High order Runge–Kutta methods revisited

John Butcher

ANODE 2023

Dedicated to Dauda Gulibur Yakubu

1. A brief history of Runge–Kutta methods (Contents)

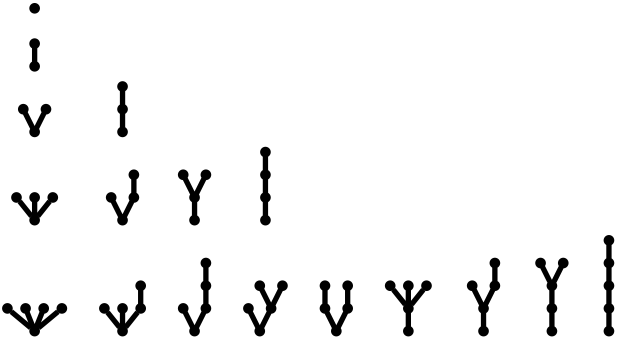
1. A brief history of Runge–Kutta methods
   - Trees and order conditions
   - Euler, Runge, Heun, Kutta, Nyström, Orders 1, 2, 3, 4, 5
   - Order barriers
   - Orders up to 10
2. Methods based on Lobatto quadrature
3. A variant of Lobatto methods
4. Sotware support

Trees and order conditions

The famous trees of Cayley, which were originally drawn upside-down, turn out to be at the centre of the theory of Runge–Kutta methods.

The number of vertices of t is the order |t|

Up to order 5, the trees are



1. A brief history of Runge–Kutta methods

For a Runge–Kutta method

$$\begin{array}{c|c} c & A \\ \hline & b^{\mathsf{T}} \end{array},$$

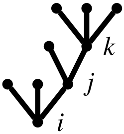
the conditions for order p are

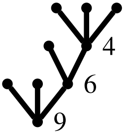
$$\Phi(\mathrm{t}) = (\mathrm{t}!)^{-1}, \qquad |\mathrm{t}| \le p, .$$

where $\Phi(\mathrm{t})$ is the elementary weight and $\mathrm{t}!$ is the factorial.

An example is

$$\sum b_i c_i^2 a_{ij} c_j a_{jk} c_k^3 \quad = \quad \frac{1}{216}$$





Euler, Runge, Heun, Kutta, Nyström, Orders 1, 2, 3, 4, 5

In this brief history, we will confine ourselves to *explicit* methods.

A little table will give us an idea when it is possible to achieve order p with s stages

p	trees	totals	s	$\frac{1}{2}s(s+1)$	authors
1	1	1	1	1	Euler
2	1	2	2	3	Runge
3	2	4	3	6	Heun
4	4	8	4	10	Kutta
			5	15	
5	9	17	6	21	Nyström

What this table doesn't tell us:

- Kutta derived two methods with order 5 but each had trivial errors. Nyström corrected one of these
- Early derivations were for a single first order equation which only required 16 order conditions
- You can guess the achievable order by comparing the number of parameters with the number of constraints.
  But this is not the true reason

Order barriers

When we get to order 6, the following happens

1. There are 37 order conditions for vector-valued problems
2. But only 36 for scalar problems
3. Huťa assumed that 8 stages (36 paremeters) were needed
4. Methods exist with 7 stages (28 parameters)

The actual number of stages required is known up to order 8

The first “order barrier" is $s \geq p + 1$ if $p \geq 5$

The second barrier is $s \geq p + 2$ if $p \geq 7$

The third barrier is $s \geq p + 3$ if $p \geq 8$

The first barrier is easy to prove

For simplicity we will assume $p = 5$

Theorem

No Runge–Kutta method exists with $s = p = 5$

Proof.

