Bull. Nov. Comp. Center, Num. Anal., 1 (1993)

Modified Runge-Kutta method

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Modern Runge-Kutta method of solving ODE bears a slight resemblance with the classical (explicit) method and is based on the transformation of the differential equation to the integral one. The contents of the mathematical theory was formulated by J.C. Butcher et all (see [1], [2]). Nevertheless, the technique of constracting fundamental equations of RK-method remained unchanged. In this paper new principles are lying in the basis of constructing fundamental equations. Some new ideas are used for solving the fundamental equations, in particular, the principle of nilpotency for explicit, diagonal and singly-implicit RK-methods is successively performed.

1. Discretization

Let an ordinary differential equation

$$\frac{\partial y}{\partial t} = f(t,y), \quad 0 \le t \le T, \quad y(0) = y_0, \tag{1}$$

be given. We aim at constructing its approximate solution y_k at the discrete points $t_k, t_k \in [0,T]$. If y_n is found, then the solution y_{n+1} at the point $t_{n+1} = t_n + \tau$ according to the Runge-Kutta method is described by the system of algebraic equations

$$\begin{aligned} \eta_0 &= y_n, \\ \eta_i &= y_n + \tau \textstyle\sum_{j=1}^{m} \beta_{ij} f_j, \quad j = 1(1)m+1, \\ y_{n+1} &= \eta_{m+1} \end{aligned} \tag{2}$$

with the notations

$$\begin{aligned} f_j &= f(\xi_j, \eta_j), \\ \xi_i &= t_n + \lambda_i \tau, \quad i = 0(1)m+1, \\ \lambda_0 &= 0, \quad \lambda_{m+1} = 1, \quad \lambda_j \le \lambda_{j+1}. \end{aligned} \tag{3}$$

The value of

$$\varepsilon_{n+1} = y(t_{n+1}) - y_{n+1} \tag{4}$$

is said to be the global truncation error, while

$$l_{n+1} = y(t_{n+1}) - \hat{y}_{n+1} \tag{5}$$

is the local truncation error. Here and in the sequel $y(t_{n+1})$ is the proximate solution of equation (1.1) at the point $t_{n+1}, \hat{y}_{n+1}$ is the solution of system (1.2) after replacement of y_n by $y(t_n)$.

Following the test function principle, we will construct the RK-scheme thus providing the exact solution of pequation (1), when $f(t,y)$ has some specific form, namely

$$f(t,y) = lt^{l-1}, \quad l = 1(1)M, \tag{6}$$

where M is some positive integer. In this case the function

$$f(t,y) = (M+1)t^M$$

could be used for the characterization of the local truncation error

$$l_{n+1} = y(t_{n+1}) - \hat{y}_{n+1} = t_{n+1}^{M+1} - t_n^{M+1} - \tau(M+1)\sum_{j=1}^{m} \beta_{M+1,j}\xi_j^M, \tag{7}$$

since it depends on the RK-scheme only and does not depend on any properties of differential equation (1).

Let us apply the test functions method for determining the parameters β_{ij}, λ_i. Equations (2) for the right-hand side, defined in (6), admit the form

$$\begin{aligned} \eta_j &= t_n^l + \tau\textstyle\sum_{j=1}^m \beta_{ij} l(t_n + \lambda_j\tau)^{l-1} \\ &= t_n^l + \textstyle\sum_{j=1}^m \sum_{k=0}^{l-1} lC_{l-1}^k \beta_{ij}\lambda_j^k \tau^{k+1} t_n^{l-k-1} \\ &= t_n^l + \textstyle\sum_{k=1}^l kC_l^k \tau^k t_n^{l-k} \sum_{j=1}^m \beta_{ij}\lambda_j^{k-1} \\ &= t_n^l + \textstyle\sum_{k=1}^l \frac{\tau^k}{k!}\frac{d^k y_n}{dt_n^k} k \sum_{j=1}^m \beta_{ij}\lambda_j^{k-1}, \end{aligned}$$

where

$$C_l^k = \frac{l!}{k!(l-k)!}$$

is the binomial coefficient. Let us constitute the difference, which is the residual g_i of the quasi-solution at the intermediate nodes ξ_i,

$$\begin{aligned} g_i &= \eta_i - \xi_i^l = \textstyle\sum_{k=1}^l \left(k\sum_{j=1}^m \beta_{ij}\lambda_j^{k-1} - \lambda_i^k\right)\frac{\tau^k}{k!}\frac{d^k y_n}{dt_n^k}, \\ & i = 1(1)m+1, \quad l = 1(1)M+1, \end{aligned} \tag{8}$$

using the above equality and definition (3). Condition $g_{m+1} = 0$ for arbitrary t_n and τ implies equalities

$$\sum_{j=1}^{m} \beta_{m+1,j}\lambda_j^{k-1} = \frac{1}{k}, \quad k = 1(1)M. \tag{9}$$

The local error is determined from (7) for $l = M + 1$. We obtain

$$\begin{aligned} l_{m+1} &= \xi_{m+1}^{M+1} - \eta_{m+1} = \sum_{j=0}^{M+1} C_{M+1}^{j} t_n^j \tau^{M+1-j} \\ &\quad - t_n^{M+1} - (M+1)\tau \sum_{i=1}^{m} \beta_{m+1,i}(t_n + \lambda_i \tau)^M \\ &= \sum_{j=0}^{M} C_{M+1}^{j} t_n^j \tau^{M+1-j} - (M+1)\tau \sum_{j=0}^{M} C_M^j t_n^j \tau^{M-j} \sum_{i=1}^{m} \beta_{m+1,i}\lambda_i^{M-j}. \end{aligned}$$

With the help of the identity

$$(M+1)C_M^j = (M-j+1)C_{M+1}^j$$

we find

$$l_{n+1} = \sum_{j=0}^{M} C_{M+1}^{j} t_n^j \tau^{M+1-j} \left(1 - (M-j+1)\sum_{i=1}^{m} \beta_{m+1,i}\lambda_i^{M-j}\right).$$

The final relation is obtained with the use of (9):

$$l_{n+1} = \left(1 - (M+1)\sum_{i=1}^{m} \beta_{m+1,i}\lambda_i^{M}\right)\tau^{M+1}. \tag{10}$$

For further analysis let us introduce the matrix and vector notations.

$$B = \begin{pmatrix} \beta_{11} & \beta_{12} & \dots & \beta_{1m} \\ \beta_{21} & \beta_{22} & \dots & \beta_{2m} \\ \dots & \dots & \dots & \dots \\ \beta_{m1} & \beta_{m2} & \dots & \beta_{mm}, \end{pmatrix}$$

$$\begin{aligned} b_i &= (\beta_{i1}, \dots, \beta_{im}), \quad i = 1(1)m+1, \\ \Lambda &= \mathrm{diag}(\lambda_1, \dots, \lambda_m), \quad h = \mathrm{diag}(1, 1/2, \dots, 1/m), \\ \eta &= (\eta_1, \dots, \eta_m)^T, \quad f = (f_1, \dots, f_m)^T, \\ g &= (g_1, \dots, g_m)^T, \quad e = (1, \dots, 1)^T, \end{aligned}$$

where B, Λ, h are matrices, b_i are row vectors and η, f, g are column vectors. In these notations equations (1.2) admit the form of

$$\begin{aligned} \eta &= y_n e + \tau B f, \\ y_{n+1} &= y_n + \tau b_{m+1} f, \end{aligned} \tag{11}$$

and equalities (1.9) - the form of

$$b_{m+1}\Lambda^{k-1}e = \frac{1}{k}, \quad k = 1(1)M. \tag{12}$$

Assuming $M \geq m$, select the first m of these equations in order to determine b_{m+1}, and represent them in the vector form

$$b_{m+1}W = e^T h, \tag{13}$$

where

$$W = \begin{pmatrix} 1 & \lambda_1 & \lambda_1^2 & \dots & \lambda_1^{m-1} \\ 1 & \lambda_2 & \lambda_2^2 & \dots & \lambda_2^{m-1} \\ \dots & \dots & \dots & \dots & \dots \\ 1 & \lambda_m & \lambda_m^2 & \dots & \lambda_m^{m-1} \end{pmatrix} \tag{14}$$

is the Vandermonde matrix.

