Runge–Kutta methods for ordinary differential equations

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- Taylor expansion of exact solution
- Taylor expansion for numerical approximation

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Introduction to Runge–Kutta methods

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The simple Euler method:

$$y_n = y_{n-1} + hf(y_{n-1}), \quad h = x_n - x_{n-1}$$

can be made more accurate by using the mid-point quadrature formula:

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The simple Euler method:

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can be made more accurate by using either the mid-point or the trapezoidal rule quadrature formula:

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In the early days of Runge–Kutta methods the aim seemed to be to find explicit methods of higher and higher order.

Later the aim shifted to finding methods that seemed to be optimal in terms of local truncation error and to finding built-in error estimators.

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A-stable methods exist in these classes.

Because of the high cost of these methods, attention moved to diagonally and singly implicit methods.

Formulation of method

In carrying out a step we evaluate s stage values

$$Y_1, \quad Y_2, \quad \dots, \quad Y_s$$

and s stage derivatives

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and the approximation at $x_1 = x_0 + h$ is found from

$$y_1 = y_0 + h \sum_{i=1}^{s} b_i F_i$$

We represent the method by a tableau:

$$
\begin{array}{c|cccc}
c_1 & a_{11} & a_{12} & \cdots & a_{1s} \\
c_2 & a_{21} & a_{22} & \cdots & a_{2s} \\
\vdots & \vdots & \vdots & & \vdots \\
c_s & a_{s1} & a_{s2} & \cdots & a_{ss} \\
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or, if the method is explicit, by the simplified tableau

$$
\begin{array}{c|ccccc}
0 & & & & & \\
c_2 & a_{21} & & & & \\
\vdots & \vdots & \vdots & \ddots & & \\
c_s & a_{s1} & a_{s2} & \cdots & a_{s,s-1} & \\
\hline
 & b_1 & b_2 & \cdots & b_{s-1} & b_s
\end{array}
$$

Examples:

$$y_1 = y_0 + \mathbf{0} hf(y_0) + \mathbf{1} hf\left(y_0 + \mathbf{\tfrac{1}{2}} hf(y_0)\right)$$

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

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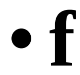
This will become increasingly complicated as we evaluate higher derivatives.

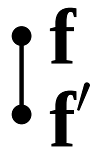
Hence we look for a systematic pattern.

Write $\mathbf{f} = f(y(x))$, $\mathbf{f}' = f'(y(x))$, $\mathbf{f}'' = f''(y(x))$, ...

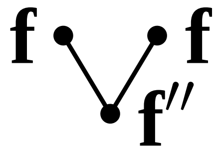
$$y'(x) = \mathbf{f}$$



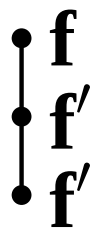
$$y''(x) = \mathbf{f}'\mathbf{f}$$



$$y'''(x) = \mathbf{f}''(\mathbf{f},\mathbf{f})$$



$$+\,\mathbf{f}'\mathbf{f}'\mathbf{f}$$



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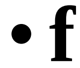

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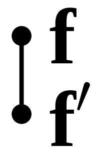

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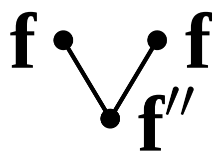
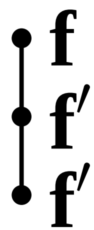


$$+ \mathbf{f}'\mathbf{f}'\mathbf{f}$$



The various terms have a structure related to rooted-trees.

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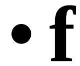

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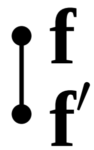

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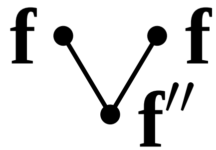

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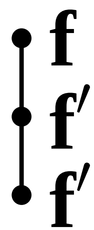
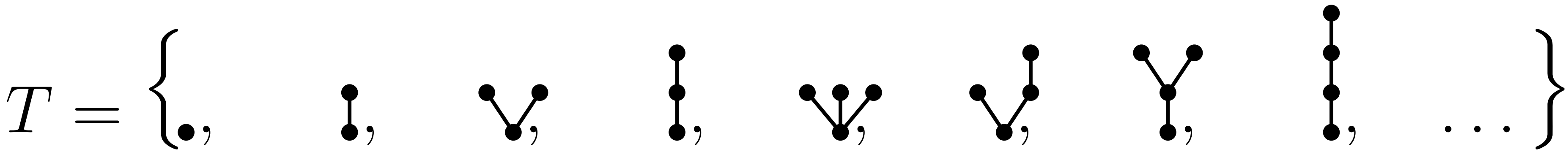


The various terms have a structure related to rooted-trees.

