Nullspaces yield a new family of explicit Runge–Kutta pairs

Jim Verner

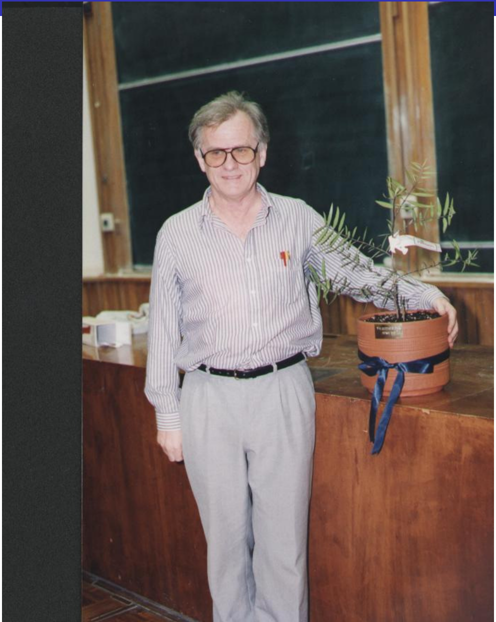
PIMS & Department of Mathematics
Simon Fraser University, Canada
jimverner@shaw.ca
http://www.math.sfu.ca/∼jverner

Abstract

Recently, John Butcher developed a MAPLE code 'Test 21' to solve the order conditions directly. This code was applied to derive 13-stage pairs of orders 7 and 8 and unexpectedly, revealed the existence of some previously unknown pairs. This talk reports formulas for directly deriving such a new parametric family.

February 24, 2023

John Butcher has developed a culture of Trees



and over the years has made many friends

who helped him create new Runge–Kutta arrays

Outline

Explicit Runge–Kutta pairs of methods

For a vector initial value problem in ordinary differential equations:

$$y = f(x, y), \quad y(x_0) = y_0,$$

Explicit Runge–Kutta pairs of methods

For a vector initial value problem in ordinary differential equations:

$$\mathrm{y} = f(x, \mathrm{y}), \quad \mathrm{y}(x_0) = \mathrm{y}_0,$$

an $s-$stage explicit Runge–Kutta **pair** is defined for a step of h as,

$$\mathrm{Y}^{[i]} = \mathrm{y}_{n-1} + h * \Sigma_{j=1}^{i-1} a_{i,j} f(x_{n-1} + c_i h, \mathrm{Y}^{[j]}), \qquad i = 1, .., s,$$

$$\mathrm{y}_n = \mathrm{y}_{n-1} + h * \Sigma_{i=1}^{s} b_i f(x_{n-1} + h, \mathrm{Y}^{[i]}), \qquad n = 1, ..,$$

$$\widehat{\mathrm{y}_n} = \mathrm{y}_{n-1} + h * \Sigma_{i=1}^{s} \widehat{b}_i f(x_{n-1} + h, \mathrm{Y}^{[i]}), \qquad n = 1, ..,$$

Explicit Runge–Kutta pairs of methods

For a vector initial value problem in ordinary differential equations:

$$\mathrm{y} = f(x, \mathrm{y}), \quad \mathrm{y}(x_0) = \mathrm{y}_0,$$

an $s-$stage explicit Runge–Kutta **pair** is defined for a step of h as,

$$\mathrm{Y}^{[i]} = \mathrm{y}_{n-1} + h * \Sigma_{j=1}^{i-1} a_{i,j} f(x_{n-1} + c_i h, \mathrm{Y}^{[j]}), \qquad i = 1, .., s,$$

$$\mathrm{y}_n = \mathrm{y}_{n-1} + h * \Sigma_{i=1}^{s} b_i f(x_{n-1} + h, \mathrm{Y}^{[i]}), \qquad n = 1, ..,$$

$$\widehat{\mathrm{y}_n} = \mathrm{y}_{n-1} + h * \Sigma_{i=1}^{s} \widehat{b}_i f(x_{n-1} + h, \mathrm{Y}^{[i]}), \qquad n = 1, ..,$$

- where $\{b_i, \widehat{b_i}, a_{i,j}, c_i\}$ are coefficients of the pair,
- $\mathrm{y_n}$ approximates $\mathrm{y}(x_n)$ to order p,
- the difference $\mathrm{y_n} - \widehat{\mathrm{y_n}}$ is an order $p-1$ estimate of the local truncation error that can be used for stepsize control.

History of explicit Runge–Kutta derivation

When did this study start?

- Long ago: The Initial Value Problem (IVP)
- 1901,1905: Runge, Kutta
- 1963: Butcher: Rooted trees yield Order Conditions

History of explicit Runge–Kutta derivation

When did this study start?

- Long ago: The Initial Value Problem (IVP)
- 1901,1905: Runge, Kutta
- 1963: Butcher: Rooted trees yield Order Conditions
- New Explicit Methods:
  - 1963-64: Butcher: methods of orders 6 and 7
  - 1967-68: Fehlberg derived *pairs* of orders 6 to 9
  - 1968-72: Cooper and JHV, Curtis: p=8, s=11 methods.
  - 1975: Curtis: p=10, s=18 methods.
  - 1974-78: JHV improved *pairs* of orders 6 to 9
  - 1978: Hairer: derived p=10, s=17 methods

History of explicit Runge–Kutta derivation

When did this study start?

- Long ago: The Initial Value Problem (IVP)
- 1901,1905: Runge, Kutta
- 1963: Butcher: Rooted trees yield Order Conditions
- New Explicit Methods:
  - 1963-64: Butcher: methods of orders 6 and 7
  - 1967-68: Fehlberg derived *pairs* of orders 6 to 9
  - 1968-72: Cooper and JHV, Curtis: p=8, s=11 methods.
  - 1975: Curtis: p=10, s=18 methods.
  - 1974-78: JHV improved *pairs* of orders 6 to 9
  - 1978: Hairer: derived p=10, s=17 methods

Since these derivations, there have been many contributions to searching and finding new methods and pairs for constructing and maintaining software to solve real IVPs.

History of explicit Runge–Kutta derivation

When did this study start?

- Long ago: The Initial Value Problem (IVP)
- 1901,1905: Runge, Kutta
- 1963: Butcher: Rooted trees yield Order Conditions
- New Explicit Methods:
  - 1963-64: Butcher: methods of orders 6 and 7
  - 1967-68: Fehlberg derived *pairs* of orders 6 to 9
  - 1968-72: Cooper and JHV, Curtis: p=8, s=11 methods.
  - 1975: Curtis: p=10, s=18 methods.
  - 1974-78: JHV improved *pairs* of orders 6 to 9
  - 1978: Hairer: derived p=10, s=17 methods

What other (explicit Runge–Kutta) methods exist?

Motivation

- **This is a study to formulate some specific new pairs.**

Motivation

- This is a study to formulate some specific new pairs.
- **Better methods would lead to improvements in software for IVPs - hence, there has since been a search for better methods.**

Motivation

- This is a study to formulate some specific new pairs.
- Better methods would lead to improvements in software for IVPs - hence, there has since been a search for better methods.
- **In 2021, John Butcher developed the MAPLE program 'Test21' which solves order conditions directly to obtain some (explicit) Runge–Kutta methods.**

Motivation

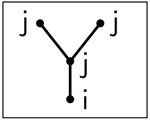
- This is a study to formulate some specific new pairs.
- Better methods would lead to improvements in software for IVPs - hence, there has since been a search for better methods.
- In 2021, John Butcher developed the MAPLE program 'Test21' which solves order conditions directly to obtain some (explicit) Runge–Kutta methods.
- **Some new R–K *pairs* were found on applying 'Test21'.**

Motivation

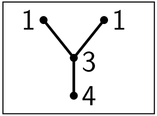
- This is a study to formulate some specific new pairs.
- Better methods would lead to improvements in software for IVPs - hence, there has since been a search for better methods.
- In 2021, John Butcher developed the MAPLE program 'Test21' which solves order conditions directly to obtain some (explicit) Runge–Kutta methods.
- **Some new R–K *pairs* were found on applying 'Test21'.**
  - These new pairs were members of a parametric family.
  - Knowledge of the structure of these new methods may yield more methods in this family.
  - The structure for these new methods may lead to **other types of new methods**.
  - Does this new family contain methods better than those already known?

