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Modified Runge-Kutta method. II

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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 constructing fundamental equations of RK-method remained unchanged. In this paper new concepts 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. In the second part of this paper the investigation of the nilpotency method is continued. The main attention is paid to the singly implicit RK-method [3]. The new set of the singly implicit RK-schemes of high accuracy was proposed.

Let us give some necessary results (with corresponding numbering) from Part I of this paper [1]. We discuss the problem of discretization of ordinary differential equation

$$\frac{\partial y}{\partial t} = f(t, y), \quad 0 \le t \le T, \quad y(0) = y_0, \tag{1.1}$$

by means of the system of nonlinear algebraic equations

$$\begin{aligned} \eta_0 &= y_n, \\ \eta_i &= y_n + \tau \sum_{j=1}^{m} \beta_{ij} f_j, \quad j = 1(1)m+1, \\ y_{n+1} &= \eta_{m+1} \end{aligned} \tag{1.2}$$

with the notations

$$\begin{aligned} f_j &= f(\xi_j, \eta_j), \\ \xi_i &= t_n + \lambda_i \tau, \quad i = 0(1)m+1, \\ \lambda_0 &= 0, \quad \lambda_{m+1} = 1, \quad \lambda_j \le \lambda_{j+1}, \end{aligned} \tag{1.3}$$

which may be presented in the vector form

$$\begin{aligned} \eta &= y_n e + \tau B f, \\ y_{n+1} &= y_n + \tau b_{m+1} f, \end{aligned} \tag{1.11}$$

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

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

The test function method leads to the following equations

$$b_{m+1} W = e^T h, \tag{1.13}$$

$$\begin{aligned} &E_j = 0, \quad j = 1(1)M, \\ &l_{n+1} = E_{M+1} \tau^{M+1}, \end{aligned} \tag{1.17}$$

where

$$E_j = 1 - j b_{m+1} \Lambda^{j-1} e, \tag{1.18}$$

where l_m is a local trancation error, M – an order of accuracy. For receiving the following set of equations

$$\begin{aligned} &b_{m+1} B^{j-1} (kB - \Lambda) \Lambda^{k-1} e = 0, \\ &\quad 2 \le j + k \le N, \quad j = 1(1)N-1, \end{aligned} \tag{1.21}$$

$$\begin{aligned} &b_{m+1} B^j \Lambda^{k-1} e = \frac{(k-1)!}{(k+j-1)!} b_{m+1} \Lambda^{k+j-1} e = (k-1)! b_{m+1} B^{k+j-1} e, \\ &\quad 2 \le k + j \le N, \quad j = 1(1)N-1, \end{aligned} \tag{1.22}$$

$$\begin{aligned} &b_{m+1} B^j \Lambda^{k-1} e = \frac{(k-1)!}{(k+j)!}, \\ &\quad k = 0(1)M - j, \quad j = 1(1)M, \end{aligned} \tag{1.23}$$

where $N \ge M$, the weak approximation principle was proposed. However, equations (1.13), (1.23) are also not enough for determining B, Λ, b_{m+1}. The characteristic polynomial of the matrix B plays the fundamental role in the theory of RK-methods.

$$Q_m(\lambda) = \lambda^m - \sum_{j=1}^{m} q_j \lambda^{m-j}. \tag{1.24}$$

The present paper establishes that the most representative class of the RK-methods of moderate accuracy is characterized by specific form of the polynomial $Q_m(\lambda)$,

$$Q_m(\lambda) = (\lambda - \mu)^m = \lambda^m + \sum_{j=1}^{m}(-1)^j C_m^j \mu^j \lambda^{m-j}, \tag{2.1}$$

connected with property of nilpotency matrix $B - \mu E$, where μ - a real number. For such matrix the following assertion takes place.

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

$$B^{m+k} = \sum_{j=1}^{m}(-1)^{j-1} C_{k+j-1}^{k} C_{k+m}^{k+j} \mu^{j+k} B^{m-j} \tag{2.3}$$

is valid.

One can use the nilpotency property of the matrix $B-\mu E$ to transform the fundamental equations (1.23) in the following way

$$\begin{gathered} b_{m+1}(B - \mu E)^j \Lambda^{k-1} e = \mu^j \frac{(k-1)!}{(k+j)!} j!\, \mathcal{L}_{k+j}^{(k)}(1/\mu), \\ k = 1(1)M - j, \quad j = 0(1)M - 1. \end{gathered} \tag{2.6}$$

The right-hand side is proportional to the k-th Laguerre polynomial derivative of the $(j+k)$-th order with respect to the variable μ^{-1}.

$$L_k(\lambda) = \sum_{j=0}^{k}(-1)^{k-j}\frac{1}{j!}C_k^j \lambda^j. \tag{2.7}$$

$$L_{k+l}^{(l)}(\lambda) = \frac{(k+l)!}{k!}\sum_{j=0}^{k}(-1)^{k-j} C_k^j \frac{\lambda^j}{(j+l)!}. \tag{2.11}$$

This yields

$$\mu^k L_{k+l}^{(l)}\Big(\frac{1}{\mu}\Big) \to \frac{1}{k!}, \tag{2.12}$$

$$\frac{\lambda}{m+1} L_{m+1}^{(1)}(\lambda) = L_{m+1}(\lambda) + L_m(\lambda). \tag{2.14}$$

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

$$L_{ind}^{(1)}\Big(\frac{1}{\mu}\Big) \neq 0 \tag{2.21}$$

and in the 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

$$L^{(1)}_{ind+1}\Big(\frac{1}{\mu}\Big) = 0, \tag{2.22}$$

the order of accuracy is equal to $ind + 1$ - the maximal achieved one.