Hence, we introduce the set of all rooted trees and some functions on this set.

Let T denote the set of rooted trees:



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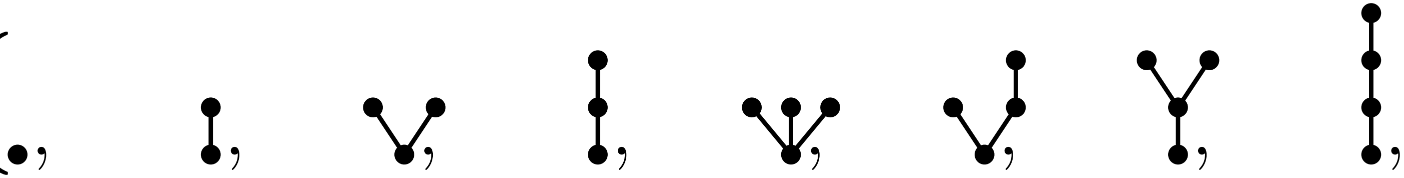
$T = \Big\{$  $\ldots \Big\}$

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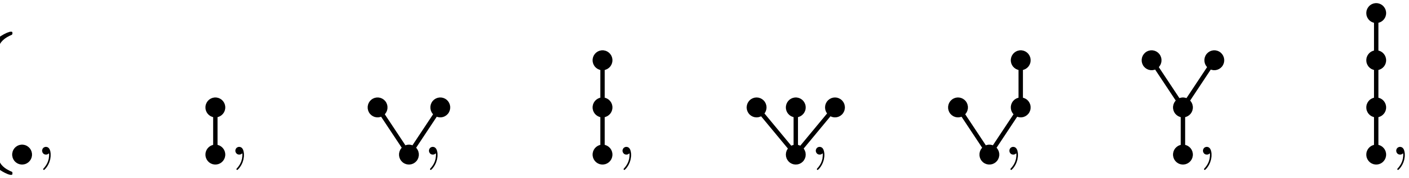
$T = \Bigg\{$  $\ldots \Bigg\}$

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In this table, t will denote a typical tree

$r(t)$	order of t = number of vertices

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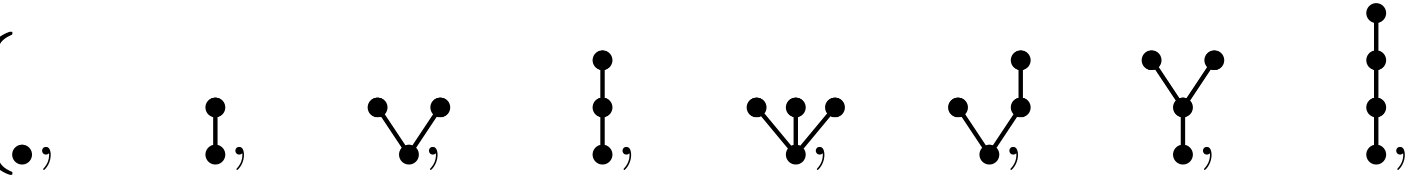
$$T = \Big\{$$  $$\ldots \Big\}$$

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$r(t)$	order of t = number of vertices
$\sigma(t)$	symmetry of t = order of automorphism group