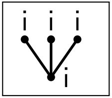
Order Conditions are generated by Rooted Trees

Two similar standard order conditions are

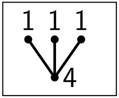


$$\Sigma_{i,j} b_i a_{i,j} c_j^2 = 1/(1*1*3*4)$$



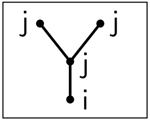


$$\Sigma_i b_i c_i^3/3 = 1/(1*1*1*4)/3$$

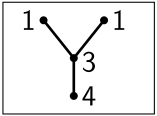


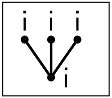
Order Conditions are generated by Rooted Trees

Two similar standard order conditions are

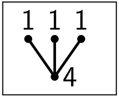


$$\Sigma_{i,j} b_i a_{i,j} c_j^2 = 1/(1 * 1 * 3 * 4)$$

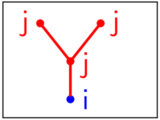




$$\Sigma_i b_i c_i^3 / 3 = 1/(1 * 1 * 1 * 4)/3$$



The difference gives a 'Singly Orthogonal Order Condition':



$$\Sigma_{i,j} b_i \left(a_{i,j} c_j^2 - \frac{c_i^3}{3}\right) = 0$$

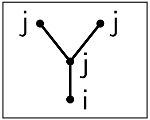
We define "stage-order" or "subquadrature" expressions as

$$q^{[k]} = (AC^{k-1} - C^k/k),$$

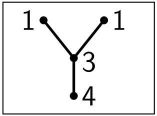
to find that vector b must be orthogonal to vector $q^{[3]}$.

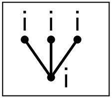
Order Conditions are generated by Rooted Trees

Two similar standard order conditions are

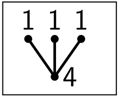


$$\Sigma_{i,j} b_i a_{i,j} c_j^2 = 1/(1*1*3*4)$$

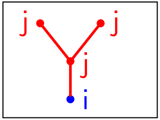




$$\Sigma_i b_i c_i^3 / 3 = 1/(1*1*1*4)/3$$



The difference gives a 'Singly Orthogonal Order Condition':



$$\Sigma_{i,j} b_i \left(a_{i,j} c_j^2 - \frac{c_i^3}{3}\right) = 0$$

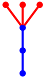
i.e. $b.q^{[3]} = 0$, and past derivations have relied on making parts of either such order conditions components equal to zero, **but more flexibility is possible**.

There are only four types of Order Conditions

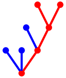
Order conditions can be partitioned into four types that exist:

- A. Quadrature  $\Sigma_i b_i c_i^4 = 1/5 = \int_0^1 c^4 dc$

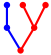
  k-1 terminal nodes each connected to the root

- B. Linear C.C. N.H.  $\Sigma_{i,j,k} b_i a_{i,j} a_{j,k} c_k^3 = 1/120$

  all terminal nodes connected to the penultimate node

- C. Linear V.C.  $\Sigma_{i,j,k} b_i c_i^2 a_{i,j} c_j a_{j,k} c_k^2 = 1/120$

  'side' subtrees of single nodes only

- D. Non-Linear  $\Sigma_{i,j,k} b_i (a_{i,j} c_j)(a_{i,k} c_k^2) = 1/36$

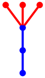
  at least two subtrees of height two or more)

There are only four types of Order Conditions

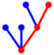
Order conditions can be partitioned into four types that exist:

- A. Quadrature  $\Sigma_i b_i c_i^4 = 1/5 = \int_0^1 c^4 dc$

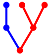
  k-1 terminal nodes each connected to the root

- B. Linear C.C. N.H.  $\Sigma_{i,j,k} b_i a_{i,j} a_{j,k} c_k^3 = 1/120$

  all terminal nodes connected to the penultimate node

- C. Linear V.C.  $\Sigma_{i,k} b_i c_i^2/2 a_{i,k} c_k^2 = 1/36$

  'side' subtrees of single nodes only

- D. Non-Linear  $\Sigma_{i,j,k} b_i (a_{i,j} c_j)(a_{i,k} c_k^2) = 1/36$

  at least two subtrees of height two or more)

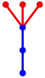
This type D becomes C if $b_i = 0$ or $\Sigma_j a_{i,j} c_j = c_i^2/2, \ i = 1..12$.

There are only four types of Order Conditions

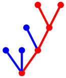
Order conditions can be partitioned into four types that exist:

- A. Quadrature  $\Sigma_i b_i c_i^4 = 1/5 = \int_0^1 c^4 dc$

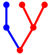
  k-1 terminal nodes each connected to the root

- B. Linear C.C. N.H.  $\Sigma_{i,j,k} b_i a_{i,j} a_{j,k} c_k^3 = 1/120$

  all terminal nodes connected to the penultimate node

- C. Linear V.C.  $\Sigma_{i,j,k} b_i c_i^2 a_{i,j} c_j a_{j,k} c_k^2 = 1/120$

  'side' subtrees of single nodes only

- D. Non-Linear  $\Sigma_{i,j,k} b_i (a_{i,j} c_j)(a_{i,k} c_k^2) = 1/36$

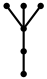
  at least two subtrees of height two or more)

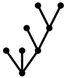
In general, we assume $b_i = 0$ or $q_i^{[2]} = q_i^{[3]} = 0, \; i = 1..12.$

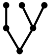
Vector-Matrix format of Standard Order Conditions

A Vector-Matrix notation is more convenient:

A. Quadrature **$Q^{[5]}=0$**  $bC^4e = 1/5$

B. Linear Constant Coefficient  $bA^2C^3e = 1/120$

C. Linear Variable Coefficient  $bC^2ACAC^2e = 1/120$

D. Non-Linear  $b(ACe).(AC^2e) = 1/36$

With retained simplifying conditions, Type D conditions collapse to type C. Hence, I will be focusing of how to solve the first three types.

Otherwise, the order conditions can be expressed using integrals:

If you work with order conditions, the following interpretation as recursive integration may be helpful - for example:

$$bCAC^3AC^2e = \int_{c=0}^{1} c \int_{\bar{c}=0}^{c} \bar{c}^3 \int_{\hat{c}=0}^{\bar{c}} \hat{c}^2 d\hat{c} d\bar{c} dc.$$

Otherwise, the order conditions can be expressed using integrals:

If you work with order conditions, the following interpretation as recursive integration may be helpful - for example:

$$bCAC^3AC^2e = \int_{c=0}^{1} c \int_{\bar{c}=0}^{c} \bar{c}^3 \int_{\hat{c}=0}^{\bar{c}} \hat{c}^2 d\hat{c} d\bar{c} dc.$$

- i.e. b is replaced by integration on [0,1],
- each A is replaced by integration on $[0, c]$,
- each C^k is replaced by the form $\bar{c}^k$.

