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Embedded (4, 5) pairs of explicit 7-stage Runge–Kutta methods with FSAL property

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Abstract

The general case of embedded (4, 5) pairs of explicit 7-stage Runge–Kutta methods with FSAL property ($a_{7j} = b_j$, $1 \le j \le 7$, $c_7 = 1$) is considered. Besides exceptional cases, the pairs form five 4-dimensional families. The pairs within two (already known) families satisfy the simplifying assumption $\sum_j a_{ij} c_j = c_i^2/2$, $i \ge 3$.

Keywords Adaptive step size control · Embedded pairs of Runge–Kutta methods

Mathematics Subject Classification 65L05 · 65L06

1 Introduction

Runge–Kutta methods (see, *e.g.*, [4, Sect. 23 and ch. 3], [14, ch. II], [1, ch. 4], [16, ch. 3]) are widely and successfully used to solve Ordinary Differential Equations (ODEs) numerically for over a century [6]. Consider a system $\mathrm{d}\boldsymbol{x}/\mathrm{d}t = \boldsymbol{f}(t, \boldsymbol{x})$. To propagate by the step size h and update the position, $\boldsymbol{x}(t) \mapsto \tilde{\boldsymbol{x}}(t+h)$, where $\tilde{\boldsymbol{x}}(t+h)$ is a numerical approximation to the exact solution $\boldsymbol{x}(t+h)$, an s-stage explicit Runge-Kutta method (which is determined by the coefficients a_{ij}, weights b_j, and nodes c_i) would compute $\boldsymbol{F}_1$, $\boldsymbol{F}_2$, ..., $\boldsymbol{F}_s$, and then $\tilde{\boldsymbol{x}}(t+h)$:[1]

$$\boldsymbol{F}_i = \boldsymbol{f}\left(t + c_i h, \boldsymbol{x}(t) + h \sum_{j=1}^{i-1} a_{ij} \boldsymbol{F}_j\right), \qquad \tilde{\boldsymbol{x}}(t+h) = \boldsymbol{x}(t) + h \sum_{j=1}^{s} b_j \boldsymbol{F}_j$$

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[1] It is natural and will be assumed that $\sum_{j=1}^{i-1} a_{ij} = c_i$. For $i = 1$ the sum is empty, so $c_1 = 0$ and $\boldsymbol{F}_1 = \boldsymbol{f}\big(t, \boldsymbol{x}(t)\big)$.

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To obtain an accurate solution with less effort, various adaptive step size strategies were developed (see, *e.g.*, [4, Sect. 33], [14, Sect. II.4], [1, Sect. 4.5], [16, ch. 6]). Typically the system of ODEs is solved in two different ways, and the step size is chosen so that the two solutions are sufficiently close. Embedded pairs of Runge–Kutta methods are computationally efficient, as the two methods within a pair have different weights, but share the nodes and the coefficients. The vectors $\boldsymbol{F}_1$, $\boldsymbol{F}_2, \cdots, \boldsymbol{F}_s$ are computed only once, and then are used in both methods.

The Butcher tableau [3] of an embedded (4, 5) pair of explicit 7-stage Runge–Kutta methods with so-called First Same As Last (FSAL) property [12, p. 17], [10] looks like

$$\begin{array}{c|ccccccc}
0 \\
c_2 & a_{21} \\
c_3 & a_{31} & a_{32} \\
c_4 & a_{41} & a_{42} & a_{43} \\
c_5 & a_{51} & a_{62} & a_{53} & a_{54} \\
c_6 & a_{61} & a_{62} & a_{63} & a_{64} & a_{65} \\
1 & b_1 & b_2 & b_3 & b_4 & b_5 & b_6 \\
\hline
 & b_1 & b_2 & b_3 & b_4 & b_5 & b_6 \\
 & d_1 & d_2 & d_3 & d_4 & d_5 & d_6 & d_7
\end{array}$$

The vector $\boldsymbol{b} = \begin{bmatrix} b_1 & b_2 & b_3 & b_4 & b_5 & b_6 & 0 \end{bmatrix}^{\mathrm{T}}$ is the weights vector of the 5th order method, and $\boldsymbol{d} = \begin{bmatrix} d_1 & d_2 & d_3 & d_4 & d_5 & d_6 & d_7 \end{bmatrix}^{\mathrm{T}}$ is the difference between the 4th and the 5th order methods weights vectors.[2] The FSAL property means that the vector $\boldsymbol{F}_1$ at the current step is equal to the already computed $\boldsymbol{F}_7$ at the previous step. It implies $c_7 = 1$ and $a_{7j} = b_j$ for all $1 \le j \le 7$; *e.g.*, $b_7 = 0$.

Let $\boldsymbol{c} = \begin{bmatrix} 0 & c_2 & c_3 & c_4 & c_5 & c_6 & 1 \end{bmatrix}^{\mathrm{T}}$ and $\boldsymbol{A} = \begin{bmatrix} a_{ij} \end{bmatrix}$ be the 7×7 matrix with a_{ij} as its matrix element in the ith row and jth column (visibly, $a_{ij} = 0$ if $i \le j$). Let $\mathbf{1}$ be the vector with all components being equal to 1. The condition $\sum_j a_{ij} = c_i$ or $\boldsymbol{A}\mathbf{1} = \boldsymbol{c}$ is assumed. Let $\boldsymbol{c}' = \boldsymbol{A}\boldsymbol{c}$, $\boldsymbol{c}'' = \boldsymbol{A}\boldsymbol{c}'$, and $\boldsymbol{c}''' = \boldsymbol{A}\boldsymbol{c}'' = \boldsymbol{A}^4\mathbf{1}$. A Runge–Kutta method of order p should satisfy the conditions $\boldsymbol{b}^{\mathrm{T}}\boldsymbol{\Phi}(\mathrm{t}) = 1/\mathrm{t}!$ for all rooted trees t with up to p vertices [4, p. 175], [5, p. 177], [14, p. 153] . For $p = 5$ these conditions are listed in Table 1, see also [4, p. 172], [5, p. 126], [14, p. 148], [11, table 1]. For a (4, 5) pair the conditions $\boldsymbol{b}^{\mathrm{T}}\boldsymbol{\Phi}(\mathrm{t}) = 1/\mathrm{t}!$ and $\boldsymbol{d}^{\mathrm{T}}\boldsymbol{\Phi}(\mathrm{t}) = 0$ are satisfied for all trees t with up to 5 and 4 vertices, respectively.

The process of Runge–Kutta methods construction is streamlined by using so-called simplifying assumptions (see, *e.g.*, [4, Sect. 321], [14, pp. 136 and 175]). The one that is important for the subject discussed here is $c_i' = \sum_j a_{ij}c_j = c_i^2/2$ for any $i \ne 2$. For a method of order at least 3 this would imply $b_2 = 0$, as $\boldsymbol{b}^{\mathrm{T}}\boldsymbol{c}' = \frac{1}{6} = \frac{1}{2}\boldsymbol{b}^{\mathrm{T}}(\boldsymbol{c} * \boldsymbol{c})$.

There is no 5-stage explicit Runge–Kutta 5th order method [3]. The general case of the 6-stage, 5th order method was considered in [8, 9], where the set of order conditions, by exclusion of variables, was drastically reduced, and methods

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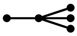
[2] Usually the 4th order method vector of weights $\boldsymbol{b} + \boldsymbol{d}$ is written in place of $\boldsymbol{d}$.

Table 1 Order conditions $\boldsymbol{b}^{\mathrm{T}}\boldsymbol{\Phi}(\mathrm{t}) = 1/\mathrm{t}!$ for rooted trees t with 1, 2, 3, 4, and 5 vertices

Order	t	$\boldsymbol{\Phi}(\mathrm{t})$	t!
1st		$\mathbf{1}$	1
2nd		$\boldsymbol{c}$	2
3rd		$\boldsymbol{c} * \boldsymbol{c}$	3
↓		$\boldsymbol{c}'$	6
4th		$\boldsymbol{c} * \boldsymbol{c} * \boldsymbol{c}$	4
↓		$\boldsymbol{c}' * \boldsymbol{c}$	8
		$\boldsymbol{A}(\boldsymbol{c} * \boldsymbol{c})$	12
		$\boldsymbol{c}''$	24
5th		$\boldsymbol{c} * \boldsymbol{c} * \boldsymbol{c} * \boldsymbol{c}$	5
↓		$\boldsymbol{c}' * \boldsymbol{c} * \boldsymbol{c}$	10
		$\big(\boldsymbol{A}(\boldsymbol{c} * \boldsymbol{c})\big) * \boldsymbol{c}$	15
		$\boldsymbol{c}'' * \boldsymbol{c}$	30
		$\boldsymbol{c}' * \boldsymbol{c}'$	20
		$\boldsymbol{A}(\boldsymbol{c} * \boldsymbol{c} * \boldsymbol{c})$	20
		$\boldsymbol{A}(\boldsymbol{c}' * \boldsymbol{c})$	40
		$\boldsymbol{A}^2(\boldsymbol{c} * \boldsymbol{c})$	60
		$\boldsymbol{c}'''$	120

The "$*$" sign denotes component-wise multiplication of vectors, *i.e.*, $(\boldsymbol{x} * \boldsymbol{y})_i = x_i y_i$

with $b_2 \neq 0$ were built. A two-dimensional family of embedded (4, 5) pairs of 6-stage Runge–Kutta methods (with $3c_2 = 2c_3$, $c_5 = 1$, and $b_2 = d_2 = d_7 = 0$) was constructed in [12]. A method suggested in [7] belongs to this family. In [11] a three-dimensional family of 7-stage pairs with FSAL property was presented (with $3c_2 = 2c_3$, $c_6 = 1$, and $b_2 = d_2 = 0$). Both families were extended to four-dimensional ones in [19]. In [21] FSAL pairs not satisfying the simplifying assumption were considered, seemingly with the aim of extending the set of pairs satisfying the order conditions and thus potentially finding a more efficient and practical pair. With the conditions solved in part analytically and in part numerically, the [21, table 1] pair was suggested.