We will show that the existence of a method with $s = p = 5$ leads to a contradiction. Evaluate the vector product uv^{T}, and impose order conditions to the result, where

$$u = \begin{bmatrix} b_5 a_{54} a_{43} \\ b_4(c_4 - c_5) a_{43} \\ b_3(c_3 - c_5)(c_3 - c_4) \end{bmatrix}, \quad v^{\mathsf{T}} = \begin{bmatrix} a_{32} c_2 & (c_3 - c_2) c_3 \end{bmatrix},$$

$$uv^{\mathsf{T}} = \begin{bmatrix} \frac{1}{120} & \frac{1}{60} - \frac{1}{24} c_2 \\ \frac{1}{30} - \frac{1}{24} c_5 & \frac{1}{15} - \frac{1}{12} c_5 - (\frac{1}{8} - \frac{1}{6} c_5) c_2 \\ \frac{1}{10} - \frac{1}{8}(c_4 + c_5) + \frac{1}{6} c_4 c_5 & \frac{1}{5} - \frac{1}{4}(c_4 + c_5) + \frac{1}{3} c_4 c_5 - (\frac{1}{4} - \frac{1}{3}(c_4 + c_5) + \frac{1}{2} c_4 c_5) c_2 \end{bmatrix}.$$

Because uv^{T} has rank 1, it is found that either $c_2 = 0$, or $c_4 = c_5 = 1$. If $c_2 = 0$, a method with $s = 4$, $p = 5$ would exist.

Therefore

$$0 = \sum b_i (1 - c_i) a_{ij} a_{jk} c_k = \frac{1}{120}.$$

Orders up to 10

As pointed out above, Huťa derived a method with $s = 8$ satisfying the order 6 conditions for a scalar problem which, fortunately, also satisfies the full order 6 conditions for vector problems.

For $p = 7$, $s = 9$ is necessary and sufficient.

Methods with $p = 8$, $s = 11$ were derived by G. J. Cooper and J. H. Verner. This was first published in Verner's 1969 thesis but hinges on both unpublished work of Cooper as well as on the collaborations between Cooper and Verner.

Methods with $p = 8$, $s = 11$, were also discovered independently by A. R. Curtis.

It has been shown that methods with $p = 8$, $s = 10$ do not exist.

A method with $p = 10$, $s = 17$ was derived by E. Hairer.

2. Methods based on Lobatto quadrature (Contents)

Examples of Lobatto methods

For even order methods, Lobatto quadrature plays an important role.

Here are some examples

$p = 2:\qquad \int_0^1 \phi(x|)dx \approx \frac{1}{2}\phi(0) + \frac{1}{2}\phi(1)$

$$\begin{array}{c|c} 0 & \\ 1 & 1 \\ \hline \frac{1}{2} & \frac{1}{2} \end{array}$$

$p = 4:\qquad \int_0^1 \phi(x)dx \approx \frac{1}{6}\phi(0) + \frac{2}{3}\phi(\frac{1}{2}) + \frac{1}{6}\phi(1)$

$$\begin{array}{c|cccc} 0 & & & & \\ \frac{1}{2} & \frac{1}{2} & & & \\ \frac{1}{2} & \frac{1}{4} & \frac{1}{4} & & \\ 1 & 0 & -1 & 2 & \\ \hline & \frac{1}{6} & 0 & \frac{2}{3} & \frac{1}{6} \end{array}$$

$p = 6:\qquad \int_0^1 \phi(x)dx \approx \frac{1}{12}\phi(0) + \frac{5}{12}\phi(\frac{1}{2} - \frac{1}{10}\sqrt{5}) + \frac{5}{12}\phi(\frac{1}{2} + \frac{1}{10}\sqrt{5}) + \frac{1}{12}\phi(1)$