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

For the complete nilpotent RK-method the equations (2.6) have the form

$$b_{m+1}(B - \mu E)^j \Lambda^{k-1} e = \mu^j \frac{(k-1)!j!}{(k+j)!} L^{(k)}_{j+k}\left(\frac{1}{\mu}\right), \qquad k = 1(1)m - j, \quad j = 0(1)m - 1, \tag{2.25}$$

$$l_{n+1} = E_{m+1}\tau^{m+1}, \tag{2.26}$$

thereto, according to (2.22),

$$E_{m+1} = m!\mu^m L^{(1)}_{m+1}\Big(\frac{1}{\mu}\Big), \tag{2.27}$$

$$b_{m+1}(B - \mu E)^{m-j}\Lambda^k e = \sum_{i=1}^{j} \theta_{ij}\lambda_i^k = g_k^j, \qquad k = 0(1)j - 1, \quad j = 1(1)m, \tag{3.6}$$

$$g_k^j = \frac{k!(m-j)!}{(m-j+k+1)!}\mu^{m-j} L^{(k+1)}_{m-j+k+1}\Big(\frac{1}{\mu}\Big), \tag{3.7}$$

$$\pi_j(\lambda) = \prod_{l=1}^{j}(\lambda - \lambda_l) = \sum_{l=0}^{j} c_{j,l}\lambda^{j-l}, \quad c_{j,0} = 1. \tag{3.10}$$

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

$$\lambda_j = \sum_{l=0}^{j-1} c_{j-1,l}\, g^{j+1}_{j-l} \Big/ \sum_{l=0}^{j-1} c_{j-1,l}\, g^{j+1}_{j-l-1}$$

be violated for all j;

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

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

$$b_{m+1}B^{m-j}\Lambda^j e = \frac{j!}{(m+j)!} - \sum_{i=0}^{j} c_{j,j-i} g_i^j, \quad j = 1(1)m, \tag{3.21}$$

thereto g_i^j *is defined in* (3.7) *and the coefficients* $c_{j,j-i}$ *are defined in* (3.10).

3. The DIRK-method (continuation)

Let us determine the maximum order of accuracy for the DIRK-method. In doing so we will assume $ind = m$. The solvability analysis of equations (3.6) shows, that the condition $N = m$ brings about a consistent, i.e., non-contradictory system (3.6). Hence, Lemma 2.6 in its first part can be applied to the complete DIRK-method and provide the order of accuracy $M = m$. In order to apply the second part of the lemma to the DIRK-method, let us prove the following assertion.

Lemma 3.5. *In order to satisfy the condition* $N = m + 1$, *it is necessary and sufficient to satisfy equalities*

$$b_{m+1}B^{m-j}\Lambda^j e = \frac{j!}{(m+1)!}(1 - E_{m+1}), \quad j = 0(1)m, \tag{3.25}$$

where

$$E_{m+1} = m!\mu^m L_{m+1}^{(1)}(1/\mu).$$

Proof. Note first, that equations (6), which are valid for $j = 1(1)m$, in the case $j = 0$ are reduced to the form $g_0^0 = 0$. Since this extension is consistent and imposes only some restriction on μ ($L_{m+1}^{(1)}(\mu^{-1}) = 0$), equations (3.21) in Lemma 3.3 might be also extended by assuming $j = 0(1)m$. Then it follows from Lemma 3.3 that equalities $\gamma_j = j\gamma_{j-1}$, $j = 1(1)m$ are necessary and sufficient for the equality $N = m + 1$ be valid, where N is the weak order of accuracy and

$$\gamma_j = \sum_{i=0}^{j} c_{j,j-1} g_i^j.$$

In this case equations (1.21) are valid for $j + k < m + 1$. Since γ_j are recursively related, we find easily that

$$\gamma_j = j!\gamma_0 = j!g_0^0 = j!\frac{\mu^m}{(m+1)!} L_{m+1}^{(1)}(1/\mu).$$

Therefore, substituting these values of γ_j into (3.21), obtain

$$b_{m+1}B^{m-j}\Lambda^j = \frac{j!}{(m+1)!} - \frac{j!}{m+1}\mu^m L^{(1)}_{m+1}(1/\mu). \qquad \square$$

The above-proved lemma contains something more than the second part of Lemma 2.6, since it determines the conditions of attaining equality $N = m+1$. Due to this fact, the following assertion is valid.

Theorem 3.5. *For the order of accuracy in the complete DIRK-method to be equal to $m+1$ ($M = m+1$), it is necessary and sufficient that relations*

$$L^{(1)}_{m+1}(1/\mu) = 0,$$
$$\lambda_1 = \mu, \quad \lambda_{j+1} = \frac{\sum_{k=0}^{j} c_{j,j-k}g^{j+1}_{k+1}}{\sum_{k=0}^{j} c_{j,j-k}g^{j+1}_{k}}, \quad j = 0(1)m-1,$$

hold simultaneously.