Increasing the number of stages (and thus the amount of computation per step) provides additional flexibility in choosing $\boldsymbol{A}$, $\boldsymbol{b}$, $\boldsymbol{c}$, and $\boldsymbol{d}$, which may be exploited to construct viable pairs that produce an accurate solution in fewer steps. In [20, Sect. 3.1] and [2] non-FSAL embedded (4, 5) pairs of 7-stage Runge–Kutta methods were suggested.

In this paper embedded (4, 5) pairs of 7-stage Runge–Kutta methods with FSAL property (this includes non-FSAL pairs of 6-stage methods) are considered, with the aim of complete classification of at least general, non-exceptional, cases. After rewriting the order conditions in terms of $\boldsymbol{c}$, $\boldsymbol{c}'$, $\boldsymbol{c}''$, $\boldsymbol{c}'''$, and a_{65}, b_6,

d_5, d_6, d_7 (Sect. 1), a pair is expressed through 6 variables: c_2, c_3, c_4, c_5, c_6, and c'_3 (Sect. 2). Lastly, pairs are classified into five 4-dimensional families (Sect. 3). The topics of choosing the magnitude of the vector $\boldsymbol{d}$ and of continuous formulas or interpolants (see, *e.g.*, [14, Sect. II.6]) are not considered.

2 Rewriting some of the order conditions in a compact form

It is convenient to express the $30 = 5_{\boldsymbol{c}=\boldsymbol{A}\boldsymbol{1}} + 17_5^{\text{th}}$ order, $\boldsymbol{b} + 8_4^{\text{th}}$ order, $\boldsymbol{d}$ conditions on an embedded pair not in terms of $\boldsymbol{A}$, $\boldsymbol{b}$, $\boldsymbol{c}$, and $\boldsymbol{d}$ ($33 = 21_{\boldsymbol{A},\boldsymbol{b}} + 5_{\boldsymbol{c}} + 7_{\boldsymbol{d}}$ degrees of freedom), but in terms of $\boldsymbol{c}$, $\boldsymbol{c}'$, $\boldsymbol{c}''$, $\boldsymbol{c}'''$, a_{65}, b_6, d_5, d_6, and d_7 ($19 = 5_{\boldsymbol{c}} + 4_{\boldsymbol{c}'} + 3_{\boldsymbol{c}''} + 2_{\boldsymbol{c}'''} + 5_{a_{65},b_6,d_{5,6,7}}$ degrees of freedom). After this (rather mechanical) change of variables the relations $\boldsymbol{c} = \boldsymbol{A}\boldsymbol{1}$, $\boldsymbol{c}' = \boldsymbol{A}\boldsymbol{c}$, $\boldsymbol{c}'' = \boldsymbol{A}\boldsymbol{c}'$, $\boldsymbol{c}''' = \boldsymbol{A}\boldsymbol{c}''$ and the order conditions $\boldsymbol{b}^{\text{T}}\big[\boldsymbol{1}\ \boldsymbol{c}\ \boldsymbol{c}'\ \boldsymbol{c}''\ \boldsymbol{c}'''\big] = \big[1\ \tfrac{1}{2}\ \tfrac{1}{6}\ \tfrac{1}{24}\ \tfrac{1}{120}\big]$, $\boldsymbol{d}^{\text{T}}\big[\boldsymbol{1}\ \boldsymbol{c}\ \boldsymbol{c}'\ \boldsymbol{c}''\big] = \big[0\ 0\ 0\ 0\big]$ will be satisfied by construction.[3] There still going to be $16 = (17-5)_5^{\text{th}}$ order, $\boldsymbol{b} + (8-4)_4^{\text{th}}$ order, $\boldsymbol{d}$ (redundant) order conditions

The condition $\boldsymbol{c} = \boldsymbol{A}\boldsymbol{1}$ and the order conditions $\boldsymbol{b}^{\text{T}}\boldsymbol{1} = 1$, $\boldsymbol{d}^{\text{T}}\boldsymbol{1} = 0$ imply

$$\begin{aligned}
a_{21} &= c_2\\
a_{31} &= c_3 - a_{32}\\
a_{41} &= c_4 - a_{42} - a_{43}\\
a_{51} &= c_5 - a_{52} - a_{53} - a_{54}\\
a_{61} &= c_6 - a_{62} - a_{63} - a_{64} - a_{65}\\
b_1 &= 1 - b_2 - b_3 - b_4 - b_4 - b_6\\
d_1 &= -d_2 - d_3 - d_4 - d_4 - d_6 - d_7
\end{aligned}$$

Five stages are not enough to satisfy all the required order conditions [3], thus $c_2 \neq 0$ (otherwise the and 1st and 2nd stages are redundant) and $b_6 \neq 0$. The relation $\boldsymbol{c}' = \boldsymbol{A}\boldsymbol{c}$ and the order conditions $\boldsymbol{b}^{\text{T}}\boldsymbol{c} = \frac{1}{2}$, $\boldsymbol{d}^{\text{T}}\boldsymbol{c} = 0$ imply

$$\begin{aligned}
a_{32} &= c'_3/c_2\\
a_{42} &= (c'_4 - a_{43}c_3)/c_2\\
a_{52} &= (c'_5 - a_{53}c_3 - a_{54}c_4)/c_2\\
a_{62} &= (c'_6 - a_{63}c_3 - a_{64}c_4 - a_{65}c_5)/c_2\\
b_2 &= (1/2 - b_3c_3 - b_4c_4 - b_5c_5 - b_6c_6)/c_2\\
d_2 &= (-d_3c_3 - d_4c_4 - d_5c_5 - d_6c_6 - d_7)/c_2
\end{aligned}$$

In what follows it is going to be assumed that the matrix elements of $\boldsymbol{A}$ right below the diagonal are non-zero: $a_{32} \neq 0$, $a_{43} \neq 0$, $a_{54} \neq 0$, and $a_{65} \neq 0$.[4] This is equivalent

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[3] The FSAL property $a_{7j} = b_j$, $1 \leq j \leq 7$ and the order conditions $\boldsymbol{b}^{\text{T}}\boldsymbol{c} = 1/2$, $\boldsymbol{b}^{\text{T}}\boldsymbol{c}' = 1/6$, $\boldsymbol{b}^{\text{T}}\boldsymbol{c}'' = 1/24$ result in $c'_7 = 1/2$, $c''_7 = 1/6$, and $c'''_7 = 1/24$.

[4] The full analysis of $a_{65}a_{54}a_{43}a_{32} = 0$ case is tedious and is not expected to result in an embedded pair of practical interest. For instance, if $a_{32} = 0$, then $c_3 = 3c_2/(8c_2 - 3)$ and $c_4 = 0$.

to $c'_3 \neq 0$, $c''_4 \neq 0$, $c'''_5 \neq 0$, and $a_{65} \neq 0$. The relations $\boldsymbol{c}'' = \boldsymbol{A}\boldsymbol{c}'$, $\boldsymbol{c}''' = \boldsymbol{A}\boldsymbol{c}''$ and the order conditions $\boldsymbol{b}^{\mathrm{T}}\left[\boldsymbol{c}' \;\; \boldsymbol{c}'' \;\; \boldsymbol{c}'''\right] = \left[\tfrac{1}{6} \;\; \tfrac{1}{24} \;\; \tfrac{1}{120}\right]$, $\boldsymbol{d}^{\mathrm{T}}\left[\boldsymbol{c}' \;\; \boldsymbol{c}''\right] = \left[0 \;\; 0\right]$ imply

$$\begin{aligned}
a_{43} &= c''_4/c'_3 \\
a_{53} &= (c''_5 - a_{54}c'_4)/c'_3 \\
a_{63} &= (c''_6 - a_{64}c'_4 - a_{65}c'_5)/c'_3 \\
b_3 &= (1/6 - b_4c'_4 - b_5c'_5 - b_6c'_6)/c'_3 \\
d_3 &= (-d_4c'_4 - d_5c'_5 - d_6c'_6 - d_7/2)/c'_3 \\
a_{54} &= c'''_5/c''_4 \\
a_{64} &= (c'''_6 - a_{65}c''_5)/c''_4 \\
b_4 &= (1/24 - b_5c''_5 - b_6c''_6)/c''_4 \\
d_4 &= (-d_5c''_5 - d_6c''_6 - d_7/6)/c''_4 \\
b_5 &= (1/120 - b_6c'''_6)/c'''_5
\end{aligned}$$