See next page

$$
\begin{array}{c|ccccccc}
0 & & & & & & & \\
\frac{5+\sqrt{5}}{10} & \frac{5+\sqrt{5}}{10} & & & & & & \\
\frac{5+\sqrt{5}}{10} & \frac{5+\sqrt{5}}{20} & \frac{5+\sqrt{5}}{20} & & & & & \\
\frac{5-\sqrt{5}}{10} & \frac{\sqrt{5}}{10} & \frac{-2+\sqrt{5}}{2} & \frac{15-7\sqrt{5}}{10} & & & & \\
\frac{5-\sqrt{5}}{10} & \frac{5+\sqrt{5}}{60} & 0 & \frac{15-7\sqrt{5}}{60} & \frac{1}{6} & & & \\
\frac{5+\sqrt{5}}{10} & \frac{5-\sqrt{5}}{60} & 0 & \frac{1}{6} & \frac{-27-11\sqrt{5}}{60} & \frac{7+3\sqrt{5}}{10} & & \\
1 & \frac{1}{6} & 0 & \frac{-25+7\sqrt{5}}{12} & \frac{17+11\sqrt{5}}{12} & -1-\sqrt{5} & \frac{5-\sqrt{5}}{2} & \\
\hline
 & \frac{1}{12} & 0 & 0 & 0 & \frac{5}{12} & \frac{5}{12} & \frac{1}{12}
\end{array}
$$

To illustrate the pattern, which also works for the $p = 8$, $s = 11$ methods of Cooper and Verner, we can highlight the most significant elements in this tableau

2. Methods based on Lobatto quadrature (continued)

$$
\begin{array}{c|c|ccccccc}
 & 0 & & & & & & & \\
1 & \frac{5+\sqrt{5}}{10} & \frac{5+\sqrt{5}}{10} & & & & & & \\
 & \frac{5+\sqrt{5}}{10} & \frac{5+\sqrt{5}}{20} & \frac{5+\sqrt{5}}{20} & & & & & \\
2 & \frac{5-\sqrt{5}}{10} & \frac{\sqrt{5}}{10} & \frac{-2+\sqrt{5}}{2} & \frac{15-7\sqrt{5}}{10} & & & & \\
 & \frac{5-\sqrt{5}}{10} & \frac{5+\sqrt{5}}{60} & 0 & \frac{15-7\sqrt{5}}{60} & \frac{1}{6} & & & \\
3 & \frac{5+\sqrt{5}}{10} & \frac{5-\sqrt{5}}{60} & 0 & \frac{1}{6} & \frac{-27-11\sqrt{5}}{60} & \frac{7+3\sqrt{5}}{10} & & \\
 & 1 & \frac{1}{6} & 0 & \frac{-25+7\sqrt{5}}{12} & \frac{17+11\sqrt{5}}{12} & -1-\sqrt{5} & \frac{5-\sqrt{5}}{2} & \\
\hline
 & & \frac{1}{12} & 0 & 0 & 0 & \frac{5}{12} & \frac{5}{12} & \frac{1}{12}
\end{array}
$$

Structure and notation

The tableau for a block Lobatto method, with the blocks shown on the left, is

$$
\begin{array}{c@{\qquad}c|cccccc}
B_0 & \mathbf{0} & & & & & & \\
B_1 & \mathbf{c}_1 & \mathbf{c}_1 & & & & & \\
B_2 & \mathbf{c}_2 & \mathbf{o}_2 & \mathbf{a}_2 & \mathbf{d}_2 & & & \\
B_3 & \mathbf{c}_3 & \mathbf{o}_3 & & \mathbf{a}_3 & \mathbf{d}_3 & & \\
B_4 & \mathbf{c}_4 & \mathbf{o}_4 & & & \mathbf{a}_4 & \mathbf{d}_4 & \\
\vdots & \vdots & \vdots & & & & \ddots & \ddots \\
B_n & \mathbf{c}_n & \mathbf{o}_n & & & & & \mathbf{a}_n \quad \mathbf{d}_n \\
\hline
 & & \mathbf{b}_0 & & & & & \mathbf{b}
\end{array}
$$

$$
\begin{aligned}
\mathbf{b} &: 1 \times n, & & \\
\mathbf{c}_m &: m \times 1, & m &= 1, 2, \ldots, n, \\
\mathbf{a}_m &: m \times (m-1), & m &= 2, 3, \ldots, n, \\
\mathbf{d}_m &: m \times m, & m &= 2, 3, \ldots, n, \\
s &= 1 + \tfrac{1}{2} n(n+1). & &
\end{aligned}
$$

The stages in block B_m have stage order m, $(m = 2, 3, \ldots, n)$.