Proof. All relations in the statement of the theorem are corollaries of the equalities $\gamma_j = 0$, $j = 0(1)m$. The first relation is equivalent to $\gamma_0 = g^0_0 = 0$ due to (3.7) and property (2.12). In order to obtain the other relations, we act similarly to the derivation of Theorem 3.1. Replace the coefficients $c_{j+1,j-i+1}$ in the condition $\gamma_{i+1} = 0$ with their recursive representations and solve the equalities with respect to λ_{j+1}, $j = 0(1)m-1$. The case $\lambda_1 = \mu$ follows from the general one for $j = 0$:

$$\begin{aligned}\lambda_1 &= \frac{g^1_1}{g^1_0} = \frac{1}{m+1}L^{(2)}_{m+1}(1/\mu)/L^{(1)}_m(1/\mu)\\ &= \mu + \mu\frac{m}{m+1}L^{(1)}_{m+1}(1/\mu)/L^{(1)}_m(1/\mu),\end{aligned}$$

if equation (2.19) for $j-l = 2$, $k-i = m+1$ is used. It remains to note only that due to separation of the roots of the polynomials $L^{(1)}_m(\lambda)$ and $L^{(1)}_{m+1}(\lambda)$, they do not simultaneously turn zero, and the requirement of completeness for the DIRK-method is compatible with the condition $M = m+1$ providing $\lambda_1 = \mu$. $\square$

Some features of the nodes λ_j of the complete DIRK-method with $M = m+1$ is given by the theorem as follows

Theorem 3.6. *For the order of accuracy of the complete DIRK-method to be equal to $m+1$, it is necessary to satisfy condition*

$$\int_0^1 \pi_m(\lambda)d\lambda = 0.$$

PROOF. Since the condition $\gamma_m = 0$ is necessary for attaining $M = m+1$, then

$$\sum_{j=0}^{m} c_{m,m-j} g_j^m = 0.$$

According to (3.7), $g_k^m = (k+1)^{-1}$ due to which the previous equality implies

$$\sum_{j=0}^{m} \frac{1}{j+1} c_{m,m-j} = 0.$$

But definition (3.10) of the polynomial $\pi_m(\lambda)$ leads to

$$\int_0^1 \pi_m(\lambda)d\lambda = \sum_{j=0}^{m} \frac{1}{j+1} c_{m,m-j}. \qquad \square$$

The simplest realization of the DIRK-method is carried out in the case $\mu = 0$. From relations (1.2) we find that

$$\begin{aligned} \eta_1 &= y_n, \\ \eta_i &= y_n + \tau \sum_{j=1}^{i-1} \beta_{ij} f(\xi_j, \eta_j), \quad i = 2(1)m+1, \\ y_{n+1} &= \eta_{m+1}, \end{aligned} \tag{3.26}$$

which implies that all the values η_i are determined explicitly. The RK-method, described by formulae (3.26), is said to be the explicit RK-method. It is obtained from the DIRK-method by the limit transition with the help of (2.12). All the algorithms of the DIRK-method are also valid for the explicit RK-method.

Since the explicit method is a particular case of the diagonally implicit one for $\mu = 0$, its stability function $R(\tau)$ is a polynomial:

$$R(\tau) = \sum_{j=0}^{m} \frac{1}{j!}\tau^j,$$

i.e., a segment of the Taylor expansion of exponent. The domain of absolute stability of $R(\tau)$ in the explicit method cannot be large and this imposes serious restrictions on the value of the stepwidth τ.

4. Singly implicit RK-method

In a more general case, a nilpotent matrix is not necessarily triangular. In order to specify the matrix B, m^2, scalar equations are required. However, one cannot obtain this number of equations at the expense of raising the order of accuracy, as it is demonstrated by Lemma 2.6. Hence, it is necessary to move in the direction of the weak order of accuracy N. But we will see that in this case the domain of the parameters j, k in (1.21) should be also reduced.

Lemma 4.1. *In the nilpotent RK-method the condition $N = m + 1$ takes place if the equation*

$$\sum_{i=0}^{m} \frac{1}{i+1} c_{m,m-i} = \frac{m!}{m+1} \mu^m L_{m+1}^{(1)}(1/\mu)$$

holds.

PROOF. Let us consider relations (1.21) for $N = m + 1$, $j = m - k + 1$:

$$b_{m+1} B^{m-k}(kB - \Lambda)\Lambda^{k-1} e = 0, \quad k = 1(1)m. \tag{4.1}$$

With the exception of the cases $k = 1$ and $k = m$, these equations do not depend on the group of equations (1.21) for $k + j \leq m$. However the equality

$$b_{m+1} B^m e = \frac{1}{m!} b_{m+1} \Lambda^m e,$$

due to the Cayley-Hamilton theorem, is expressed by means of the indicated group, hence, it must be consistent with the latter. According to (2.3), (1.23) and (2.11)

$$b_{m+1} B^m e = \frac{1}{(m+1)!} - \frac{1}{m+1} \mu^m L_{m+1}^{(1)}(1/\mu).$$

Thereto, (3.10) and (1.23) yield

$$b_{m+1} \Lambda^m e = -\sum_{i=0}^{m-1} \frac{1}{i+1} c_{m,m-i} = \frac{1}{m+1} - \sum_{i=0}^{m} \frac{1}{i+1} c_{m,m-i}.$$

