cases} \frac{h^4}{24} \left(\frac{x-a}{h}\right)^4 & \text{for } x \in [a,a+\beta h], \\ \frac{h^4}{24} \left(\left(\frac{x-a}{h}\right)^4 - 2\left(\frac{x-a}{h}\right)^3 + \frac{6}{3+\sqrt{3}} \left(\frac{x-a}{h}\right)^2 + \left(2+\sqrt{3}\right) \left(\frac{x-a}{h}\right) + \frac{1}{27+15\sqrt{3}} \right) \\ & \text{for } x \in (a+\beta h,a+(1-\beta)h), \\ \frac{h^4}{24} \left(\frac{x-a}{h}-1\right)^4 & \text{for } x \in [a+(1-\beta)h,a+h]. \end{cases}$$

Its graph is given in Figure 4 below.

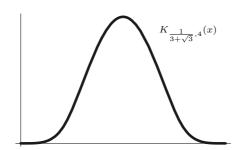


Fig. 4. Graph of the Peano kernel $K_{\frac{1}{3+\sqrt{3}},4}(x)$

A simple calculation leads to the relation

$$\int_{a}^{b} K_{\frac{1}{3+\sqrt{3}},4}(x) \, dx = \frac{nh^5}{4320} = \frac{(b-a)h^4}{4320}.$$

For $f \in C^4([a, b])$, we thus obtain the following estimate:

$$E^{\frac{1}{3+\sqrt{3}}}(f) = \frac{(b-a)h^4}{4320}f^{(4)}(\xi), \qquad \xi \in [a,b].$$
 (11)

Example 1. Consider the integral

$$J := \int_{\frac{1}{4\pi}}^{\frac{1}{\pi}} f(x) \, dx$$

where $f(x) := \frac{\cos \frac{1}{x} - x \sin \frac{1}{x}}{2x\sqrt{1 - x \sin \frac{1}{x}}}$ (Fig. 1). It is easy to verify by a direct calculation that the primitive function of f(x) is the function $F(x) = \sqrt{1 - x \sin \frac{1}{x}}$, so that J = 0.

Consequently, the value $Q^{\beta}(f)$ (Tab. 1) is equal to the error for the quadrature formula.

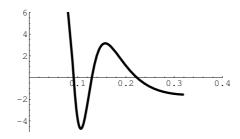


Fig. 5. Graph of the function f(x) in Example 1

Table 1 Values of the error of Q^{β} for the integral J

	$\beta = \frac{1}{6}$	$\beta = \frac{1}{3}$	$\beta = \frac{1}{3 + \sqrt{3}}$
n = 10	5.463635e - 3	-6.398709e - 3	2.099473e - 3
n = 40	3.385498e - 5	-5.428245e-5	6.210446e-6

3. APPLICATIONS

In this section we demonstrate some applications of the family Q^{β} . We will take into account cubature formulas, integral equations and ordinary differential equations.

3.1. CONSTRUCTION OF THE PRODUCT CUBATURE FORMULA

If $Q(f) = \sum_{i=0}^{m} a_i f(t_i)$ is a quadrature formula of the r-th order for the integral $I(f) = \int_0^1 f(t) dt$, then

$$\widetilde{Q}(F) = \sum_{i_1=0}^{m} \dots \sum_{i_n=0}^{m} a_{i_1} a_{i_2} \dots a_{i_n} F(t_{i_1}, t_{i_2}, \dots, t_{i_n})$$

defines so called product cubature formula for the integral

$$\widetilde{I}(F) = \int_{[0,1]^n} F(x) \, dx$$

where $F: \mathbb{R}^n \supset [0,1]^n \to \mathbb{R}$. It is proved (see [5]) that this cubature formula is of the r-th order too. An integral $\int_{\Omega} F(x) dx$ where $F : \mathbb{R}^n \supset \Omega \to \mathbb{R}$, $x = (x_1, \dots, x_n)$ and Ω is a regular domain may be reduced to an integral over cube $[0,1]^n$ by a change of variables. For example, for a double integral $\iint_{\Omega} F(x_1, x_2) dx_1 dx_2$, where $\Omega = \{x = (x_1, x_2) : a \leq x_1 \leq b, \varphi(x_1) \leq x_2 \leq \psi(x_1)\} \subset \mathbb{R}^2$, we can do it by substitution $x_1(s_1, s_2) = (1 - s_1)a + s_1b, x_2(s_1, s_2) = (1 - s_2)\varphi(x_1(s_1, s_2)) + s_2\psi(x_1(s_1, s_2))$. So, if we put Q^{β^*} instead of Q with $\beta^* = \frac{1}{3 + \sqrt{3}}$, then the suitable product cubature

formula Q^{β^*} is of the fourth order.