Now a_{ij}, b_j, d_j, where $2 \le i \le 7, 1 \le j \le 4$, and b_5 are expressed through $\boldsymbol{c}$, $\boldsymbol{c}'$, $\boldsymbol{c}''$, $\boldsymbol{c}'''$, a_{65}, b_6, d_5, d_6, and d_7. The variables b_5 and c'''_6 are interchangeable:

$$\begin{aligned}
b_5 =& (1/120 - b_6c'''_6)/c'''_5 \quad \longleftrightarrow \quad c'''_6 = (1/120 - b_5c'''_5)/b_6 \\
a_{64} =& (c'''_6 - a_{65}c''_5)/c''_4 = (1/120 - b_5c'''_5)/b_6c''_4 - a_{65}c''_5/c''_4
\end{aligned} \tag{1}$$

The following notation will be useful, where $4 \le m \le 7$ and $1 \le n \le 3$:[5]

$$\begin{aligned}
\gamma_{m,c^{n+1}} &= c'_3c_m(c^n_m - c^n_2) - c'_mc_3(c^n_3 - c^n_2) \\
\gamma_{m,c'c^n} &= c'_m(c^n_m - c^n_3) \\
\gamma_{m,c'^2} &= c'_m(c'_m - c'_3) \\
\gamma_{m,c''c} &= c''_m(c_m - c_4) \\
\lambda_{m,*} &= c''_4\gamma_{m,*} - c''_m\gamma_{4,*}, \qquad * = c^{n+1}, c'c^n, c'^2, c''c \\
\gamma_{Ac^2} &= c''_4c_3(c_3 - c_2) \\
\mu_{m,c^{n+1}} &= \gamma_{m,c^{n+1}} + 4c''_m\big(c_3(c^n_3 - c^n_2) + 3c'_3(c^n_2 - \tfrac{2}{n+2})\big) \\
\mu_{m,c'c^n} &= \gamma_{m,c^nc'} + 4c''_m(c^n_3 - \tfrac{3}{n+3}) \\
\mu_{m,c'^2} &= \gamma_{m,c'^2} + 4c''_m(c'_3 - \tfrac{3}{10}) \\
\mu_{m,c''c} &= c''_m(c_m - \tfrac{4}{5}) \\
\eta_{c^{n+1}} &= c_3(c^n_3 - c^n_2) + 4c'_3(c^n_2 - \tfrac{3}{4n+2}) \\
\eta_{c'c} &= c_3 - \tfrac{3}{5} \\
\eta_{Ac^2} &= c'_3(c_2 - \tfrac{2}{5})
\end{aligned}$$

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[5] Further derivation was done in interaction with computer algebra system Wolfram Mathematica 8.0, mainly using commands **`Solve`** to symbolically solve linear equations, **`Simplify`**, and (in Sect. 3) **`Factor`**.

The remaining 12 order conditions for the 5th order method, with the exception of $\boldsymbol{b}^{\mathrm{T}}\big((\boldsymbol{A}(\boldsymbol{c} * \boldsymbol{c})) * \boldsymbol{c}\big) = \frac{1}{15}$, could be written as

$$\operatorname{rank}\begin{bmatrix} b_6 & 1/120 \\ \lambda_{5,c^2} + 5c'''_5\mu_{4,c^2} & c'''_6\lambda_{5,c^2} - c'''_5\lambda_{6,c^2} \\ \lambda_{5,c^3} + 5c'''_5\mu_{4,c^3} & c'''_6\lambda_{5,c^3} - c'''_5\lambda_{6,c^3} \\ \lambda_{5,c^4} + 5c'''_5\mu_{4,c^4} & c'''_6\lambda_{5,c^4} - c'''_5\lambda_{6,c^4} \\ \lambda_{5,c'c} + 5c'''_5\mu_{4,c'c} & c'''_6\lambda_{5,c'c} - c'''_5\lambda_{6,c'c} \\ \lambda_{5,c'c^2} + 5c'''_5\mu_{4,c'c^2} & c'''_6\lambda_{5,c'c^2} - c'''_5\lambda_{6,c'c^2} \\ \lambda_{5,c'^2} + 5c'''_5\mu_{4,c'^2} & c'''_6\lambda_{5,c'^2} - c'''_5\lambda_{6,c'^2} \\ \lambda_{5,c''c} + 5c'''_5\mu_{4,c''c} & c'''_6\lambda_{5,c''c} - c'''_5\lambda_{6,c''c} \\ \gamma_{4,c^2} + 5c''_4\eta_{c^2} & -a_{65}\lambda_{5,c^2} \\ \gamma_{4,c^3} + 5c''_4\eta_{c^3} & -a_{65}\lambda_{5,c^3} \\ \gamma_{4,c'c} + 5c''_4\eta_{c'c} & -a_{65}\lambda_{5,c'c} \\ \gamma_{Ac^2} + 5c''_4\eta_{Ac^2} & -a_{65}c'''_5\gamma_{4,c^2} \end{bmatrix} = 1 \tag{2}$$

Currently the whole vector $\boldsymbol{b}$ is expressed through $\boldsymbol{c}$, $\boldsymbol{c}'$, $\boldsymbol{c}''$, $\boldsymbol{c}'''$, a_{65}, and b_6. Any but the 1st row in this 12×2 matrix gives the solution for b_6 in the corresponding order condition $\boldsymbol{b}^{\mathrm{T}}\boldsymbol{\Phi}(\mathrm{t}) = 1/\mathrm{t}!$. From the second to eighth row these conditions can be rewritten as[6]

$$\underbrace{\overbrace{\begin{bmatrix}\mu_{4,*} & \mu_{5,*} & \mu_{6,*}\end{bmatrix}\begin{bmatrix}1 & -c''_5 & -c''_6 \\ 0 & c''_4 & 0 \\ 0 & 0 & c''_4\end{bmatrix}}^{[\,\mu_{4,*}\ \lambda_{5,*}\ \lambda_{6,*}\,]}\mathrlap{\overbrace{\phantom{\begin{bmatrix}5c'''_5 & 0 \\ 1 & c'''_6 \\ 0 & -c'''_5\end{bmatrix}\begin{bmatrix}1/120 \\ -b_6\end{bmatrix}}}^{c'''_5[\,1/24\ b_5\ b_6\,]^{\mathrm{T}}}}\begin{bmatrix}5c'''_5 & 0 \\ 1 & c'''_6 \\ 0 & -c'''_5\end{bmatrix}}_{[\,\lambda_{5,*}+5c'''_5\mu_{4,*}\ \ c'''_6\lambda_{5,*}-c'''_5\lambda_{6,*}\,]}\begin{bmatrix}1/120 \\ -b_6\end{bmatrix} = [\,0\,] \tag{3}$$

For the 4th and 5th order methods in the pair to produce distinct solutions, the vector $\boldsymbol{d}$ is non-zero. The following four combinations should be equal to zero:

$$\begin{aligned} c'_3c''_4\,\boldsymbol{d}^{\mathrm{T}}(\boldsymbol{c} * \boldsymbol{c}) &= d_5\lambda_{5,c^2} + d_6\lambda_{6,c^2} + d_7\lambda_{7,c^2} \\ c'_3c''_4\,\boldsymbol{d}^{\mathrm{T}}(\boldsymbol{c} * \boldsymbol{c} * \boldsymbol{c}) &= d_5\lambda_{5,c^3} + d_6\lambda_{6,c^3} + d_7\lambda_{7,c^3} \\ c''_4\,\boldsymbol{d}^{\mathrm{T}}(\boldsymbol{c}' * \boldsymbol{c}) &= d_5\lambda_{5,c'c} + d_6\lambda_{6,c'c} + d_7\lambda_{7,c'c} \\ c'_3c''_4\,\boldsymbol{d}^{\mathrm{T}}\boldsymbol{A}(\boldsymbol{c} * \boldsymbol{c}) &= d_5c'''_5\gamma_{4,c^2} + d_6(c'''_6\gamma_{4,c^2} + a_{65}\lambda_{5,c^2}) \\ &\quad + d_7\big(\lambda_{5,c^2} + 5c'''_5\gamma_{4,c^2} - 120b_6(c'''_6\lambda_{5,c^2} - c'''_5\lambda_{6,c^2})\big)/120c'''_5 \end{aligned}$$

The condition $\boldsymbol{b}^{\mathrm{T}}(\boldsymbol{c} * \boldsymbol{c}) = \frac{1}{3}$ implies $120b_6(c'''_6\lambda_{5,c^2} - c'''_5\lambda_{6,c^2}) = \lambda_{5,c^2} + 5c'''_5\mu_{4,c^2}$, which simplifies the coefficient at d_7 in $\boldsymbol{d}^{\mathrm{T}}\boldsymbol{A}(\boldsymbol{c} * \boldsymbol{c})$. As the conditions on the vector $\boldsymbol{d}$ are linear and homogeneous, it can be rescaled by any non-zero factor. Such a rescaling just recalibrates the measure of closeness between the two solutions in the adaptive step size scheme.

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[6] Also $b_4\mu_{4,*} + b_5\mu_{5,*} + b_6\mu_{6,*} = 0$, as $b_4 = (1/24 - b_5c''_5 - b_6c''_6)/c''_4$.