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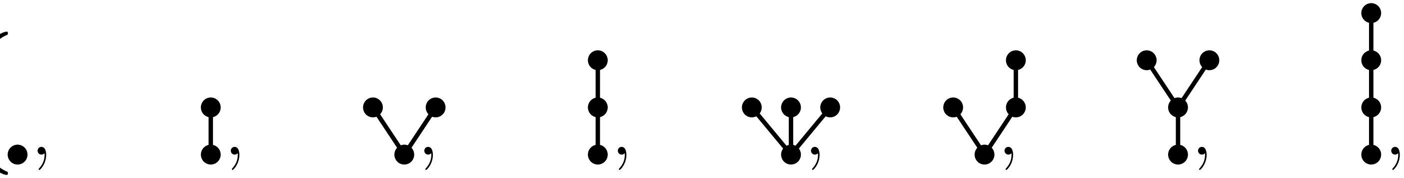
$T = \Big\{$  $\ldots \Big\}$

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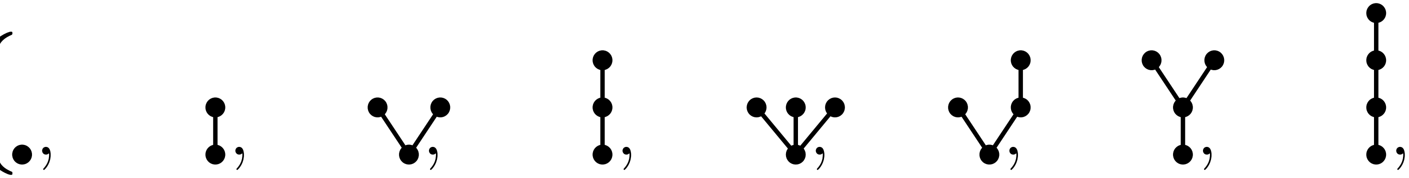
$T = \Big\{$  $\ldots \Big\}$

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$\alpha(t)$	number of ways of labelling with an ordered set

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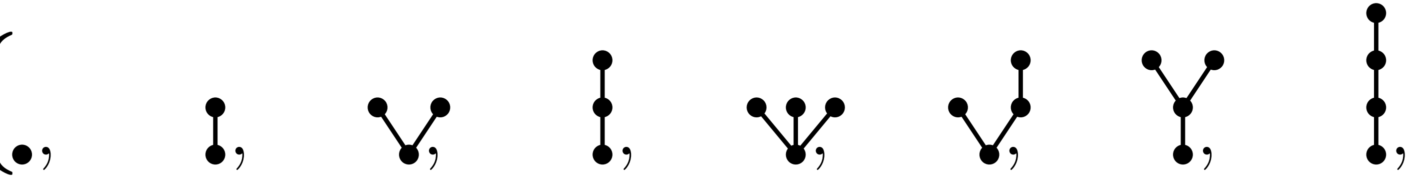
$T = \{$  $\ldots \}$

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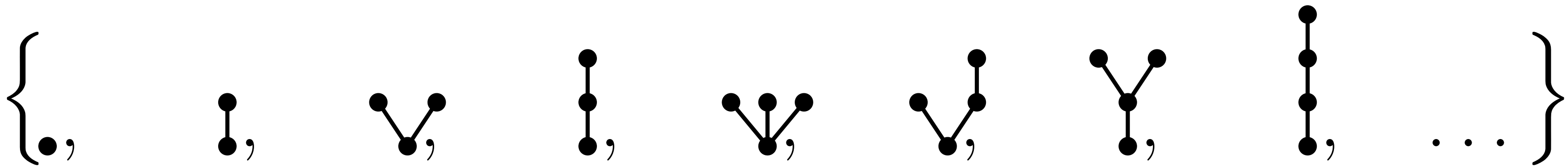
$T =$ 

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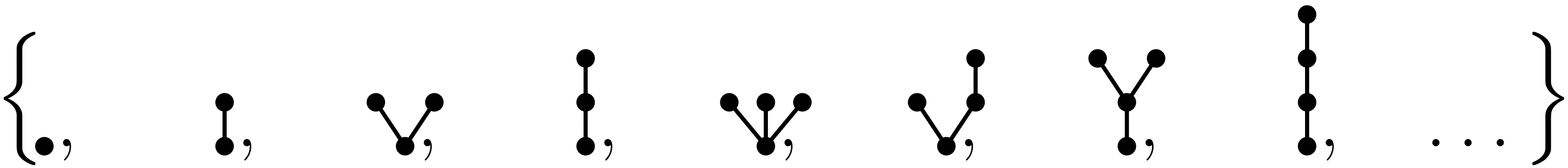
$T =$ 