Equations (12) are obtained by analyzing the test functions behaviour at the point t_{n+1}. One may expect that the analysis of these functions at the intermediate nodes $\xi_j, j = 1(1)m$ will bring about new equations with respect to the parameters β_{ij}, λ_i. However it is not so. Let us present the corresponding calculations. Since

$$\frac{dg_i}{dt_n} = \frac{d\eta_i}{dt_n} - f_i = \sum_{k=1}^{l} \frac{d^{k+1}y_n}{dt_n^{k+1}} \left(k \sum_{j=1}^{m} \beta_{ij}\lambda_j^{k-1} - \lambda_i^k \right) \frac{\tau^k}{k!},$$

expression

$$\begin{aligned} \frac{dg}{dt_n} &= \frac{d\eta}{dt_n} - f = \sum_{k=1}^{l-1}(kB - \Lambda)\Lambda^{k-1}e\frac{\tau^k}{k!}\frac{d^{k+1}y_n}{dt_n^{k+1}} \\ &= \sum_{k=1}^{M}(kB - \Lambda)\Lambda^{k-1}e\frac{\tau^k}{k!}\frac{d^{k+1}y_n}{dt_n^{k+1}} \end{aligned} \tag{15}$$

for $l = 2(1)M+1$ is a polynomial of order $l-2$ with respect to t_n. Substitute f from (15) into (11):

$$\eta = y_n e + \tau B\frac{d\eta}{dt_n} - \tau B\frac{dg}{dt_n},$$

$$y_{n+1} = y_n + \tau b_{m+1} \frac{d\eta}{dt_n} - \tau b_{m+1} \frac{dg}{dt_n}.$$

In order to eliminate $d\eta/dt_n$ from the second equation, differentiate the first one:

$$\frac{d^{k-1}\eta}{dt_n^{k-1}} = \frac{d^{k-1}y_n}{dt_n^{k-1}} e + \tau B \frac{d^k\eta}{dt_n^k} - \tau B \frac{d^k g}{dt_n^k},$$

multiply it by $(\tau B)^{k-2}$ and sum up with respect to k from 2 to $M+1$. Obtain

$$\frac{d\eta}{dt_n} = \sum_{k=1}^{M} (\tau B)^{k-1} \frac{d^k y_n}{dt_n^k} e - \sum_{k=2}^{M} (\tau B)^{k-1} \frac{d^k g}{dt_n^k} + (\tau B)^M \frac{d^{M+1}\eta}{dt_n^{M+1}},$$

thereto, for the test functions according to (8) holds

$$\frac{d^{M+1}\eta}{dt_n^{M+1}} = \frac{d^{M+1}y_n}{dt_n^{M+1}} = e, \quad \frac{d^{M+1}g}{dt_n^{M+1}} = 0.$$

Then

$$y_{n+1} = y_n + \sum_{j=1}^{M+1} b_{m+1} B^{j-1} e \frac{d^j y_n}{dt_n^j} \tau^j - \sum_{j=1}^{M} b_{m+1} B^{j-1} \frac{d^j g}{dt_n^j} \tau^j. \qquad (16)$$

With regard to relation (15), the second sum on the right-hand side admits the form

$$\begin{aligned}
&\sum_{j=1}^{M} b_{m+1} B^{j-1} \frac{d^j g}{dt_n^j} \tau^j \\
&= \sum_{j=1}^{M} b_{m+1} B^{j-1} \sum_{k=1}^{M-j+1} (kB - \Lambda)\Lambda^{k-1} e \frac{\tau^{k+j}}{k!} \frac{d^{k+j} y_n}{dt_n^{k+j}} \\
&= \sum_{i=2}^{M+1} \tau^i \frac{d^i y_n}{dt_n^i} \sum_{j=1}^{i-1} \frac{1}{(i-j)!} b_{m+1} B^{j-1}((i-j)B - \Lambda)\Lambda^{i-j-1} e \\
&= \sum_{i=2}^{M+1} \tau^i \frac{d^i y_n}{dt_n^i} \sum_{j=1}^{i-1} \frac{1}{(i-j-1)!} b_{m+1} B^j \Lambda^{i-j-1} e \\
&\quad - \sum_{j=1}^{i-1} \frac{1}{(i-j)!} b_{m+1} B^{j-1} \Lambda^{i-j} e.
\end{aligned}$$

In the second sum, over j, we introduce substitution $j-1 \to j$, which makes clear that both sums differ in the limits of summation only. Thus

$$\sum_{j=1}^{M} b_{m+1} B^{j-1} \frac{d^j g}{dt_n^j} \tau^j = \sum_{i=1}^{M+1} \tau^i \frac{d^i y_n}{dt_n^j} \left(b_{m+1} B^{i-1} e - \frac{1}{(i-1)!} b_{m+1} \Lambda^{i-1} e \right),$$

which yields

$$y_{n+1} = y_n + \sum_{i=1}^{M+1} \frac{\tau^i}{(i-1)!} \frac{d^i y_n}{dt_n^i} b_{m+1} \Lambda^{i-1} e$$

and comparing this representation with the Taylor expansion of the polynomial $y(t_{n+1})$ of the order less or equal to $M+1$,

$$y(t_{n+1}) = y_n + \sum_{i=1}^{M+1} \frac{1}{i!} \tau^i \frac{d^i y_n}{dt_n^i}$$

for arbitrary τ, we return to relations (12) and (10), which can be rewritten in the form

$$\begin{aligned} E_j &= 0, \quad j = 1(1)M, \\ l_{n+1} &= E_{M+1} \tau^{M+1}, \end{aligned} \tag{17}$$

where

$$E_j = 1 - j b_{m+1} \Lambda^{j-1} e. \tag{18}$$

Equations (12) for given $\lambda_i, i = 1(1)m$, determine only the row vector b_{m+1}. We also have to evaluate some m^2 elements of the matrix B. Moreover, the elements λ_i are also to be specified. Therefore, the test functions approach in the Runge-Kutta method is insufficient. In order to obtain new relations, it is necessary to restrict the behaviour of the test functions at the intermediate nodes ξ_i. To this end, we apply again representation (16). Summands

$$b_{m+1} B^{j-1} \frac{d^{j-1}}{dt_n^{j-1}} \left(\frac{d\eta}{dt_n} - f \right), \quad j = 1(1)N-1, \tag{19}$$

where N is some positive integer, are some residual functionals of solution at the intermediate nodes if η is considered some approximation to solution. Let us require η_i to be a weak approximation of the solution of equation (1) at the intermediate node ξ_i, at least, for test functions (6) when $l = 1(1)N$, i.e., annihilate summands (19). Combined with relations (15), it results in equation

$$\begin{gathered} b_{m+1} B^{j-1} \textstyle\sum_{k=1}^{l-j} (kB - \Lambda) \Lambda^{k-1} e \frac{\tau^k}{k!} \frac{d^{k+j} y_n}{dt_n^{k+j}} = 0, \\ l = 2(1)N, \quad j = 1(1)N-1. \end{gathered} \tag{20}$$

the number N will be said to be the order of weak approximation.

