Explicit Runge-Kutta methods for the numerical solution of linear inhomogeneous IVPs

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Abstract

Runge-Kutta methods for the numerical solution of inhomogeneous linear initial value problems with constant coefficients are considered.

A general procedure to construct explicit s-stage RK methods with order s, for the class of IVP under consideration, depending on the nodes $c_i, i = 1, \ldots, s$ is presented. This procedure only requires the solution of succcessive linear equations in the elements of the matrix $\mathbf{A}$ and avoids the solution of non linear equations.

We obtain several RK schemes with number of stages $s = 5, \ldots, 8$ and maximal order $p = s$ for the class of problems under consideration. Finally, some numerical experiments to test the behaviour of the new RK schemes are presented.

Keywords:
Initial value problem, Linear inhomogeneous, Runge–Kutta, Order conditions

1 Introduction

We consider Initial Value Problems (IVPs) for d-dimensional differential systems of linear inhomogeneous equations given by the equations

$$\begin{aligned} \frac{dy}{dt} &= y'(t) = D\, y(t) + f(t), \qquad t \in [t_0, t_0 + T], \\ y(t_0) &= y_0 \in \mathbb{R}^d, \end{aligned} \tag{1}$$

where $D \in \mathbb{R}^{d \times d}$ is a constant matrix and $f : \mathbb{R} \to \mathbb{R}^d$ is a sufficiently smooth function in the interval of interest.

We approximate the solution $y = y(t)$ of (1) at $t = t_0 + h$ by means of an s-stage explicit Runge-Kutta (RK) method given by

$$y_1 = y_0 + \sum_{j=1}^{s} b_j\, K_j, \tag{2}$$

where the stage vectors $K_j \in \mathbb{R}^d$, $j = 1, \ldots, s$ are computed recursively from the equations

$$K_j = h\, D \left[y_0 + \sum_{k=1}^{j-1} a_{jk}\, K_k \right] + h\, f(t_0 + c_j h), \quad j = 1, \ldots, s. \tag{3}$$

Here $b_j, c_j, a_{jk}, (k = 1, \ldots, j-1)$, $j = 1, \ldots, s$ are real constant coefficients appropriately choosen that define the method.

It is usual to specify the RK method (2), (3) by the Butcher [1] tableau

$$\begin{array}{c|ccccc} c_1 & 0 & & & & \\ c_2 & a_{21} & 0 & & & \\ c_3 & a_{31} & a_{32} & 0 & & \\ \vdots & & & & & \\ c_s & a_{s1} & a_{s2} & \ldots & a_{s,s-1} & 0 \\ \hline & b_1 & b_2 & \ldots & & b_s \end{array} \quad \equiv \quad \begin{array}{c|c} \mathbf{c} & \mathbf{A} \\ \hline & \mathbf{b}^T \end{array} \tag{4}$$

Clearly the s-stage explicit RK method (4) depends on $s + s + s(s-1)/2 = s(s+3)/2$ constant real parameters.

In the derivation of RK methods it is usual to choose the coefficients (4) so that for all IVP under consideration (here of type (1)) the local error LE satisfies

$$LE = y(t_0 + h) - y_1 = \mathcal{O}(h^{p+1}), \qquad (h \to 0), \tag{5}$$

with the highest positive integer p and in this case the method is said to have order p. Also in many problems it is necessary to take into account some stability properties of (2),(3) that depend on the coefficients of the method (4).

The study of the order of RK methods for non linear differential systems is a well established theory after the early papers of Butcher that can be seen e.g. in the books Butcher [1] and Hairer-Norsett-Wanner [3]. However this theory is carried out under the simplifying condition on the coefficients

$$\sum_{k=1}^{j-1} a_{jk} = c_j, \quad j = 1, \ldots, s. \tag{6}$$

This condition is essential in the derivation of RK methods for non linear systems because it allows us to reduce the solution of a d-dimensional non autonomous differential IVP to an equivalent $(d+1)$-dimensional autonomous problem and then the theory is developed for autonomous problems.

As remarked by several authors such as Zingg and Chrisholm [6] and Simos and Tsitouras [5] the number of order conditions for the linear case is smaller than in the non linear case and this extra freedom allows us to derive new special methods. Furthermore, as shown in [6] there are some practical applications that lead to this type of linear problems and therefore such special methods will be useful in this context.

Here in contrast with [6] and [5] we will derive the order conditions of the methods (2), (3) without the simplifying condition (6). In this case we have additional freedom in the available parameters (4) and this leads to new methods for problems (1) with properties to be considered below.

The paper is organized as follows: In Section 2 we give a direct derivation of the order conditions on the coefficients (4) of the method (2), (3) to attain an order $p \leq s$ without the simplifying assumption (6). Note that under this simplifying assumption these conditions can be obtained from the general theory of order of RK methods [1], [3] considering only the rooted trees associated to the special class of problems (1). Some consequences of these conditions are also given.

In Section 3 we present a procedure to construct explicit s-stage RK methods with general order s. This procedure starts from a quadrature rule in $[0,1]$ with nodes $c_i, i = 1, \ldots, s$ and weights $b_j, j = 1, \ldots, s$ with degree of precision at least $s-1$ and then we substitute the non linear equations in the elements a_{ik}, $s \geq i > k \geq 1$ of $\mathbf{A}$ by some equivalent linear equations. Hence the construction procedure only requires the solution of successive linear systems in the elements a_{ij}, $s \geq i > j \geq 1$ of $\mathbf{A}$ and avoids the solution of non linear equations. Several low order examples are presented. In Section 4 some explicit RK methods and maximal order $p = s$ obtained following the algorithm given in Section 3 are given. It is worth to note that when the nodes c_i are rational numbers, the coefficients a_{ik} and b_i are also rational. Also, a six-stage sixth-order explicit RK method, with optimized Euclidean norm of the coefficients of the principal term of the local error is deduced. Finally, in Section 5 several numerical experiments are presented to test the behaviour of the new sixth-order method.

2 Order conditions

In this section we present a direct derivation of the conditions on the coefficients (4) of an s-stage explicit RK method (2), (3) to attain a given order p.

For the series expansion of the exact solution of (1) at $t = t_0 + h$ in powers of h, it follows from (1) that the derivatives of $y(t)$ can be written in the form

$$y^{(k)}(t) = D^k\, y(t) + \sum_{i=0}^{k-1} D^{k-i-1}\, f^{(i)}(t), \quad k = 1, 2, \ldots \tag{7}$$

and then putting $f_0^{(i)} = f^{(i)}(t_0)$ and $D^n y_0 = D^n y(t_0)$ the Taylor series expansion of the solution of (1) at $t = t_0$ is

$$y(t_0 + h) = y_0 + \sum_{n \geq 1} \frac{h^n}{n!}\, D^n\, y_0 + \sum_{n \geq 1} \frac{h^n}{n!} \left(\sum_{i=0}^{n-1} D^{n-i-1}\, f_0^{(i)} \right). \tag{8}$$

Clearly in the right hand side of (8) the first terms are the expansion of the homogeneous solution of (1)

$$y_H(t_0 + h) = \exp(h\, D)\; y_0, \tag{9}$$

whereas the last term corresponds to the particular solution

$$y_P(t_0 + h) = \exp(hD) \int_0^h \exp(-\tau D)\, f(t_0 + \tau)\, \mathrm{d}\tau. \tag{10}$$

Rearranging the last term of (8), $y_P(t_0 + h)$ can be written also in the form

$$y_P(t_0 + h) = \left(\sum_{n \geq 1} \frac{h^n}{n!} D^{n-1}\, f_0 \right) + \left(\sum_{n \geq 2} \frac{h^n}{n!} D^{n-2}\, f_0^{(1)} \right) + \left(\sum_{n \geq 3} \frac{h^n}{n!} D^{n-3}\, f_0^{(2)} \right) + \ldots \tag{11}$$

For the series expansion of the RK method (2), (3) we introduce some auxiliary notations

$$\mathbf{K} = \begin{pmatrix} K_1 \\ K_2 \\ \vdots \\ K_s \end{pmatrix} \in \left(\mathbb{R}^d\right)^s, \quad \mathbf{e} = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \in \mathbb{R}^s, \quad \omega_{i,k} = \mathbf{b}^T\, \mathbf{A}^i\, \mathbf{c}^k, \quad i \geq 0,\; k \geq 0, \tag{12}$$

and taking into account that $\mathbf{A}$ is a strictly lower triangular matrix and $\mathbf{A}^s = 0$, $\omega_{i,k} = 0$ for all $i \geq s$.