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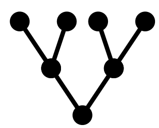
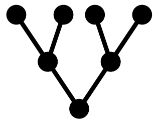
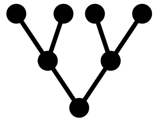
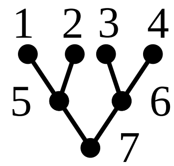
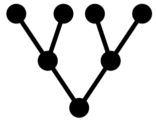
We will give examples of these functions based on $t =$ 

$t =$ 

$t =$ 

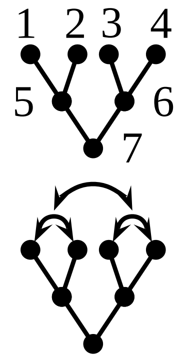
$r(t) = 7$

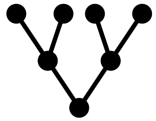


$$t =$$ 

$$r(t) = 7$$

$$\sigma(t) = 8$$



$t =$ 

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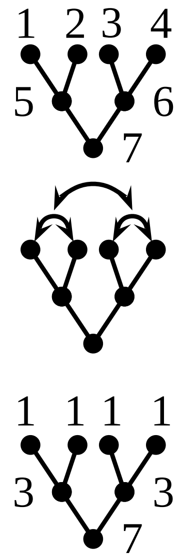
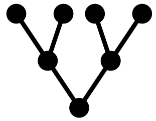
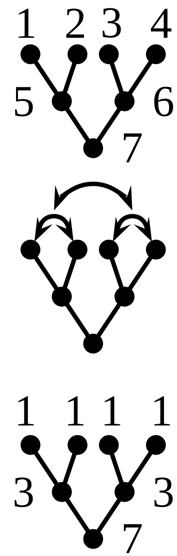


$t =$ 



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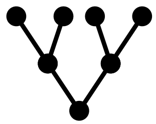
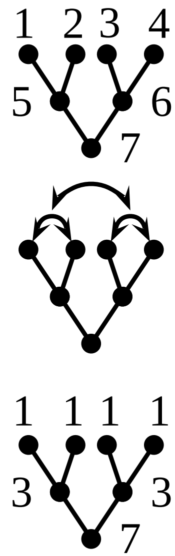
$$\alpha(t) = \frac{r(t)!}{\sigma(t)\gamma(t)} = 10$$

$$t = $$ 



$$r(t) = 7$$

$$\sigma(t) = 8$$

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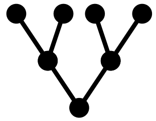
$$\alpha(t) = \frac{r(t)!}{\sigma(t)\gamma(t)} = 10$$

$$\beta(t) = \frac{r(t)!}{\sigma(t)} = 630$$

$$t =$$



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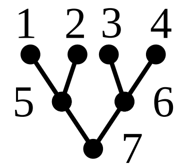

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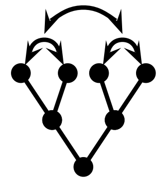

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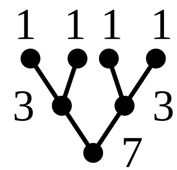

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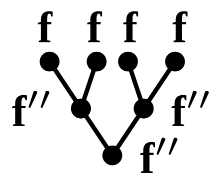
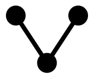
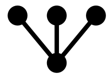
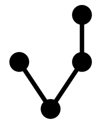
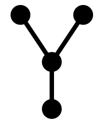
$$F(t) = \mathbf{f}''\big(\mathbf{f}''(\mathbf{f},\mathbf{f}),\mathbf{f}''(\mathbf{f},\mathbf{f})\big)$$