Equating these two expressions, we come to the statement of the lemma. □

We see that choosing λ_i, $i = 1(1)m$, and μ according to Lemma 4.1, one can obtain the weak order of accuracy equal to $m + 1$. One cannot achieve in the general case a higher weak approximation order. Indeed, let us consider the condition $N \geq m+2$. In this case, equation of Lemma 4.1 is complemented, in particular, with the following:

$$b_{m+1}B^{m+k}(B-\Lambda)e = 0,$$
$$b_{m+1}((m+k+1)B-\Lambda)\Lambda^{m+k}e = 0, \quad k \geq 0.$$

Powers B^{m+k} are expressed with the help of formula (2.3). Powers Λ^{m+k} are reduced similarly with the help of formula (3.10). It is easy to establish the following relations for the case $N = m+2$:

$$\begin{aligned} b_{m+1}B^{m+1}e &= \frac{1}{(m+2)!} - \frac{1}{m+2}\mu^{m+1}L^{(1)}_{m+2}(1/\mu) \\ &\quad -\mu^{m+1}L^{(1)}_{m+1}(1/\mu), \\ b_{m+1}B^{m}\Lambda e &= \frac{1}{(m+2)!} - \frac{1}{m+2}\mu^{m+1}L^{(1)}_{m+2}(1/\mu) \\ &\quad -\mu^{m+1}L^{(1)}_{m+1}(1/\mu); \end{aligned} \tag{4.2}$$

$$\begin{aligned} \frac{1}{m!}b_{m+1}B\Lambda^{m}e &= \frac{1}{(m+2)!} + \frac{c_{m,1}}{m(m+1)}\mu^{m}L^{(1)}_{m+1}(1/\mu) \\ &\quad -\frac{1}{m!}\sum_{i=0}^{m}\frac{c_{m,m-i}}{(i+1)(i+2)}, \\ \frac{1}{(m+1)!}b_{m+1}\Lambda^{m+1}e &= \frac{1}{(m+2)!} - \frac{1-c_{m,1}}{(m+1)^2}\mu^{m}L^{(1)}_{m+1}(1/\mu) \\ &\quad +\frac{1}{(m+1)!}\sum_{i=0}^{m}\frac{c_{m,m-i}}{(i+1)(i+2)}. \end{aligned} \tag{4.3}$$

The left-hand sides of equations (4.3) must be identical. In the condition $L^{(1)}_{m+1}(\mu^{-1}) = 0$, it is possible only when the equations

$$\sum_{i=0}^{m}\frac{c_{m,m-i}}{(i+1)(i+2)} = 0$$

take place, which means that $M = m+2$. But the second equality from (4.2) implies that the equality

$$m!b_{m+1}B^{m}\Lambda e = b_{m+1}B\Lambda^{m}e$$

cannot be valid in the same conditions, since $L^{(1)}_{m+2}(\mu^{-1}) \neq 0$, i.e., N is a fortiori less than $m+2$. Thus, in order not to lose the nilpotency property of the matrix $B-\mu E$, we will restrict ourselves to the case $M \leq N \leq m+1$, but in order to obtain a sufficient number of equations, we will consider truncated scheme (1.21), in which the powers of the matrices B and Λ do not exceed m:

$$b_{m+1}B^{j-1}(kB-\Lambda)\Lambda^{k-1}e = 0, \qquad j = 1(1)m, \quad k = 1(1)l. \tag{4.4}$$

Let us now introduce the following

Definition 1. The nilpotent RK-method with the conditions $M \leq N \leq m+1$ and auxiliary conditions (4.4) for $l = m-1, m$ will be said to be the singly implicit RK-method.

In order to apply Lemmas 2.6 and 4.1, it is necessary to check now whether the nilpotency index of the matrix $B-\mu E$ in the singly implicit RK-method is equal to m, i.e., the singly implicit RK-method is complete. But since the technique of the further analysis is essentially connected with the Frobenius matrix F,

$$F = \begin{pmatrix} 0 & 1 & & \cdots & 1 \\ \vdots & 0 & 1 & & \vdots \\ & & \ddots & \ddots & \\ 0 & & \cdots & 0 & 1 \\ p_m & & \cdots & p_2 & p_1 \end{pmatrix} \tag{4.5}$$

let us consider some of its properties first.

The Frobenius matrix is characterized by the following property. Each of its eigenvalues, notwithstanding its multiplicity, has only one eigenvector. This follows from the fact, that the matrix $\lambda E - F$ has the rank $m-1$ independently of λ. In order to convince ourselves in that, it is sufficient to cross out the first column and the last row of the matrix. Let us prove this fact in a more general form.

If λ_i, $i = 1(1)m$ are eigenvalues of the matrix F, then

$$|\lambda E - F| = \pi_m(\lambda) = \prod_{i=1}^{m}(\lambda - \lambda_i) = \lambda^m - \sum_{i=1}^{m} p_i \lambda^{m-i} \tag{4.6}$$

is the characteristic polynomial of the matrix F. Let us define this fact in a more general form.