Here are the conditions on the vector $\boldsymbol{d}$ combined with Eq. (3) for $*= c^2$, c^3, and $c'c$, and also with the last four rows of the matrix in Eq. (2):[7]

$$\begin{bmatrix} 1/120 & 0 & b_6 a_{65} & 0 & 0 \\ 0 & 1/24 & b_5 & b_6 & 0 \\ 0 & 0 & d_5 & d_6 & d_7 \end{bmatrix} \boldsymbol{M} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boldsymbol{M} = \begin{bmatrix} \gamma_{4,c^2} + 5c''_4\eta_{c^2} & \gamma_{4,c^3} + 5c''_4\eta_{c^3} & \gamma_{4,c'c} + 5c''_4\eta_{c'c} & \gamma_{Ac^2} + 5c''_4\eta_{Ac^2} \\ \mu_{4,c^2} & \mu_{4,c^3} & \mu_{4,c'c} & c''_4\eta_{c^2} \\ \lambda_{5,c^2} & \lambda_{5,c^3} & \lambda_{5,c'c} & c'''_5\gamma_{4,c^2} \\ \lambda_{6,c^2} & \lambda_{6,c^3} & \lambda_{6,c'c} & c'''_6\gamma_{4,c^2} + a_{65}\lambda_{5,c^2} \\ \lambda_{7,c^2} & \lambda_{7,c^3} & \lambda_{7,c'c} & (\gamma_{4,c^2} - \mu_{4,c^2})/24 \end{bmatrix} \tag{4}$$

As $c''_4\eta_{c^2}/24 + b_5c'''_5\gamma_{4,c^2} + b_6(c'''_6\gamma_{4,c^2} + a_{65}\lambda_{5,c^2}) = (\gamma_{4,c^2} + 5c''_4\eta_{c^2})/120 + b_6a_{65}\lambda_{5,c^2} = 0$, the matrix element in the 2nd row and the 4th column of the product in Eq. (4) is equal to zero. All the columns of $\boldsymbol{M} = \left[m_{ij}\right]$ are orthogonal to any row of the 3×5 matrix in Eq. (4) whose rank is 3, thus $\operatorname{rank}\boldsymbol{M} \le 2$. The 1st and 3rd rows of $\boldsymbol{M}$ are proportional to each other.

The order conditions that are not taken into account in Eq. (4) are $\boldsymbol{b}^{\mathrm{T}}\left[(\boldsymbol{c} * \boldsymbol{c} * \boldsymbol{c} * \boldsymbol{c}) \;\; (\boldsymbol{c}' * \boldsymbol{c} * \boldsymbol{c}) \;\; \left(\left(\boldsymbol{A}(\boldsymbol{c} * \boldsymbol{c})\right) * \boldsymbol{c}\right) \;\; (\boldsymbol{c}'' * \boldsymbol{c}) \;\; (\boldsymbol{c}' * \boldsymbol{c}')\right] = \left[\tfrac{1}{5} \;\; \tfrac{1}{10} \;\; \tfrac{1}{15} \;\; \tfrac{1}{30} \;\; \tfrac{1}{20}\right]$.

3 Expressing a pair through c_2, c_3, c_4, c_5, c_6, and c'_3

The first two rows of Eq. (4) are used to express a_{65}, b_5, b_6, and c'''_5 (and thus also c'''_6, see Eq. (1)) through $\boldsymbol{c}$, $\boldsymbol{c}'$, and $\boldsymbol{c}''$:

$$b_5 = -\frac{1}{24}\frac{\mu_{4,c^2}\lambda_{6,c'c} - \mu_{4,c'c}\lambda_{6,c^2}}{\lambda_{5,c^2}\lambda_{6,c'c} - \lambda_{5,c'c}\lambda_{6,c^2}}, \qquad c'''_5 = \frac{m_{31}m_{14}}{\gamma_{4,c^2}m_{11}} = \frac{\lambda_{5,c^2}(\gamma_{Ac^2} + 5c''_4\eta_{Ac^2})}{\gamma_{4,c^2}(\gamma_{4,c^2} + 5c''_4\eta_{c^2})}$$

$$b_6 = \frac{1}{24}\frac{\mu_{4,c^2}\lambda_{5,c'c} - \mu_{4,c'c}\lambda_{5,c^2}}{\lambda_{5,c^2}\lambda_{6,c'c} - \lambda_{5,c'c}\lambda_{6,c^2}}, \qquad a_{65} = -\frac{m_{11}}{120b_6m_{31}} = -\frac{\gamma_{4,c^2} + 5c''_4\eta_{c^2}}{120b_6\lambda_{5,c^2}}$$

The element m_{44} of the matrix $\boldsymbol{M}$ is equal to $m_{44} = c'''_6\gamma_{4,c^2} + a_{65}\lambda_{5,c^2} = \gamma_{4,c^2}\left(\frac{1}{120} - b_5c'''_5\right)/b_6 - (\gamma_{4,c^2} + 5c''_4\eta_{c^2})/120b_6 = -(m_{24}/24 + b_5m_{34})/b_6$, which is compatible with the 2nd row of Eq. (4).

---

[7] In the case of an embedded pair of 6-stage Runge–Kutta methods, *i.e.*, $d_7 = 0$, the rank of the matrix $\boldsymbol{M}$ without the 5th row should be equal to 1.

By performing the following elementary row and column operations (the order is important) the matrix $\boldsymbol{M}$ is brought to a simpler form:

$$\begin{aligned}
\boldsymbol{M}_{*2} &\leftarrow \boldsymbol{M}_{*2} - (c_2 + c_3)\boldsymbol{M}_{*1} \\
\boldsymbol{M}_{(m-2)*} &\leftarrow \big(\boldsymbol{M}_{(m-2)*} + c''_m \boldsymbol{M}_{1*}\big)/c''_4, \qquad m = 5, 6, 7 \\
\boldsymbol{M}_{2*} &\leftarrow (\boldsymbol{M}_{1*} - \boldsymbol{M}_{2*})/c''_4 \\
\boldsymbol{M}_{5*} &\leftarrow (\boldsymbol{M}_{2*} - 3\boldsymbol{M}_{5*})/c_2 \\
\boldsymbol{M}_{2*} &\leftarrow \boldsymbol{M}_{2*} + 2(1 - 4c_2)\boldsymbol{M}_{5*} \\
\begin{bmatrix} \boldsymbol{M}_{2*} \\ \boldsymbol{M}_{5*} \end{bmatrix} &= \begin{bmatrix} c_3(c_3 - c_2) & 2c_2 & c_3 & c'_3 c_2 \\ c'_3 & -c_3 & 0 & 0 \end{bmatrix}
\end{aligned}$$

These operations do not destroy the proportionality of the 1st and 3rd rows.

The matrix $\boldsymbol{M}$ depends on c'_4, c'_5, and c'_6 in a linear way. The 2nd and 5th rows of the transformed $\boldsymbol{M}$ do depend on c_2, c_3, and c'_3 only. The first three columns of $\boldsymbol{M}$ form a rank-deficient matrix if

$$c'_m = \frac{c'_3 c_3 c_m^2 (c_m - c_2) + 3c''_m (c_3 - c_2)(c_3^2 - 2c'_3)}{c_3^3 (c_m - c_2) - c_2 (c_m - c_3)(c_3^2 - 2c'_3)}, \quad m = 4, 5, 6 \tag{5}$$

Note that the expression (5) for c'_m is valid for any $1 \le m \le 7$. Indeed, for $m = 1$ and $m = 2$ the Eq. (5) gives $c'_1 = c'_2 = 0$ due to $c_1 = c''_1 = 0$ and $c_m - c_2 = c''_2 = 0$, respectively. For $m = 3$ due to $c_m - c_3 = c''_3 = 0$ the Eq. (5) is reduced to a tautology $c'_3 = c'_3$. For $m = 7$, as $c_7 = 1$ and $c''_7 = 1/6$, the expression gives $c'_7 = 1/2$. Also if $c'_3 = c_3^2/2$, then the Eq. (5) gives $c'_m = c_m^2/2$ whenever $c_m \ne c_2$.

Below $\boldsymbol{M} = \big[m_{ij}\big]$ stands for the already transformed matrix. It is of rank 2, as $m_{51}m_{24} - m_{21}m_{54} = c'^2_3 c_2 \ne 0$. Since $m_{53} = m_{54} = 0$ and $m_{23} = c_3$, $m_{24} = c'_3 c_2$, the following linear combinations $q_i = c'_3 c_2 m_{i3} - c_3 m_{i4}$, where $i = 1$, 3, 4, should be equal to zero. The equation $q_1 = 0$ is linear in c''_4, with the solution

$$\begin{aligned}
c'_4 &= \frac{c'_3 c_4^2 (c_4 - c_2)\big(c_3^2 (c_3 - c_2) + c'_3 (3c_2 - 2c_3)\big)}{c_4\big(2c'^2_3 c_2 + c_3 (c_3 - c_2)^2 (c_3^2 - 2c'_3)\big) - c'_3 c_2 c_3 \big(2c'_3 - c_3 (c_3 - c_2)\big)} \\
c''_4 &= \frac{c'^2_3 c_2 c_4^2 (c_4 - c_2)(c_4 - c_3)}{c_4\big(2c'^2_3 c_2 + c_3 (c_3 - c_2)^2 (c_3^2 - 2c'_3)\big) - c'_3 c_2 c_3 \big(2c'_3 - c_3 (c_3 - c_2)\big)}
\end{aligned}$$

The numerator of q_3 is bilinear in c''_4 and c''_5. With c''_4 being already set, the variable c''_5 is determined from effectively a linear equation $q_3 = 0$. This results in $q_4 = 0$ and $\boldsymbol{M}$ being of rank 2, also rank $\big[\boldsymbol{M}_{1*}^{\mathrm{T}}\ \ \boldsymbol{M}_{3*}^{\mathrm{T}}\big] = 1$. The variable c''_6 is found from a linear equation “the numerator of $\big(\boldsymbol{b}^{\mathrm{T}}(\boldsymbol{c} * \boldsymbol{c} * \boldsymbol{c} * \boldsymbol{c}) - 1/5\big)'' = 0$.