Also, for $f : \mathbb{R} \to \mathbb{R}^d$ and a vector $\mathbf{u} = (u_1, u_2, \ldots, u_s)^T \in \mathbb{R}^s$ we denote by $f(\mathbf{u})$ the (ds)-dim vector with components

$$f(\mathbf{u}) = \begin{pmatrix} f(u_1) \\ f(u_2) \\ \vdots \\ f(u_s) \end{pmatrix} \in \left(\mathbb{R}^d\right)^s. \tag{13}$$

With these notations the equation (2) may be written as

$$y_1 = y_0 + \sum_{j=1}^{s} b_j \; K_j = y_0 + \left(\mathbf{b}^T \otimes I_d\right) \; \mathbf{K}, \tag{14}$$

where I_d is the identity matrix of order d and $\otimes$ the standard Kronecker product and (3) becomes

$$\mathbf{K} = h\,(\mathbf{e} \otimes D\; y_0) + h\;\; (\mathbf{A} \otimes D)\;\; \mathbf{K} + h\; f(t_0\; \mathbf{e} + h\; \mathbf{c}). \tag{15}$$

From (15) it follows that

$$\mathbf{K} \;\; = \left[I_{ds} - h\;\; (\mathbf{A} \otimes D)\right]^{-1} \left[h\;(\mathbf{e} \otimes D\; y_0) + h\;\;\; f(t_0\; \mathbf{e} + h\; \mathbf{c})\right], \tag{16}$$

and, taking into account that $\mathbf{A}$ is a lower triangular matrix,

$$\left[I_{ds} - h\;\; (\mathbf{A} \otimes D)\right]^{-1} = \sum_{j=1}^{s} h^{j-1}\; (\mathbf{A} \otimes D)^j, \tag{17}$$

and assuming that f is sufficiently smooth

$$f(t_0\; \mathbf{e} + h\; \mathbf{c}) = (\mathbf{e} \otimes f_0) + \sum_{i \geq 1} \frac{h^i}{i!} \;\; \left(\mathbf{c}^i \otimes f_0^{(i)}\right). \tag{18}$$

Substituting (16)–(17) and (18) into (14) we arrive to

$$y_1 = \widetilde{y}_H + \widetilde{y}_P, \tag{19}$$

with

$$\widetilde{y}_H = y_0 + \sum_{j=1}^{s} h^j \;\omega_{j-1,0}\; D^j\; y_0, \tag{20}$$

and

$$\widetilde{y}_P = \sum_{i \geq 0} \frac{h^{i+1}}{i!} \;\; \left(\sum_{j=1}^{s} \omega_{j-1,i}\; h^{j-1}\; D^{j-1}\; f_0^{(i)} \right), \tag{21}$$

where here again $\widetilde{y}_H$ is the numerical contribution to the homogeneous solution and $\widetilde{y}_P$ that corresponding to the particular solution.

The expressions (19), (20) and (21) define the series expansion of the numerical solution in powers of the step size h.

From (5) the local error becomes

$$LE = y(t_0 + h) - y_1 = \left[y_H(t_0 + h) - \widetilde{y}_H\right] + \left[y_P(t_0 + h) - \widetilde{y}_P\right] \tag{22}$$

with

$$y_H(t_0 + h) - \widetilde{y}_H = \sum_{n \geq 1} h^n \;\; \left(\frac{1}{n!} - \omega_{n-1,0}\right) \;\; D^n\; y_0 \tag{23}$$

and

$$
\begin{aligned}
y_P(t_0+h) - \widetilde{y}_P &= \sum_{n\geq 1} \frac{h^n}{n!} \left(\sum_{i=0}^{n-1} D^{n-i-1} f_0^{(i)} \right) \\
&- \sum_{n\geq 1} \frac{h^n}{(n-1)!} \left(\sum_{j=1}^{s} \omega_{j-1,n-1} h^{j-1} D^{j-1} f_0^{(n-1)} \right).
\end{aligned} \tag{24}
$$

From (22), (23), (24) it follows at once that the order p is always $\leq s$ and we conclude

Theorem 2.1.

1. *The order p of the s-stage method (2), (3) is $\leq s$.*

2. *The conditions of order $p \leq s$ are*

$$
\omega_{i,k} \equiv \boldsymbol{b}^T \boldsymbol{A}^i \boldsymbol{c}^k = \frac{k!}{(i+k+1)!}, \qquad 0 \leq i+k \leq p-1. \tag{25}
$$

Proof. The proof is direct taking into account (23) and that $\omega_{i,k} = 0$, for $i \geq s$. Then, it follows from (24)

$$
y_P(t_0+h) - \widetilde{y}_P = \sum_{n\geq 1} h^n \sum_{k=0}^{n-1} \left(\frac{1}{n!} - \frac{\omega_{n-k-1,k}}{k!} \right) D^{n-k-1} f_0^{(k)}.
$$

□

Remark 1.

According to (25) the number of conditions of the s-stage method (2), (3) for order $p = s$ are $s(s+1)/2$ whereas the number of free parameters is $s(s+3)/2 = s(s+1)/2 + s$ i.e., we have s free parameters. Then, it is expected that for all s there will be methods with maximum order s and this circumvent the order barriers of explicit RK methods for non linear IVPs, in which $p < s$ for $s \geq 5$.

Remark 2.

The order of the s-stage method (2), (3) depends on the available parameters through the real constants $\omega_{i,k}$. Moreover for a method with order $p \leq s$ the principal term of the local error LE (22) is

$$
\begin{aligned}
PTLE &= h^{p+1} \left(\frac{1}{(p+1)!} - \omega_{p,0} \right) D^{p+1} y_0 \\
&+ h^{p+1} \sum_{i=0}^{p} \left(\frac{1}{(p+1)!} - \frac{\omega_{p-i,i}}{i!} \right) D^{p-i} f_0^{(i)},
\end{aligned} \tag{26}
$$

where again the first term is the contribution due to the homogeneous part of the solution and the second one to the non homogeneous term.

Remark 3.

Under the simplifying condition (6) $\mathbf{A}\,\mathbf{e} = \mathbf{c}$, the conditions of order p

$$
\omega_{i,0} = \mathbf{b}^T \mathbf{A}^i \mathbf{c}^0 = \mathbf{b}^T \mathbf{A}^i \mathbf{e} = \frac{1}{(i+1)!}, \quad i = 1, \ldots, p-1, \tag{27}
$$

are identical to

$$\omega_{i-1,1} = \mathbf{b}^T\ \mathbf{A}^{i-1}\ \mathbf{c} = \frac{1}{(i+1)!}, \quad i = 1, \ldots, p-1. \tag{28}$$

Therefore the number of order conditions is reduced, because either (27) or else (28) can be skipped.

Remark 4.

The above theory of order for explicit methods (2), (3) can be easily extended to implicit RK methods with s stages. In this case, the expansion (17) becomes

$$[I_{ds} - h\ (\mathbf{A} \otimes D)]^{-1} = \sum_{i \geq 0} h^i\ (\mathbf{A} \otimes D)^i, \tag{29}$$

and (20) and (21) become, respectively

$$\begin{aligned} \widetilde{y}_H &= y_0 + \sum_{n \geq 1} h^n\ \omega_{n-1,0}\ D^n y_0, \\ \widetilde{y}_P &= \sum_{i,k \geq 0} \frac{h^{i+k+1}}{k!}\ \omega_{i,k}\ D^j\ f_0^{(k)}. \end{aligned} \tag{30}$$

The conditions of order p are again

$$\omega_{i,k} = \frac{k!}{(i+k+1)!}, \qquad 0 \leq i+k \leq p-1. \tag{31}$$

Now, since the condition $\omega_{k,0} = 0$ for $k \geq s$ does not hold anymore, we do not have the limitation of order $p \leq s$. However taking into account that the maximum degree of precision of the underlying quadrature

$$\omega_{0,k} = \mathbf{b}^T\ \mathbf{c}^k = \frac{1}{k+1}$$

is $(2s-1)$ the order p is bounded by $p \leq 2s$.

Another interesting consequence of Theorem 2.1 will be stated in the following

Corollary 2.1. *Let* $(\boldsymbol{A}, \boldsymbol{b}, \boldsymbol{c})$ *an* s*-stage explicit RK method (2)–(3) of order* s *satisfying*

$$c_1 = 0, \qquad b_s\ a_{ss-1}\ \ldots a_{32} \neq 0. \tag{32}$$

Then, the coefficients satisfy the simplifying assumption $\boldsymbol{A}\boldsymbol{e} = \boldsymbol{c}$.

Proof. Let $\mathbf{d} = \mathbf{A}\ \mathbf{e} - \mathbf{c} = (d_1, d_2, \ldots, d_s)^T$. Clearly the condition $c_1 = 0$ implies that $d_1 = 0$.

Next, from the order conditions

$$\omega_{i,0} = \mathbf{b}^T\ \mathbf{A}^i\ \mathbf{c}^0 = \mathbf{b}^T\ \mathbf{A}^i\ \mathbf{e} = \frac{1}{(i+1)!}, \quad i = 1, \ldots, s-1, \tag{33}$$

and

$$\omega_{i-1,1} = \mathbf{b}^T\ \mathbf{A}^{i-1}\ \mathbf{c} = \frac{1}{(i+1)!}, \quad i = 1, \ldots, s-1, \tag{34}$$

we get

$$\mathbf{b}^T\ \mathbf{A}^{i-1}\ \mathbf{d} = \mathbf{b}^T\ \mathbf{A}^{i-1}\ (\mathbf{A}\ \mathbf{e} - \mathbf{c}) = 0, \quad i = 1, \ldots, s-1. \tag{35}$$

Then, by taking into account that $\mathbf{A}$ is lower triangular the last equation of (35) becomes

$$d_s\ b_s\ a_{ss-1}\ \ldots a_{32} = 0,$$

that, by virtue of (32), implies $d_s = 0$.