Achieving block order

Define the "quadrature matrix" $\mathbf{q}_m$ $(m \times (m-1))$ so that

$$\mathbf{q}_m \mathbf{c}_{m-1}^{i-1} = \tfrac{1}{i}\mathbf{c}_m^i, \quad i = 1, 2, \ldots m$$

Define the "interpolation matrix" $\mathbf{p}_m$ $(m \times (m-1))$ so that

$$\mathbf{p}_m \mathbf{c}_{m-1}^{i-1} = \mathbf{c}_{m-1}^i, \quad i = 1, 2, \ldots m$$

with the final row zero.

Theorem

The stages in block B_m have stage order m, $(m = 2, 3, \ldots, n)$ iff

$$\mathbf{a}_m = \mathbf{q}_m - \mathbf{d}_m \mathbf{p}_m.$$

2. Methods based on Lobatto quadrature (continued)

Trees and order conditions

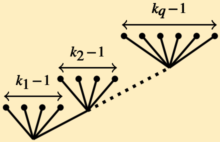
Recall the standard conditions for order p

$$\Phi(\mathrm{t}) = \frac{1}{\mathrm{t}!}, \qquad |\mathrm{t}| \leq p. \tag{*}$$

Theorem

If the block stage order conditions are satisfied then (*) *needs to hold only for trees of the form*

$$t = [k_1, k_2, \ldots, k_q] :=$$



These conditions reduce to equations in $\mathbf{d}_2, \ldots, \mathbf{d}_n$.

Denote $\mathbf{C}_m = \operatorname{diag} \mathbf{c}_m$, then $\Phi(\mathrm{t})$ can be evaluated recursively by

$$\Phi(\mathrm{t}) = \mathbf{b}\mathbf{C}_n^{k_1-1}\boldsymbol{\phi}_{n,2}, \tag{1}$$

$$\begin{aligned}\boldsymbol{\phi}_{m,i} &= \mathbf{a}_m\mathbf{C}_{m-1}^{k_i-1}\boldsymbol{\phi}_{m-1,i+1} + \mathbf{d}_m\mathbf{C}_m^{k_i-1}\boldsymbol{\phi}_{m,i+1} \\ &= \mathbf{q}_m\mathbf{C}_{m-1}^{k_i-1}\boldsymbol{\phi}_{m-1,i+1} - \mathbf{d}_m\mathbf{p}_m\mathbf{C}_{m-1}^{k_i-1}\boldsymbol{\phi}_{m-1,i+1} + \mathbf{d}_m\mathbf{C}_m^{k_i-1}\boldsymbol{\phi}_{m,i+1},\end{aligned} \tag{2}$$

$$\begin{aligned}\boldsymbol{\phi}_{m,q} &= \mathbf{a}_m\mathbf{c}_{m-1}^{k_q-1} + \mathbf{d}_m\mathbf{c}_m^{k_q-1} \\ &= \mathbf{q}_m\mathbf{c}_{m-1}^{k_q-1} - \mathbf{d}_m\mathbf{p}_m\mathbf{c}_{m-1}^{k_q-1} + \mathbf{d}_m\mathbf{c}_m^{k_q-1}.\end{aligned} \tag{3}$$

with

$$\mathrm{t}! = k_q(k_q + k_{q-1})\cdots(k_q + k_{q-1} + \cdots + k_1).$$

For methods in which $\mathbf{c}_{m-1}$ is a permutation of the first $m-1$ elements of $\mathbf{c}_m$, the interpolation is exact and (3) reduces to

$$\boldsymbol{\phi}_{m,q} = \mathbf{q}_m\mathbf{c}_{m-1}^{k_q-1}.$$

Wider choice of $\mathbf{c}_2$

It is possible, at least for $n = 3$, to choose the components of $\mathbf{c}_2$ other than from the first 2 components of c_3. For example,

