High order Runge–Kutta methods

Theory, History, Recent Results

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Abstract

For a given initial value problem $y'(x) = f(x, y)$, $y(x_0) = y_0$, an s-stage Runge–Kutta method computes the approximate solution after a step of length h by the equations

$$X_i = x_0 + hc_i, Y_i = y_0 + h\sum_{j=1}^{i-1} a_{ij}F_j, F_i = f(X_i, Y_i),$$

$$y_1 = y_0 + h\sum_{j=1}^{s} b_jF_j.$$

It is usual to specify a particular methods by its tableau, shown here for the famous Kutta method

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

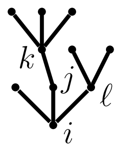
Runge–Kutta methods were invented 130 years ago and have had a steady development as higher and higher orders have been discovered. In the table on the right, the authors are shown for the first contribution, or for a significant contribution, to the discovery of a Runge–Kutta method with order p. Also N_p is the number of conditions for order p and V_s is the number of free parameters in an s-stage method.

p	N_p	s	V_s	Authors	
2	2	2	3	Runge[a]	
3	4	3	6	Heun[b]	
4	8	4	10	Kutta[c]	
5	17	6	21	Kutta,	Nyström[d]
6	37	7	28	Hut'a[e] ($s = 8$),	Butcher[f] ($s = 7$)
7	85	9	45	Butcher[g]	
8	200	11	66	Verner[h], Curtis[i],	Cooper and Verner[j]
9	486	15	120	Verner[k]	
10	1205	16	136	Hairer[l],	Zhang[m]

[a]Runge, C.: Über die numerische Auflösung von Differentialgleichungen. Math. Ann. **46**, 167–178 (1895)
[b]Heun, K., Neue Methode zur approximativen Integration der Differentialgleichungen einer unabhängigen Veränderlichen. Z. Math. Phys. **45**, 23–38 (1900)
[c]Kutta, W.: Beitrag zur näherungsweisen Integration totaler Differentialgleichungen. Z. Math. Phys. **46**, 435–453 (1901)
[d]Nyström, E.J.: Über die numerische Integration von Differentialgleichungen. Acta Soc. Sci. Fennicae **50** (13), 1–55 (1925)
[e]Hut'a, A., Une amélioration de la méthode de Runge–Kutta-Nyström pour la résolution numérique des équations différentielles du premier ordre. Acta Fac. Nat. Univ. Comenian. Math. **1**, 201–224 (1956)
[f]Butcher, J.C.: On Runge–Kutta processes of high order, J. Aust. Math. Soc. **4**, 179-194 (1964)
[g]Butcher, J.C.: Numerical Methods for Ordinary Differential Equations (Third Edition), Wiley (2016)
[h]Verner, J.H.: Numerical Solution of Differential Equations. Ph.D. thesis, Univ. of Edinburgh, (1969)
[i]Curtis, A.R., An eighth order Runge–Kutta method with eleven function evaluations. Numer. Math. 16, 268–277 (1970)
[j]Cooper, G.J. and Verner J.H., Some explicit Runge–Kutta methods of high order. SIAM J. Numer. Anal. 9, 389–405 (1972)
[k]Verner, J.H.: The derivation of high order Runge–Kutta methods. Univ. Auckland Dept. Math. Report Series **93**, 27 pages (1976)
[l]Hairer, E.: A Runge–Kutta method of order 10. J. Inst. Math. Appl. 21, 47–59 (1978)
[m]Zhang, D.K. An explicit 16-stage RungeKutta method of order 10 discovered by numerical search. Numer Algor (2024)

T will denote the set of trees. The use of trees, such as , . . . , is an essential component in the analysis of Runge–Kutta methods. In particular, order of accuracy p, is satisfied if $\Phi(t) = 1/t!$ for $|t| \le p$, where $\Phi(t)$ is the "elementary weight" and $t!$ is the factorial of t.

For the following example tree, attach labels i, j, k, ℓ to certain vertices.