Example 2. Let us calculate the double integral

$$I := \iint_{\Omega} e^{-(x^2 + y^2)} dx \, dy,$$

where Ω is the circle of radius 3 with centre at the origin. Its value can be computed by passing to polar coordinates. The exact value of the integral is $\pi(1-e^{-9}) \approx$ $3.141\,204\,950\,255\,893\,570\,3$. The application of cubature formula Q^{β} yields results with the error $(I - Q^{\beta})$. In Table 2, we give some exemplary values.

Error arising if the cubature formula Q^{β} is applied to computing integral I

	$\beta = \frac{1}{6}$	$\beta = \frac{1}{3}$	$\beta \frac{1}{3+\sqrt{3}}$
n = 10	6.249007e-6	-3.258042e-5	-7.661622e - 6
n = 30	1.775033e - 6	-5.495439e - 6	-7.692695e-7

3.2. AN APPLICATION TO FREDHOLM INTEGRAL EQUATIONS

Let us consider the one-dimensional Fredholm equation of second kind in the form

$$\lambda u(x) - \int_{a}^{b} k(x, y)u(y) \, dy = f(x) \qquad x \in [a, b],$$
 (12)

where k and f are continuous functions, and $\lambda \in \mathbb{R} \setminus \{0\}$. The Nyström method of solving this equation (see [1,4]) consists in replacing the integral appearing in equation (12) by a quadrature formula and equalizing both the sides of (12) in its nodes. We will here apply the quadrature formula Q^{β} .

Let us adopt the notations

$$\mu_{2j} = a + jh + \beta h \quad \mu_{2j+1} = a + (j+1)h - \beta h$$

$$z_{2j} \approx u(\mu_{2j}) \qquad z_{2j+1} \approx u(\mu_{2j+1}) \qquad j = 0, 1, \dots, n-1.$$

The Nyström method constructed by using quadrature formula Q^{β} leads to a system of 2n algebraic equations:

$$\begin{cases} \lambda z_{2j} - \frac{h}{2} \sum_{l=0}^{n-1} \left(k(\mu_{2j}, \mu_{2l}) z_{2l} + k(\mu_{2j}, \mu_{2l+1}) z_{2l+1} \right) = f(\mu_{2j}), \\ \lambda z_{2j+1} - \frac{h}{2} \sum_{l=0}^{n-1} \left(k(\mu_{2j+1}, \mu_{2l}) z_{2l} + k(\mu_{2j+1}, \mu_{2l+1}) z_{2l+1} \right) = f(\mu_{2j+1}) \end{cases}$$
(13)

 $(j=0,1,\ldots,n-1)$ in 2n unknowns z_k $(k=0,1,\ldots,2n-1)$. We denote the matrix of this system by A_{2n} . A discrete solution z_k $(k=0,1,\ldots,2n-1)$ may be extended onto the whole interval [a,b] to the function

$$z(x) = \frac{1}{\lambda} \left(f(x) + \frac{h}{2} \sum_{j=0}^{n-1} \left(k(x, \mu_{2j}) z_{2j} + k(x, \mu_{2j+1}) z_{2j+1} \right) \right).$$

In [1], an asymptotic error estimation of this method and the bound of $cond(A_{2n})$ in a general case are given. Some generalization to non-continuous kernels is also given. These results may be transferred on to our particular case.