Remark 1. The condition of weak approximation (20) can be extended to the region of negative orders of the differentiation operator (i.e., to the region of the integration operators of the corresponding multiplicity), by introduction of $j = 0, -1$, etc. This extension will be used in Section 6.1.

Due to an arbitrary choice of τ, relation (20) implies

$$\begin{aligned} &b_{m+1} B^{j-1}(kB - \Lambda)\Lambda^{k-1} e = 0, \\ &2 \le j + k \le N, \quad j = 1(1)N-1, \end{aligned} \tag{21}$$

and one can derive sequentially

$$\begin{aligned} b_{m+1} B^j \Lambda^{k-1} e &= (1/k) b_{m+1} B^{j-1} \Lambda^k e = \frac{1}{k(k+1)} b_{m+1} B^{j-2} \Lambda^{k+1} e \\ &= \ldots = \frac{(k-1)!}{(k+j-1)!} b_{m+1} \Lambda^{k+j-1} e. \end{aligned}$$

Therefore,

$$\begin{aligned} b_{m+1} B^j \Lambda^{k-1} e &= \tfrac{(k-1)!}{(k+j-1)!} b_{m+1} \Lambda^{k+j-1} e \\ &= (k-1)! b_{m+1} B^{k+j-1} e, \\ 2 \le k + j &\le N, \quad j = 1(1)N-1. \end{aligned} \tag{22}$$

Assuming $M \le N$, with the help of (12) we derive the fundamental equations of the Runge-Kutta method:

$$\begin{aligned} b_{m+1} B^j \Lambda^{k-1} e &= \tfrac{(k-1)!}{(k+j)!}, \\ k = 0(1)M - j, & \qquad j = 1(1)M. \end{aligned} \tag{23}$$

Therefore, in order to evaluate the parameters of the RK-schemes, one can apply equations (23), and for $N > M$ - equations (22) as well. The relationship between m, M and N is not *a priori* fixed and may be arbitrary. We restrict ourselves to consideration of such RK-schemes, for which inequalities $N \ge M \ge m$ take place. As we will see later, the precise relations between these numbers are defined by the form of the matrix B. Thus, the analysis of the RK-schemes is essentially connected with the analysis of the matrices B. The circumstance that equations (23) are not generally sufficient for evaluation of b_{m+1}, B, Λ, makes us to impose certain restrictions on the form of the matrix B. In the sequel, we will consider the characteristic polynomial of the matrix B:

$$Q_m(\lambda) = \lambda^m - \sum_{j=1}^{m} q_j \lambda^{m-j} \tag{24}$$

and identity

$$B^m = \sum_{j=1}^{m} g_j B^{m-j}. \tag{25}$$

following the Hamilton-Cayley theorem.

2. Nilpotent RK-methods

A large group of the RK-schemes is based on the property of matrix nilpotency. Let μ be some real number. The matrix $B - \mu E$ is said to be nilpotent, if for some positive integer l the equality $(B - \mu E)^l = 0$ holds.

It is evident, that if $(B - \mu E)^l = 0$, then $(B - \mu E)^{l+1} = 0$. Positive integer ind is said to be the nilpotency index of the matrix $b - \mu E$, if $(B - \mu E)^{ind} = 0$, but $(B - \mu E)^{ind-1} \neq 0$. The nilpotency index does not exceed the order of the matrix , i.e., $ind \leq m$. Indeed, the matrix $B - \mu E$ cannot be nilpotent if at least one of its eigenvalues is non-zero. Otherwise, if all the eigenvalues are equal to zero, then its characteristic polynomial is λ^m and the Hamilton-Cayley theorem yields $(B - \mu E)^m = 0$. The nilpotency index coincides with the order of the minimum matrix polynomial. If $ind = m$, i.e., the minimum polynomial coincides with the characteristic polynomial, the matrix is said to be complete. If the matrix $B - \mu E$ is complete, then the matrix B is also complete with the characteristic polynomial $(\lambda - \mu)^m$, i.e., with m-multiple eigenvalue μ.

Only one eigenvector U_1 corresponds to a complete nilpotent matrix $B - \mu E$. This vector belongs to the set of the adjoint vectors U_i of height i, satisfying the equation $U_i(B - \mu E)^i = 0$ under condition $U_i(B - \mu E)^{i-1} \neq 0$, $i = 1(1)ind$. These relations define a recursive connection $U_{i+1}(B - \mu E) = U_i$, $U_1(B - \mu E) = 0$. The vectors U_i are linearly independent.

Definition. *The RK-method with nilpotent matrix $B - \mu E$ is said to be the nilpotent RK-method.*

According to (1.24), the characteristic polynomial of the matrix B of the nilpotent RK-method is

$$Q_m(\lambda) = (\lambda - \mu)^m = \lambda^m + \sum_{j=1}^{m} (-1)^j C_m^j \mu^j \lambda^{m-j}, \tag{1}$$

hence

$$q_j = (-1)^{j-1} C_m^j \mu^j, \quad j = 1(1)m. \tag{2}$$

The powers of such a matrix are of a specific form, established by the following assertion.

Lemma 2.1. *For $k \geq 0$ representation*

$$B^{m+k} = \sum_{j=1}^{m} (-1)^{j-1} C_{k+j-1}^{k} C_{k+m}^{k+j} \mu^{j+k} B^{m-j}. \tag{3}$$

is valid.

Proof. Representations (1.25) and (2) imply

$$B^m = \sum_{j=1}^{m} (-1)^{j-1} C_m^j \mu^j B^{m-j}, \tag{4}$$

i.e., representation (3) for $k = 0$. Multiply (3) by B, eliminate B^m by means of (4) and apply identity

$$C_{k+m}^{k+1} C_m^j - C_{k+j}^{k} C_{k+m}^{k+j+1} = C_{k+j}^{k+1} C_{k+m+1}^{k+j+1}, \tag{5}$$

which can be directly verified. The equality obtained coincides with (3) after substitution of k instead of $k+1$. Therefore, all the requirements of the induction method are justified and the assertion of the lemma is proved. □

Let us employ the nilpotency property of the matrix $B - \mu E$ and transform fundamental relations (1.23). Multiplying equalities

$$(B - \mu E)^j = \sum_{i=0}^{j} C_j^i (-\mu)^i B^{j-i}$$

by b_{m+1} on the left and by $\Lambda^{k-1} e$ on the right, find from (1.23) that

$$\begin{aligned} b_{m+1}(B - \mu E)^j \Lambda^{k-1} e &= \sum_{i=0}^{j} C_j^i \frac{(k-1)!}{(k+j-i)!} (-\mu)^i \\ &= (-\mu)^j (k-1)! \sum_{i=0}^{j} C_j^i \frac{1}{(i+k)!} (-1/\mu)^i. \end{aligned}$$

The sum on the right-hand side to within a factor is the k-th Laguerre polynomial derivative of the $(j+k)$-th order with respect to the variable μ^{-1}. Therefore,

$$b_{m+1}(B-\mu E)^j\Lambda^{k-1}e = \mu^j\tfrac{(k-1)!}{(k+j)!}j!\mathcal{L}_{k+j}^{(k)}(1/\mu),\qquad k=1(1)M-j,\quad j=0(1)M-1. \tag{6}$$

These relations enable us to ascertain the nature of the vector b_{m+1}.