$$
\begin{array}{c|ccccccc}
0 & & & & & & & \\
\frac{1}{3} & \frac{1}{3} & & & & & & \\
\frac{1}{3} & \frac{1}{6} & \frac{1}{6} & & & & & \\
1 & -\frac{1}{2} & -\frac{9}{2} & 6 & & & & \\
\frac{5-\sqrt{5}}{10} & \frac{5+\sqrt{5}}{50} & 0 & \frac{75-21\sqrt{5}}{200} & \frac{5-3\sqrt{5}}{200} & & & \\
\frac{5+\sqrt{5}}{10} & \frac{5-\sqrt{5}}{50} & 0 & \frac{75+21\sqrt{5}}{200} & \frac{5+3\sqrt{5}}{200} & 0 & & \\
1 & 0 & 0 & -\frac{15}{4} & -\frac{1}{4} & \frac{5+\sqrt{5}}{2} & \frac{5-\sqrt{5}}{2} & \\
\hline
 & \frac{1}{12} & 0 & 0 & 0 & \frac{5}{12} & \frac{5}{12} & \frac{1}{12}
\end{array}
$$

A detailed analysis yields the condition on $\mathbf{c}_2$ to obtain order 6:

$$
(\mathbf{c}_2)_2 = \frac{(\mathbf{c}_2)_1}{15(\mathbf{c}_2)_1^2 - 10(\mathbf{c}_2)_1 + 2}.
$$

4. Sotware support (Contents)

A 1970 program

On 1 January 1970, the same day as the UNIX era began, Jim Verner and I wrote a code for testing the order of a Runge–Kutta method.

We developed the algorithm in Algol and Jim wrote the working version in APL.

In 2022, Jim translated the program from APL into Maple.

An account of this work can be found in “Our first B-series program", by John Butcher and Jim Verner, https://jcbutcher.com/1970

A 2021 program

An algorithm from “B-series: Algebraic Analysis of Numerical Methods, Springer 2021" has been implemented as test21. This has a similar function to test70.

Derivation and testing of Lobatto methods

Using a Maple program based on test21, specifically targeted to the analysis and derivation of Lobatto methods, a new derivation of the pioneering methods of Cooper and Verner has been found.

As an illustration of how this works, look at the derivation of an order 6 method. This is followed by a sample order 8 derivation

Command	Output
prep(12, 21, 1);	
test(2);	1: [2, 4] 0
test(3);	1: [2, 1, 3] 1
sol(3);	"solution found"
fix(3);	∅
test(4);	1: [2, 1, 1, 2] 1
sol(2);	"solution found"
fix(2);	∅
test(5);	no trees

4. Sotware support (continued)

Command	Output
prep(123, 321, 21, 1);	
test(2);	1: [2, 6] 0
	2: [2, 5] 0
	3: [3, 5] 0
test(3);	1: [2, 1, 5] 1
	2: [2, 2, 4] 1
	3: [2, 1, 4] 1
	4: [3, 1, 4] 1
sol(4);	"solution found"
fix(4);	$\emptyset$
test(4);	1: [2, 1, 1, 4] 1
	2: [2, 1, 2, 3] 1
	3: [2, 2, 1, 3] 1
	4: [2, 1, 1, 3] 1
	5: [3, 1, 1, 3] 1
sol(3);	"solution found"
fix(3);	$\emptyset$
test(5);	1: [2, 1, 1, 1, 3] 0
	2: [2, 1, 1, 2, 2] 0
	3: [2, 1, 2, 1, 2] 0
	4: [2, 2, 1, 1, 2] 1
	5: [2, 1, 1, 1, 2] 0
	6: [3, 1, 1, 1, 2] 1
sol(2);	"solution found"
fix(2);	$\emptyset$
test(6);	1: [2, 1, 1, 1, 1, 2] 0
test(7);	no trees

Tree of the day

According to Wagner, Tanhäuser was given a sign that his sins were forgiven when his walking staff sprouted leaves and flowers.

In the 1940s, something similar happened to a fence post standing in Lake Wānaka.

The Wānaka Willow is now the most photographed tree in New Zealand.