Lemma 4.2. *Let* $d = \mathrm{diag}(d_1, ..., d_m)$ *be a diagonal matrix. Then the determinant of the matrix* $\lambda E - dF$ *has the following form*

$$|\lambda E - dF| = \lambda^m - \sum_{i=0}^{m-1} \Big(\prod_{j=i+1}^{m} d_j \Big) p_{m-i} \lambda^i, \qquad (4.7)$$

where the product is assumed to be equal to one, if the upper limit is less than the lower one.

PROOF. Consider the determinant of the $(j+1)$-th order

$$\Delta_j(\lambda) = \begin{vmatrix} \lambda & -d_1 & & & & \\ & \lambda & -d_2 & & & \\ & & \ddots & \ddots & & \\ & & & \lambda & -d_j & \\ -d_m p_m & & \dots & & -d_m p_{m-j+1} & -d_m p_{m-j} \end{vmatrix}.$$

Uncovering its last column, find

$$\Delta_j(\lambda) = -d_m p_{m-j} \lambda^j + d_j \Delta_{j-1}(\lambda).$$

Since

$$\Delta_1(\lambda) = -d_m(\lambda p_{m-1} + d_1 p_m),$$

the induction easily justifies the representation

$$\Delta_j(\lambda) = -d_m \sum_{i=0}^{j} \Big(\prod_{k=i+1}^{j} d_k \Big) p_{m-i} \lambda^i.$$

But the determinant $\Delta_{m-1}(\lambda)$ differs from $|\lambda E - dF|$ only in the missing summand λ at the intersection of the m-th row and the m-th column, due to which

$$|\lambda E - dF| = \lambda^m + \Delta_{m-1}(\lambda). \qquad \square$$

It follows from (4.6), that $W_{k\bullet} F^T = \lambda_k W_{k\bullet}$, $k = 1(1)m$, $W_{k\bullet}$ is the k-th row of the Vandermonde matrix. Thus, if all the eigenvalues of the Frobenius matrix are different, representation

$$WF^T = \Lambda W \qquad (4.8)$$

takes place. Raising the matrix dF^T to a power, one has to keep in mind the representation as follows:

Lemma 4.3. *There holds*

$$(dF)^j = \sum_{i=1}^{m-j} \prod_{k=i}^{i+j-1} d_k e_i e_{i+j}^T + \sum_{i=m-j+1}^{m} e_i r_i^{(j)}, \tag{4.9}$$

where $r^{(i)}$ are some row vectors, the sum is considered to equal zero, when the upper limit is less than the lower one.

Proof. The assertion of the lemma is evident for $j = 0, 1$. Let us assume it to be valid for $j = k \le m - 1$. Then, taking into account $e_i^T e_l = \delta_{il}$, find

$$(dF)^{k-1} = \Big(\sum_{i=2}^{m} d_{i-1} e_{i-1} e_i^T + e_m r_m^{(1)}\Big)\Big(\sum_{l=1}^{m-k} \prod_{t=l}^{l+k-1} d_t e_l e_{l+k}^T + \sum_{l=m-k+1}^{m} e_l r_l^{(k)}\Big)$$
$$= \sum_{i=2}^{m-k} \prod_{l=i-1}^{i+k-1} d_l e_{i-1} e_{i+k}^T + \sum_{i=m-k+1}^{m} d_{i-1} e_{i-1} r_i^{(k)} + e_m r_m^{(1)} (dF)^k.$$

Changing the summation index (from $i - 1$ to i), obtain representation (4.9) in the notations

$$r_i^{(k+1)} = d_i r_{i+1}^{(k)}, \quad i = m - k(1)m - 1,$$
$$r_m^{(k+1)} = r_m^{(1)} (dF)^k. \qquad \square$$

Corollary 1. *Find for $d = E$ from Lemma 4.3*

$$F^j = \sum_{i=1}^{m-j} e_i e_{i+j}^T + \sum_{i=m-j+1}^{m} e_i r_i^{(j)}, \quad j = 0(1)m, \tag{4.10}$$

where

$$r_i^{(j+1)} = r_{i+1}^{(i)}, \quad i = m - j + 1(1)m - 1,$$
$$r_m^{(j+1)} = r_m^{(1)} F^j.$$

If $d = h$ then

$$(F^T h)^j = \sum_{i=1}^{m-j} \frac{1}{j!} e_{i+j} e_i^T + \sum_{i=m-j+1}^{m} (r_i^{(j)})^T e_i^T, \tag{4.11}$$

with the appropriate definition of $r_i^{(j)}$.