Lemma 2.2. *The vector b_{m+1} is the left adjoint vector of height ind for the matrix B, defined in (1), if and only if μ^{-1} is not a root of the polynomial $\mathcal{L}_{ind}^{(1)}(\lambda)$.*

Proof. If b_{m+1} is the adjoint vector of height ind, then $b_{m+1}(B-\mu E)^{ind-1} \neq 0$. By definition (6)

$$b_{m+1}(B-\mu E)^{ind-1}e = \frac{\mu^{ind-1}}{ind!}\mathcal{L}_{ind}^{(1)}(1/\mu).$$

In the next section some properties of the Laguerre polynomials will be studied, particularly (12), according to which the right-hand side of the given equality may not turn to zero for $\mu = 0$. Hence, the assertion of the lemma is valid. □

Therefore, in the conditions of Lemma 2.2, the vector b_{m+1} is the adjoint vector of height ind, hence the vectors $U_i = b_{m+1}(B-\mu E)^{ind-i}, i = 1(1)ind$, are linearly independent. Note that weak approximation conditions (1.21) are the relations of $V_k = (kB-\Lambda)\Lambda^{k-1}e$ being orthogonal to $r_j = b_{m+1}B^{j-1}, j = 1(1)N-k$.

Lemma 2.3. *In the nilpotent RK-method the vectors $r_j = b_{m+1}B^{j-1}, j = 1(1)ind$, are linearly independent.*

Proof. The vectors $U_{ind-j+1} = b_{m+1}(B-\mu E)^{j-1}$ for the nilpotent matrix $B-\mu E$ are linearly independent, since they are adjoint vectors of height $ind-j+1$. Since

$$U_{ind-j+1} = \sum_{i=1}^{j}(-\mu)^{j-i}C_{j-1}^{i-1}r_i$$

and the coefficient of r_j is equal to one, then the transformation of the vectors U_{m-j+1} into the vectors r_j, $j = 1(1)ind$ is carried out with the help of a lower triangle matrix of the order ind with the unit diagonal, i.e., non-degenerate. It provides validity of the lemma. □

Consider some properties of the Laguerre polynomials $L_k(\lambda)$

$$L_k(\lambda) = \sum_{j=0}^{k} (-1)^{k-j} \frac{1}{j!} C_k^j \lambda^j. \tag{7}$$

It is easy to check, that they satisfy the recursive relations

$$\begin{aligned} L_{-1}(\lambda) &= 0, \\ L_0(\lambda) &= 1, \\ (k+1)L_{k+1}(\lambda) &= (\lambda - 2k - 1)L_k(\lambda) - kL_{k-1}(\lambda), \end{aligned} \tag{8}$$

and this implies that the roots $\lambda_i^{(k)}, L_k(\lambda_i^{(k)}) = 0, i = 1(1)k$, arranged in ascending order, are real, single and satisfy separation condition

$$\lambda_i^{(k+1)} < \lambda_i^{(k)} < \lambda_{i+1}^{(k+1)}, \quad i = 1(1)k. \tag{9}$$

By the sequential differentiation of representation (7), evaluate

$$L_k^{(l)}(\lambda) = \sum_{j=l}^{k} (-1)^{k-j} \frac{1}{(j-l)!} C_k^j \lambda^{j-l}, \tag{10}$$

and, also,

$$L_{k+l}^{(l)}(\lambda) = \frac{(k+l)!}{k!} \sum_{j=0}^{k} (-1)^{k-j} C_k^j \frac{\lambda^j}{(j+l)!}. \tag{11}$$

This yields

$$\mu^k L_{k+l}^{(l)} \left(\frac{1}{\mu}\right) \to \frac{1}{k!}, \tag{12}$$

for $\mu \to 0$.

The Laguerre polynomials satisfy also relations

$$L_k^{(1)}(\lambda) + L_{k+1}^{(1)}(\lambda) = L_k(\lambda), \tag{13}$$

$$L_k(\lambda) + L_{k+1}(\lambda) = \frac{\lambda}{k+1} L_{k+1}^{(1)}(\lambda), \tag{14}$$

which is easily checked with the help of identities

$$\begin{aligned} C_k^j + C_k^{j-1} &= C_{k+1}^j, \\ (j+1)C_k^{j+1} &= kC_{k-1}^j. \end{aligned} \tag{15}$$

Lemma 2.4. *The polynomials* $L_k^{(j)}(\lambda)$ *satisfy the recurrent relations*

$$\begin{aligned} L_{j-1}^{(j)}(\lambda) &= 0, \\ L_j^{(j)}(\lambda) &= 1, \\ (k-j+1)L_{k+1}^{(j)}(\lambda) &= (\lambda - 2k + j - 1)L_k^{(j)}(\lambda) - kL_{k-1}^{(j)}(\lambda), \quad k \geq j. \end{aligned} \tag{16}$$

In particularly, the conditions $L_k^{(1)}(\nu_i^{(k)}) = 0$, imply inequalities

$$\nu_i^{(k+1)} < \nu_i^{(k)} < \nu_{i+1}^{(k+1)}, \quad i = 1(1)k. \tag{17}$$

Lemma 2.5. *The inequalities*

$$\lambda_i^{(m)} < \nu_i^{(m+1)}, \quad i = 1(1)m, \tag{18}$$

are valid.

Proof. From Lemma 4.3 the polynomial

$$\frac{\lambda}{m+1} L_{m+1}^{(1)}(\lambda) = L_{m+1}(\lambda) + L_m(\lambda) \tag{19}$$

of order $n+1$ has the roots $\nu_i^{(m+1)}$, $i = 1(1)m$, $\nu_0^{(m+1)} = 0$, which are separated by the roots $\lambda_i^{(m)}$. The coefficients of polynomials $L_{k+1}^{(l)}(\lambda)$ in representation (11) have an alternative sign, therefore the value $\nu_i^{(m+1)}$, $\lambda_i^{(m)}$, $i = 1(1)m$, will be real and positive. □

Equations (6) define the nilpotent RK-method. Let us find the discretization order of this method. This is proved to be essentially connected with the nilpotency index of the matrix $B - \mu E$.