Otherwise, the order conditions can be expressed using integrals:

If you work with order conditions, the following interpretation as recursive integration may be helpful - for example:

$$bCAC^3AC^2e = \int_{c=0}^{1} c \int_{\bar{c}=0}^{c} \bar{c}^3 \int_{\hat{c}=0}^{\bar{c}} \hat{c}^2 d\hat{c} d\bar{c} dc.$$

- i.e. b is replaced by integration on [0,1],
- each A is replaced by integration on $[0, c]$,
- each C^k is replaced by the form $\bar{c}^k$.

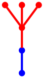
Some multiples of these forms can be expressed using specific nodes as convenient.

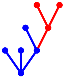
Such expressions are utilized in proving some order conditions.

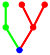
Vector-Matrix Singly Orthogonal Order Conditions

Combining *each* Standard Order Condition with an earlier one yields a "Singly Orthogonal Order Condition" (SOOC) from which constants have been eliminated:

A. Quadrature 5  - 4  $b(5C^4 - 4C^3)e = 0$

B. Linear Constant Coefficient  $bAq^{[4]} = 0$

C. Linear Variable Coefficient  $bC^2ACq^{[3]} = 0$

D. Non Linear  $b(ACe.q^{[3]}) = 0$

The "subquadratures" $q^{[k]} = (AC^{k-1} - C^k/k)e$, show that SOOCs constrain coefficient expressions by orthogonality.

How many SOOC.s of each type are there?

Type / *Order* p	A	B	C	D		N_p	
(1)	(1)				=	(1)	$(\Sigma b_i = 1)$
2	1				=	1	$\Sigma b_i(1-2c_i) = 0$
3	1	1			=	2	.
4	1	2	1		=	4	.
5	1	3	4	1	=	9	.
6	1	4	11	4	=	20	.
7	1	5	26	16	=	48	.
8	1	6	57	51	=	115	.
— — —	— —	— —	— —	— —		— —	
Totals	8	21	99	72	=	200	-1

All but (1) can be expressed as a S.O. Order Condition.

How many SOOC.s of each type are there?

Type / Order p	A	B	C	D		N_p	
(1)	(1)				$=$	(1)	$(\Sigma b_i = 1)$
2	1				$=$	1	$\Sigma b_i(1 - 2c_i) = 0$
3	1	1			$=$	2	.
4	1	2	1		$=$	4	.
5	1	3	4	1	$=$	9	.
6	1	4	11	4	$=$	20	.
7	1	5	26	16	$=$	48	.
8	1	6	57	51	$=$	115	.
Totals	8	21	99	72	$=$	200	-1

Moreover, by suppressing (1) and 2, $(\Sigma N_p) - 2$ order conditions can be written as SOOCs with neither b_1 nor c_1 present.

How many SOOC.s of each type are there?

Type / *Order p*	*A*	*B*	*C*	*D*		N_p	
(1)	(1)				=	(1)	$(\Sigma b_i = 1)$
2	1				=	1	$\Sigma b_i(1-2c_i) = 0$
3	1	1			=	2	.
4	1	2	1		=	4	.
5	1	3	4	1	=	9	.
6	1	4	11	4	=	20	.
7	1	5	26	16	=	48	.
8	1	6	57	51	=	115	.
Totals	8	21	99	72	=	200	-1

For (13,7-8) methods, we have seen that $q_i^{[k]} = 0, \; k = 2, 3$ or $b_i = 0$ otherwise imply conditions D collapse to conditions C. Next, we show how conditions A and B are satisfied.

There exist (p,p) methods for linear C.C. problems

Theorem 1: For non-homogeneous linear constant coefficient initial value problems, there exist p-stage methods of order p.

Proof.

(This skeleton will be expanded to derive (s,p) methods for more general problems.)

There exist (p,p) methods for linear C.C. problems

Theorem 1: For non-homogeneous linear constant coefficient initial value problems, there exist p-stage methods of order p.

Proof.

(This skeleton will be expanded to derive (s,p) methods for more general problems.)

(a) For p distinct nodes c_i, there is a unique solution of

$$\sum_{i=1}^{p} b_i c_i^{k-1} = \frac{1}{k}, \qquad k = 1, .., p.$$

There exist (p,p) methods for linear C.C. problems

Theorem 1: For non-homogeneous linear constant coefficient initial value problems, there exist p-stage methods of order p.

Proof.

(This skeleton will be expanded to derive (s,p) methods for more general problems.)

(a) For p distinct nodes c_i, there is a unique solution of

$$\Sigma_{i=1}^{p} b_i c_i^{k-1} = \frac{1}{k}, \qquad k = 1, .., p.$$

(b) More generally, for p distinct nodes c_i, $L_{p+2-k,i} = bA_i^{k-1}$, $i = p-k+1..1$, $k = 1, .., p$, uniquely satisfy

$$\Sigma_{i=1}^{p+1-k} L_{p+2-k,i} c_i^{j-1} = \frac{(k-j)!}{k!}, \; j = 1, .., p-k.$$

Coefficients $a_{i,j}$ are obtained using a back-substitution with $L_{p+2-i,j}$.

There exist (p,p) methods for linear C.C. problems

Theorem 1: For non-homogeneous linear constant coefficient initial value problems, there exist p-stage methods of order p.

Proof.

(This skeleton will be expanded to derive (s,p) methods for more general problems.)

(a) For p distinct nodes c_i, there is a unique solution of

$$\Sigma_{i=1}^{p} b_i c_i^{k-1} = \frac{1}{k}, \qquad k = 1, .., p.$$

(b) More generally, for p distinct nodes c_i, $L_{p+2-k,i} = bA_i^{k-1}$, $i = p-k+1..1$, $k = 1, .., p$, uniquely satisfy

$$\Sigma_{i=1}^{p+1-k} L_{p+2-k,i} c_i^{j-1} = \frac{(k-j)!}{k!}, \; j = 1, .., p-k.$$

Coefficients $a_{i,j}$ are obtained using a back-substitution with $L_{p+2-i,j}$. (a) and (b) satisfy all conditions of type A and B. □

Back-substitution to get $a_{i,j}$

$L_{i,j}$ form a triangular array:

$$L = \begin{array}{c|cccccc} c_1 & & & & & & \\ c_2 & L_{2,1} & & & & & \\ . & \cdots & & & & & \\ c_p-1 & L_{p-1,1} & L_{p-1,2} & .. & L_{p-1,p-2} & & \\ c_s & L_{p,1} & L_{p,2} & .. & L_{p,p-2} & L_{p,p-1} & \\ \hline & L_{p+1,1} & L_{p+1,2} & .. & L_{p+1,p-2} & L_{p+1,p-1} & L_{p+1,p} \end{array}$$

and observing $b_i = L_{p+1,i}$, $a_{p,i} = (L_{p,i} - \Sigma b_j a_{j,i})/b_p$, ... we substitute up the back diagonals of L to get

$$\begin{array}{c|cccccc} c_1 & & & & \Downarrow & & \\ c_2 & a_{2,1} & & & & & \\ . & \cdots & & & & & \\ c_p-1 & a_{p-1,1} & a_{p-1,2} & .. & a_{p-1,p-2} & \nwarrow & \\ c_p & a_{p,1} & a_{p,2} & .. & a_{p,p-2} & a_{p,p-1} & \\ \hline & b_1 & b_2 & .. & b_{p-2} & b_{p-1} & b_p \end{array}$$