The row vectors $r_m^{(j)}$ admit a simple interpretation. According to (4.8),

$$F^j (W_{k\bullet})^T = \lambda_k^j (W_{k\bullet})^T$$

or

$$\sum_{i=1}^{m-j} \lambda_k^{i+j-1} e_i + \sum_{i=m-j+1}^{m} e^i r_i^{(j)} (W_{k\bullet})^T = \lambda_k^j (W_{k\bullet})^T.$$

Multiplying the equality obtained by e_l^T, $l = m - j + 1(1)m$ from the left, find

$$r_l^{(j)} (W_{k\bullet})^T = \lambda_k^{l+j-1},$$

whence

$$\lambda_k^{m+j} = r_m^{(j+1)} (W_{k\bullet})^T.$$

Let $r_m^{(j+1)} = \left(p_m^{(j)}, p_{m-1}^{(j)}, \ldots, p_1^{(j)}\right)$, $p_i^{(0)} = p_i$, $i = 1(1)m$. Then

$$\lambda_k^{m+j} = \sum_{i=0}^{m-1} p_{m-i}^{(j)} \lambda_k^i, \quad k = 1(1)m,$$

or

$$\Lambda^{m+j} = \sum_{i=0}^{m-1} p_{m-i}^{(j)} \Lambda^i, \quad j \geq 0. \tag{4.12}$$

Therefore, the $(m+j)$-th power of the matrix Λ is a linear combination of m lower powers, and the last row of the $(j+1)$-th power of the Frobenius matrix contains the coefficients of this linear combination.

Let us try, as before, to obtain the nilpotent RK-method with the maximum nilpotency index. The choice of nodes affect, though slightly, the nilpotency index in the DIRK-method.

Let us distinguish a class of singly implicit methods, for which this effect is missing.

Definition 2. A singly implicit RK-method with non-degenerate matrices Λ and W and the conditions $L_m^{(1)}(\mu^{-1}) \neq 0$ and $C(m-1)$ is said to be a transformed RK-method.

The transformed RK-method is characterized by following

Theorem 4.1. *In order the vector b_{m+1} in the singly implicit RK-method with the non-degenerate matrices Λ, W and the condition $L_m^{(1)}$ $(\mu^{-1}) \neq 0$ to be the adjoint vector of height m, it is necessary and sufficient to satisfy the condition $C(m-1)$.*

PROOF. Assume that the vector b_{m+1} is the adjoint vector of height m for the matrix B. Then (4.4) implies directly Condition C $(m-1)$ due to linear independence of the vectors $b_{m+1}B^{j-1}$, $j = 1(1)m$.

In order to prove the sufficiency, let us assume Condition $C(m-1)$ to hold, due to which

$$kBW_{\bullet k} = \Lambda W_{\bullet k}, \quad k = 1(1)m-1.$$

Evidently, the unknown vector $BW_{\bullet m}$ in the assumption $|\Lambda| \neq 0$ may be represented as $mBW_{\bullet m} = D\Lambda W_{\bullet m}$, where D is some diagonal matrix. With the help of this representation Condition $C(m-1)$ may be defined in the following matrix form

$$BW = \Lambda(Wh + (D-E)W_{\bullet m}e_m^T h) = (\Lambda W + (D-E)\Lambda W_{\bullet m}e_m^T)h.$$

Since the matrix W is non-degenerate, let us carry out the similarity transformation and define the matrix $\widetilde{B} = W^{-1}BW$. The characteristic polynomials of the matrices $\widetilde{B}$ and B coincide. We obtain

$$\widetilde{B} = W^{-1}BW = (W^{-1}\Lambda W + ze_m^T)h = (F^T + ze_m^T)h = F_z^T h, \tag{4.13}$$

where

$$z = W^{-1}\Lambda(D-E)W_{\bullet m}, \tag{4.14}$$

is, generally, an unknown vector and F_z is the Frobenius matrix of the form (4.5), where p_{m-i} is replaced with $p_{m-i} + z_{i+1}$, $i = 0(1)m-1$, thereto z_i are the components of the vector z. Hence, the characteristic polynomial of the matrix B is $|\lambda E - F_z^T h|$. In the conditions of the theorem relations (1.13) imply $b_{m+1} = e^T hW^{-1}$, thus

$$\begin{aligned} b_{m+1}&(B-\mu E)^{m-1} \\ &= e^T hW^{-1}(B-\mu E)^{m-1} = e^T h(\widetilde{B}-\mu E)^{m-1}W^{-1} \\ &= e^T h(F_z^T h - \mu E)^{m-1}W^{-1} = e^T h\sum_{i=0}^{m-1}(-\mu)^{m-i-1}C_{m-1}^i (F_z^T h)^i W^{-1}. \end{aligned}$$

In order to show that $b_{m+1}(B-\mu E)^{m-1} \neq 0$ independently of the choice of the non-degenerate matrix W, it is sufficient to calculate the first component of the vector $b_{m+1}(B-\mu E)^{m-1}W$. According to Lemma 4.3, taking into account that $d = h$, obtain

$$\begin{aligned} b_{m+1}(B-\mu E)^{m-1}We_1 &= \sum_{j=0}^{m-1}(-\mu)^{m-j-1}C_{m-1}^{j}e^T h(F_z^T h)^j e_1 \\ &= \sum_{j=0}^{m-1}(-\mu)^{m-j-1}C_{m-1}^{j}\frac{1}{j!}e^T h e_{j+1} \\ &= \mu^{m-1}\sum_{j=0}^{m-1}(-1)^{m-j-1}C_{m-1}^{j}\frac{(1/\mu)^j}{(j+1)!} \\ &= (1/m)\mu^{m-1}L_m^{(1)}\Big(\frac{1}{\mu}\Big) \neq 0, \end{aligned}$$

whence, in view of non-degeneracy of the matrix W, conclude that $b_{m+1}(B-\mu E)^{m-1} \neq 0$, i.e., $(B-\mu E)^{m-1} \neq 0$. Hence, the nilpotency index of the matrix $B-\mu E$ is equal to m, and the vector b_{m+1} is the adjoint vector of height m. □