Lemma 2.6. *The discretization order of the nilpotent RK-method defined by (6) under condition*

$$L_{ind}^{(1)}\left(\frac{1}{\mu}\right) \neq 0 \tag{20}$$

and in case of solubility of equations (1.23), is equal to the nilpotency index, i.e., $M = ind$. *If* $N \geq ind + 1$, *then under additional condition*

$$L_{ind+1}^{(1)}\left(\frac{1}{\mu}\right) = 0, \tag{21}$$

the order of accuracy is equal to $ind + 1$. *Equality is impossible.*

Proof According to relations (1.17), (1.18), (1.21), obtain in the conditions of the lemma

$$\begin{aligned} E_j &= 1 - jb_{m+1}\Lambda^{j-1}e = 1 - j!b_{m+1}B^{j-1}e, \\ & \quad j = 1(1)N, \end{aligned} \tag{22}$$

$$\begin{aligned} E_j &= 0, \quad j = 1(1)M, \\ E_{M+1} &= 1 - (M+1)b_{m+1}\Lambda^M e. \end{aligned} \tag{23}$$

Equalities (22) may take place only in case of their consistency. As soon as, according to Lemma 2.2, the vectors $r_j = b_{m+1}B^{j-1}, j = 1(1)ind$, are linearly independent if (20) holds, no additional relations are imposed on equalities $r_j e = (j!)^{-1}, j = 1(1)ind$. Their solvability signifies $E_j = 0, j = 1(1)ind$. Another situation occurs if the vectors $r_l, l = ind + 1(1)N$ are involved. The nilpotency property

$$B^l = -\sum_{i=1}^{l}(-\mu)^l C_l^i B^{l-i}$$

imposes a certain relationship on the vectors $r_j, j = 1(1)ind + 1$, thus

$$\begin{aligned} E_{ind+1} &= 1 + (ind+1)!\sum_{i=1}^{ind}(-\mu)^i C_{ind}^i b_{m+1}B^{ind-i}e \\ &= (ind+1)!\mu^{ind}\sum_{i=0}^{ind}(-1)^{ind-i}C_{ind}^i\frac{1}{(i+1)!}\left(\frac{1}{\mu}\right)^i, \end{aligned}$$

or, in accordance with (11),

$$E_{ind+1} = ind!\mu^{ind}L_{ind+1}^{(1)}\left(\frac{1}{\mu}\right). \tag{24}$$

This expression is derived with the help of the second form of representation of E_j in (22), i.e., with the use of the weak approximation and condition $N \geq M$. The condition $E_{ind+1} = 0$ cannot be satisfied for $\mu = 0$ by virtue of (12) and is attained only under condition (21). In this case $M \geq ind + 1$. Otherwise, if condition (21) is not satisfied, then $E_{ind+1} \neq 0$ and $M = ind$.

Let us make clear then if equality $M = ind + 2$ is possible. Since $E_j = 0, j = 1(1)ind + 1$, similarly to E_{ind+1}, evaluate applying the nilpotency property, assuming $N \geq M$,

$$E_{ind+2} = (ind+1)!\mu^{ind+1}L_{ind+2}^{(1)}\left(\frac{1}{\mu}\right).$$

By virtue of the roots of the polynomials $L^{(1)}_{ind+1}(\lambda)$ and $L^{(1)}_{ind+2}(\lambda)$ and being separated, simultaneous annihilation of E_{ind+1} and E_{ind+2} is impossible. Thus, (21) implies $M = ind + 1, N \geq M$

Therefore, taking care of a better approximation, one has to choose a matrix with the nilpotency index m, i.e., a complete one. In this case the row vector b_{m+1} is determined by definition of $\lambda_i, i = 1(1)m$ as it follows from (1.13).

Definition. *The nilpotent RK-method is said to be complete if the matrix B is complete.*

With regard to Lemma 4, one may write down equations (6) for the complete RK-method for $M = m$ in the form

$$\begin{gathered} b_{m+1}(B-\mu E)^j\Lambda^{k-1}e = \mu^j\tfrac{(k-1)!j!}{(k+j)!}L^{(k)}_{j+k}\left(\tfrac{1}{\mu}\right), \\ k = 1(1)m-j, \quad j = 0(1)m-1. \end{gathered} \tag{25}$$

The local trancation error is determined by the value

$$l_{n+1} = E_{m+1}\tau^{m+1}, \tag{26}$$

thereto, according to (22),

$$E_{m+1} = m!\mu^m L^{(1)}_{m+1}\left(\frac{1}{\mu}\right). \tag{27}$$

Let us express with the help of q_j the stability function $R(\tau)$

$$R(\tau) = 1 + \tau b_{m+1}(E-\tau B)^{-1}e.$$

For this purpose, define sequence

$$\begin{aligned} \varphi_0 &= 1, \\ \varphi_k &= \tau^{-1}\varphi_{k-1} - q_k, \quad k = 1(1)m, \end{aligned}$$

or

$$\begin{aligned} \varphi_0 &= 1, \\ \tau^k\varphi_k &= 1 - \textstyle\sum_{j=1}^m q_j\tau^j, \quad k = 1(1)m, \end{aligned} \tag{28}$$

which is the Horner sequence of the polynomial $Q_m(\lambda)$ at the point $\lambda = \tau^{-1}$. It is easy to check that the sequence of polynomials defined this way satisfies the relation

$$(1-\tau\lambda)^{-1} = \frac{1}{\tau\varphi_m}\sum_{j=0}^{m-1}\varphi_j\lambda^{m-j-1},$$

thus, according to the Cayley-Hamilton theorem,

$$R(\tau) = 1 + \frac{1}{\varphi_m}\sum_{k=0}^{m-1} \varphi_k b_{m+1} B^{m-k-1} e$$

or

$$R(\tau) = 1 + \frac{1}{\varphi_m}\sum_{k=0}^{m-1} \varphi_k b_{m+1} B^{m-k-1} e = \frac{1}{\varphi_m}\sum_{k=0}^{m} \frac{\varphi_k}{(m-k)!}.$$

The transformation is carried out with regard to (1.23). As soon as due to (28)

$$\begin{aligned}
\tau^m \sum_{k=0}^{m} \frac{\varphi_k}{(m-k!} &= \sum_{k=0}^{m} \frac{\tau^{m-k}}{(m-k)!} - \sum_{k=1}^{m}\sum_{j=1}^{k} q_j \frac{\tau^{m-k+j}}{(m-k)!} \\
&= \sum_{k=0}^{m} \frac{\tau^{m-k}}{(m-k)!} - \sum_{k=1}^{m}\sum_{j=0}^{k-1} q_{k-j} \frac{\tau^{m-j}}{(m-k)!} \\
&= \sum_{j=0}^{m} \frac{\tau^{m-j}}{(m-j)!} - \sum_{j=0}^{m-1} \tau^{m-j} \sum_{k=j-1}^{m} \frac{q_{k-j}}{(m-k)!} \\
&= 1 + \sum_{j=1}^{m} \frac{\tau^j}{j!} - \sum_{j=1}^{m} \tau^j \sum_{k=m-j+1}^{m} \frac{q_{k+j-m}}{(m-k)!},
\end{aligned}$$

then

$$R(\tau) = \frac{1 + \sum_{j=1}^{m} \tau^j \left(\frac{1}{j!} - \sum_{k=1}^{j} \frac{q_k}{(j-k)!}\right)}{1 - \sum_{k=1}^{m} q_k \tau^k}.$$

is valid.

In the diagonally implicit and singly implicit methods the characteristic polynomial is defined by equalities (2.1), (2.2), thus

$$\begin{aligned}
R(\tau) &= \frac{\sum_{j=0}^{m} \tau^j \sum_{k=0}^{j} (-1)^k \binom{m}{k} \frac{\mu^k}{(j-k)!}}{(1-\mu^m \tau)^m} \\
&= \frac{\sum_{j=0}^{m} (\mu\tau)^j L_m^{(m-j)}(1/\mu)}{(1-\mu\tau)^m}
\end{aligned}$$

RK-method is said to be L-stable, if $R(\tau) \to 0$ at $\tau \to -\infty$. Therefore, the following assertion is valid.