Next, considering $\mathbf{b}^T\ \mathbf{A}^{s-2}\ \mathbf{d} = 0$ we get

$$d_{s-1}\ b_s\ a_{ss-1}\ \ldots a_{43} = 0,$$

that implies $d_{s-1} = 0$. This reasoning can be repeated for $\mathbf{b}^T\ \mathbf{A}^k\ \mathbf{d} = 0$ with $k = s-3, \ldots, 1$ and then we get $d_{s-2} = \ldots = d_2 = 0$ and then $\mathbf{d} = \mathbf{0}$.

Finally, observe that in the conditions (32) we may assume that $b_s \neq 0$ because otherwise the s-stage method (2), (3) could be reduced to an $(s-1)$ stage RK method. □

3 The construction of s-stage methods of order s.

First of all observe that among the order conditions we have the s conditions

$$\omega_{0,i} = \mathbf{b}^T\ \mathbf{A}^0\ \mathbf{c}^i = \mathbf{b}^T\ \mathbf{c}^i = \frac{i!}{(i+1)!}, \qquad i = 0, \ldots s-1, \tag{36}$$

which imply that the quadrature rule

$$\int_0^1 g(t)\ \mathrm{d}t \simeq \sum_{j=1}^{s} b_j\ g(c_j),$$

with the s nodes $c_j, j = 1, \ldots, s$, and the weights $b_j, j = 1, \ldots, s$, has degree of precision $\geq (s-1)$ or, equivalently, it is exact for all polynomials of degree $\leq (s-1)$. Because of this, it is natural to start the construction of RK methods from a quadrature rule with degree of precision $\geq (s-1)$. Another point is that there exist an extensive knowledge on the theory of quadrature rules that can be used at this point, in particular it is known that the degree of precision of a quadrature rule with s nodes is $\leq (2s-1)$ and the formulas with highest degree $(2s-1)$ are the Gauss formulas where the nodes are the zeros of Legendre polynomials in $[0, 1]$ and the weights satisfy

$$\omega_{0,i} = \mathbf{b}^T\ \mathbf{c}^i = \frac{1}{i+1}, \quad i = 0, 1, \ldots 2s-1. \tag{37}$$

Starting with the nodes and weights of a quadrature formula in $[0, 1]$ with s nodes we will obtain the $s(s-1)/2$ coefficients $a_{ij}, s \geq i > j \geq 1$ of the lower triangular matrix $\mathbf{A}$ from the remaining order conditions

$$\mathbf{b}^T\ \mathbf{A}^j\ \mathbf{c}^k = \frac{k!}{(k+j+1)!}, \qquad 1 \leq j + k \leq s-1. \tag{38}$$

Clearly (38) are also $s(s-1)/2$ equations in the same number of unknowns a_{ij}, but the main difficulty comes from the fact that the equations of (38), $j \geq 2$, are nonlinear and, therefore, we cannot ensure the existence of its solution. However, as we will show in the sequel, we will propose a suitable elimination process that reduces the resolution of (38) to solve successive linear systems in the coefficients a_{ij}. Therefore, except some finite number of conditions on **b** and **c**, we may generate solutions of order s. To make clear this elimination process we will start considering the simple case $s = 3$.

Let

$$\mathbf{b} = (b_1, b_2, b_3)^T, \quad \mathbf{c} = (c_1, c_2, c_3)^T, \tag{39}$$

be the coefficients and nodes of a quadrature rule with three nodes in $[0, 1]$ with degree of precision ≥ 2. Hereafter, we will denote by Conik the order condition $\mathbf{b}^T\ \mathbf{A}^i\ \mathbf{c}^k - k!/(i + k + 1)! = 0$. The remaining conditions that must be satisfied by the elements of the lower triangular matrix **A** are:

$$\begin{aligned} \text{Con10}: &\qquad \mathbf{b}^T\ \mathbf{A}\ \mathbf{c}^0 - 1/2! = 0, \\ \text{Con20}: &\qquad \mathbf{b}^T\ \mathbf{A}^2\ \mathbf{c}^0 - 1/3! = 0, \\ \text{Con11}: &\qquad \mathbf{b}^T\ \mathbf{A}\ \mathbf{c}^1 - 1/3! = 0. \end{aligned} \tag{40}$$

Then Con10 and Con11 are linear in the a_{ik}

$$\begin{aligned} &b_2 a_{21} + b_3(a_{31} + a_{32}) - 1/2 = 0, \\ &b_2 a_{21} c_1 + b_3(a_{31} c_1 + a_{32} c_2) - 1/6 = 0. \end{aligned} \tag{41}$$

These equations can be solved in the elements a_{21} and a_{32} of the first subdiagonal of **A** and give

$$a_{21} = \frac{1 - 6a_{31}b_3c_1 - 3c_2 + 6a_{31}b_3c_2}{6b_2(c_1 - c_2)}, \quad a_{32} = \frac{-1 + 3c_1}{6b_3(c_1 - c_2)}. \tag{42}$$

Now a_{32} depends only on the elements of the underlying quadrature rule and a_{21} is an affine function of a_{31}.

Next, we consider the quadratic equation

$$\text{Con20}: \quad b_3 a_{32} a_{21} - (1/6) = 0, \tag{43}$$

and we substitute a_{32} and a_{21} from (42) into this equation (43). We have now an affine function of a_{31} with the solution

$$a_{31} = \frac{-1 - 6b_2c_1^2 + 3c_2 - 6b_2c_2^2 + 3c_1(1 + (-3 + 4b_2)c_2)}{6b_3(-1 + 3c_1)(c_1 - c_2)}. \tag{44}$$

Finally, substituting a_{31} from (44) into the the first equation of (42) we get

$$a_{21} = \frac{c_1 - c_2}{-1 + 3c_1}. \tag{45}$$

Then the equations (45), (44) and the second of (42) determine the elements of matrix **A** in terms of the nodes and coefficients of the underlying quadrature rule.

Observe that the unique solution of the successive linear systems is possible provided that the determinant of their coefficients is nonzero. Here in view of the resulting formulas we must assume

$$b_3 \neq 0, \quad c_1 \neq 1/3, \quad c_1 \neq c_2. \tag{46}$$

Then, we conclude that for all quadrature rules with three nodes in $[0, 1]$ satisfying (46) and with degree of precision ≥ 2, there exist a three-stage explicit RK method (2)–(3) for linear inhomogeneous systems with order three.

Some examples are reported below.

1. Gauss type methods

With the nodes and coefficients of the three-point quadrature rule,

$$\mathbf{b} = \left(\frac{5}{18}, \frac{8}{18}, \frac{5}{18}\right)^T, \ \mathbf{c} = \left(\frac{1}{2} - \frac{\sqrt{15}}{10}, \frac{1}{2}, \frac{1}{2} + \frac{\sqrt{15}}{10}\right)^T,$$
$$a_{21} = \frac{\sqrt{15}+9}{22}, \quad a_{31} = \frac{7\sqrt{15}-36}{55}, \quad a_{32} = \frac{9}{5} - \sqrt{\frac{3}{5}}, \tag{47}$$

one obtains a method with order three, with degree of precision 5 that does not satisfy the simplifying condition $\mathbf{A}\,\mathbf{e} = \mathbf{c}$.

2. Lobatto type methods

With the nodes and coefficients of the three-point quadrature rule,

$$\mathbf{b} = \left(\frac{1}{6}, \frac{4}{6}, \frac{1}{6}\right)^T, \quad \mathbf{c} = \left(0, \frac{1}{2}, 1\right)^T,$$
$$a_{21} = \frac{1}{2}, \quad a_{31} = -1, \quad a_{32} = 2, \tag{48}$$

one obtains again a method with order three, with degree of precision 3 and it satisfies $\mathbf{A}\,\mathbf{e} = \mathbf{c}$.

3. Radau IIA type methods

Considering the nodes and coefficients of the three-point quadrature rule,

$$\mathbf{b} = \left(\frac{16-\sqrt{6}}{36}, \frac{16+\sqrt{6}}{36}, \frac{1}{9}\right)^T, \ \mathbf{c} = \left(\frac{4-\sqrt{6}}{10}, \frac{4+\sqrt{6}}{10}, 1\right)^T,$$
$$a_{21} = \frac{2(9+\sqrt{6})}{25}, \quad a_{31} = -\frac{3+\sqrt{6}}{4}, \quad a_{32} = \frac{9-\sqrt{6}}{4}. \tag{49}$$

We have a method with order three, the underlying quadrature formula has degree of precision 4, which does not satisfy the simplifying condition $\mathbf{A}\,\mathbf{e} = \mathbf{c}$.