The expressions for c'_5, c''_5, and c'''_5 (and especially for c'_6, c''_6, c'''_6, a_{65}, b_6, d_5, d_6, and d_7) are too bulky to be included in this paper.

Some combinations of the variables can be written in a relatively compact form. For example, here is the expression for stability function $R(z)$ that determines the region of absolute stability (see, *e.g.*, [4, Sect. 238], [1, Sect. 4.4],):[8]

$$R(z) = 1 + z\boldsymbol{b}^{\mathrm{T}}(\boldsymbol{I} - z\boldsymbol{A})^{-1}\mathbf{1} = 1 + z + \tfrac{1}{2}z^2 + \tfrac{1}{6}z^3 + \tfrac{1}{24}z^4 + \tfrac{1}{120}z^5 + b_6 a_{65} c_5''' z^6$$

$$b_6 a_{65} c_5''' = -\frac{\gamma_{Ac^2} + 5c_4''\eta_{Ac^2}}{120\gamma_{4,c^2}} = \frac{c_4}{120}\left(1 - \frac{5c_3' c_2}{2c_3' - c_3(c_3 - c_2)}\right)$$

Here $\boldsymbol{I}$ is the identity matrix.

4 Five families of embedded pairs

With $\boldsymbol{c}', \boldsymbol{c}'', \boldsymbol{c}''', a_{65}$, and b_6 expressed through $\boldsymbol{c}$ and c_3', and all but four order conditions being met; the three conditions $\boldsymbol{b}^{\mathrm{T}}\left[(\boldsymbol{c}' * \boldsymbol{c} * \boldsymbol{c}) \quad \left(\left(\boldsymbol{A}(\boldsymbol{c} * \boldsymbol{c})\right) * \boldsymbol{c}\right) \quad (\boldsymbol{c}'' * \boldsymbol{c})\right] = \left[\tfrac{1}{10} \;\; \tfrac{1}{15} \;\; \tfrac{1}{30}\right]$ are satisfied when[9],[10]

$$c_4 = \frac{c_3' c_2\left(2c_3' - c_3(c_3 - c_2)\right)}{\left(2c_3'(1 - 2c_2) - c_3(c_3 - c_2)\right)^2 + 4c_3'^2 c_2^2} \tag{6}$$

or

$$c_6 = 1 \tag{7}$$

If the node c_4 is chosen according to Eq. (6), then the 3rd and 4th rows of the untransformed matrix $\boldsymbol{M}$ are proportional to each other, which results in $d_7 = 0$ and effectively a pair of 6-stage Runge–Kutta methods. The last remaining order condition $\boldsymbol{b}^{\mathrm{T}}(\boldsymbol{c}' * \boldsymbol{c}') = \frac{1}{20}$ is met in three cases:

$$\begin{aligned}
\text{type A:}\quad & c_3' = c_3^2/2 \\
\text{type B:}\quad & c_3' = 3(c_3 - c_2)(c_2 + c_3 - 4c_2c_3)\big/2\left(3 - 12c_2 + 10c_2^2\right) \\
\text{type C:}\quad & \big[3Z(12,15,20) - 3(c_2 + c_3)Z(33,40,50) + 2c_2c_3Z(138,165,200)\big] \\
& \cdot c_3^2(c_3 - c_2)^2 - \big[(12 + 50c_2^2)\left(Z(12,15,20) - c_3Z(33,40,50)\right) \\
& - 3c_2Z(207,260,350) + 2c_2c_3Z(852,1035,1300)\big]c_3'c_3(c_3 - c_2) \\
& + \big[(2 + 10c_2c_3)Z(12,15,20) - 15c_2Z(3,4,6) - 2c_3Z(33,40,50)\big] \\
& \cdot 2(3 - 12c_2 + 10c_2^2)c_3'^2 = 0
\end{aligned}$$

---

[8] Compare with [11, Eq. (3.2)], and [19, Eq. (16)] (the latter contains a sign error), where $c_3' = c_3^2/2$.

[9] They are also satisfied when $(c_3 - c_2)(c_3^2 - 2c_3') = 0$, $c_3^2(c_3 - c_2) - c_3'c_2 = 0$, and $c_3^2(c_3 - c_2) + 2c_3'c_2 = 0$, respectively. Not satisfying any of Eq. (6) and Eq. (7) would imply $c_3'c_2 = 0$ then.

[10] Compare with [12, Eq. (20)], [11, Eq. (3.3)], [19, p. 1173, Corollary 1].

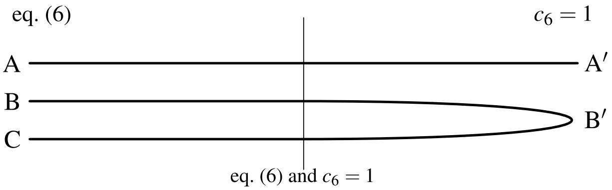

Fig. 1 Schematic depiction of the five families. The left half contains non-FSAL pairs of 6-stage methods, on the right are pairs of 7-stage methods with FSAL property

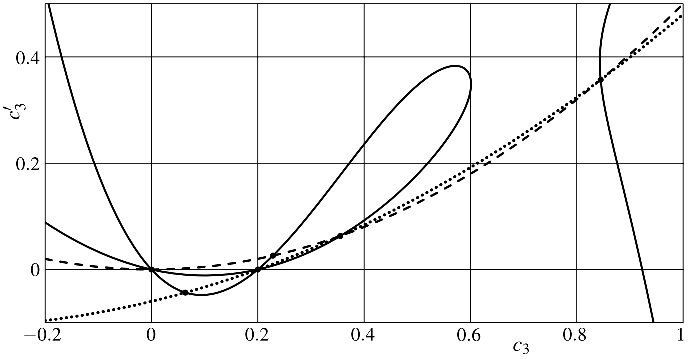

Fig. 2 A two-dimensional cut through the six-dimensional space $(c_2, c_3, c_4, c_5, c_6, c_3')$. Here $c_2 = 1/5$ and $c_5 = 4/5$. The nodes c_4 and c_6 are set according to the eqs. (6) and (7), respectively. The dashed, dotted, and solid curves correspond to pairs of type A, B, and C, respectively. The equations for the curves are (A) $c_3' = c_3^2/2$, (B) $c_3' = 3(5c_3 - 1)(1 + c_3)/50$, and (C) $c_3' = c_3(5c_3 - 1)\big[13 - 12c_3 \pm (73 - 208c_3 + 144c_3^2)^{1/2}\big]/20$. All the three curves intersect at $c_3 = \big(6 \pm 6^{1/2}\big)/10$, or when $3 - 12c_3 + 10c_3^2 = 0$. The type C curve intersects twice with the ones of type A and B at $(c_3, c_3') = (0, 0)$ and $(c_3, c_3') = (c_2, 0)$, respectively. (At these four points some of the matrix elements of $\boldsymbol{A}$ are infinite, so they do not correspond to any embedded pairs.) The structure of intersections stays the same even when only one of the eqs. (6) and (7) is satisfied

where $Z(\alpha_0, \alpha_1, \alpha_2) = \alpha_0 - \alpha_1(c_5 + c_6) + \alpha_2 c_5 c_6$. The left-hand side in the condition for embedded pairs of type C is bilinear in c_5 and c_6. Formulas for embedded pairs of type A are available in Appendix A (see also [19, app.]); for pairs of type B see Appendix B.

If $c_6 = 1$, then the condition $\boldsymbol{b}^{\mathrm{T}}(\boldsymbol{c}' * \boldsymbol{c}') = \frac{1}{20}$ is met in two cases:

type A’: $c_3' = c_3^2/2$

type B’: a bulky expression (which is a polynomial of $c_2, c_3, c_4, c_5,$ and c_3' with degrees $8, 17, 3, 2,$ and $8,$ respectively) is equal to zero

Table 2 A comparison of ten embedded (4, 5) pairs

	$10^4 \times T_6$	$10^3 \times T_7$	$\max_{ij}\lvert a_{ij}\rvert$	$\min_j b_j$	$b_6 a_{65} c_5'''$
[12, table III]	33.557...	6.7653...	8	−0.18	1/2080
[7, Eq. (5)]	9.4828...	1.3689...	2.5925...	0.0978...	1/800
[11, table 2]	3.9908...	3.9557...	11.595...	−0.3223...	1/600
[21, table 1]	1.3851...	2.1124...	12.920...	−3.2900...	1/698.
[2]	0.2216...	0.2126...	1.1637...	0.0086...	N/A
Type B, Table 3	8.9041...	1.2159...	1.6014...	−0.3077...	7/5440
Type A′, Table 4	1.2239...	1.9225...	10.435...	−2.9044...	3/2080
Type B′, $c_3 = 0$, Table 5	7.6950...	1.6029...	3.1358...	−0.0182...	1/720
Type B′, $c_3 = c_2$, Table 6	18.132...	2.7565...	19.285...	0.0416...	1/960
Type B′, Table 7	5.6328...	1.0199...	5.8955...	−0.1160...	1/600

The first five are from the literature. The Fehlberg (also available in [13, table 1]), Cash–Karp, Dormand–Prince, and Tsitouras pairs are of type A, A, A′, and B′, respectively. The $\min_j b_j$ column shows the minimal value of a non-zero weight. The quantity $b_6 a_{65} c_5'''$ is the coefficient at z^6 in the stability function $R(z)$. The stability region is most extended when its value is around 1/1280 [17, fig. 2]. The Bogacki–Shampine pair is non-FSAL and uses 7 stages, so its absolute stability region is not determined by the value of $b_6 a_{65} c_5'''$