Example 3. Consider the integral equation

$$\lambda u(x) - \int_{0}^{1} e^{xy} u(y) \, dy = f(x) \qquad x \in [0, 1],$$

with $\lambda=2$. Since the norm of the integral operator in this equation is equal to $e-1\approx 1.72$ then the integral equation is uniquely solvable for any given $f\in C[0,1]$. For example: the function $u_1(x)=e^x$ is the solution for $f(x)=2e^x+\frac{1-e^{x+1}}{x+1}$ and the function $u_2(x)=e^{-x}\cos x$ is the solution for $f(x)=2e^{-x}\cos x-\frac{1-x+e^{x-1}\left((x-1)\cos 1+\sin 1\right)}{2+(x-2)x}$. By applying formulas (13) with n=5 and $\beta=\frac{1}{3+\sqrt{3}}$ we obtain results with maximum errors on quadrature Q^β in the nodal points 1.76997e-5 in the first case and 5.835e-7 in the second case.

3.3. A METHOD OF SOLVING ORDINARY DIFFERENTIAL EQUATIONS

We consider the Cauchy initial problem

$$x' = f(t, x), \quad x(t_0) = x_0 \quad \text{for} \quad t \in I = [t_0, T],$$
 (14)

where $x: I \to \mathbb{R}^n$, $f: I \times \Omega \to \mathbb{R}^n$, with a domain $\Omega \subset \mathbb{R}^n$. We suppose f to be continuous in the set $I \times \Omega$ and satisfy a Lipschitz condition there, with a constant L > 0, with respect to the second variable, i.e., $||f(t,x) - f(t,\tilde{x})|| \le L ||x - \tilde{x}||$ for each $t \in I$ and $x, \tilde{x} \in \Omega$. These assumptions guarantee that problem (14) has exactly one solution defined in a right-hand neighbourhood of the point t_0 .

On the interval $[t_0, T]$, we introduce a uniform net $t_i = t_0 + ih$, i = 0, 1, ..., N, where $N \in \mathbb{N} \setminus \{0, 1\}$ is a given number and $h = \frac{T - t_0}{N}$.

Definition 1. We define an explicit one-step scheme of the form

$$x_{i+1} = x_i + h\Phi_f(h, t_i, x_i), \qquad i = 0, 1, \dots, N,$$
 (15)

where Φ_f is a function depending on f, and x_i denotes an approximate value of the solution x of equation (14) at the nodal point t_i (see [2]).

We consider scheme (15) in which

$$\Phi_{f}(h, t_{i}, x_{i}) := \frac{1}{2} f\left(t_{i} + \beta h, x_{i} + \beta h f\left(t_{i} + \beta \frac{h}{2}, x_{i} + \beta \frac{h}{2} f(t_{i}, x_{i})\right)\right) + \frac{1}{2} f\left(t_{i} + (1 - \beta)h, x_{i} + (1 - \beta)h f\left(t_{i} + (1 - \beta)\frac{h}{2}, x_{i} + (1 - \beta)\frac{h}{2} f(t_{i}, x_{i})\right)\right), \tag{16}$$

where $\beta = \frac{1}{3+\sqrt{3}}$.

Now we assume that the function f is sufficiently smooth. From (15) and the expansion of function x(t+h) into a Taylor series it follows that

$$\Phi_f(h,t,x) = x'(t) + \frac{h}{2}x''(t) + \frac{h^2}{6}x^{(3)}(t) + \frac{h^3}{24}x^{(4)}(t) + \dots$$

From (14), after suitable differentiations, we get

$$\Phi_f(h,t,x) = f + \frac{h}{2}(f_t + f_x f) + \frac{h^2}{6}(f_t f_x + f(f_x)^2 + f_{tt} + 2f f_{tx} + f^2 f_{xx}) +
+ \frac{h^3}{24} \left(3f_t f_{tx} + 3f f_t f_{xx} + f_t (f_x)^2 + 5f f_x f_{tx} + 4f^2 f_x f_{xx} +
+ f(f_x)^3 + f_x f_{tt} + f_{ttt} + 3f f_{ttx} + 3f^2 f_{txx} + f^3 f_{xxx} \right) + \dots$$
(17)