Now, for the case $s = 4$ we start with a quadrature rule with four nodes in $[0, 1]$ and degree of precision ≥ 3 given by the nodes and coefficients

$$\mathbf{b} = (b_1, b_2, b_3, b_4)^T, \quad \mathbf{c} = (c_1, c_2, c_3, c_4)^T. \tag{50}$$

The order conditions, that are linear in the elements of matrix $\mathbf{A} = (a_{ij})$ are:

$$\begin{aligned} \text{Con10} &: \mathbf{b}^T\,\mathbf{A}\,\mathbf{c}^0 - 1/2! = 0, \\ \text{Con11} &: \mathbf{b}^T\,\mathbf{A}\,\mathbf{c}^1 - 1/3! = 0, \\ \text{Con12} &: \mathbf{b}^T\,\mathbf{A}\,\mathbf{c}^2 - 2!/4! = 0. \end{aligned} \tag{51}$$

These conditions can be recast in matrix form as:

$$\mathbf{b}^T\ \mathbf{A}\ \left[\ \mathbf{e}\mid\mathbf{c}\mid\mathbf{c}^2\ \right] = (1/2, 1/6, 1/12).$$

By adding the identity $\mathbf{b}^T\ \mathbf{A}\ \mathbf{e}_4 = 0$ with $\mathbf{e}_4^T = (0,0,0,1)$ we have:

$$\mathbf{b}^T\ \mathbf{A}\ \left[\ \mathbf{e}\mid\mathbf{c}\mid\mathbf{c}^2\mid\mathbf{e}_4\right] = (1/2, 1/6, 1/12, 0) = \mathbf{d}_1^T. \tag{52}$$

Now assumning that $\boldsymbol{\Omega}_1 = [\ \mathbf{e}\mid\mathbf{c}\mid\mathbf{c}^2\mid\mathbf{e}_4]$ is non singular, (52) is equivalent to

$$\mathbf{b}^T\ \mathbf{A}\ = \mathbf{d}_1^T\ \boldsymbol{\Omega}_1^{-1} = \boldsymbol{\mu}_1^T, \tag{53}$$

where $\boldsymbol{\mu}_1^T = (\mu_{11}, \mu_{12}, \mu_{13}, 0)$ with μ_{1j} rational functions of the nodes c_j given by

$$\begin{aligned}
\mu_{11} &= \frac{1-2c_3-2c_2+6c_2c_3}{12(c_1-c_2)(c_1-c_3)}, \\
\mu_{12} &= \frac{-1+2c_1+2c_3-6c_1c_3}{12(c_1-c_2)(c_2-c_3)}, \\
\mu_{13} &= \frac{1-2c_1-2c_2+6c_1c_2}{12(c_1-c_3)(c_2-c_3)}.
\end{aligned} \tag{54}$$

Next, we consider the quadratic conditions in the elements of $\mathbf{A}$

$$\begin{aligned}
\text{Con20} &: \mathbf{b}^T\ \mathbf{A}^2\ \mathbf{c}^0 - 1/3! = 0, \\
\text{Con21} &: \mathbf{b}^T\ \mathbf{A}^2\ \mathbf{c} - 1!/4! = 0,
\end{aligned} \tag{55}$$

that can be written (by adding the identities $\mathbf{b}^T\ \mathbf{A}^2\ \mathbf{e}_3 = 0$ and $\mathbf{b}^T\ \mathbf{A}^2\ \mathbf{e}_4 = 0$) in the matrix form

$$\mathbf{b}^T\ \mathbf{A}^2\,[\ \mathbf{e}\mid\mathbf{c}\mid\mathbf{e}_3\mid\mathbf{e}_4\ ] = (1/6, 1/24, 0, 0) = \mathbf{d}_2^T. \tag{56}$$

Assuming again that $\boldsymbol{\Omega}_2 = [\ \mathbf{e}\mid\mathbf{c}\mid\mathbf{e}_3\mid\mathbf{e}_4\ ]$ is nonsingular these quadratic equations can be written equivalently as

$$\mathbf{b}^T\ \mathbf{A}^2 = \mathbf{d}_2^T\ \boldsymbol{\Omega}_2^{-1} = \boldsymbol{\mu}_2^T, \tag{57}$$

where $\boldsymbol{\mu}_2^T = (\mu_{21}, \mu_{22}, 0, 0)$ with μ_{21} and μ_{22} given by

$$\mu_{21} = \frac{1-c_2}{24(c_1-c_2)}, \qquad \mu_{22} = \frac{-1+c_1}{24(c_1-c_2)}. \tag{58}$$

Now, by using (53) the vector equation (57) is equivalent to

$$\boldsymbol{\mu}_1^T\ \mathbf{A} = \boldsymbol{\mu}_2^T, \tag{59}$$

that is linear in the components of $\mathbf{A}$.

Finally, we consider the cubic condition in $\mathbf{A}$

$$\text{Con30}: \quad \mathbf{b}^T\ \mathbf{A}^3\ \mathbf{c}^0 - 1!/4! = 0, \tag{60}$$

that can be written in the equivalent form

$$\mathbf{b}^T\ \mathbf{A}^3\,[\ \mathbf{e}\mid\mathbf{e}_2\mid\mathbf{e}_3\mid\mathbf{e}_4\ ] = (1/24, 0, 0, 0) = \mathbf{d}_3^T, \tag{61}$$

and, since that $\boldsymbol{\Omega}_3 = [\ \mathbf{e}\mid\mathbf{e}_2\mid\mathbf{e}_3\mid\mathbf{e}_4\ ]$ is non singular we have

$$\mathbf{b}^T\ \mathbf{A}^3 = \mathbf{d}_3^T\ \boldsymbol{\Omega}_3^{-1} = \boldsymbol{\mu}_3^T, \tag{62}$$

with $\boldsymbol{\mu}_3^T = (w_{31}, 0, 0, 0)$, $\mu_{31} = 1/24$. Again by using (57), we have the linear equation equivalent to the cubic equation

$$\boldsymbol{\mu}_2^T\, \mathbf{A} = \boldsymbol{\mu}_3^T. \tag{63}$$

Thus, under the assumption that $\boldsymbol{\Omega}_1$ and $\boldsymbol{\Omega}_2$ are nonsingular, the conditions for order four are equivalent to (53), (59), (63), i.e.,

$$\begin{aligned} b_2 a_{21} + b_3 a_{31} + b_4 a_{41} &= \mu_{11}, \\ b_3 a_{32} + b_4 a_{42} &= \mu_{12}, \\ b_4 a_{43} &= \mu_{13}, \\ \mu_{12} a_{21} + \mu_{13} a_{31} &= \mu_{21}, \\ \mu_{13} a_{32} &= \mu_{22}, \\ \mu_{22} a_{21} &= \mu_{31}, \end{aligned} \tag{64}$$

where μ_{ij} are rational functions of the nodes c_j. These equations define easily all a_{ij}. In fact, first of all for the elements of the first subdiagonal of $\mathbf{A}$, a_{21}, a_{32} and a_{43} we have:

$$a_{21} = \frac{\mu_{31}}{\mu_{22}}, \quad a_{32} = \frac{\mu_{22}}{\mu_{13}}, \quad a_{43} = \frac{\mu_{13}}{b_4}. \tag{65}$$

Next, for the second subdiagonal,

$$a_{31} = \frac{\mu_{21}}{\mu_{13}} - \frac{\mu_{12}}{\mu_{13}}\, a_{21}, \quad a_{42} = \frac{\mu_{12}}{b_4} - \frac{b_3}{b_4}\, a_{32}, \tag{66}$$

and, finally,

$$a_{41} = \frac{\mu_{11}}{b_4} - \frac{b_2}{b_4} a_{21} - \frac{b_3}{b_4} a_{31}. \tag{67}$$

The above procedure provides, for a quadrature rule with four nodes in $[0, 1]$ and degree of precision ≥ 3, an explicit fourth order RK method for linear inhomogeneous IVPs provided that the rational functions that appear in the explicit solution (65), (66) and (67) are well defined. However, as we will see in the next examples, there exist quadrature rules with degree of precision ≥ 3 that lead to infinite solutions in the a_{ij}, and others that have no solution. In any case, since the set of quadrature rules with four nodes and degree of precision ≥ 3 depend on four parameters (there are 8 parameters of $\mathbf{b}$ and $\mathbf{c}$ with four order conditions), there exist a variety of four dimensional quadrature rules with degree of precision ≥ 3. In this setting, the additional requirements to solve the systems in the elements of $\mathbf{A}$ is a finite set of zero-dimensional conditions on the components of $\mathbf{b}$ and $\mathbf{c}$ and, therefore there exist an infinite set of fourth-order explicit RK methods for linear inhomogeneous IVPs.

Example 1. Consider e.g. the quadrature rule defined by

$$\mathbf{b} = \left(\frac{1}{6}, \frac{2}{6}, \frac{2}{6}, \frac{1}{6} \right)^T, \quad \mathbf{c} = \left(0, \frac{1}{2}, \frac{1}{2}, 1 \right)^T. \tag{68}$$

In the linear equations corresponding to conditions Con10, Con11 and Con12, the last two are dependent and there is an infinite set of solutions for the unknowns a_{21}, a_{32} and a_{43}. By taking a_{32} as parameter, we get:

$$a_{21} = \frac{1}{2} \left(1 - 2a_{31} - a_{41} \right), \quad a_{43} = 2 - 2a_{32} - a_{42}. \tag{69}$$

Then, the conditions Con20 and Con21 of second order in a_{ij} define a_{31} and a_{42}, and, finally the third order equation gives a_{41}. Then putting $a_{32} = 1/2 + \lambda$ we have a family of fourth order methods with b and c given by (68), and matrix $\mathbf{A}$ as follows:

$$\mathbf{A} = \begin{pmatrix} 0 & & & \\ 1/2 & 0 & & \\ -\lambda & 1/2+\lambda & 0 & \\ 2\lambda & -4\lambda^2/(1+2\lambda) & 1/(1+2\lambda) & 0 \end{pmatrix}. \tag{70}$$

Observe that $\lambda \neq -1/2$ implies $a_{32} \neq 0$, whereas for $\lambda = 0$ we have the classical fourth order RK method.