Table 3 An embedded pair of type B

0						
$\frac{1}{6}$	$\frac{1}{6}$					
$\frac{7}{32}$	$\frac{67}{512}$	$\frac{45}{512}$				
$\frac{33}{68}$	$\frac{224787}{903992}$	$-\frac{1233765}{903992}$	$\frac{180960}{112999}$			
$\frac{3}{4}$	$\frac{921}{3496}$	$-\frac{552447}{1136200}$	$\frac{125664}{316825}$	$\frac{103173}{179075}$		
$\frac{7}{8}$	$\frac{13}{13984}$	$-\frac{5604237}{49992800}$	$\frac{2246076}{3485075}$	$-\frac{1822723}{189103200}$	$\frac{371}{1056}$	
	$\frac{1}{9}$	$-\frac{59508}{193375}$	$\frac{2281472}{3882375}$	$\frac{1920983}{7492875}$	$\frac{437}{5355}$	$\frac{76912}{283815}$
	0	$\frac{2349}{700}$	$-\frac{832}{175}$	$\frac{83521}{31800}$	$-\frac{377}{168}$	$\frac{377}{371}$

[11] Formulas for embedded pairs of type A′ are available in [19, app.]. For pairs of type B′ the expressions are simplified in the cases $c_3 = 0$ (see Appendix C) and $c_3 = c_2$ (see Appendix D).[12]

The connections between pairs of types A, A′ (that are derived in [19]), B, C, and B′ are shown in Figs. 1 and 2. The new pairs presented in this paper are listed in the lower half of Table 2. They were selected by generally following the perceptive reasoning in [22, p. 785], [11, Sect. 3], [2, p. 20]. As in [11], the local error was estimated through the ℓ^2-norms of elementary differentials vectors:

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[11] If instead of c_3' the variable $g_3' = c_3'/c_3(c_3 - c_2)$ is used, then the degrees are 6, 2, 3, 2, and 8.

[12] Pairs form a set of codimension 2 in the 6-dimensional space $(\boldsymbol{c}, c_3')$. In Fig. 2 the curves in the cut have codimension 1, as at least one of the eqs. (6) and (7) (in fact, both) is satisfied.

Table 4 An embedded pair of type A$'$ which is structurally similar to the [21, table 1] pair of type B$'$ (in the latter one should read $\tilde{b}_7 = -\frac{1}{66}$, also the presented vector $\tilde{\boldsymbol{b}}$ is the difference vector $\boldsymbol{d}$)

0							
$\frac{1}{5}$	$\frac{1}{5}$						
$\frac{21}{65}$	$\frac{21}{338}$	$\frac{441}{1690}$					
$\frac{9}{10}$	$\frac{639}{392}$	$-\frac{729}{140}$	$\frac{1755}{392}$				
$\frac{39}{40}$	$\frac{4878991}{1693440}$	$-\frac{16601}{1792}$	$\frac{210067}{28224}$	$-\frac{1469}{17280}$			
1	$\frac{13759919}{4230954}$	$-\frac{2995}{287}$	$\frac{507312091}{61294590}$	$-\frac{22}{405}$	$-\frac{7040}{180687}$		
1	$\frac{1441}{14742}$	0	$\frac{114244}{234927}$	$\frac{118}{81}$	$-\frac{12800}{4407}$	$\frac{41}{22}$	
	$\frac{1441}{14742}$	0	$\frac{114244}{234927}$	$\frac{118}{81}$	$-\frac{12800}{4407}$	$\frac{41}{22}$	
	$-\frac{1}{273}$	0	$\frac{2197}{174020}$	$-\frac{4}{15}$	$\frac{1280}{1469}$	$-\frac{33743}{52712}$	$\frac{127}{4792}$
θ	1	0	0	0	0	0	0
θ^2	$-\frac{4489}{1638}$	0	$\frac{35152}{8701}$	$-\frac{118}{9}$	$\frac{48000}{1469}$	$-\frac{246}{11}$	$\frac{3}{2}$
θ^3	$\frac{21170}{7371}$	0	$-\frac{1441232}{234927}$	$\frac{2596}{81}$	$-\frac{339200}{4407}$	$\frac{574}{11}$	-4
θ^4	$-\frac{2540}{2457}$	0	$\frac{202124}{78309}$	$-\frac{472}{27}$	$\frac{60800}{1469}$	$-\frac{615}{22}$	$\frac{5}{2}$

The last 4 rows contain coefficients for the 4th order continuously differentiable interpolant $\tilde{\boldsymbol{x}}(t + \theta h) = \boldsymbol{x}(t) + h \sum_j \beta_j(\theta)\boldsymbol{F}_j = \boldsymbol{x}(t) + h \sum_j \boldsymbol{F}_j \sum_k \beta_{kj}\theta^k$, *e.g.*, $\beta_7(\theta) = \frac{3}{2}\theta^2 - 4\theta^3 + \frac{5}{2}\theta^4$

Table 5 An embedded pair of type B$'$ with $c_3 = 0$

0							
$\frac{4}{15}$	$\frac{4}{15}$						
0	$\frac{6}{7}$	$-\frac{6}{7}$					
$\frac{1}{2}$	$-\frac{11}{384}$	$\frac{21}{32}$	$-\frac{49}{384}$				
$\frac{4}{5}$	$\frac{4}{75}$	$-\frac{6}{35}$	$\frac{14}{75}$	$\frac{128}{175}$			
1	$\frac{81}{224}$	$\frac{4917}{1568}$	$-\frac{33}{32}$	$-\frac{132}{49}$	$\frac{275}{224}$		
1	$\frac{41}{384}$	$\frac{3375}{9856}$	$-\frac{7}{384}$	$\frac{4}{21}$	$\frac{125}{384}$	$\frac{7}{132}$	
	$\frac{41}{384}$	$\frac{3375}{9856}$	$-\frac{7}{384}$	$\frac{4}{21}$	$\frac{125}{384}$	$\frac{7}{132}$	
	$\frac{1}{40}$	$\frac{405}{616}$	$-\frac{7}{40}$	$-\frac{32}{35}$	$\frac{5}{8}$	$-\frac{56}{55}$	$\frac{4}{5}$

$$T_p^2 = \sum_{\text{rooted trees t of order } p} \tau^2(\mathrm{t}), \qquad \tau(\mathrm{t}) = \frac{1}{\sigma(\mathrm{t})}\left(\boldsymbol{b}^{\mathrm{T}}\boldsymbol{\Phi}(\mathrm{t}) - \frac{1}{\mathrm{t}!}\right)$$

Here $\sigma(\mathrm{t})$ is the order of the symmetry group of the tree t (see, *e.g.*, [4, p. 154], [5, p. 58]). First, the local error T_6 was minimized with inequality constraints $\max_{ij} |a_{ij}| < M$ (for some limit M) and $\min_j b_j > -3$. Then the pair were chosen close to the optimum, with representation of coefficients a_{ij} requiring a small number of digits. The pair of type A$'$ in Table 4 was constructed to be a close analogue of [21, table 1] pair, which is of type B$'$.

The efficiency curves or work-precision diagrams of six pairs (three from literature and three new ones) are shown in Fig. 3. The performance of type B$'$ pair in

Table 6 An embedded pair of type B$'$ with $c_3 = c_2$

0							
$\frac{1}{4}$	$\frac{1}{4}$						
$\frac{1}{4}$	$-\frac{11}{20}$	$\frac{4}{5}$					
$\frac{1}{3}$	$\frac{1}{9}$	$\frac{43}{216}$	$\frac{5}{216}$				
$\frac{4}{5}$	$\frac{66}{125}$	$-\frac{593}{250}$	$-\frac{19}{50}$	$\frac{378}{125}$			
1	$-\frac{7}{2}$	$\frac{151}{8}$	$\frac{25}{8}$	$-\frac{135}{7}$	$\frac{25}{14}$		
1	$\frac{5}{48}$	0	0	$\frac{27}{56}$	$\frac{125}{336}$	$\frac{1}{24}$	
	$\frac{5}{48}$	0	0	$\frac{27}{56}$	$\frac{125}{336}$	$\frac{1}{24}$	
	$\frac{11}{8}$	$\frac{8}{3}$	$-\frac{40}{3}$	$\frac{297}{28}$	$-\frac{125}{56}$	$-\frac{1}{12}$	1

Although $1/5 = c_3' \neq c_3^2/2 = 1/32$, the weight $b_3 = 0$ and $c_m' = c_m^2/2$ for $m > 3$. Thus, the Dominant Stage-Order (DSO) [23, Eq. (5)] of the 5th order method is equal to 2. As $d_2 \neq 0$, the 4th order method has DSO $= 1$

Table 7 is the worst. With the exception of problem A4, the type B pair in Table 3 is the second-worst. The efficiency of [2] pair shows the potential benefit of adding a stage. The performance of the three other pairs, [11, table 2], [21, table 1], and Table 4, is comparable. (See [21, table 2] for the comparison of [11, table 2] and [21, table 1] pairs on all the 25 problems from [15].)