Detail on this back-substitution:

In particular, with $b_p = L_{p+1,p}$ and $L_{q,q-1}$, we first "back-compute" with $L_{q,q-1}$ from the lower-right corner:

$$
\begin{array}{c|cccccc}
c_1 & & & & & & \\
c_2 & L_{2,1} & & & & & \\
. & \dots & & & & & \\
c_{p-1} & L_{p-1,1} & L_{p-1,2} & .. & L_{p-1,s-2} & & \\
c_p & L_{p,1} & L_{p,2} & .. & L_{p,p-2} & L_{p,p-1} & \\
\hline
 & L_{p+1,1} & & .. & L_{p+1,p-2} & L_{p+1,p-1} & L_{p+1,p}
\end{array}
$$

to get $a_{q,q-1} = (L_{q,q-1})/L_{q+1,q}, \;\; q = p, .., 1,$

$$
\begin{array}{c|cccccc}
c_1 & & & & \Downarrow & & \\
c_2 & a_{2,1} & & & & & \\
. & & .. & \nwarrow & & & \\
c_{p-1} & . & . & .. & a_{p-1,p-2} & & \\
c_p & . & . & .. & . & a_{p,p-1} & \\
\hline
 & . & . & .. & . & . & b_p
\end{array}
$$

Next diagonal of back-substitution:

Next, with $L_{q,q-2}$, we back-compute up the next diagonal:

$$
\begin{array}{c|cccccc}
c_1 & & & & & & \\
c_2 & L_{2,1} & & & & & \\
. & \dots & & & & & \\
c_{p-1} & L_{p-1,1} & .. & L_{p-1,p-3} & L_{p-1,p-2} & & \\
c_p & L_{p,1} & L_{p,2} & .. & L_{p,p-2} & L_{p,p-1} & \\
\hline
 & L_{p+1,1} & & .. & L_{p+1,p-2} & L_{p+1,p-1} & L_{p+1,p}
\end{array}
$$

to get $\Downarrow$

$$a_{q,q-2} = (L_{q,q-1} - L_{q+1,q-1} * a_{q-1,q-2})/L_{q+1,q}, \;\; q = p-1, .., 1,$$

$$
\begin{array}{c|cccccc}
c_1 & & & & & & \\
c_2 & a_{2,1} & \nwarrow & \nwarrow & & & \\
. & & & & & & \\
c_{p-1} & . & .. & a_{p-1,p-3} & a_{p-1,p-2} & & \\
c_p & & . & .. & a_{p,p-2} & a_{p,p-1} & \\
\hline
 & . & . & .. & . & b_{p-1} & b_p
\end{array}
$$

Next diagonal of back-substitution:

Next, with $L_{q,q-2}$, we back-compute up the next diagonal:

$$
\begin{array}{c|cccccc}
c_1 & & & & & & \\
c_2 & L_{2,1} & & & & & \\
. & \dots & & & & & \\
c_{p-1} & L_{p-1,1} & .. & L_{p-1,p-3} & L_{p-1,p-2} & & \\
c_p & L_{p,1} & L_{p,2} & .. & L_{p,p-2} & L_{p,p-1} & \\
\hline
 & L_{p+1,1} & & .. & L_{p+1,p-2} & L_{p+1,p-1} & L_{p+1,p}
\end{array}
$$

to get $\Downarrow$

$$a_{q,q-2} = (L_{q,q-1} - L_{q+1,q-1} * a_{q-1,q-2})/L_{q+1,q}, \;\; q = p-1, .., 1,$$

$$
\begin{array}{c|cccccc}
c_1 & & & & & & \\
c_2 & a_{2,1} & & & & & \\
. & \nwarrow & \nwarrow & \nwarrow & & & \\
c_{p-1} & . & .. & a_{p-1,p-3} & a_{p-1,p-2} & & \\
c_p & \textit{and so on} & . & .. & a_{p,p-2} & a_{p,p-1} & \\
\hline
 & . & . & .. & . & b_{p-1} & b_p
\end{array}
$$

This gives a (p,p)-method for N.H. linear C.C. IVPs.

Here is an example of a restricted (6,6) method

This is a 6-stage method of order 6 for N.H. linear C.C. IVPs:

$$
\begin{array}{c|cccccc}
0 & & & & & & \\
\frac{1}{4} & \frac{1}{4} & & & & & \\
\frac{1}{2} & -\frac{1}{2} & 1 & & & & \\
\frac{3}{5} & -\frac{79}{125} & \frac{28}{25} & \frac{14}{125} & & & \\
\frac{3}{4} & \frac{1}{32} & \frac{15}{28} & -\frac{3}{8} & \frac{125}{224} & & \\
1 & \frac{4}{7} & -\frac{36}{49} & \frac{18}{7} & -\frac{125}{49} & \frac{8}{7} & \\
\hline
 & \frac{7}{90} & \frac{16}{45} & \frac{2}{15} & 0 & \frac{16}{45} & \frac{7}{90}
\end{array}
$$

Here is an example of a restricted (6,6) method

This is a 6-stage method of order 6 for N.H. linear C.C. IVPs:

$$
\begin{array}{c|cccccc}
0 & & & & & & \\
\frac{1}{4} & \frac{1}{4} & & & & & \\
\frac{1}{2} & -\frac{1}{2} & 1 & & & & \\
\frac{3}{5} & -\frac{79}{125} & \frac{28}{25} & \frac{14}{125} & & & \\
\frac{3}{4} & \frac{1}{32} & \frac{15}{28} & -\frac{3}{8} & \frac{125}{224} & & \\
1 & \frac{4}{7} & -\frac{36}{49} & \frac{18}{7} & -\frac{125}{49} & \frac{8}{7} & \\
\hline
 & \frac{7}{90} & \frac{16}{45} & \frac{2}{15} & 0 & \frac{16}{45} & \frac{7}{90}
\end{array}
$$

To implement this method with stepsize control, it is possible to derive an embedded method of order 5 with one more stage.

Let's turn now to Nullspaces: β_i = Left Nullspaces

Definition

For each i, we define β_i to be a matrix of s columns whose rows are left parts of SOOCs of products up to i coefficients.

β_i may contain b and other rows as appropriate.

Let's turn now to Nullspaces: β_i = Left Nullspaces

Definition

For each i, we define β_i to be a matrix of s columns whose rows are left parts of SOOCs of products up to i coefficients.

β_i may contain b and other rows as appropriate. One possible choice for β_4 is,

$$\hat{\beta}_4 = \begin{bmatrix} \text{b} \\ \text{bC} \\ \text{bCC} \\ \text{bCCC} \\ \text{bAA} \\ \text{bAAA} \end{bmatrix}$$

but this matrix could contain more rows such as bCCA.

Let's turn now to Nullspaces: β_i = Left Nullspaces

Definition

For each i, we define β_i to be a matrix of s columns whose rows are left parts of SOOCs of products up to i coefficients.

β_i may contain b and other rows as appropriate. One possible choice for β_4 is,

$$\hat{\beta}_4 = \begin{bmatrix} \mathrm{b} \\ \mathrm{bC} \\ \mathrm{bCC} \\ \mathrm{bCCC} \\ \mathrm{bAA} \\ \mathrm{bAAA} \end{bmatrix}$$

but this matrix could contain more rows such as bCCA.

We might use $\bar{\beta}_i$ to designate a maximal number of different rows.

α_j = Right Nullspaces

Definition

Analogously, for each j, we define α_j to be a matrix of s rows whose columns are right parts of SOOCs of products up to j coefficients,

and we use $\bar{\alpha}_j$ to designate a maximal number of different columns.