For this specific tree,

$$\Phi(t) = \sum b_i c_i a_{ij} a_{jk} c_k^3 a_{i\ell} c_\ell^2 \text{ and}$$

$$t! = 4 \cdot 5 \cdot 3 \cdot 10 = 600$$

The purpose behind deriving method of increasingly high order is to reduce the local truncation error, given by $\|y(x_1) - y_1\| = O(h^{p+1})$ which in turn reduces the global truncation error given by $\|y(x_n) - y_n\| = O(h^p)$.

The history summarised in the table above contains some interesting details and surprises. For example, a crucial step in Kuta's derivation of 4th order methods is to show that $c_4 = 1$ is a consequence of the order conditions. Kutta was the first to find 5th order methods but his published paper contained typesetting errors which were not corrected for more than 30 years.

The 6th order method derived by Hut'a was for the scalar problem $y' = f(x, y)$ for which there are only 31 order conditions instead of 37 in the general vector-based theory. But, surprisingly, the missing 6 equations are also satisfied . Furthermore, this can be done with 7 instead of 8 stages.

Even in the last few years there has been a new surprise: The 10th order method of Hairer with 17 stages held the world record for 50 years, but has now been surpassed by the 16 stage method of Zhang.

B-series make it possible to write down Taylor series in a systematic way.

For example, given the initial value problem $y'(x) = f(y(x)), y(x_0) = y_0$, we want to know the Taylor series for the flow $y(x_0 + h)$ and, for camparison, we want to know the Taylor series for y_1 as computed by a specific Runge–Kutta method.

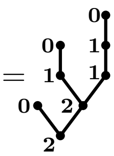
For a tree t, the "elementary differentials" evaluated at y_0 are defined recursively by

$$F(\tau)y_0 = fy_0,$$
$$F([t_1 t_2 \cdots t_n])y_0 = f^{(n)}F(t_1)F(t_2)\cdots F(t_n)y_0.$$

To illustrate this concept, the trees to order 4, with shorthand numbers shown are given below, with an 8th order example also shown

$F(\,.\,) = f$	0
$F($$) = f'f$	10
$F($$) = f''ff$	200
$F($$) = f'f'f$	110
$F($$) = f^{(3)}fff$	3000
$F($$) = f''ff'f$	2010
$F($$) = f'f''ff$	1200
$F($$) = f'f'f'f$	1110

Order 8 example

$t =$ 

$F(t) = f''ff''f'ff'f'f$

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Let a be a function $T \cup \{\varnothing\} \to \mathbb{R}$.

The B-series $B_h(a)$ is defined by

$$B_h(a)(y_0) = a(\varnothing)y_0 + \sum_{t\in T} \frac{h^{|t|}}{\sigma(t)} a(t)F(t)y_0.$$

Here are three examples:

(1) The Taylor series for the flow $a(\varnothing) = 1, a(t) = 1/t!$.
(2) The Taylor series for a Runge–Kutta approximation $a(\varnothing) = 1, a(t) = \Phi(t)$.
(3) The truncation error for a Runge–Kutta approximation $a(\varnothing) = 0, a(t) = 1/t! - \Phi(t)$.

B-series manipulations can be carried out in the Hopf Algebra of rooted trees which is not included in this abstract or the lecture.

However, in joint work with Helmut Podhaisky, it has been realised that symbolic manipulation can be avoided by using a function f which can be treated as though it were a differential equation problem .

The technique hinges on the fact that if

$$B_h(b)y_0 = hf(B_h(a)y_0),$$

then

$$b(\varnothing) = 0, b(t * t') = b(t)a(t').$$

Based on this observation, a code has been written to define a procedure f which can be used in simplified B-series experiments.

For a given Runge–Kutta method it is possible to evaluate the stages, the stage derivatives and output value. We are able to compute, not numerical values, but what is effectively a truncated B-series.

The experiment is applied to the classical method of Kutta:

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

The results will be displayed during the lecture.