Example 2. Consider the quadrature rule defined by

$$\mathbf{b} = \left(\frac{1}{6}, \frac{2}{3}, \frac{1}{2}, -\frac{1}{3}\right)^T, \quad \mathbf{c} = \left(0, \frac{1}{2}, 1, 1\right)^T, \tag{71}$$

that has degree of precision three. The equations corresponding to the first order conditions Con10, Con11 and Con12 have the solution

$$a_{21} = \frac{1}{4}(1 - 3a_{31} + 2a_{41}), \quad a_{32} = \frac{2}{3}(1 + a_{42}), \quad a_{43} = 0. \tag{72}$$

Substituting (72) into the equation corresponding to the second order condition Con22 it turns out to be incompatible. Hence it does not exist a fourth order method associated to the quadrature rule (71).

Finally, we describe the construction of s-stage explicit RK methods with order s for the linear inhomogeneous IVP (1), starting from a quadrature rule with s nodes in $[0, 1]$ and degree of precision $\geq (s-1)$. Let the nodes and coefficients of this quadrature rule given by:

$$\mathbf{c} = (c_1, c_2, \ldots, c_s)^T, \qquad \mathbf{b} = (b_1, b_2, \ldots, b_s)^T. \tag{73}$$

The main point here is to show that the non linear system of the order conditions in the $s(s-1)/2$ elements a_{ij}, $s \geq i > j \geq 1$ of matrix $\mathbf{A}$ may be reduced (under some conditions on the quadrature rule) to a set of linear systems.

At first, we consider the $(s-1)$ order conditions for order s that are linear in $\mathbf{A}$,

$$\begin{array}{ll} \text{Con10}: & \mathbf{b}^T\,\mathbf{A}\,\mathbf{c}^0 = 0!/2!, \\ \text{Con11}: & \mathbf{b}^T\,\mathbf{A}\,\mathbf{c}^1 = 1!/3!, \\ \text{Con12}: & \mathbf{b}^T\,\mathbf{A}\,\mathbf{c}^2 = 2!/4!, \\ \quad\cdots & \quad\cdots \\ \text{Con1}\,(s-2): & \mathbf{b}^T\,\mathbf{A}\,\mathbf{c}^{s-2} = (s-2)!/s!, \end{array} \tag{74}$$

that can be written in the matrix form

$$\mathbf{b}^T\,\mathbf{A}\,\left[\mathbf{e} \mid \mathbf{c} \mid \ldots \mid \mathbf{c}^{s-2}\right] = \left(\frac{1}{2!}, \frac{1}{3!}, \ldots, \frac{(s-2)!}{s!}\right). \tag{75}$$

By adding the identity $\mathbf{b}^T\,\mathbf{A}\,\mathbf{e}_s = 0$, the $(s-1)$-dim system (75) is equivalent to the s-dim system

$$\mathbf{b}^T\,\mathbf{A}\,\mathbf{\Omega}_1 = \mathbf{d}_1^T, \tag{76}$$

with

$$\boldsymbol{\Omega}_1 = \left[\mathbf{e} \mid \mathbf{c} \mid \ldots \mid \mathbf{c}^{s-2} \mid \mathbf{e}_s\right], \quad \mathbf{d}_1^T = \left(\frac{1}{2!}, \frac{1}{3!}, \ldots, \frac{(s-2)!}{s!}, 0\right). \tag{77}$$

Assuming that $\boldsymbol{\Omega}_1$ is a nonsingular matrix, (76) is equivalent to

$$\mathbf{b}^T \mathbf{A} = \mathbf{d}_1^T \boldsymbol{\Omega}_1^{-1} = \boldsymbol{\mu}_1^T, \tag{78}$$

where $\boldsymbol{\mu}_1^T = (\mu_{11}, \mu_{12}, \ldots, \mu_{1,s-1}, 0)$, with the μ_{1i} rational functions of the nodes.

Next, we consider the $(s-2)$ quadratic equations in $\mathbf{A}$. With similar notations as above, they can be written as:

$$\mathbf{b}^T \mathbf{A}^2 \left[\mathbf{e} \mid \mathbf{c} \mid \ldots \mid \mathbf{c}^{s-3}\right] = \left(\frac{1}{3!}, \frac{1}{4!}, \ldots, \frac{(s-3)!}{s!}\right). \tag{79}$$

With the notations

$$\boldsymbol{\Omega}_2 = \left[\mathbf{e} \mid \mathbf{c} \mid \ldots \mid \mathbf{c}^{s-3} \mid \mathbf{e}_{s-1} \mid \mathbf{e}_s\right], \quad \mathbf{d}_2^T = \left(\frac{1}{3!}, \frac{1}{4!}, \ldots, \frac{(s-3)!}{s!}, 0, 0\right) \tag{80}$$

Equation (79) is written in the equivalent form

$$\mathbf{b}^T \mathbf{A}^2 \boldsymbol{\Omega}_2 = \mathbf{d}_2^T. \tag{81}$$

Assuming that $\boldsymbol{\Omega}_2$ is nonsingular, and taking into account (78), we have

$$\boldsymbol{\mu}_1^T \mathbf{A} = \mathbf{b}^T \mathbf{A}^2 = \mathbf{d}_2^T \boldsymbol{\Omega}_2^{-1} = \boldsymbol{\mu}_2^T, \tag{82}$$

with $\boldsymbol{\mu}_2^T = (\mu_{21}, \mu_{22}, \ldots, \mu_{2,s-2}, 0, 0)$, that is a linear equation in the elements a_{ij} equivalent to the quadratic equation (81).

This process can be repeated for the higher order terms in $\mathbf{A}$, thus obtaining

$$\begin{array}{rcll} \boldsymbol{\mu}_2^T \mathbf{A} & = & \boldsymbol{\mu}_3^T, & \boldsymbol{\mu}_3^T = \mathbf{d}_3^T \boldsymbol{\Omega}_3^{-1} = (\mu_{31}, \mu_{32}, \ldots, \mu_{3,s-3}, 0, 0, 0), \\ \vdots & & \vdots & \vdots \\ \boldsymbol{\mu}_{s-2}^T \mathbf{A} & = & \boldsymbol{\mu}_{s-1}^T, & \boldsymbol{\mu}_{s-1}^T = \mathbf{d}_{s-1}^T \boldsymbol{\Omega}_i^{-1} = (\mu_{s-1,1}, 0, \ldots, 0). \end{array} \tag{83}$$

Observe that if the nodes $c_1, \ldots, c_{s-1}$ are distinct between them, the successive matrices $\boldsymbol{\Omega}_i$ are nonsingular and the corresponding vectors $\boldsymbol{\mu}_i^T = \mathbf{d}_i^T \boldsymbol{\Omega}_i^{-1}$ are uniquely determined.

For the existence and uniqueness of solution of the linear system composed by the equations $\mathbf{b}^T \mathbf{A} = \boldsymbol{\mu}_1^T$, $\boldsymbol{\mu}_i^T \mathbf{A} = \boldsymbol{\mu}_{i+1}^T$, $i = 2, \ldots, s-2$ in a_{ik}, it can be cast as the matricial linear system $(s-1) \times (s-1)$

$$\mathbf{W} \widehat{\mathbf{A}} = \mathbf{V}, \tag{84}$$

$$\mathbf{W} = \begin{pmatrix} \mu_{s,s-2} & 0 & \ldots & 0 \\ \vdots & & \ddots & \\ \mu_{12} & \ldots & \mu_{1,s-1} & 0 \\ b_2 & \ldots & b_{s-1} & b_s \end{pmatrix}, \widehat{\mathbf{A}} = \begin{pmatrix} a_{21} & 0 & \ldots & 0 \\ a_{31} & a_{32} & \ldots & 0 \\ \vdots & & \ddots & 0 \\ a_{s1} & a_{s2} & \ldots & a_{s,s-1} \end{pmatrix}, \mathbf{V} = \begin{pmatrix} \mu_{s-1,1} & 0 & \ldots & 0 \\ \vdots & & \ddots & \\ \mu_{21} & \ldots & \mu_{2,s-2} & 0 \\ \mu_{11} & \ldots & \mu_{1,s-2} & \mu_{1,s-1} \end{pmatrix}, \tag{85}$$

and this triangular linear system has a unique solution if and only if $b_s \prod_{i=2}^{s-1} \mu_{s-i,i} \neq 0$ (see Example 2 above).

The solution of this linear system can be carried out as in the above case $s = 4$, and by using the same reasoning for all values of s, as a result, there exist infinitely many explicit RK methods of order s for the linear inhomogeneous IVP (1).

Remark. Note that given the non-confluent nodes $c_1, \ldots, c_{s-1}$, the resulting method can be obtained by a code (symbolic or numeric) in which the vectors $\boldsymbol{\mu}_i$, $i = 1, \ldots, s-1$ are computed from (78), (82) and (83) and, after checking that the elements of the diagonal of $\mathbf{W}$ do not vanish, the elements a_{ik} are obtained from (84).

For the case of repeated nodes, if a method exists, it is possible to design a similar algorithm for the linear equations $\boldsymbol{\mu}_i^T \boldsymbol{\Omega}_i = \mathbf{d}_i^T$ that can introduce additional free parameters and there is an infinite set of solutions, as in Example 1 above.