5 Conclusions

In pairs of 7-stage explicit Runge–Kutta methods, the FSAL property implies $c_6 = 1$ and the condition $D(1)$: $\sum_i b_i a_{ij} = b_j(1 - c_j)$ (see, e.g., [4, p. 189], [14, Eqs. (5.6)], [5, pp. 173 and 193]), regardless of whether the simplifying assumption is satisfied (type A$'$) or not (type B$'$). There are pairs of 8-stage methods with FSAL property and $c_7 \neq 1$, *e.g.*, the [18, fig. 3] pair has $\boldsymbol{c}^{\mathrm{T}} = \begin{bmatrix} 0 & \frac{1}{6} & \frac{1}{4} & \frac{1}{2} & \frac{1}{2} & \frac{9}{14} & \frac{7}{8} & 1 \end{bmatrix}$.

The simplifying assumption $c_i' = \sum_j a_{ij} c_j = c_i^2/2$, where $i \neq 2$, introduces additional redundancy in the order conditions, and the number of free parameters in the families of pairs of types A and A$'$ (that do satisfy the assumption) is the same as for B, B$'$, and C (that do not satisfy the assumption). Not assuming the simplifying assumption does not increase the dimension of the set of pairs satisfying the order conditions. The pairs of types A$'$ and B$'$ form different 4-dimensional submanifolds of the space of matrices $\boldsymbol{A}$, with a 3-dimensional intersection.

From numerical experiments, the part of type B$'$ pairs set that contains efficient pairs is close to the set of type A$'$ pairs. For example, in [21, table 1] pair the weight $b_2 = \frac{1}{100}$ is small, and $a_{32} c_2 / (c_3^2/2) = 1.0102...$ is close to 1. It is hard to expect a good pair of type B$'$ without a counterpart of type A$'$.

Table 7 An embedded pair of type B′

0				
$\frac{1}{5}$	$\frac{1}{5}$			
$\frac{1}{4}$	$\frac{1}{8}$	$\frac{1}{8}$		
$\frac{3}{5}$	$\frac{141}{575}$	$-\frac{228}{115}$	$\frac{1344}{575}$	
c_5	$-\frac{c_5(860c_5^3-1077c_5^2+379c_5-48)}{3(39c_5-5)}$	$\frac{c_5(5c_5-1)(1340c_5^2-1367c_5+277)}{2(39c_5-5)}$	$-\frac{16c_5(5c_5-1)(4c_5-1)(73c_5-55)}{7(39c_5-5)}$	
1	$\frac{113c_5^2-35c_5-40}{c_5(285-319c_5)}$	$-\frac{4(2845c_5^2-2999c_5+654)}{(5c_5-1)(285-319c_5)}$	$\frac{384(168c_5^2-193c_5+52)}{7(4c_5-1)(285-319c_5)}$	
1	$\frac{31c_5-5}{288c_5}$	$-\frac{125(3-c_5)}{768(5c_5-1)}$	$\frac{8(7c_5+3)}{63(4c_5-1)}$	
	$\frac{31c_5-5}{288c_5}$	$-\frac{125(3-c_5)}{768(5c_5-1)}$	$\frac{8(7c_5+3)}{63(4c_5-1)}$	
	$\frac{5(43c_5-33)}{216c_5}$	$\frac{175(43c_5-33)}{288(5c_5-1)}$	$-\frac{152(43c_5-33)}{189(4c_5-1)}$	
c_5	$\frac{115c_5(5c_5-1)(4c_5-1)(5c_5-3)}{42(39c_5-5)}$			
1	$-\frac{460(35c_5^2-55c_5+22)}{7(5c_5-3)(285-319c_5)}$	$\frac{24(1-c_5)(39c_5-5)}{c_5(5c_5-1)(4c_5-1)(5c_5-3)(285-319c_5)}$		
1	$\frac{2875(7c_5-5)}{8064(5c_5-3)}$	$\frac{39c_5-5}{96c_5(5c_5-1)(4c_5-1)(5c_5-3)(1-c_5)}$	$\frac{285-319c_5}{2304(1-c_5)}$	
	$\frac{2875(7c_5-5)}{8064(5c_5-3)}$	$\frac{39c_5-5}{96c_5(5c_5-1)(4c_5-1)(5c_5-3)(1-c_5)}$	$\frac{285-319c_5}{2304(1-c_5)}$	
	$\frac{575(43c_5-33)}{1512(5c_5-3)}$	$-\frac{(39c_5-5)(43c_5-33)}{72c_5(5c_5-1)(4c_5-1)(5c_5-3)(1-c_5)}$	$-\frac{5(285-319c_5)}{864(1-c_5)}$	1
0.000				
0.200	0.200			
0.250	0.125	0.125		
0.600	0.245	−1.983	2.337	

Table 7 (continued)

0.814	−0.107	2.416	−2.110	0.615			
1.000	0.304	−4.967	5.896	−1.014	0.782		
1.000	0.086	−0.116	0.490	0.232	0.249	0.059	
	0.086	−0.116	0.490	0.232	0.249	0.059	
	0.056	0.392	−0.707	0.706	−0.657	−0.791	1.000

The parameters are $c_2 = 1/5$, $c_3 = 1/4$, $c'_3 = 1/40$, and $c_4 = 3/5$. All the conditions up to the 5th order are satisfied but $\boldsymbol{b}^{\mathrm{T}}(\boldsymbol{c}' * \boldsymbol{c}') - 1/20 = (289c_5^2 + 2586c_5 - 2295)/6900(39c_5 - 5)(285 - 319c_5) = 0$, which leads to $c_5 = 3\bigl(8\sqrt{4054} - 431\bigr)/289 = 0.81351...$ (The other choice $c_5 = -9.76...$ would result in $T_6 = 0.045...$, $T_7 = 0.30...$, and $|a_{52}| > 8.9 \times 10^4$.) At the bottom is the Butcher tableau rounded to the nearest thousandth

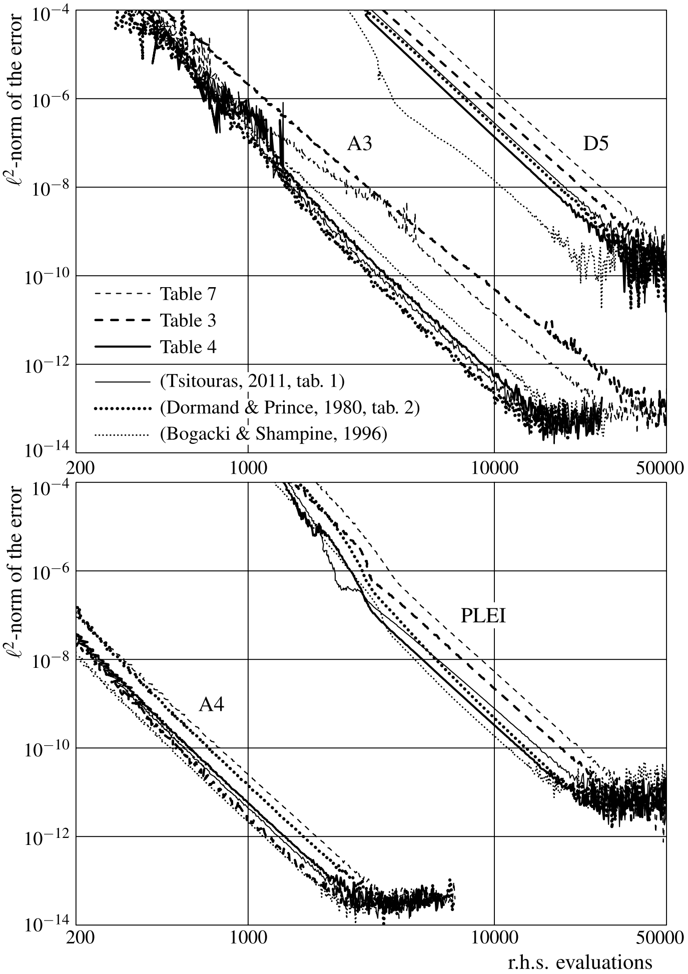

Fig. 3 Efficiency curves for problems A3, A4 [15, p. 617], D5 [15, p. 620], and PLEI [14, p. 245]: the pair in Table 3 (dashed curve), Table 7 (thin dashed curve), Table 4 (solid curve), and [21, table 1] (thin solid curve), [11, table 2] (dotted curve), and [2] (thin dotted curve) pairs. The adaptive step size scheme $h \leftarrow 0.9h\big(\text{ ATOL } /E\big)^{1/5}$ was used. (The starting step size $h_0 = 10^{-6}$ was swiftly corrected by the adaptive step size control.) Here ATOL is the absolute error tolerance, and E is the ℓ^2-norm of the difference vector between the two solutions within a pair. The steps with $E >$ ATOL were rejected, but they were still contributing to the number of the r.h.s. evaluations. For A3, A4, and D5 problems the maximal value of the ℓ^2-norm of the error $\|\tilde{\boldsymbol{x}}(t) - \boldsymbol{x}(t)\|_2$ along the whole trajectory $0 \le t \le 20$ is plotted. For PLEI the ℓ^2-norm of the error was measured at the end of the integration interval $t = 3$, using only 14 components of $\boldsymbol{x}$ that correspond to the coordinates of the stars