α_j will not contain $\mathrm{e} = [1, \ldots, 1]^t$, but could contain $(I - 2C)\mathrm{e}$ and for $j > 1$, $(2C - 3C^2)\mathrm{e}$ and/or $\mathrm{q}^{[2]}$.

α_j = Right Nullspaces

Definition

Analogously, for each j, we define α_j to be a matrix of s rows whose columns are right parts of SOOCs of products up to j coefficients,

and we use $\bar{\alpha}_j$ to designate a maximal number of different columns.

α_j will not contain $\mathrm{e} = [1, ..., 1]^t$, but could contain $(I - 2C)\mathrm{e}$ and for $j > 1$, $(2C - 3C^2)\mathrm{e}$ and/or $\mathrm{q}^{[2]}$.

We'll see an example of α_2 soon. An example of α_3 is

$$\hat{\alpha}_3 = [(2\mathrm{C} - 3\mathrm{C}^2)\mathrm{e}, \mathrm{q}^{[2]}, (3\mathrm{C}^2 - 4\mathrm{C}^3)\mathrm{e}, \mathrm{Aq}^{[2]}, \mathrm{q}^{[3]}].$$

We observe now that any matrices β_i and α_j are mutually orthogonal whenever $1 < i + j \le p$. Hence, each contains vectors in the Nullspace of the other.

The Nullspace Theorem

From these definitions, we have the following:

Theorem 2: For an s-stage method of order p, it is necessary that

$$\beta_i . \alpha_j = 0, \quad 1 < i + j \leq p.$$

To derive methods, we might try to characterize coefficients of a method that possesses such orthogonality properties. To this end, I have studied the orthogonality properties of some new methods found using Test21. Eventually, I found that matrix A of such methods has a very special two-parameter partitioning.

Nullspaces for low order Runge–Kutta methods

As an example, consider three-stage methods of general order three:

1. $\widetilde{\mathrm{Q}}^{[1]} = \Sigma_{i=1}^{3} b_i - 1 \qquad = 0$
2. $\widetilde{\mathrm{Q}}^{[1]} - 2\widetilde{\mathrm{Q}}^{[2]} = \Sigma_{i=1}^{3} \mathrm{b_i}(1 - 2c_i) \qquad = 0$
3. $2\widetilde{\mathrm{Q}}^{[2]} - 3\widetilde{\mathrm{Q}}^{[3]} = [\mathrm{b}_2 \quad \mathrm{b}_3] \begin{bmatrix} c_2(2-3c_2) \\ c_3(2-3c_3) \end{bmatrix} \qquad = 0$
4. $\mathrm{b}.\widetilde{\mathrm{q}}^{[2]} = 0$

Four solutions exist (see Butcher, 2021, p. 63)

Nullspaces for low order Runge–Kutta methods

As an example, consider three-stage methods of general order three:

1. $\widetilde{Q}^{[1]} = \Sigma_{i=1}^{3} b_i - 1 \qquad = 0$
2. $\widetilde{Q}^{[1]} - 2\widetilde{Q}^{[2]} = \Sigma_{i=1}^{3} \mathrm{b_i}(1 - 2c_i) \qquad = 0$
3. $2\widetilde{Q}^{[2]} - 3\widetilde{Q}^{[3]} = [\mathrm{b}_2 \quad \mathrm{b}_3]\begin{bmatrix} c_2(2-3c_2) \\ c_3(2-3c_3)\end{bmatrix} \qquad = 0$
4. $\mathrm{b}.\widetilde{\mathrm{q}}^{[2]} = 0$

Four solutions exist (see Butcher, 2021, p. 63)

We observe that

$$\beta_1 = \begin{bmatrix} b_1 & b_2 & b_3 \end{bmatrix} \quad \textit{and} \quad \alpha_2 = \begin{bmatrix} 1 & 0 & 0 \\ 1-2c_2 & c_2(2-3c_2) & q_2^{[2]} \\ 1-3c_3 & c_3(2-3c_3) & q_3^{[2]} \end{bmatrix};$$

these are orthogonal and $\mathrm{b} \neq 0$, so that α_2 has rank 2. Hence, α_2 contains a row or column of zeros, or else has linear dependence, and this leads to the four solutions that exist.

What is known about (13,7-8) Runge–Kutta pairs?

- The 12-stage method of order 8 is derived first:
- For this, split an (8,8) method for N.H. C.C. linear problems **after column 1**, by moving values $L_{p+2-k,j},\ j = 2..8$ to $L_{s+2-k,j}, j = 6..s$ for $s = 12$, and then insert new values $\mathrm{L}_{\mathrm{s+2-k,j}} = 0 \quad (\mathrm{i.e.b_j} = \mathrm{L}_{13,\mathrm{j}} = 0, \mathrm{bA_j} = \mathrm{L}_{12,\mathrm{j}} = 0, ..\ \mathrm{j} = 2, 3, 4, 5.)$

What is known about (13,7-8) Runge–Kutta pairs?

- The 12-stage method of order 8 is derived first:
- For this, split an (8,8) method for N.H. C.C. linear problems **after column 1**, by moving values $L_{p+2-k,j},\ j = 2..8$ to $L_{s+2-k,j}, j = 6..s$ for $s = 12$, and then insert new values $\mathrm{L_{s+2-k,j} = 0}$ $\quad$ $\mathrm{(i.e. b_j = L_{13,j} = 0, bA_j = L_{12,j} = 0, .. j = 2, 3, 4, 5.)}$
- On stages 2..9, impose stage-order conditions $q^{[k]} = 0$, and additional constraints on nodes and coefficients so that remaining conditions of type C are satisfied.
- Assign $b_i = L_{13,i}, i = 1..12$, and after computing coefficients from stages 2 to 9, use a back substitution algorithm on $L_{s+2-k,j}$ to compute $a_{i,j}$, j=i-1..1, i=12,11,10.

What is known about (13,7-8) Runge–Kutta pairs?

- The 12-stage method of order 8 is derived first:
- For this, split an (8,8) method for N.H. C.C. linear problems **after column 1**, by moving values $L_{p+2-k,j},\ j = 2..8$ to $L_{s+2-k,j}, j = 6..s$ for $s = 12$, and then insert new values $\mathrm{L_{s+2-k,j}} = 0$ $\quad(\mathrm{i.e.b_j} = \mathrm{L_{13,j}} = 0, \mathrm{bA_j} = \mathrm{L_{12,j}} = 0, ..\ \mathrm{j} = 2, 3, 4, 5.)$
- On stages 2..9, impose stage-order conditions $q^{[k]} = 0$, and additional constraints on nodes and coefficients so that remaining conditions of type C are satisfied.
- Assign $b_i = L_{13,i}, i = 1..12$, and after computing coefficients from stages 2 to 9, use a back substitution algorithm on $L_{s+2-k,j}$ to compute $a_{i,j}$, j=i-1..1, i=12,11,10.
- Then, **the embedded method of order 7** is obtained from similar values $\hat{L}_{i,j}$ using another back-substitution.

Properties of the New Methods

On computation with some new methods of order 8, I found

- $\bar{\beta}_4$ is 18×12, has four columns of zeros, and rank $= 6$.
- $\bar{\beta}_4$ is spanned by the rows of $\hat{\beta}_4$. (Linear independence is needed.)