Finally, we state a consequence of the above equations on the choice of the nodes:

Corollary 3.1. *Consider a s-stage explicit RK method that does not satisfy $\boldsymbol{A}\boldsymbol{e} = \boldsymbol{c}$. If $c_1 = 1/s$, then there does not exist RK method of order $p = s$.*

Proof. This easily follows from the last equation of (83) □

4 Some high order methods

Due to the fact that there exist quadrature rules with arbitrary high precision degree, it is always possible to obtain explicit Runge-Kutta methods for the numerical solution of linear inhomogeneous IVPs with any number of stages and maximal order $p = s$ for this class of problems. In this section we give several examples of RK schemes for $s = 5, \ldots, 8$, obtained following the algorithm given in the previous section.

In Appendix A we give the Butcher tableau of methods with 5, 6, 7 and 8 stages. They are collected in Tables 2 to 9. If the nodes are rational (algebraic) numbers, then all coefficients have an exact rational (algebraic) expression.

Concerning the choice of the nodes in the s-stage explicit RK methods with maximal order s we have the possibility to use the free parameters to improve some properties of the method. First of all since all s-stage explicit RK methods with order s have the same polynomial of stability $P(z) = \sum_{j=0}^{s} z^j/j!$, the free parameters cannot be used to improve the linear stability of these methods. On the other hand due to the connection between the nodes and coefficients of a RK method with the same nodes and weights of a quadrature rule we may select the nodes and coefficients taking into account the quadrature rule. Thus, for the s Gauss nodes in $[0, 1]$ we will have RK methods with order s that satisfy the additional conditions $\omega_{0,i} = \mathbf{b}^T \mathbf{c}^i = 1/(i + 1)$, $i \leq 2s - 1$. Here the main drawback is that the nodes (and also the remaining coefficients of the RK method) are algebraic numbers and the exact expression becomes complicated for high values of s.

A particular simple choice of nodes are the Newton-Côtes type nodes that are equally spaced in $[0, 1]$. In the case $c_i = i/(s - 1)$, $i = 0, \ldots, s - 1$ with even s from the theory of quadrature rules we know that all $b_i > 0$ and the formula has degree of precision s, consequently the corresponding RK methods satisfy $\mathbf{Ae} = \mathbf{c}$, and the a_{ik} are simple rational numbers.

Another possibility is to use the free parameters to minimize the principal term of the local truncation error (26) with $p = s$. Then, we may consider the Euclidean norm of the coefficients given by the vector

$$\mathbf{C}_{s+1}^T = \frac{1}{(s+1)!}(1, \ldots, 1) - \left(\omega_{s0}, \omega_{s0}, \frac{\omega_{s-1,1}}{1!}, \frac{\omega_{s-2,2}}{2!}, \ldots, \frac{\omega_{0,s}}{s!}\right) \in \mathbb{R}^{s+2}.$$

Since $\omega_{s,0} = \mathbf{b}^T \mathbf{A}^s \mathbf{e} = 0$ the first two components of $\mathbf{C}_{s+1}$ are constant, we minimize the Euclidean norm of the coefficients of the terms that depend on the nodes.

Moreover, if $c_1 = 0$ then $\mathbf{Ae} = \mathbf{c}$ and also $\omega_{s-1,1} = \mathbf{A}^{s-1}\mathbf{c} = 0$. Therefore, we minimize the Euclidean norm of

$$\widehat{\mathbf{C}}_{s+1}^T = \frac{1}{(s+1)!}(1, \ldots, 1) - \left(\frac{\omega_{s-2,2}}{2!}, \ldots, \frac{\omega_{0,s}}{s!}\right) \in \mathbb{R}^{s-1}. \tag{86}$$

This approach has been used in the derivation of a six-stage sixth-order RK method with $c_1 = 0$, selecting $c_2, \ldots, c_6$ so that they minimize (86). After this process of minimization, we obtain an easy set of values, rounding the optimized solution. This new method is given in Table 7 in Appendix. In Table 6 we give the Euclidean norm of the error coefficient sof the new method together with that of the Côtes one, Zingg and Chrisholm method [6] and the method obtained using the Gauss quadrature. We can see in the table that all the methods have a similar value of the error coefficient,

Table 1: Summary of six-stage sixth-order RK methods

method	$\mathbf{c}^T$	$\|\mathrm{C}_{s+1}\|$	$\|\widehat{\mathrm{C}}_{s+1}\|$
RK6 new	$(0, 1/6, 1/2, 2/3, 4/5, 1)$	3.53×10^{-4}	8.30×10^{-5}
Cotes	$(0, 1/6, 2/6, 3/6, 4/6, 5/6)$	3.57×10^{-4}	9.51×10^{-5}
Zingg	$(0, 3/20, 9/25, 57/100, 3/4, 9/10)$	3.58×10^{-4}	1.02×10^{-4}
Gauss	based on the Gauss nodes in [0,1]	3.30×10^{-4}	—

5 Numerical experiments

We present here some numerical experiments with the methods included in Table 1 and also the efficient six-stage, fifth-order DoPri5 [2]. The Euclidean norm of all the coefficients of its PTLE is 3.99×10^{-4}.

We have considered the following test problems:

(I) C2 test problem of the DETEST package [4]

$$\begin{cases} y_1' = -y_1, \ t \in [0, 20] \\ y_i' = (i-1)y_{i-1} - iy_i, \ i = 2, \ldots, 9, \\ y_{10}' = 9y_9, \\ \\ y_1(0) = 1, y_i(0) = 0, \ i = 2, \ldots, 10, \quad h = \dfrac{1}{5 \times 2^i}, \ i = 0, \ldots, 5. \end{cases}$$

(II) Simple scalar test problem

$$\begin{cases} y' = -2y + \mathrm{e}^{-t}\cos(6t), \ t \in [0, 40], \quad y(0) = 1, \\ h = \dfrac{1}{5 \times 2^{i-2}}, \ i = 0, \ldots, 4. \end{cases}$$

(III) Inhomogeneous linear system

Starting from the wave equation [5] given by

$$\begin{aligned} &\frac{\partial^2 x}{\partial t^2} = 4\frac{\partial^2 x}{\partial r^2} + \sin t \cdot \cos\left(\frac{\pi x}{100}\right), \qquad 0 \le r \le 100, \qquad t \in [0, 40\pi], \\ &\frac{\partial x}{\partial r}(t, 0) = \frac{\partial x}{\partial r}(t, 100) = 0, \\ &x(0, r) = 0, \frac{\partial x}{\partial t}(0, r) = \frac{100^2}{4\pi^2 - 100^2}\cos\frac{\pi r}{100}, \end{aligned}$$

with exact solution

$$x(t, r) = \frac{100^2}{4\pi^2 - 100^2} \cdot \sin(t) \cdot \cos\frac{\pi r}{100},$$

we semi-discretize $\frac{\partial^2 x}{\partial r^2}$ with fourth-order symmetric differences at internal points and one-sided differences of the same order at the boundaries obtaining the system:

$$\begin{bmatrix} x_1'' \\ x_2'' \\ x_{N+1}'' \end{bmatrix} = \frac{4}{(\Delta r)^2} \begin{bmatrix} -\frac{415}{72} & 8 & -3 & \frac{8}{9} & -\frac{1}{8} & 0 & \cdots & \\ \frac{257}{144} & -\frac{10}{3} & \frac{7}{4} & -\frac{2}{9} & \frac{1}{48} & 0 & \cdots & \\ -\frac{1}{12} & \frac{4}{3} & -\frac{5}{2} & \frac{4}{3} & -\frac{1}{12} & & & \vdots \\ 0 & & \ddots & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & & & -\frac{1}{12} & \frac{4}{3} & -\frac{5}{2} & \frac{4}{3} & -\frac{1}{12} \\ & \cdots & 0 & \frac{1}{48} & -\frac{2}{9} & \frac{7}{4} & -\frac{10}{3} & \frac{257}{144} \\ & \cdots & 0 & -\frac{1}{8} & \frac{8}{9} & -3 & 8 & -\frac{415}{72} \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_{N+1} \end{bmatrix}$$

$$+ \sin t \cdot \begin{bmatrix} \cos\left(\frac{0 \cdot \Delta r}{100} \cdot \pi\right) \\ \cos\left(\frac{1 \cdot \Delta r}{100} \cdot \pi\right) \\ \vdots \\ \cos\left(\frac{N \cdot \Delta r}{100} \cdot \pi\right) \end{bmatrix}.$$

By choosing the spatial step size $\Delta r = 5$, we arrive at a constant coefficient linear system with $N = 20$. Then, $x_1 \approx x(t, 0), x_2 \approx x(t, \Delta r), \ldots, x_{21} \approx u(t, 20\Delta r)$. Clearly, it is necessary to convert the above system to a first order system doubling the dimension. The time step sizes used are $h = \dfrac{4\pi}{3 \times 2^i}$, $i = 1, \ldots, 4$ and for computing the global error at each step, we have used the code DOPRI853 [3] at stringent tolerance.