Lemma 2.7. *The maximal achieved order of accuracy of L-stable nilpotent RK-method is equal to the nilpotent index ($M = ind$) and always less than m.*

Proof. The condition of L-stability implies the equality $L_m(\frac{1}{\mu}) = 0$. In this case $L_{m-1}(\frac{1}{\mu}) \neq 0$ and $L_m^{(1)}(\frac{1}{\mu}) \neq 0$ is valid. Sequently, the assertion of the lemma follows from Lemma 2.6. □

3. The DIRK-method

From all matrices B satisfying definition (2.1) let us first consider the lower triangular one

$$B = \begin{pmatrix} \mu & & & & \\ \beta_{21} & \mu & & 0 & \\ \beta_{31} & \beta_{32} & \mu & & \\ \vdots & & \ddots & \ddots & \\ \beta_{m1} & \beta_{m2} & \dots & \beta_{m,m-1} & \mu \end{pmatrix} \tag{1}$$

Definition. *The nilpotent RK-method with lower triangular matrix B is said to be the DIRK-method (diagonally implicit RK method).*

Elements $\beta_{i,i-j}, i = j+1(1)m$, form j-th diagonal of the matrix B. The only element of $(m-1)$-th diagonal is β_{m1}.

Definition. *j-th diagonal will be said to be the boundary one, if all the elements above this diagonal are equal to zero, i.e., $\beta_{i+k,i-j} = 0, i = j+1(1)m, k > 0$.*

According to the definition, the first diagonal is the boundary one in the matrix $B - \mu E$, if $\beta_{i,i-1} \neq 0$ at least for one i (which isassumed below).

Lemma 3.1. *j-th diagonal is the boundary one for the matrix $(B - \mu E)^j$. The element w_{kl}^j at the intersection of k -th row and l-th column of this matrix is equal to*

$$w_{kl}^j = \sum_{p=l+j-1}^{k-1} \beta_{kp} \sum_{q=l+j-2}^{p-1} \beta_{pq} \dots \beta_{xy} \sum_{z=l+1}^{y-1} \beta_{yz}\beta_{zl}, \tag{2}$$

with $j-1$-fold summation.

It follows from (2), in particular, that $w_{kl}^j = 0$, if $k < l + j$, since the upper summation limit becomes less than the lower one. Therefore, the elements $w_{j+l,l}^j$ constitute the boundary diagonal and are equal to

$$w_{j+l,l}^j = \prod_{i=l+1}^{l+j} \beta_{i,i-1}, \quad l = 1(1)m - j. \tag{3}$$

Lemma 3.2. *For the nilpotency index of the matrix $B - \mu E$ to be equal to m, it is necessary and sufficient to satisfy conditions*

$$\beta_{i,i-1} \neq 0, \quad i = 2(1)m. \tag{4}$$

Proof. Let the nilpotency index of the matrix $B - \mu E$ be equal to m. Then

$$w_{m-1}^{m-1} = \prod_{i=2}^{m} \beta_{i,i-1} \neq 0, \tag{5}$$

is the only element of the boundary diagonal of the matrix $(B - \mu E)^{m-1}$. This implies the necessity. If $\beta_{i,i-1} \neq 0, i = 2(1)m$, then the same equality implies also the sufficiency. □

The preceding analysis requires the solvability of equations (2.25), which is related, in particular, to the choice of μ and the nodes $\lambda_i, i = 1(1)m$. In order to study the solvability, assume $N = m$ and introduce a row-vector $\Theta(j) = (\theta_{1j}, \ldots, \theta_{jj})$, such that

$$(\theta_{1j}, \ldots, \theta_{jj}, 0, \ldots, 0) = b_{m+1}(B - \mu E)^{m-j},$$

and system (2.25) is represented in the form

$$\begin{gathered} b_{m+1}(B - \mu E)^{m-j} \Lambda^k e = \textstyle\sum_{i=1}^{j} \theta_{ij} \lambda_i^k = g_k^j, \\ k = 0(1)j-1, \quad j = 1(1)m, \end{gathered} \tag{6}$$

thereto

$$g_k^j = \frac{k!(m-j)!}{(m-j+k+1)!} \mu^{m-j} L_{m-j+k+1}^{(k+1)} \left(\frac{1}{\mu} \right). \tag{7}$$

For a fixed j, these relations define a system of equations with the Vandermonde matrix W_j of the order j,

$$W_j = \begin{pmatrix} 1 & \lambda_1 & \ldots & \lambda_1^{j-1} \\ 1 & \lambda_2 & \ldots & \lambda_2^{j-1} \\ \ldots & \ldots & \ldots & \ldots \\ 1 & \lambda_j & \ldots & \lambda_j^{j-1} \end{pmatrix} \tag{8}$$

with the determinant

$$|W_j| = |W_{j-1}| \pi_{j-1}(\lambda_j), \tag{9}$$

where

$$\pi_j(\lambda) = \prod_{l=1}^{j} (\lambda - \lambda_l) = \sum_{l=0}^{j} c_{j,l} \lambda^{j-l}, \quad c_{j,0} = 1, \tag{10}$$

and the right-hand side

$$G(j) = (g_0^j, \ldots, g_{j-1}^j). \tag{11}$$

Therefore, equations (6) may be rewritten in the vector form

$$\Theta(j)W_j = G(j), \quad j = 1(1)m. \tag{12}$$

In the assumption that all λ_i are different, $|W_j| \neq 0$ according to (9) and $\Theta(j)$ are uniquely determined from (12). Particularly, the elements $\beta_{m+1,i}$ are found, since

$$\Theta(m) = b_{m+1}. \tag{13}$$

If the matrix $B - \mu E$ is to have the nilpotency index equal to m, the nodes $\lambda_i, i = 1(1)m$ should be subject to some conditions. According to Lemma 3.2, the elements, $\beta_{i,i-1}, i = 2(1)m$, being non-zero is the necessary and sufficient condition for the equality $ind = m$. Since j-th column of the matrix $(B - \mu E)^{m-j}$ is $w_{mj}^{m-j} e_m$, where e_m is m-th column of the unit matrix E,

$$\theta_{jj} = \beta_{m+1,m} w_{mj}^{m-j}$$

and, by virtue of (3),

$$\theta_{jj} = \prod_{l=j}^{m} \beta_{l+1,l}.$$

Therefore, if $\beta_{m+1,m} \neq 0$, then θ_{jj} should turn to zero for no $j, j = 1(1)m$. Since θ_{jj} are determined from the solution of system (6) with the fixed right-hand side (if some μ is chosen), then the matrices of these systems, i.e., the nodes $\lambda_j, j = 2(1)m$ should be selected that as to provide θ_{jj} being non-zero. Let us find some necessary conditions for the latter. According to the Cramer rule, equation (6) yields

$$\theta_{j+1,j+1} = \frac{\Delta_{j+1}}{|W_{j+1}|}, \quad j = 1(1)m - 1, \tag{14}$$