Properties of the New Methods

On computation with some new methods of order 8, I found

- $\bar{\beta}_4$ is 18×12, has four columns of zeros, and rank $= 6$.
- $\bar{\beta}_4$ is spanned by the rows of $\hat{\beta}_4$. (Linear independence is needed.)
- $P_4(C) = I - 20C + 90C^2 - 140C^3 + 70C^4$ and $\mathrm{q}^{[4]}$ are Nullvectors of $\bar{\beta}_4$. Hence, Nullspace $(\bar{\beta}_4)$ is spanned by $\{\mathrm{e_i},\ \mathrm{i} = 2..5,\ \mathrm{P_4(C)},\ \mathrm{q}^{[4]}\}$.
- If $c_6 = 1/2$, then Rank (Columns 6 to 12 of $\bar{\beta}_4$)=5, and $\mathrm{q}^{[4]}$ is a Nullvector of this submatrix.

Properties of the New Methods

On computation with some new methods of order 8, I found

- $\bar{\beta}_4$ is 18×12, has four columns of zeros, and rank $= 6$.
- $\bar{\beta}_4$ is spanned by the rows of $\hat{\beta}_4$. (Linear independence is needed.)
- $P_4(C) = I - 20C + 90C^2 - 140C^3 + 70C^4$ and $\mathrm{q}^{[4]}$ are Nullvectors of $\bar{\beta}_4$. Hence, Nullspace $(\bar{\beta}_4)$ is spanned by $\{\mathrm{e_i},\ \mathrm{i} = 2..5,\ \mathrm{P_4(C)},\ \mathrm{q}^{[4]}\}$.
- If $c_6 = 1/2$, then Rank (Columns 6 to 12 of $\bar{\beta}_4$)=5, and $\mathrm{q}^{[4]}$ is a Nullvector of this submatrix.
- Rank of $\alpha_4 = 5$. (I expected this rank to be six.)
- Non-trivial columns of α_4 are $\mathrm{P_4(C)}$ and $\mathrm{q}^{[4]}\}$.

Properties of the New Methods

On computation with some new methods of order 8, I found

- $\bar{\beta}_4$ is 18×12, has four columns of zeros, and rank $= 6$.
- $\bar{\beta}_4$ is spanned by the rows of $\hat{\beta}_4$. (Linear independence is needed.)
- $P_4(C) = I - 20C + 90C^2 - 140C^3 + 70C^4$ and $\mathrm{q}^{[4]}$ are Nullvectors of $\bar{\beta}_4$. Hence, Nullspace $(\bar{\beta}_4)$ is spanned by $\{\mathrm{e_i},\ \mathrm{i} = 2..5,\ \mathrm{P_4(C)},\ \mathrm{q}^{[4]}\}$.
- If $c_6 = 1/2$, then Rank (Columns 6 to 12 of $\bar{\beta}_4$)=5, and $\mathrm{q}^{[4]}$ is a Nullvector of this submatrix.
- Rank of $\alpha_4 = 5$. (I expected this rank to be six.)
- Non-trivial columns of α_4 are $\mathrm{P_4(C)}$ and $\mathrm{q}^{[4]}\}$.

Observe that $\mathrm{q}^{[4]} = 0$ used in known (12,8) methods is relaxed so that lhis vector lies in the Nullspace of $\bar{\beta}_4$.

Outline of New (12,8) Methods

Almost Theorem 3: Compute for a 12-stage method:

1. 12 nodes with $c_1, c_6, .., c_{12}$ distinct confined by $c_3 = 2c_4/3, \quad c_5 = (4c_4 - 3c_6)/(c_6(6c_4 - 4c_6))$, and for $\pi(c) = c(c-c_6)(c-c_7)(c-c_8)$, c_9 is chosen so that
$$\Big[\int_0^1 \pi(c)\frac{(c-1)^2}{2!}\,dc\Big]\Big[\int_0^1 \pi(c)(c-c_9)\frac{(c-1)^2}{2!}\,dc\Big] = \Big[\int_0^1 \pi(c)\frac{(c-1)^3}{3!}\,dc\Big]\Big[\int_0^1 \pi(c)(c-c_9)\frac{(c-1)}{1!}\,dc\Big].$$
2. Choose stages 2 to 9 so that $q_i^{[k]} = 0, \; k = 1,2,3$.
3. Constrain stage 9 so that $\Sigma_i b_i c_i^2 a_{i,j} = 0, \; j = 4,5$.
4. Choose remaining parameters so $\bar{\beta}_4$ is orthogonal to $q^{[4]}$.
5. $L_{i,j}$ (with $L_{i,j} = 0, \; j = 2..5$) and back-substitution, for the weights b_i and stages 12 to 10.

Then, the method has order 8.

Partial proof

Proof.

Conditions A and B follow from $q^{[k]}, k = 1, 2, 3$, and $L_{i,j}$. Also, values for $q_i^{[k]}$ force Conditions D to collapse to Conditions C . To establish Conditions C, formulas among A, C, b are used:

- $L_{i,j}$ with $i = 13, 12$ imply $bA = b(I - C)$
- post-multiplication of bA-b(I-C) by A,C,AA,CC,AC,CA
- $bCCA * q^{[4]} = 0$

These imply bAC, bCA, bCAA, bACC lie in the rowspace of $\hat{\beta}_4$; bAAC, bCAC, bACA, added to linear combinations of $C^k, \ k = 0..4$ can be shown to be orthogonal to $q^{[4]}$ by direct computation. These imply most of Conditions C hold. □

This will leave one arbitrary coefficient in row 8 of A (selected as $a_{8,7}$).As well, under further constraints, $a_{7,6}$ is arbitrary.

Algorithm for Known (12,8) methods

- Stage 2: $q_2^{[1]} = 0 \implies a_{2,1} = c_2$.
- Stage 3: $q_3^{[1]} = q_3^{[2]} = 0$.
- Stage 4: $a_{4,2} = 0,\ q_4^{[k]} = 0, k = 1,2,3.$
- Stage 5: $a_{5,2} = 0, q_5^{[k]} = 0, k = 1,2,3.$
- Stage 6: $a_{6,2} = a_{6,3} = 0, q_6^{[k]} = 0, k = 1,2,3,4.$
- Stage 7: $a_{7,2} = a_{7,3} = 0, q_7^{[k]} = 0, k = 1,2,3,4.$
- Stage 8: $a_{8,2} = a_{8,3} = 0, a_{8,4}, q_8^{[k]} = 0, k = 1,2,3,4.$
- Stage 9: $a_{9,2} = a_{9,3} := 0, q_9^{[k]} = 0, k = 1,2,3,4.$
  $L_{13,10}(c_{10} - c_{12})(c_{10} - c_{11})\Sigma_{j=k+1}^{9} L_{11,j} a_{j,k}$
  -$L_{11,10}\Sigma_{j=k+1}^{9} L_{13,j}(c_j - c_{12})(c_j - c_{11}) a_{j,k} = 0, \quad k = 4,5.$
- Stages 12..10 and b_i: Observe $b_i = L_{13,i}, i = 1..12$, and use back-substitution on $L_{14-k,i}, k = 2..4,\ i = 13-k,..,1$ to get $a_{14-k,i},\quad k = 2..4,\ i = 13-k..1$.