These functions are easy to compute up to order 4 trees:

t								
$r(t)$	1	2	3	3	4	4	4	4
$\sigma(t)$	1	1	2	1	6	1	2	1
$\gamma(t)$	1	2	3	6	4	8	12	24
$\alpha(t)$	1	1	1	1	1	3	1	1
$\beta(t)$	1	2	3	6	4	24	12	24
$F(t)$	$\mathbf{f}$	$\mathbf{f}'\mathbf{f}$	$\mathbf{f}''(\mathbf{f},\mathbf{f})$	$\mathbf{f}'\mathbf{f}'\mathbf{f}$	$\mathbf{f}^{(3)}(\mathbf{f},\mathbf{f},\mathbf{f})$	$\mathbf{f}''(\mathbf{f},\mathbf{f}'\mathbf{f})$	$\mathbf{f}'\mathbf{f}''(\mathbf{f},\mathbf{f})$	$\mathbf{f}'\mathbf{f}'\mathbf{f}'\mathbf{f}$

The formal Taylor expansion of the solution at $x_0 + h$ is

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By comparing these formulae term by term, we will obtain conditions for a specific order of accuracy.

Taylor expansion for numerical approximation

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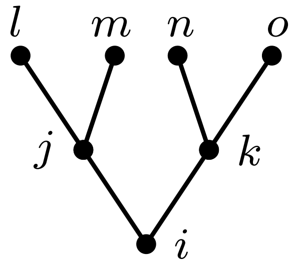
$t =$ 

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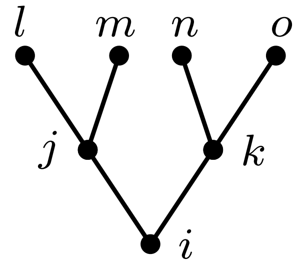
$t =$ 

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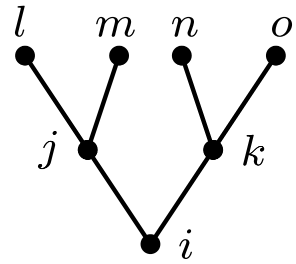
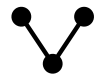
$t =$ 

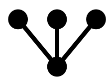
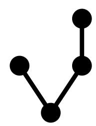
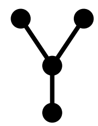
$$\Phi(t) = \sum_{i,j,k,l,m,n,o=1}^{s} b_i a_{ij} a_{ik} a_{jl} a_{jm} a_{kn} a_{ko}$$

Simplify by summing over l, m, n, o:

$$\Phi(t) = \sum_{i,j,k=1}^{s} b_i a_{ij} c_j^2 a_{ik} c_k^2$$

Now add $\Phi(t)$ to the table of functions:

t				
$r(t)$	1	2	3	3
$\alpha(t)$	1	1	1	1
$\beta(t)$	1	2	3	6
$\Phi(t)$	$\sum b_i$	$\sum b_i c_i$	$\sum b_i c_i^2$	$\sum b_i a_{ij} c_j$

t				
$r(t)$	4	4	4	4
$\alpha(t)$	1	3	1	1
$\beta(t)$	4	24	12	24
$\Phi(t)$	$\sum b_i c_i^3$	$\sum b_i c_i a_{ij} c_j$	$\sum b_i a_{ij} c_j^2$	$\sum b_i a_{ij} a_{jk} c_k$

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$$y_1 = y_0 + \sum_{t \in T} \frac{h^{r(t)}}{\sigma(t)} \Phi(t) F(t)(y_0)$$

Order conditions

To match the Taylor series

$$y(x_0 + h) = y_0 + \sum_{t \in T} \frac{h^{r(t)}}{\sigma(t)\gamma(t)} F(t)(y_0)$$

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Order 2:

$$\begin{aligned} b_1 + b_2 &= 1 \\ b_2 c_2 &= \tfrac{1}{2} \end{aligned}$$

$$\begin{array}{c|cc} 0 & & \\ c_2 & c_2 & \\ \hline & 1 - \frac{1}{2c_2} & \frac{1}{2c_2} \end{array} \qquad \begin{array}{c|cc} 0 & & \\ \frac{1}{2} & \frac{1}{2} & \\ \hline & 0 & 1 \end{array} \qquad \begin{array}{c|cc} 0 & & \\ 1 & 1 & \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

Order 3:

$$\begin{aligned} b_1 + b_2 + b_3 &= 1 \\ b_2 c_2 + b_3 c_3 &= \tfrac{1}{2} \\ b_2 c_2^2 + b_3 c_3^2 &= \tfrac{1}{3} \\ b_3 a_{32} c_2 &= \tfrac{1}{6} \end{aligned}$$