Corollary 2. *The singly implicit RK-method with the non-degenerate matrices W, Λ and the conditions $L_m^{(1)}(1/\mu) \neq 0$ and $C(m-1)$ is complete.*

As soon as the characteristic polynomials of the matrices B and $\widetilde{B}$ coincide, relations (2.1) and (1.3) and Lemma 4.2 with $D = h$ bring about the following equality

$$\begin{aligned} Q_m(\lambda) = \lambda^m - \sum_{i=1}^{m} q_i\lambda^{m-i} &= |\lambda E - F_z^T h| \\ &= \lambda^m - \sum_{i=1}^{m}\frac{(m-i)!}{m!}(p_i + z_{m-i+1})\lambda^{m-i}, \end{aligned}$$

from which we find

$$q_i = \frac{(m-i)!}{m!}(p_i + z_{m-i+1}), \quad i = 1(1)m. \tag{4.15}$$

Expressing q_i through (2.1) leads us to a limitation on the coefficients $p_i + z_{m-i+1}$:

$$p_i + z_{m-i+1} = (-1)^{i-1}\frac{m!}{(m-i)!}C_m^i\mu^i, \quad i = 1(1)m. \tag{4.16}$$

This makes clear that fixing a vector z, we thus specify the nodes λ_i, $i = 1(1)m$. In the simplest case $z = 0$ relations (4.15) and (4.16) admit the form

$$q_i = \frac{(m-i)!}{m!} p_i, \quad i = 1(1)m, \tag{4.17}$$

$$p_i = (-1)^{i-1} \frac{m!}{(m-i)!} C_m^i \mu^i, \quad i = 1(1)m. \tag{4.18}$$

Relations (4.13) are reduced in the meantime to the form $BW = \Lambda W h$, i.e., to Condition $C(m)$.

Definition 3. RK-method is said to be a collocation one, if it satisfies Condition $C(m)$.

As we have already stated, Condition $C(m)$ means that the values η_i approximate the solution of differential equation at the nodes ξ_i, $i = 1(1)m$ with the order m. For the collocation RK-method relation (4.17) is defining, for the nilpotent collocation method the same role is played by (4.18). It is essential that restriction (4.18) should not affect non-degeneracy of the matrices W and Λ.

Theorem 4.2. *In the nilpotent RK-method the intermediate nodes λ_j satisfy relation*

$$L_m\Big(\frac{\lambda_j}{\mu}\Big) = 0, \quad j = 1(1)m, \tag{4.19}$$

and thus the matrices W and Λ are non-degenerate.

PROOF. Applying representation (4.18), calculate the characteristic polynomial $\pi_m(\lambda)$ of the matrix Λ:

$$\begin{aligned}\pi_m(\lambda) &= \sum_{j=0}^{m} (-1)^j C_m^j \frac{m!}{(m-j)!} \mu^j \lambda^{m-j} \\ &= m! \mu^m \sum_{j=0}^{m} (-1)^{m-j} C_m^j \frac{1}{j!} (\lambda/\mu)^j,\end{aligned}$$

i.e., according to (2.7),

$$\pi_m(\lambda) = m! \mu^m L_m(\lambda/\mu),$$

which implies the assertion of the theorem. □

Corollary 3. *In order the nilpotent collocation method to be complete, it is necessary and sufficient to satisfy the condition $L_m^{(1)}(\mu^{-1}) \neq 0$.*

The class of transformed RK-schemes is not exhausted by collocation schemes. Relation (4.16) implies that the characteristic polynomial of a transformed RK-method in the most general case has the form

$$\pi_m(\lambda) = m!\mu^m L_m(\lambda/\mu) + \sum_{i=1}^{m} z_i \lambda^{i-1}. \tag{4.20}$$

The coefficients z_i, $i = 1(1)m$ define a polynomial of the order $m - 1$ and should be chosen so that the polynomial $\pi_m(\lambda)$ has single real roots on the interval [0,1] (at least, mainly). These requirements could be provided non-trivially (as in the case of collocation methods) by setting, for instance,

$$z_{m-1}(\lambda) = \sum_{i=1}^{m} z_i \lambda^{i-1} = \text{const}\, L_{m-1}(\lambda/\mu). \tag{4.21}$$

In order to understand why is it so, let us make the following statement.