Algorithm for Known (12,8) methods

- Stage 2: $q_2^{[1]} = 0 \implies a_{2,1} = c_2$. SO=1
- Stage 3: $q_3^{[1]} = q_3^{[2]} = 0$. SO=2
- Stage 4: $a_{4,2} = 0,\ q_4^{[k]} = 0, k = 1, 2, 3.$ SO=3
- Stage 5: $a_{5,2} = 0, q_5^{[k]} = 0, k = 1, 2, 3.$ SO=3
- Stage 6: $a_{6,2} = a_{6,3} = 0, q_6^{[k]} = 0, k = 1, 2, 3, 4.$ SO=4
- Stage 7: $a_{7,2} = a_{7,3} = 0, q_7^{[k]} = 0, k = 1, 2, 3, 4.$ SO=4
- Stage 8: $a_{8,2} = a_{8,3} = 0, a_{8,4}, q_8^{[k]} = 0, k = 1, 2, 3, 4.$ SO=4
- Stage 9: $a_{9,2} = a_{9,3} := 0, q_9^{[k]} = 0, k = 1, 2, 3, 4.$ SO=4

  $L_{13,10}(c_{10} - c_{12})(c_{10} - c_{11})\Sigma_{j=k+1}^{9} L_{11,j} a_{j,k}$
  -$L_{11,10}\Sigma_{j=k+1}^{9} L_{13,j}(c_j - c_{12})(c_j - c_{11}) a_{j,k} = 0, \quad k = 4, 5.$
- Stages 12..10 and b_i: Observe $b_i = L_{13,i}, i = 1..12$, and use back-substitution on $L_{14-k,i}, k = 2..4,\ i = 13 - k, .., 1$ to get $a_{14-k,i}, \quad k = 2..4,\ i = 13 - k..1$.

Algorithm for New (12,8) methods - reduce SO

- Stage 2: $q_2^{[1]} = 0 \implies a_{2,1} = c_2.$ SO=1
- Stage 3: $q_3^{[1]} = q_3^{[2]} = 0.$ SO=2
- Stage 4: $a_{4,2} = 0,\ q_4^{[k]} = 0, k = 1, 2, 3.$ SO=3
- Stage 5: $a_{5,2} = 0, q_5^{[k]} = 0, k = 1, 2, 3.$ SO=3
- Stage 6: $a_{6,2} = a_{6,3} = 0, q_6^{[k]} = 0, k = 1, 2, 3, 4.$ SO=4
- Stage 7: $a_{7,2} = a_{7,3} = 0, a_{7,6}, q_7^{[k]} = 0, k = 1, 2, 3$ >SO=3
- Stage 8: $a_{8,2} = a_{8,3} = 0, a_{8,7}, q_8^{[k]} = 0, k = 1, 2, 3$ >SO=3
- Stage 9: $a_{9,2} = a_{9,3} := 0, q_9^{[k]} = 0, k = 1, 2, 3$ >SO=3

  $L_{13,10}(c_{10} - c_{12})(c_{10} - c_{11})\Sigma_{j=k+1}^{9} L_{11,j} a_{j,k}$
  $-L_{11,10}\Sigma_{j=k+1}^{9} L_{13,j}(c_j - c_{12})(c_j - c_{11})a_{j,k} = 0, \quad k = 4, 5.$
- Stages 12..10 and b_i: Observe $b_i = L_{13,i}, i = 1..12$, and use back-substitution on $L_{14-k,i}, k = 2..4,\ i = 13 - k, .., 1$ to get $a_{14-k,i}, \quad k = 2..4,\ i = 13 - k..1.$

But to get order 8 more is needed to replace $q^{[4]} = 0$.

Structure of New Pairs

Theorem 4: Assume $\{b,\ \hat{b},\ A,\ c\}$, yield a traditional (13,7-8) pair. For $c_6 = 1/2$, and any other value of $a_{7,6} = \widehat{a_{76}}$, and possibly a different value of $a_{8,7} = \widehat{a_{87}}$, define four vectors by

- R1 is the solution of $a_{7,2} = a_{7,3} = 0,\ a_{7,6} = \widehat{a_{76}}$, $q_7^{[k]} = 0,\ k = 1, 2, 3.$
- V1 is the solution of $V1_7 = 1$, and $\hat{\beta}_4.V1 = 0$.

Structure of New Pairs

Theorem 4: Assume $\{b,\ \hat{b},\ A,\ c\}$, yield a traditional (13,7-8) pair. For $c_6 = 1/2$, and any other value of $a_{7,6} = \widehat{a_{76}}$, and possibly a different value of $a_{8,7} = \widehat{a_{87}}$, define four vectors by

- R1 is the solution of $a_{7,2} = a_{7,3} = 0,\ a_{7,6} = \widehat{a_{76}}$, $q_7^{[k]} = 0,\ k = 1, 2, 3.$
- V1 is the solution of $V1_7 = 1$, and $\hat{\beta}_4.V1 = 0$.
- R2 is the solution of $a_{8,2} = a_{8,3} = 0,\ a_{8,7} = \widehat{a_{87}}$, $q_8^{[k]} = 0,\ k = 1, 2, 3,\ q_8^{[4]} = V1_8 * q_7^{[4]}/V1_7$.
- V2 is the solution of $V2_8 = 1$, and $\hat{\beta}_3.V2 = 0$.

Structure of New Pairs

Theorem 4: Assume $\{b,\ \hat{b},\ A,\ c\}$, yield a traditional (13,7-8) pair. For $c_6 = 1/2$, and any other value of $a_{7,6} = \widehat{a_{76}}$, and possibly a different value of $a_{8,7} = \widehat{a_{87}}$, define four vectors by

- R1 is the solution of $a_{7,2} = a_{7,3} = 0,\ a_{7,6} = \widehat{a_{76}}$, $q_7^{[k]} = 0,\ k = 1, 2, 3.$
- V1 is the solution of $V1_7 = 1$, and $\hat{\beta}_4.V1 = 0.$
- R2 is the solution of $a_{8,2} = a_{8,3} = 0,\ a_{8,7} = \widehat{a_{87}}$, $q_8^{[k]} = 0,\ k = 1, 2, 3,\ q_8^{[4]} = V1_8 * q_7^{[4]}/V1_7.$
- V2 is the solution of $V2_8 = 1$, and $\hat{\beta}_3.V2 = 0.$

Then for each $\widehat{a_{76}}$ and $\widehat{a_{87}}$, and

$$\hat{\mathrm{A}} = \mathrm{A} + \mathrm{V1.R1}\widehat{\mathrm{a}_{76}} + \mathrm{V2.R2}\widehat{\mathrm{a}_{87}},$$

(Vi.Ri is an outer product) $\{\mathrm{b},\ \hat{\mathrm{b}},\ \hat{\mathrm{A}},\ \mathrm{c}\}$ yields a new (13,7-8) pair.

Structure of New Pairs (Continued)

Proof.

For $c_6 = 1/2$, the matrix for V1 has rank 5, so V1 is a right Nullvector of $\bar{\beta}_4$. Also, R1 is a left Nullvector of $\bar{\alpha}_4$. The matrix for V2 has rank 4, and so V2 is a right Nullvector of $\bar{\beta}_3$. As well, R2 is a left Nullvector of $\bar{\alpha}_3$. These seem sufficient to prove that coefficients $\{b,\ bh,\ \hat{A},\ c\}$ yield a (13,7-8) pair. □

Structure of New Pairs (Continued)

Proof.

For $c_6 = 1/2$, the matrix for V1 has rank 5, so V1 is a right Nullvector of $\bar{\beta}_4$. Also, R1 is a left Nullvector of $\bar{\alpha}_4$. The matrix for V2 has rank 4, and so V2 is a right Nullvector of $\bar{\beta}_3$. As well, R2 is a left Nullvector of $\bar{\alpha}_3$. These seem sufficient to prove that coefficients $\{b,\ bh,\ \hat{A},\ c\}$ yield a (13,7-8) pair. □

For each traditional (13,7-8) pair with $c_6 = 1/2$ and a value of $a_{8,7}$, this yields a new family of such pairs in the parameter $a_{7,6}$. While we have exchanged the freedom to choose an arbitrary value for c_6 to make $a_{7,6}$ a parameter, we have derived a new family of pairs.