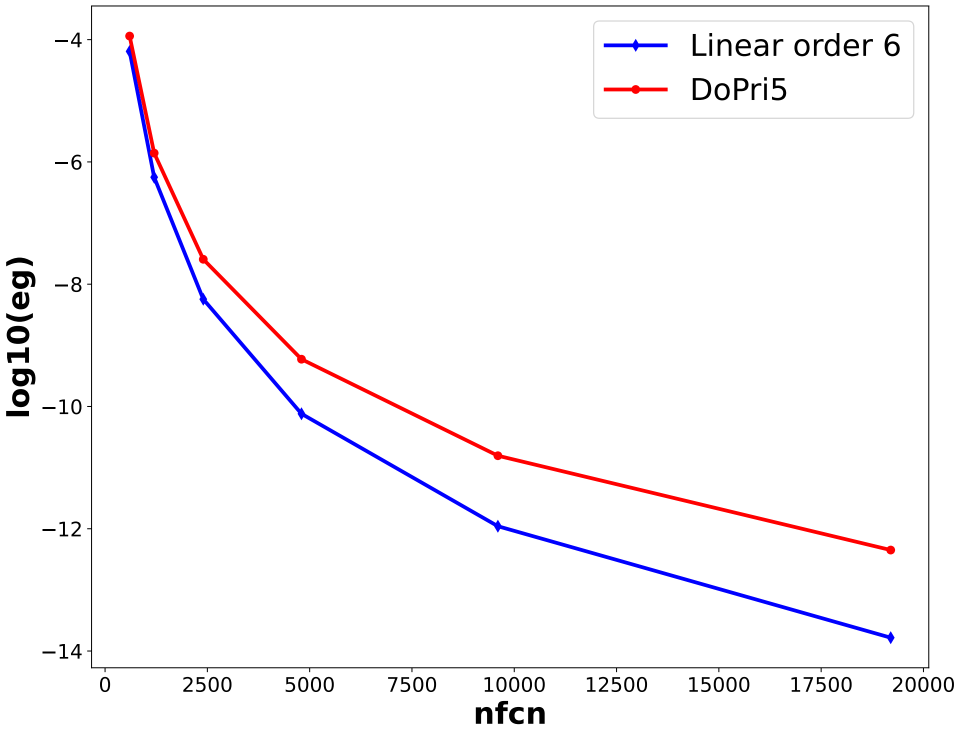

Figure 1: Efficiency plot for problem I. All RK methods give the same results

In Figures 1, 2, 3 we show efficiency plots, computing the maximum global error $(\log_{10}(\max \|y(t_n) - y_n\|))$ over the whole integration interval and plotted against the number of required function evaluations.

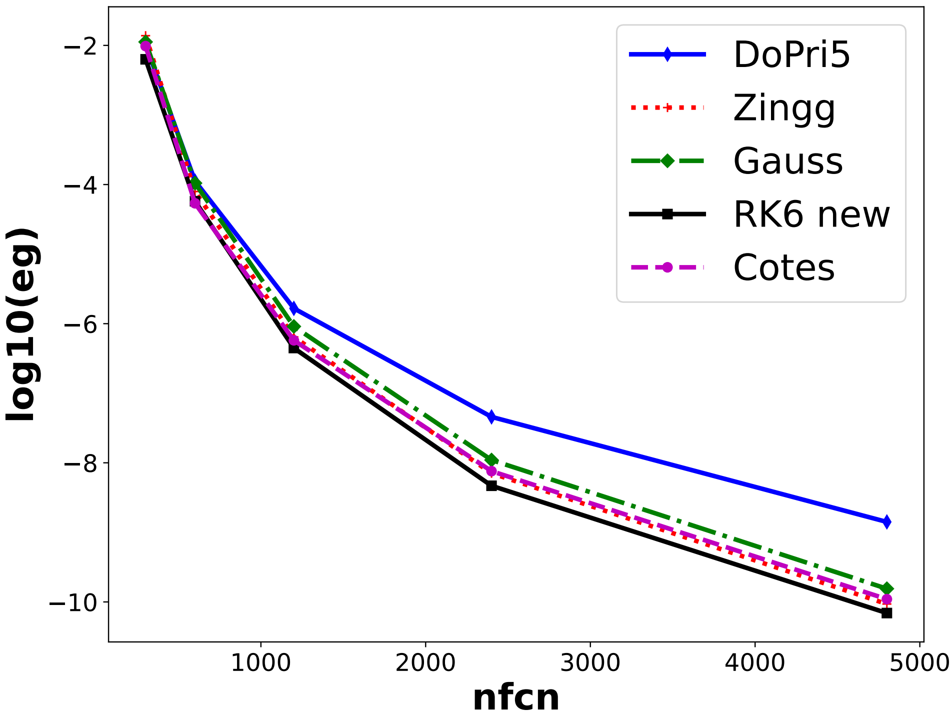

Figure 2: Efficiency plot for problem II.

From the numerical results obtained in Figures 1, 2 and 3, it follows that for the problems under consideration, the efficiency of the RK methods developed for linear problems is clearly superior to the standard DoPri5. In problem I, where $f(t) = 0$, all RK methods designed for the numerical integration of inhomogeneous problems give the same numerical results.

Also, the differences between the methods for the numerical integration of inhomogeneous IVPs are small, being the optimized method deduced in the previous section the most efficient.

6 Conclusions

For the class of linear inhomogeneous IVPs, the order conditions of explicit RK methods have been obtained by a direct derivation without using the standard Butcher theory of B-series. The order conditions given in Section 2 do not assume the standard simplifying condition $\mathbf{Ae} = \mathbf{c}$ and hold true for general implicit RK methods.

By using the close connection of these order conditions with those which appear in the theory of degree of precision of quadrature rules, we have proposed an algorithm for the direct construction of s-stage explicit RK methods that only requires the solution of $s(s-1)/2$ linear systems in the elements a_{ik}, $s \geq i > k \geq 1$ of matrix $\mathbf{A}$.

Thus, our algorithm avoids the treatment of non-linear algebraic equations in the available parameters a_{ik} by substituting these equations by equivalent linear equations obtained after suitable reduction.

As an application of the proposed algorithm, the coefficients of several RK methods with orders less than nine have been obtained.

It is found that when the available parameters of the nodes c_i are taken as rational numbers (as in the case in Newton-Côtes quadrature rules) the algorithm leads to explicit

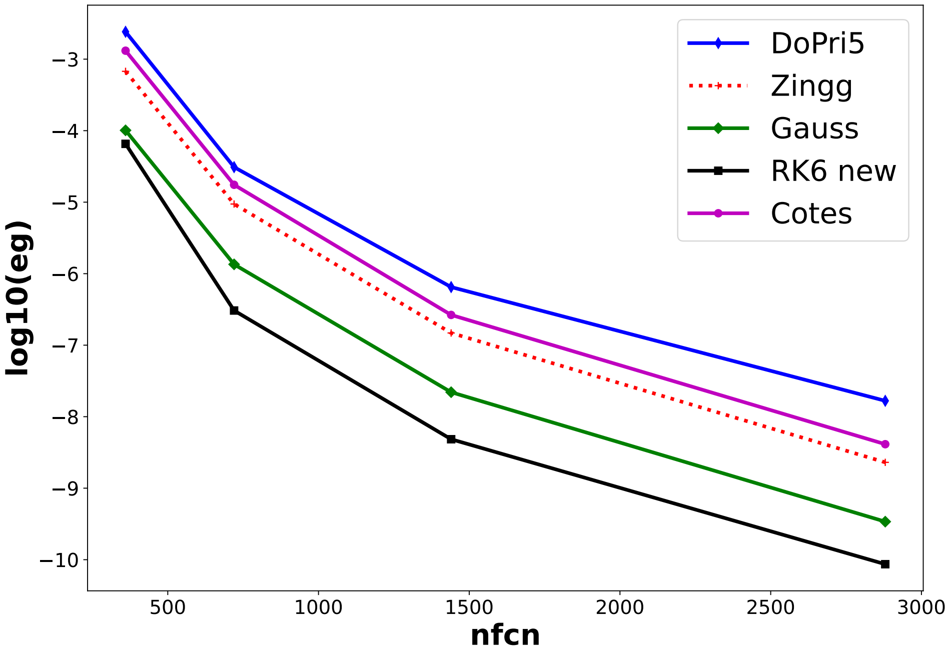

Figure 3: Efficiency plot for problem III.

RK methods with nice rational coefficients.

Finally, the results of some numerical experiments to compare the behaviour of several 6-stages methods have been presented.

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Appendix

Table 2: Five-stage RK based on the Lobatto's nodes (here $r = \sqrt{21}$). This scheme verifies $\mathbf{Ae} = \mathbf{c}$. The Euclidean norm of the principal term of the local error is 2.50×10^{-3}.

0	0				
$\frac{7-r}{14}$	$\frac{7-r}{14}$				
$\frac{1}{2}$	$\frac{5-11r}{136}$	$\frac{63+11r}{136}$			
$\frac{7+r}{14}$	$\frac{1687+491r}{3332}$	$-\frac{3}{476}(137+25r)$	$\frac{42+4r}{49}$		
1	$\frac{-967+33r}{204}$	$\frac{2527+411r}{612}$	$-\frac{2}{9}(5+2r)$	$\frac{7}{18}(7-r)$	
	$\frac{1}{20}$	$\frac{49}{180}$	$\frac{16}{45}$	$\frac{49}{180}$	$\frac{1}{20}$

Table 3: Five-stage RK Newton-Côtes type based on five equidistant nodes contained in $[0,1]$. This scheme does not verify $\mathbf{Ae} = \mathbf{c}$. The Euclidean norm of the principal term of the local error is 2.02×10^{-3}.