Theorem 4.3. *Let two polynomials $P_m(\lambda)$, $P_{m-1}(\lambda)$, of the order m and $m - 1$ respectively with real single roots μ_i, $i = 1(1)m$, ν_i, $i = 1(1)m - 1$ ordered by ascendance be specified, i.e., $\mu_i < \mu_{i+1}$, $i = 1(1)m-1$, $\nu_i < \nu_{i+1}$, $i = 1(1)m - 2$. Assume in addition that the roots ν_i separate the roots μ_i, i.e.,*

$$\mu_i < \nu_i < \mu_{i+1}.$$

Then the polynomial $R_m(\lambda)$ of the order m,

$$R_m(\lambda) = P_m(\lambda) + cP_{m-1}(\lambda), \tag{4.22}$$

where c is an arbitrary real constant, has real single roots λ_i, $i = 1(1)m$, separated by the roots ν_i, i.e.,

$$\lambda_i < \nu_i < \lambda_{i+1}.$$

PROOF. The polynomials $R_m(\lambda)$ and $P_m(\lambda)$ have the same order and both tend to $+\infty$. Moreover, (4.22) implies

$$R_m(\nu_i) = P_m(\nu_i), \quad i = 1(1)m - 1.$$

Since the open interval (ν_i, ν_{i+1}), $i = 1(1)m - 1$, contains a root of the polynomial $P_m(\lambda)$, it has the opposite signs at the points ν_i and ν_{i+1}. Hence, $R_m(\lambda)$ has the opposite signs at the ends, i.e., the root lies inside the interval (ν_i, ν_{i+1}), $i = 1(1)m - 2$. The polynomials $P_m(\lambda)$ and thus $R_m(\lambda)$ also have one root each inside the intervals $(-\infty, \nu_1)$ and (ν_{m-1}, ∞). □

Representation (4.20) combined with (4.21) provides for the necessary properties of the polynomial $\pi_m(\lambda)$ due to the separation of the roots of the polynomials $L^m(\lambda)$ and $L_{m-1}(\lambda)$. But the polynomial $z_{m-1}(\lambda)$ may be represented in a more general form. In the assumption

$$\mu_i < \nu_i < \mu_{i+1}, \quad i = 1(1)m-1, \tag{4.23}$$

the polynomial $\pi_m(\lambda)$,

$$\pi_m(\lambda) = m!\mu^m L_m(\lambda/\mu) + cL_{m-1}(\lambda/\nu), \tag{4.24}$$

where c is an arbitrary real number,

$$L_m(\mu_i\mu^{-1}) = 0, \qquad i = 1(1)m,$$
$$L_{m-1}(\nu_i\nu^{-1}) = 0, \quad i = 1(1)m-1,$$

and ν satisfies relations (4.23), also has the real roots λ_i, $i = 1(1)m$, satisfying property

$$\lambda_i < \nu_i < \lambda_{i+1}, \quad i = 1(1)m-1. \tag{4.25}$$

Representation (4.24) provides for the most general transformed RK-method from all those considered. So, for $\nu = \mu$ obtain (4.20), (4.21) and for $c = 0$ obtain (4.18), i.e., the collocation RK-method.

Let us establish the order of accuracy of the transformed RK-methods. Lemma 2.6 implies

Theorem 4.4. *The order of accuracy of the transformed RK-method is equal to m.*

In order to apply the second part of Lemma 2.6, one should address to Lemma 2.1, which implies that in order to satisfy $N = m+1$, it is necessary and sufficient that

$$\begin{aligned}\mu^m L^{(1)}_{m+1}(1/\mu) &= \frac{m+1}{m!}\sum_{i=0}^{m}\frac{c_{m,m-i}}{i+1}\\ &= \frac{m+1}{m!}\left(-\sum_{i=0}^{m-1}\frac{p_{m-i}}{i+1}+\frac{1}{m+1}\right).\end{aligned} \tag{4.26}$$

This equality admits a simpler form in application to the transformed RK-method. Substituting p_{m-i} from (4.16) to the right-hand side, find

$$\begin{aligned}\mu^m L^{(1)}_{m-1}(1/\mu) &= \frac{m+1}{m!}\left(\frac{1}{m+1}+\mu^m\sum_{i=0}^{m-1}(-1)^{m-i}\frac{m!}{(i+1)!}C^i_m(1/\mu)^i\sum_{i=0}^{m}\frac{z_i}{i}\right)\\ &= \mu^m L^{(1)}_{m+1}(1/\mu)+\frac{m+1}{m!}\sum_{i=1}^{m}\frac{z_i}{i},\end{aligned}$$

which implies

Theorem 4.5. *In order to satisfy the condition $N = m + 1$ in the transformed RK-method, it is necessary and sufficient that*

$$\sum_{i=1}^{m} \frac{z_i}{i} = 0. \tag{4.27}$$

Now we can state the conditions, in which the order of accuracy is equal to $m + 1$.

Theorem 4.6. *In order that the disretization order M in the transformed RK-method defined by* (4.24) *be equal to $m+1$, it is necessary and sufficient that*

$$L_{m+1}^{(1)}(1/\mu) = cL_m^{(1)}(1/\nu) = 0. \tag{4.28}$$

PROOF. For the collocation method $c = 0$, thus the statement of the theorem is a simple corollary of Lemma 2.6. If $c \neq 0$, by Theorem 4.5, in order to attain $N = m + 1$, it is necessary and sufficient to satisfy (4.27), which is nothing else but the equality

$$\int_0^1 \sum_{i=1}^{m} z_i \lambda^{i-1} d\lambda = 0,$$

or, by (4.21),

$$\int_0^1 L_{m-1}(\lambda/\nu) d\lambda = 0.$$

The left-hand side of this equality is equal to $L_m^{(1)}(1/\nu)$. In the meantime the left equality in (4.28) is a corollary of Lemma 2.6. □

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