where

$$\Delta_{j+1} = \begin{vmatrix} 1 & \lambda_1 & \ldots & \lambda_1^j \\ \multicolumn{4}{c}{\dotfill} \\ 1 & \lambda_j & \ldots & \lambda_j^j \\ g_0^{j+1} & g_1^{j+1} & \ldots & g_j^{j+1} \end{vmatrix},$$

thus $\theta_{j+1,j+1}$, if and only if $\Delta_{j+1} = 0$. The determinant Δ_{j+1} differs from $|W_{j+1}|$ in the last row only, and can be easily calculated. According to (9), (10)

$$|W_{j+1}| = |W_j| \sum_{l=0}^{j} c_{j,l} \lambda_{j+1}^{j-1},$$

which is the expansion of the determinant with respect to the last row. Therefore, replacing the last row only, find

$$\Delta_{j+1} = |W_j| \sum_{l=0}^{j} c_{j,l} g_{j-1}^{j+1}.$$

Thus, for the single nodes λ_i, $i = 1(1)m$ in order to satisfy the equality $\theta_{j+1,j+1} = 0$, it is necessary and sufficient to satisfy condition

$$\sum_{l=0}^{j} c_{j,l} g_{j-l}^{j+1} = 0, \quad j = 1(1)m-1. \tag{15}$$

Since

$$\pi_j(\lambda) = (\lambda - \lambda_j)\pi_{j-1}(\lambda),$$

then

$$\begin{aligned} c_{j,0} &= 1, \\ c_{j,i} &= c_{j-1,i} - \lambda_j c_{j-1,i-1}, \quad i = 1(1)j, \\ c_{j-1,j} &= 0, \end{aligned}$$

and the substitution of these relations into (15) brings about equality

$$\lambda_j = \frac{\sum_{l=0}^{j-1} c_{j-1,l} g_{j-1}^{j+1}}{\sum_{l=0}^{j-1} c_{j-1,l} g_{j-l-1}^{j+1}}, \tag{16}$$

which is necessary and sufficient for $\theta_{j+1,j+1} = 0, j = 1(1)m-1$. This fact is expressed in

Theorem 3.1. *For the triangular nilpotent matrix $B - \mu E$ with single λ_i, $i = 1(1)m$ to have the nilpotency index equal to m and the vector b_{m+1} to be the adjoint vector of height m, it is necessary and sufficient that*

1) condition (16) be violated for all j;

2) $L_m^{(1)}(1/\mu) \neq 0$.

In the meantime, condition (16) is the condition of λ_j being a multiple node, $\lambda_j = \lambda_{j+1}$, for all the other being single. Indeed, in this case $|W_{j+1}| = 0$, since $\pi_j(\lambda_{j+1}) = 0$, and the Kronecker-Capelli theorem requires the equality of the ranks of the extended matrix and the basic one for a solution of system (12) to exist, thus it is necessary to satisfy the condition $\Delta_{j+1} = 0$, i.e., condition (16). More precise conditions of the existence of multiple roots and an algorithm of their calculation is contained in

Theorem 3.2. *For the triangular nilpotent matrix $B-\mu E$ with $m-2$ single roots and one double, $\lambda_k = \lambda_{k+1}, 2 \leq k \leq m-1$, to have the nilpotency index equal to m and the vector b_{m+1} to be its adjoint vector of height m, it is necessary and sufficient to satisfy simultaneously the conditions:*

1) equality (16) holds for $j = k$, but does not take place for $j = 2(1)k-1$;

2) for $j = k+2(1)m$ equalities

$$\lambda_j = \frac{\sum_{i=0}^{j-1} c_{j-1,i} \sum_{l=i}^{j-1} \lambda_{k+1}^{l-i} g_{j-l-1}^{j+1}}{\sum_{i=0}^{j-1} c_{j-1,i-1} \sum_{l=i}^{j-1} \lambda_{k+1}^{l-i} g_{j-l-1}^{j+1}}$$

are valid;

3) $L_m^{(1)}(1/\mu) \neq 0$.

In the sequel, we restrict ourselves to the case of the single nodes $\lambda_i, i = 1(1)m$ and assume that they are chosen with regard to Theorem 3.1.

Equations (2.25) are essentially non-linear. Even after the calculation of the elements θ_{ij} from equations (6), this non-linearity still takes place. Thus it is important to construct an algorithm providing the solution of system (6) in case the number μ and the nodes $\lambda_i, i = 1(1)m$ are properly chosen (i.e., in accordance with Theorem 3.1 or Theorem 3.2). In the notations of Lemma 3.1

$$\theta_{j-i,j} = \sum_{l=m-i}^{m} \beta_{m+1,l} w_{l,j-i}^{m-j}, \quad j = 1(1)m, \quad i = 0(1)j-1. \tag{17}$$

From the same Lemma let us derive equalities

$$w_{l,j-i}^{m-j} = \sum_{k=m-i-1}^{l-1} \beta_{lk} w_{k,j-i}^{m-j-1}, \quad l = m-i(1)m. \tag{18}$$

Relations (17),(18) will be used as the basis for the solution of system (6). First of all, $\beta_{m+1,i}$, $i = 1(1)m$, are found, as it was established in (13).

Elements of the matrix $B-\mu E$ are found in the following way. We make replacements in (18) $j \to j+l, i \to i+l, l \to m-l$ and present equations (17),(18) in the form

$$\begin{aligned} w_{m,j-i}^{m-j} &= \left(\theta_{j-i,j} - \textstyle\sum_{l=m-i}^{m-1} \beta_{m+1,l} w_{l,j-i}^{m-j}\right) \beta_{m+1,m}, \\ & \quad j = i+1(1)m-1, \\ w_{m-l-1,j-i}^{m-j-l-1} &= \left(w_{m-l,j-i}^{m-j-l} - \textstyle\sum_{k=m-i-l-1}^{m-l-2} \beta_{m-l,k} w_{k,j-i}^{m-j-l-1}\right) / \beta_{m-l,m-l-1}, \\ & \quad j = i+1(1)m-l-2, \quad l = 0(1)m-i-3, \\ & \quad i = 0(1)m-2, \end{aligned} \tag{19}$$

where, as usual, it is assumed that the sum is equal to zero, if the upper limit is less than the lower one.

The solution is attained stage by stage. At first, the stage $i = 0$ is carried out:

$$\begin{aligned} w_{m,j}^{m-j} &= \theta_{jj}/\beta_{m+1,m}, \quad j = 1(1)m-1, \\ w_{m-l-1,j}^{m-j-l-1} &= w_{m-l,j}^{m-j-l}/\beta_{m-l,m-l-1}, \quad j = 1(1)m-l-2, \; l = 0(1)m-3. \end{aligned}$$

Meanwhile the k-th diagonals of the matrices $(B - \mu E)^k, k = 1(1)m - 1$ are calculated consecutively. Therefore, at zero stage we have already calculated the elements $\beta_{j,j-1}, j = m + 1(-1)2$.

Consider the i-th stage, $i = 1(1)m - 2$. At the preceding stages, the values w_{lk}^j are determined. At the i-th stage, the elements w_{lk}^j should be calculated, i.e., the elements of $(j + i)$-th diagonal of the matrix $(B - \mu E)^j, j = 1(1)m - i - 1$. In particular, $(i + 1)$-th diagonal of the matrix $B - \mu E$ is calculated. Therefore, after i stages the first $i + 1$ diagonals of the matrix $B - \mu E$, which differs from B in the main diagonal μE only, are determined.

