International Conference on Advances in Differential Equations and Numerical Analysis (ADENA2020)
Indian Institute of Technology Guwahati, October 12 - 14, 2020

Runge–Kutta methods and B-series

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ABSTRACT

In 1895 an important discovery was made [1]. It became possible to obtain second order Runge–Kutta methods. A few years later Heun [2] and Kutta [3] raised the order to 3 and 4 and eventually to 5 [4] and 6 [5].

A Runge–Kutta method for a *scalar* initial value problem

$$y'(x) = f(x, y(x)), \quad y(x_0) = y_0, \tag{1}$$

computes $y_1 \approx y(x_0 + h)$ by first computing $Y_i \approx y(x_0 + hc_i)$, $i = 1, 2, \ldots, s$, These, and y_1 itself are found in turn from the formulae

$$Y_i = y_0 + h \sum_{j<i} a_{ij} f(x_0 + hc_j, Y_j), \quad i = 1, 2, \ldots, s,$$
$$y_1 = y_0 + h \sum_{i=1}^{s} b_i f(x_0 + hc_i, Y_i)$$

The parameters in these formulae are chosen to get a good approximation. For convenience, they are often arranged in a tableau as follows

$$\begin{array}{c|c} c & A \\ \hline & b^{\mathrm{T}} \end{array} = \begin{array}{c|ccccc} 0 & & & & & \\ c_2 & a_{21} & & & & \\ c_3 & a_{31} & a_{32} & & & \\ \vdots & \vdots & \vdots & \ddots & & \\ c_s & a_{s1} & a_{s2} & \cdots & a_{s,s-1} & \\ \hline & b_1 & b_2 & \cdots & b_{s-1} & b_s \end{array}$$

The number of stages is s and the number of free parameters is $S := \frac{1}{2}s(s+1)$. The aim of Runge, and the people who followed him, was to make the order p of the method as high as possible because this gives greater efficiency if a high accuracy is required.

Two famous examples are

$$\begin{array}{c|cc} 0 & & \\ 1 & 1 & \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array} \qquad \text{(Runge, } s = p = 2\text{)}$$

$$\begin{array}{c|cccc} 0 & & & & \\ \frac{1}{2} & \frac{1}{2} & & & \\ \frac{1}{2} & 0 & \frac{1}{2} & & \\ \hline & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} \end{array} \qquad \text{(Kutta, } s = p = 4\text{)}$$

The number of conditions for order p will be written as $Q(p)$. We have ben following the lead of Runge and the other the pioneers, and considering a single scalar problem. However, for a *vector-valued* problem of arbitrary dimension, there can be more than $Q(p)$ conditions for order p. Denote the number of conditions in the vector case by $P(p)$.

Some of this information is shown in Table 1.

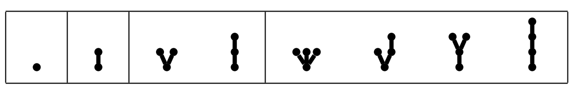
Table 1: Order information for a Runge–Kutta method

s	1	2	3	4	5	6	7	8
$S(s)$	1	3	6	10	15	21	28	36
p	1	2	3	4	5	6	7	8
$Q(p)$	1	2	4	8	16	31	?	?
$P(p)$	1	2	4	8	17	37	85	200

It was once assumed that if $S(s) < Q(p)$ then it is not possible to obtain an order p method with just s stages. But this is not true.

The value of $P(p)$ is now known to be equal to the number of rooted trees with up to p vertices. To illustrate what trees look like, the 8 trees up to order 4 are shown in Table 2

Table 2: Rooted trees to order 4



The analysis of order is a very simple idea: simply compare the Taylor series for the solution to the initial value problem in powers of h tand the Taylor series for he numerical approximation also in powers of h. If the series are identical to within $O(h^{p+1})$ then the order is p.

The theory of B-series provides the missing details. The key fact is that each of the series we need to compare, can be written in terms which exactly correspond to trees.

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