$\frac{1}{6}$	0				
$\frac{2}{6}$	1				
$\frac{3}{6}$	$\frac{16}{11}$	$\frac{1}{11}$			
$\frac{4}{6}$	$\frac{171}{16}$	$-\frac{1}{11}$	$\frac{11}{16}$		
$\frac{5}{6}$	$-\frac{761}{2904}$	$-\frac{174}{121}$	$\frac{93}{88}$	$\frac{8}{33}$	
	$\frac{11}{20}$	$-\frac{7}{10}$	$\frac{13}{10}$	$-\frac{7}{10}$	$\frac{11}{20}$

Table 4: Six-stage RK Newton-Côtes type based on six equidistant nodes contained in $[0,1]$. This scheme does not verify $\mathbf{Ae} = \mathbf{c}$. The Euclidean norm of the principal term of the local error is 2.90×10^{-4}.

$$
\begin{array}{c|cccccc}
\frac{1}{7} & 0 & & & & & \\
\frac{2}{7} & 1 & & & & & \\
\frac{3}{7} & \frac{25}{16} & \frac{1}{16} & & & & \\
\frac{4}{7} & \frac{337}{320} & -\frac{359}{320} & \frac{4}{5} & & & \\
\frac{5}{7} & -\frac{4441}{6140} & -\frac{17593}{6140} & \frac{2918}{1535} & \frac{40}{307} & & \\
\frac{6}{7} & -\frac{36035983}{30012320} & -\frac{71843719}{30012320} & \frac{2464508}{937885} & -\frac{175904}{187577} & \frac{307}{611} & \\
\hline
 & \frac{611}{1440} & -\frac{151}{480} & \frac{281}{720} & \frac{281}{720} & -\frac{151}{480} & \frac{611}{1440}
\end{array}
$$

Table 5: Six-stage RK Newton-Côtes type based on six equidistant nodes contained in $[0,1]$. This scheme satisfies $\mathbf{Ae} = \mathbf{c}$. The Euclidean norm of the principal term of the local error is 2.20×10^{-4}.

$$
\begin{array}{c|cccccc}
0 & 0 & & & & & \\
\frac{1}{6} & \frac{1}{6} & & & & & \\
\frac{2}{6} & 0 & \frac{1}{3} & & & & \\
\frac{3}{6} & -\frac{1}{10} & \frac{3}{10} & \frac{3}{10} & & & \\
\frac{4}{6} & -\frac{11}{135} & \frac{16}{45} & \frac{1}{45} & \frac{10}{27} & & \\
\frac{5}{6} & \frac{197}{1485} & \frac{83}{495} & \frac{68}{495} & -\frac{4}{297} & \frac{9}{22} & \\
\hline
 & 0 & \frac{11}{20} & -\frac{7}{10} & \frac{13}{10} & -\frac{7}{10} & \frac{11}{20}
\end{array}
$$

Table 6: Six-stage RK closed Newton-Côtes type based on six equidistant nodes contained in $[0,1]$. This scheme satisfies $\mathbf{Ae} = \mathbf{c}$. The Euclidean norm of the principal term of the local error is 3.50×10^{-4}.

$$
\begin{array}{c|cccccc}
0 & 0 & & & & & \\
\frac{1}{5} & \frac{1}{5} & & & & & \\
\frac{2}{5} & -\frac{1}{10} & \frac{1}{2} & & & & \\
\frac{3}{5} & -\frac{1}{5} & \frac{2}{5} & \frac{2}{5} & & & \\
\frac{4}{5} & \frac{1}{5} & \frac{7}{15} & -\frac{8}{15} & \frac{2}{3} & & \\
1 & \frac{4}{19} & -\frac{20}{19} & \frac{50}{19} & -\frac{30}{19} & \frac{15}{19} & \\
\hline
 & \frac{19}{288} & \frac{25}{96} & \frac{25}{144} & \frac{25}{144} & \frac{25}{96} & \frac{19}{288}
\end{array}
$$

Table 7: Six-stage optimized RK. The Euclidean norm of the principal term of the local error is 3.53×10^{-4}.

$$
\begin{array}{c|cccccc}
0 & 0 & & & & & \\
\frac{1}{6} & \frac{1}{6} & & & & & \\
\frac{1}{2} & -\frac{1}{2} & 1 & & & & \\
\frac{2}{3} & \frac{2}{3} & -\frac{2}{3} & \frac{2}{3} & & & \\
\frac{4}{5} & \frac{994}{625} & -\frac{228}{125} & \frac{532}{625} & \frac{114}{625} & & \\
1 & -\frac{639}{136} & \frac{2115}{323} & -\frac{5}{17} & -\frac{30}{17} & \frac{3125}{2584} & \\
\hline
 & \frac{23}{480} & \frac{126}{475} & \frac{2}{5} & -\frac{9}{80} & \frac{625}{1824} & \frac{17}{300}
\end{array}
$$

Table 8: Six-stage RK based on the Gauss nodes in $[0, 1]$ with sixteen digits of accuracy. This scheme does not verify $\mathbf{Ae} = \mathbf{c}$. The Euclidean norm of the principal term of the local error is 3.30×10^{-4}.

$a_{21} = 0.17008855137744719$	$c_1 = 0.033765242898423986$
$a_{31} = -0.036888940300067292$	$c_2 = 0.16939530676686774$
$a_{32} = 0.45240489953000035$	$c_3 = 0.38069040695840155$
$a_{41} = 0.23830851952634143$	$c_4 = 0.61930959304159845$
$a_{42} = -0.28170661126540363$	$c_5 = 0.83060469323313226$
$a_{43} = 0.66726065151020145$	$c_6 = 0.96623475710157601$
$a_{51} = -0.064893941725909717$	$b_1 = 0.085662246189585173$
$a_{52} = 0.71939718201543294$	$b_2 = 0.18038078652406930$
$a_{53} = -0.59024734998626291$	$b_3 = 0.2339569672863455$
$a_{54} = 0.68879062122934539$	$b_4 = 0.2339569672863455$
$a_{61} = 0.22838119153891675$	$b_5 = 0.18038078652406930$
$a_{62} = -0.33378343949486307$	$b_6 = 0.08566224618958517$
$a_{63} = 1.2619397331911941$	
$a_{64} = -0.56068125856425523$	
$a_{65} = 0.45845099889945668$	

Table 9: Seven-stage RK based on seven equidistant nodes in $[0, 1]$. This scheme does not verify $\mathbf{Ae} = \mathbf{c}$. The Euclidean norm of the principal term of the local error is 3.64×10^{-5}.

$$
\begin{array}{c|ccccccc}
\frac{1}{8} & 0 & & & & & & \\
\frac{1}{4} & 1 & & & & & & \\
\frac{3}{8} & \frac{18}{11} & \frac{1}{22} & & & & & \\
\frac{1}{2} & 1 & -\frac{17}{11} & 1 & & & & \\
\frac{5}{8} & -\frac{1168}{869} & -\frac{362}{79} & \frac{226}{79} & \frac{11}{158} & & & \\
\frac{3}{4} & -\frac{315985}{123398} & -\frac{307194}{61699} & \frac{25468}{5609} & -\frac{7915}{5609} & \frac{79}{142} & & \\
\frac{7}{8} & \frac{1805971}{1233980} & \frac{25721299}{11352616} & \frac{5712577}{2580140} & -\frac{17708727}{5160280} & \frac{759}{710} & \frac{213}{920} & \\
\hline
 & \frac{92}{189} & -\frac{106}{105} & \frac{244}{105} & -\frac{2459}{945} & \frac{244}{105} & -\frac{106}{105} & \frac{92}{189}
\end{array}
$$

Table 10: Eight-stage RK based on equidistant nodes in $[0,1]$. This scheme satisfies $\mathbf{Ae} = \mathbf{c}$. The Euclidean norm of the principal term of the local error is 4.91×10^{-6}

0	0							
$\frac{1}{7}$	$\frac{1}{7}$							
$\frac{2}{7}$	$-\frac{1}{21}$	$\frac{1}{3}$						
$\frac{3}{7}$	$-\frac{1}{5}$	$\frac{13}{35}$	$\frac{9}{35}$					
$\frac{4}{7}$	$-\frac{73}{455}$	$\frac{227}{455}$	$-\frac{69}{455}$	$\frac{5}{13}$				
$\frac{5}{7}$	$\frac{183}{455}$	$\frac{103}{455}$	$-\frac{241}{455}$	$\frac{11}{39}$	$\frac{1}{3}$			
$\frac{6}{7}$	$\frac{22171}{33215}$	$-\frac{9169}{33215}$	$-\frac{16557}{33215}$	$\frac{1149}{949}$	$-\frac{57}{73}$	$\frac{39}{73}$		
1	$-\frac{7697}{3755}$	$\frac{46249}{48815}$	$\frac{202377}{48815}$	$-\frac{53893}{9763}$	$\frac{3633}{751}$	$-\frac{1533}{751}$	$\frac{511}{751}$	
	$\frac{751}{17280}$	$\frac{3577}{17280}$	$\frac{49}{640}$	$\frac{2989}{17280}$	$\frac{2989}{17280}$	$\frac{49}{640}$	$\frac{3577}{17280}$	$\frac{751}{17280}$