In the previous sections, equations for calculation of the matrix $B - \mu E$ and the vector b_{m+1}, an algorithm of their solution for given matrix Λ were obtained with the help of the triangular property of a nilpotent matrix, and thereto the conditions on Λ were indicated, in which the nilpotency index of the matrix $B - \mu E$ is equal to m. In the meantime, Theorem 3.1 is more likely to demonstrate us, which way one should not choose the matrix Λ. In order to answer the question, how it is be chosen, it is necessary to proceed with the analysis of equations (1.21). As it has been already mentioned, equations (1.21) are the orthogonality relations of the vector $v_k = (kB - \Lambda)\Lambda^{k-1}e$ to the vectors $r_j = b_{m+1}B^{j-1}$

$$r_j v_k = 0, \quad j = 1(1)N - k, \quad k = 1(1)N - 1, \tag{20}$$

thereto it was established in Lemma 2.3 that the vectors $r_j, j = 1(1)ind$ are linearly independent. In particular, the vector $v_1 = (B - \Lambda)e$ is orthogonal to $N - 1$ vectors r_j. Since $N \geq ind$, as it is required by Lemma 2.6, v_1 is orthogonal at least to $ind - 1$ linearly independent vectors of the space $\mathbf{R}_m$. Assuming $ind = m$, let us show that v_1 is orthogonal also to the vector r_m, i.e., to the entire space $\mathbf{R}_m$, which is possible only if $v_1 = 0$. Let us prove some preliminary assertion.

Lemma 3.3. *In the DIRK-method the following relations are valid:*

$$b_{m+1}B^{m-j}\Lambda^j e = \frac{j!}{(m+1)!} - \sum_{i=0}^{j} c_{j,j-i} g_i^j, \quad j = 1(1)m, \tag{21}$$

thereto g_i^j is defined in (7) and the coefficients $c_{j,j-i}$ are defined in (10).

Proof. Similarly to (6), write down

$$\begin{aligned} b_{m+1}(B-\mu E)^{m-j}\Lambda^j e &= \sum_{i=1}^{j}\theta_{ij}\lambda_i^j \\ &= -\sum_{l=1}^{j}c_{j,l}\sum_{i=1}^{j}\theta_{ij}\lambda_i^{j-l} = -\sum_{l=1}^{j}c_{j,l}g_{j-l}^j \\ &= g_i^j - \sum_{i=0}^{j}c_{j,j-i}g_i^j. \end{aligned}$$

It remains to check that

$$b_{m+1}B^{m-j}\Lambda^j e = b_{m+1}(B-\mu E)^{m-j}\Lambda^j e - g_j^i + \frac{j!}{(m+1)!},$$

applying for this purpose relations (1.23), (7) and (2.11). □

Lemma 3.4. *Equality $\lambda_1 = \mu$ is sufficient for the relation*

$$b_{m+1}B^{m-1}(B-\Lambda)e = 0$$

in the DIRK-method. If the vector b_{m+1} is the adjoint one of height m, this condition is also necessary.

Proof. It follows from (21) for $j = 0, 1$ that

$$\begin{aligned} b_{m+1}B^{m-1}(B-\Lambda)e &= g_1^1 + c_{1,1}g_0^1 - g_0^0 \\ &= \mu^{m-1}\left(\frac{(m-1)!}{(m+1)!}L_{m+1}^{(2)}(1/\mu) + c_{1,1}\frac{(m-1)!}{m!}L_m^{(1)}(1/\mu)\right. \\ &\quad \left. - \mu\frac{m!}{(m+1)!}L_{m+1}^{(1)}(1/\mu)\right). \end{aligned}$$

Assuming $i = -1, j \div l = 2$ in (2.19), obtain the relation

$$(1/\mu)L_{m+1}^{(2)}(1/\mu) = (m+1)L_m^{(1)}(1/\mu) + mL_{m+1}^{(1)}(1/\mu),$$

with which help we find

$$b_{m+1}B^{m-1}(B-\Lambda)e = (1/m)(\mu + c_{1,1})\mu^{m-1}L_m^{(1)}(1/\mu).$$

By definition, $c_{1,1} = -\lambda_1$. □

Now we can answer the question, if the values $\eta_i, i = 1(1)m$ are at least to some extent the solutions of equation (1.1) at the nodes ξ_i. Equality (1.8) implies $\eta_i = \xi_i^l$ for $f_i = l\xi_i^{l-1}, i = 1(1)m, l = 1(1)L$ if and only if the Butcher condition $C(L)$ is satisfied:

$$B\Lambda^{k-1}e = (1/k)\Lambda^k e, \quad k = 1(1)L.$$

In this case, equation (1.8) assumes the form

$$\eta_i = \xi_i^l + \sum_{k=L+1}^{l} \left(k \sum_{j=1}^{m} \beta_{ij}\lambda_j^{k-1} - \lambda_j^k \right) \frac{\tau^k}{k!} \frac{dy_n}{dt_n^k}, \quad l = 1(1)M + 1.$$

Theorem 3.3. *In the complete DIRK-method, condition $C(1)$, i.e.,*

$$\sum_{j=1}^{i} \beta_{ij} = \lambda_i, \quad i = 1(1)m \tag{22}$$

holds when the conditions $\lambda_1 = \mu, L_m^{(1)}(\mu^{-1}) \neq 0$ are satisfied simultaneously (thereto the first condition is also necessary).

Proof. If both conditions are satisfied, then by virtue of Lemmas 2.2 and 3.4 the vector $v_1 = (B - \Lambda)e$ is orthogonal to m linearly independent vectors $r_j = b_{m+1}B^{j-1}, j = 1(1)m$, i.e., it is equal to zero, which signifies (22). If (22) holds, then $\beta_{11} = \lambda_1$ and $\beta_{11} = \mu$. □

Therefore the desire to obtain Condition $C(1)$ enables us to determine λ_1 and, moreover, carry out the correctness control of the calculation of elements of the matrix B.

Theorem 3.4. *In the complete DIRK-method, Condition $C(2)$ is impossible for any value of μ.*

Proof. Notice first of all, that Condition $C(2)$ implies $C(1)$. Therefore it is sufficient to prove the functionals

$$I_j = b_{m+1}B^{m-j}(2B - \Lambda)\Lambda e, \quad j = 1, 2,$$

not to turn to zero simultaneously, thus the vector $v_2 = (2B - \Lambda)\Lambda e$ might not be equal to zero. We have

$$I_1 = \mu[(m-1)I_2 + \mu^m L_m^{(1)}(1/\mu)], \tag{23}$$

and

$$I_2 = \frac{1}{m(m-1)}\mu^{m-1}L_m^{(2)}(1/\mu) - (m-1)(\lambda_2 - 2\mu)L_m^{(1)}(1/\mu)). \qquad (24)$$

It follows from (24), that if $\mu = 0$, then $I_1 = 0, I_2 = -\lambda_2(m!)^{-1} \neq 0$. If $\mu \neq 0$, then $I_2 = 0$ implies the equality $I_1 = m^{-1}\mu^{m+1}L_m^{(1)}(\mu^{-1})$, by which $I_1 \neq 0$ according to the conditions of the theorem. □

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