Formulas for pairs of type A

$$
\begin{aligned}
c_4 &= c_3 \big/ 2(1 - 4c_3 + 5c_3^2) \\
c'_m &= c_m^2/2, \qquad m = 3, 4, 5, 6 \\
c''_m &= c_m(c_m - c_3)(c_3 + c_m - 4c_3c_m) \big/ 2\big(3 - 12c_3 + 10c_3^2\big), \qquad m = 4, 5, 6 \\
c'''_5 &= c_3c_5(c_5 - c_3)(c_5 - c_4) \big/ 4(3 - 12c_3 + 10c_3^2) \\
g &= 8c_3 - 15c_3^2 - 4c_5(1 - 4c_3 + 5c_3^2) + 2c_6(2 - 13c_3 + 20c_3^2) \\
c'''_6 &= \frac{g\,c_6(c_6 - c_3)(c_6 - c_4)}{4(3 - 12c_3 + 10c_3^2)(8 - 15c_3 - 10c_5 + 20c_3c_5)} \\
b_6a_{65}c'''_5 &= c_4(2 - 5c_3)/240 \\
b_6c'''_6 &= g/480(c_6 - c_5)\big(1 - 4c_3 + 5c_3^2\big) \\
b_2 &= d_2 = d_7 = 0 \\
d_5c_5(c_5 - c_3)(c_5 - c_4) &+ d_6c_6(c_6 - c_3)(c_6 - c_4) = 0
\end{aligned}
$$

Note that $\boldsymbol{c}'$, $\boldsymbol{c}''$, $\boldsymbol{c}'''$, and b_6 do not depend on c_2. As $b_2 = d_2 = 0$, the whole vectors $\boldsymbol{b}$ and $\boldsymbol{d}$ do not depend on c_2. The coefficients a_{ij} and the weights b_j, d_j are obtained using formulas in the beginning of Section 1, *e.g.*, $b_5 = (1/120 - b_6c'''_6)/c'''_5$.

Formulas for pairs of type B

$$
\begin{aligned}
g &= (3 - 12c_2 + 10c_2^2)(3 - 12c_3 + 10c_3^2) + 15(c_2 + c_3 - 4c_2c_3)^2 \\
c_4 &= 3(3 - 10c_2c_3)(c_2 + c_3 - 4c_2c_3) \big/ 2g \\
c'_m &= 3(c_m - c_2)(c_2 + c_m - 4c_2c_m) \big/ 2\big(3 - 12c_2 + 10c_2^2\big), \qquad m = 3, 4, 5, 6 \\
h_m &= 3c_2 + 3c_3 + 3c_m - 12c_2c_3 - 12c_2c_m - 12c_3c_m + 38c_2c_3c_m \\
c''_m &= \frac{(c_m - c_2)(c_m - c_3)\, h_m}{2\big(3 - 12c_2 + 10c_2^2\big)\big(3 - 12c_3 + 10c_3^2\big)}, \qquad m = 4, 5, 6 \\
c'''_5 &= \frac{3(c_5 - c_2)(c_5 - c_3)(c_5 - c_4)(c_2 + c_3 - 4c_2c_3)}{4\big(3 - 12c_2 + 10c_2^2\big)\big(3 - 12c_3 + 10c_3^2\big)} \\
p &= 24 - 45c_2 - 45c_3 + 100c_2c_3 - 10\big[3 - 6c_2 - 6c_3 + 14c_2c_3\big]c_5 \\
q &= 3(c_2 + c_3 - 4c_2c_3)(24 - 45c_2 - 45c_3 + 100c_2c_3) \\
&\quad - \big[4\big(3 - 12c_2 + 10c_2^2\big)\big(3 - 12c_3 + 10c_3^2\big) + 60(c_2 + c_3 - 4c_2c_3)^2\big]c_5 \\
&\quad + \big[4\big(3 - 12c_2 + 10c_2^2\big)\big(3 - 12c_3 + 10c_3^2\big) \\
&\qquad\qquad - 30(c_2 + c_3 - 4c_2c_3)(3 - 8c_2 - 8c_3 + 22c_2c_3)\big]c_6 \\
c'''_6 &= \frac{(c_6 - c_2)(c_6 - c_3)(c_6 - c_4)q}{4\big(3 - 12c_2 + 10c_2^2\big)\big(3 - 12c_3 + 10c_3^2\big)p} \\
b_6a_{65}c'''_5 &= (c_2 + c_3 - 4c_2c_3)(6 - 15c_2 - 15c_3 + 40c_2c_3) \big/ 160g \\
b_6c'''_6 &= q \big/ 480(c_6 - c_5)g \\
b_1 &= 1/9 \\
d_1 &= d_7 = 0 \\
d_5(c_5 - c_2)(c_5 - c_3)(c_5 - c_4) &+ d_6(c_6 - c_2)(c_6 - c_3)(c_6 - c_4) = 0
\end{aligned}
$$

Formulas for pairs of type B′, $c_3 = 0$

$$c_3 = 0$$

$$c_6 = 1$$

α_{lmn}	$l=0$		$l=1$		$l=2$		$l=3$	
	$m=0$	$m=1$	$m=0$	$m=1$	$m=0$	$m=1$	$m=0$	$m=1$
$n=0$	144	180	180	228	72	93	9	12
$n=1$	360	940	512	940	222	366	30	48
$n=2$	200	1100	340	960	162	360	24	48

$$g = 5(c_2^2 + 4c_4^2)c_5(3 - 5c_5) - c_2c_4 \sum_{l=0}^{3}\sum_{m=0}^{1}\sum_{n=0}^{2}(-1)^{l+m+n}\alpha_{lmn}(5c_2)^l c_4^m c_5^n$$

$$p = 3 - 5c_2 - 5c_4 + 10c_2c_4$$

$$q = 12 - 15c_2 - 15c_4 - 15c_5 + 20c_2c_4 + 20c_2c_5 + 20c_4c_5 - 30c_2c_4c_5$$

$$c_3' = 3g \big/ 2(6 - 15c_2 - 10c_5 + 30c_2c_5)pq$$

$$c_4' = 3c_4(c_4 - c_2)/2$$

$$c_5' = 3(c_5 - c_2)\big(c_5 + c_4(2 - 5c_2 - 5c_5 + 10c_2c_5)\big) \big/ 2p$$

$$c_6' = 3(1 - c_2)\big(4 - 7c_4 - 5c_5 + 5c_2c_4 + 10(1 - c_2)c_4c_5\big) \big/ 2q$$

$$c_m'' = c_m'c_m/3, \qquad m = 4, 5, 6$$

$$c_5''' = c_4c_5(c_5 - c_2)(c_5 - c_4)(2 - 5c_2)/4p$$

$$c_6''' = (1 - c_2)(1 - c_4)(2 - 2c_4 - 2c_5 + 5c_2c_4)/4q$$

$$b_6a_{65}c_5''' = c_4(2 - 5c_2)/240$$

$$b_6c_6''' = (2 - 2c_4 - 2c_5 + 5c_2c_4)/240(1 - c_5)$$

$$d_5 = p\big(c_2c_4 + (c_2 - 2c_4)(3 - 5c_5) + 15c_2(1 - c_2)c_4(1 - 2c_5)\big)$$

$$d_6 = qc_5(c_5 - c_2)(c_5 - c_4)\big(4c_4 - 2c_2 - 14c_2c_4 + 15c_2^2c_4\big) \big/ (1 - c_2)(1 - c_4)$$

$$d_7 = 15c_5(c_5 - c_2)(c_5 - c_4)(1 - c_5)\big(c_2 - 2c_4 + 8c_2c_4 - 10c_2^2c_4\big)$$

Formulas for pairs of type B′, $c_3 = c_2$

$$\begin{aligned}
&c_3 = c_2\\
&c_4 = (3 - 5c_5) \big/ 5(1 - 2c_5)\\
&c_6 = 1\\
&c'_m = c_m^2/2, \qquad m = 4, 5, 6\\
&c''_4 = c_4^2(c_4 - c_2)/2\\
&c''_5 = c_5(c_5 - c_2)\big(c_5 + c_4(2 - 5c_2 - 5c_5 + 10c_2c_5)\big) \big/ 2p\\
&c''_6 = (1 - c_2)\big(4 - 7c_4 - 5c_5 + 5c_2c_4 + 10(1 - c_2)c_4c_5\big) \big/ 2q\\
&b_1 = (1 - 8c_5 + 10c_5^2)/12c_5(5c_5 - 3)\\
&b_2 = b_3 = 0\\
&b_4 = 125(2c_5 - 1)^4/12(5c_5 - 2)(5c_5 - 3)(3 - 10c_5 + 10c_5^2)\\
&b_5 = 1/12c_5(1 - c_5)(3 - 10c_5 + 10c_5^2)\\
&b_6 = -(3 - 12c_5 + 10c_5^2)/12(1 - c_5)(5c_5 - 2)\\
&d_5 = -(1 - c_2)(5c_5 - 3)(6 - 15c_2 - 10c_5 + 30c_2c_5) \big/ 3c_5(3 - 10c_5 + 10c_5^2)\\
&d_6 = \big(12 - 52c_2 + 45c_2^2 - 5c_5(4 - 18c_2 + 15c_2^2)\big)(3 - 12c_5 + 10c_5^2) \big/ 3(5c_5 - 2)\\
&d_7 = (1 - c_5)\big(6 - 29c_2 + 30c_2^2 - 10c_5(1 - 5c_2 + 5c_2^2)\big)
\end{aligned}$$

See Appendix C for the expressions for p, q, c'''_5, c'''_6, and $b_6a_{65}c'''_5$. The whole vector $\boldsymbol{b}$ depends on c_5 only.

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Declarations

Conflict of interest Not applicable.

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