Structure of New Pairs (Continued)

Proof.

For $c_6 = 1/2$, the matrix for V1 has rank 5, so V1 is a right Nullvector of $\bar{\beta}_4$. Also, R1 is a left Nullvector of $\bar{\alpha}_4$. The matrix for V2 has rank 4, and so V2 is a right Nullvector of $\bar{\beta}_3$. As well, R2 is a left Nullvector of $\bar{\alpha}_3$. These seem sufficient to prove that coefficients $\{b,\ bh,\ \hat{A},\ c\}$ yield a (13,7-8) pair. □

For each traditional (13,7-8) pair with $c_6 = 1/2$ and a value of $a_{8,7}$, this yields a new family of such pairs in the parameter $a_{7,6}$. While we have exchanged the freedom to choose an arbitrary value for c_6 to make $a_{7,6}$ a parameter, we have derived a new family of pairs.

A code for obtaining pairs of this new type is similar to that for the traditional pairs. When $c_6 = 1/2$, I have used this code to optimize over the range of arbitrary nodes, $a_{7,6}$ and $a_{8,7}$.

Are there efficient pairs within the new family?

Criteria accepted for determining good pairs usually requires that the 2-norm of the Local Truncation Error is small for the propagating method.

Pair	*Nodes*	LTE_2	*D*	*Stab.*
$EE-JHV(1978)$	$0, 1/4, 1/12$	$3.82E-05$	5.98	$(-5.07, 0]$
$Fam-JHV(1979)$	$0, 2/27, 1/9$	$9.82e-06$	15.64	$(-5.00, 0]$
$HNW(DP)(1991)$	$0, .158, .237$	$2.24E-06$	43.48	$(-5.49, 0]$
$SS(1993)$	$0, 19/250, 1/10$	$1.08E-06$	27.30	$(-5.68, 0]$
$MAPLE(2000)$	$0, .054, .102$	$1.55E-06$	20.18	$(-5.84, 0]$
$Eff.-JHV(2010)$	$0, 1/20, 341/3200$	$2.82E-07$	123.37	$(-5.86, 0]$

Are there efficient pairs within the new family?

Criteria accepted for determining good pairs usually requires that the 2-norm of the Local Truncation Error is small for the propagating method.

Pair	*Nodes*	LTE_2	*D*	*Stab.*
$EE - JHV(1978)$	$0, 1/4, 1/12$	$3.82E-05$	5.98	$(-5.07, 0]$
$Fam - JHV(1979)$	$0, 2/27, 1/9$	$9.82e-06$	15.64	$(-5.00, 0]$
$HNW(DP)(1991)$	$0, .158, .237$	$2.24E-06$	43.48	$(-5.49, 0]$
$SS(1993)$	$0, 19/250, 1/10$	$1.08E-06$	27.30	$(-5.68, 0]$
$MAPLE(2000)$	$0, .054, .102$	$1.55E-06$	20.18	$(-5.84, 0]$
$Eff. - JHV(2010)$	$0, 1/20, 341/3200$	$2.82E-07$	123.37	$(-5.86, 0]$
Improvement	(2023)	$2.73E-07$	123.75	$(-5.81, 0]$

Are there efficient pairs within the new family?

Criteria accepted for determining good pairs usually requires that the 2-norm of the Local Truncation Error is small for the propagating method.

Pair	*Nodes*	LTE_2	*D*	*Stab.*
$EE - JHV(1978)$	$0, 1/4, 1/12$	$3.82E-05$	5.98	$(-5.07, 0]$
$Fam - JHV(1979)$	$0, 2/27, 1/9$	$9.82e-06$	15.64	$(-5.00, 0]$
$HNW(DP)(1991)$	$0, .158, .237$	$2.24E-06$	43.48	$(-5.49, 0]$
$SS(1993)$	$0, 19/250, 1/10$	$1.08E-06$	27.30	$(-5.68, 0]$
$MAPLE(2000)$	$0, .054, .102$	$1.55E-06$	20.18	$(-5.84, 0]$
$Eff. - JHV(2010)$	$0, 1/20, 341/3200$	$2.82E-07$	123.37	$(-5.86, 0]$
Improvement	(2023)	$2.73E-07$	123.75	$(-5.81, 0]$
$New - JHV(2023)$	$0, 1/1000, 1/6$	$3.67E-06$	48.52	$(-4.29, 0]$

What have we learned?

1. An algorithm for deriving methods for N.H. linear C.C. IVPs.
2. That there exist undiscovered parametric families of explicit R–K pairs for general IVPs.
3. Algorithms for deriving these new methods.
4. Better methods have been known for over a decade.

What have we learned?

1. An algorithm for deriving methods for N.H. linear C.C. IVPs.
2. That there exist undiscovered parametric families of explicit R–K pairs for general IVPs.
3. Algorithms for deriving these new methods.
4. Better methods have been known for over a decade.

What else can we study?

1. A more complete proof of order of the new pairs.
2. Why is Rank(α_4) only equal to 5?
3. Explore orthogonality properties of lower and higher order explicit methods.
4. Can these tools be used for deriving General Linear Methods?

What have we learned?

1. An algorithm for deriving methods for N.H. linear C.C. IVPs.
2. That there exist undiscovered parametric families of explicit R–K pairs for general IVPs.
3. Algorithms for deriving these new methods.
4. Better methods have been known for over a decade.

What else can we study?

1. A more complete proof of order of the new pairs.
2. Why is Rank(α_4) only equal to 5?
3. Explore orthogonality properties of lower and higher order explicit methods.
4. Can these tools be used for deriving General Linear Methods?

Thank you for listening

But wait! I wanted to mention one more thing...

This week Paul Muir and Ray Spitiri provided me with a link to an Undergraduate Thesis by David K. Zhang. This thesis may be found at

https://arxiv.org/abs/1911.00318

The thesis discusses the use of Machine Learning that David K. Zhang utilized to obtain approximate coefficients for some (16-10) methods. John has been searching for such methods for over 40 years. For two methods displayed in the Appendices, coefficients are recorded in 70 decimal digit floating point form.

A challenge

I have applied a MAPLE version of the code John and I wrote in 1970 to find that coefficients of the first method displayed satisfies the order conditions to 68 digits.

I have also applied a few of the tools I have described above to show for this first method that β_4 is orthogonal to each of $q^{[4]}$, $q^{[5]}$, $q^{[6]}$, and as well to each of three polynomials of degrees 4,5, and 6 that are analogs of $P_4(C)$ defined above. It might be hoped that such tools may lead to a precise characterization of such methods having exact coefficients.

A challenge

I have applied a MAPLE version of the code John and I wrote in 1970 to find that coefficients of the first method displayed satisfies the order conditions to 68 digits.

I have also applied a few of the tools I have described above to show for this first method that β_4 is orthogonal to each of $q^{[4]}$, $q^{[5]}$, $q^{[6]}$, and as well to each of three polynomials of degrees 4,5, and 6 that are analogs of $P_4(C)$ defined above. It might be hoped that such tools may lead to a precise characterization of such methods having exact coefficients.

Perhaps some of you may wish to do some studies of this. I also hope that I have given John a new perspective on this problem he has studied for so many years.

HAPPY BIRTHDAY JOHN