Let us take the value of (17) at the point (h, t_i, x_i) . Subtracting this from the Taylor series expansion of the right-hand side of (16), we get

$$\left(\frac{1}{96}f_{tt}f_x + \frac{1}{48}ff_{tx}f_x + \frac{1}{24}f(f_x)^2 + \frac{1}{24}f_t(f_x)^2 + \frac{1}{96}f^2f_xf_{xx}\right)h^3 + O(h^4), \quad (18)$$

thus, method (16) is of the third order. The local error of the method, r_i , defined by the formula

$$r_i = x(t_i + h) - x(t_i) - h\Phi(h, t_i, x(t_i)),$$

with $x(\cdot)$ being an exact solution of equation (14), is equal to

$$r_i = \left(\frac{1}{96}f_{tt}f_x + \frac{1}{48}ff_{tx}f_x + \frac{1}{24}f(f_x)^2 + \frac{1}{24}f_t(f_x)^2 + \frac{1}{96}f^2f_xf_{xx}\right)h^4 + O(h^5), \quad (19)$$

having noticed that the function f and all of its partial derivatives appearing in this formula, are calculated at the point $(t_i, x(t_i))$. Figure 6 illustrates the domain of stability for scheme (15)–(16). It is interesting that this stability domain is the same

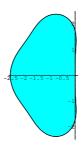


Fig. 6. Domain of stability for scheme (15)–(16)

as for the explicit Runge-Kutta method of the third order:

$$x_{i+1} = x_i + \frac{h}{9} \left(2K_1 + 3K_2 + 4K_3 \right),$$

$$K_1 = f(t_i, x_i), \quad K_2 = f\left(t_i + \frac{h}{2}, x_i + \frac{h}{2}K_1\right), \quad K_3 = f\left(t_i + \frac{3}{4}h, x_i + \frac{3}{4}hK_2\right).$$
(20)

Example 4. It is known that the system of equations (three-body gravitational problem):

$$\begin{split} x_1 &= x_3, \\ x_2 &= x_4, \\ x_3 &= x_1 + 2x_4 - (1 - \mu) \frac{x_1 + \mu}{D_1} - \mu \frac{x_1 - 1 + \mu}{D_2}, \\ x_4 &= x_2 + 2x_3 - (1 - \mu) \frac{x_2}{D_1} - \mu \frac{x_2}{D_2}, \end{split}$$

where $D_1 = ((x_1 + \mu)^2 + x_2^2)^{3/2}$, $D_2 = ((x_1 - 1 + \mu)^2 + x_2^2)^{3/2}$, $\mu = \frac{1}{81.45}$ with initial conditions $(x_1, x_2, x_3, x_4)(0) = (0.994, 0, 0, -2.00158510637908252240537862224)$ has a periodical solution with period T = 17.065216560157965588917206249. Solving this system by methods (15)–(16), (20) with step size $h = \frac{T}{n}$ we obtain the following results (Tab. 3).

Table 3 Value of $x_2(T)$

	Method (15)–(16)	Method (20)
n = 100000	-0.000207	-0.000126
n = 150000	-0.000063	-0.000038

The exact value $x_2(T)$ is equal to 0.

REFERENCES

- [1] K. Atkinson, W. Han, *Theoretical Numerical Analysis*, A Functional Analysis Framework, Springer–Verlag, New York, 2001.
- [2] E. Hairer, S.P. Nørsett, G. Wanner, Solving Ordinary Differential Equations I, Nonstiff Problems, Springer, New York, 1993.
- [3] D. Kincaid, W. Cheney, Numerical Analysis, Mathematics of Scientific Computing, 3rd ed., The University of Texas at Austin, Brooks/Cole-Thomson Learning, 2002.
- [4] E. Nyström, Über die praktische Auflösung von Integralgleichungen mit Anwendungen auf Randwertaufgaben, Acta Math., **54** (1930), 185–204.
- [5] A.H. Stroud, Approximate Calculation of Multiple Integrals, Prentice-Hall, Englewood Cliffs, New Jersey, 1971.

Bogusław Bożek bozek@uci.agh.edu.pl

AGH University of Science and Technology Faculty of Applied Mathematics al. Mickiewicza 30, 30-065 Cracow, Poland

Wiesław Solak solak@uci.agh.edu.pl

AGH University of Science and Technology Faculty of Applied Mathematics al. Mickiewicza 30, 30-065 Cracow, Poland

Zbigniew Szydełko

AGH University of Science and Technology Faculty of Applied Mathematics al. Mickiewicza 30, 30-065 Cracow, Poland

Received: January 4, 2007. Revised: November 7, 2007. Accepted: November 11, 2007.