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$$\begin{array}{c|ccc} 0 & & & \\ \frac{1}{2} & \frac{1}{2} & & \\ 1 & -1 & 2 & \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array} \qquad \begin{array}{c|ccc} 0 & & & \\ \frac{2}{3} & \frac{2}{3} & & \\ \frac{2}{3} & 0 & \frac{2}{3} & \\ \hline & \frac{1}{4} & \frac{3}{8} & \frac{3}{8} \end{array} \qquad \begin{array}{c|ccc} 0 & & & \\ \frac{2}{3} & \frac{2}{3} & & \\ 0 & -1 & 1 & \\ \hline & 0 & \frac{3}{4} & \frac{1}{4} \end{array}$$

Order 4:

$$b_1 + b_2 + b_3 + b_4 = 1 \tag{1}$$

$$b_2c_2 + b_3c_3 + b_4c_4 = \frac{1}{2} \tag{2}$$

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To solve these equations, treat c_2, c_3, c_4 as parameters, and solve for b_1, b_2, b_3, b_4 from (1), (2), (3), (5).

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Result: $c_4 = 1$.

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Lemma 1 *Let U and V be 3×3 matrices such that*

$$UV = \begin{bmatrix} w_{11} & w_{12} & 0 \\ w_{21} & w_{22} & 0 \\ 0 & 0 & 0 \end{bmatrix} \textit{ where } \begin{bmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{bmatrix} \textit{ is non-singular}$$

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We will apply this result with a specific choice of U and V.

Let

$$U = \begin{bmatrix} b_2 & b_3 & b_4 \\ b_2 c_2 & b_3 c_3 & b_4 c_4 \\ \sum_i b_i a_{i2} & \sum_i b_i a_{i3} & \sum_i b_i a_{i4} \\ -b_2(1-c_2) & -b_3(1-c_3) & -b_4(1-c_4) \end{bmatrix}$$

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$$V = \begin{bmatrix} c_2 & c_2^2 & \sum_j a_{2j} c_j - \frac{1}{2} c_2^2 \\ c_3 & c_3^2 & \sum_j a_{3j} c_j - \frac{1}{2} c_3^2 \\ c_4 & c_4^2 & \sum_j a_{4j} c_j - \frac{1}{2} c_4^2 \end{bmatrix}$$

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then

$$UV = \begin{bmatrix} \frac{1}{2} & \frac{1}{3} & 0 \\ \frac{1}{3} & \frac{1}{4} & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

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Kutta classified all solutions to the fourth order conditions.
In particular we have his famous method:

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

Order barriers

We will review what is achievable up to order 8.

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$M_s = s(s+1)/2$ is the number of free parameters to satisfy the order conditions for the required s stages.

p	N_p	s	M_s
1	1	1	1
2	2	2	3
3	4	3	6
4	8	4	10
5	17	6	21
6	37	7	28
7	115	9	45
8	200	11	66

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$$U = \begin{bmatrix} \widehat{b}_2 & \widehat{b}_3 & \widehat{b}_4 \\ \widehat{b}_2 c_2 & \widehat{b}_3 c_3 & \widehat{b}_4 c_4 \\ \sum_i \widehat{b}_i a_{i2} & \sum_i \widehat{b}_i a_{i3} & \sum_i \widehat{b}_i a_{i4} \\ -\frac{1}{2}\widehat{b}_2(1-c_2) & -\frac{1}{2}\widehat{b}_3(1-c_3) & -\frac{1}{2}\widehat{b}_4(1-c_4) \end{bmatrix}$$

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By modifying the details slightly, we can prove that $s = p > 5$ is never possible.

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The proof that $s = p + 2$ is impossible when $p \geq 8$ is much more complicated.

Algebraic interpretation

We will introduce an algebraic system which represents individual Runge-Kutta methods and also compositions of methods.

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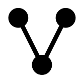
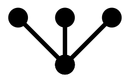
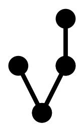
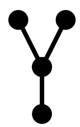
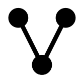
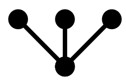
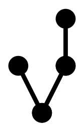
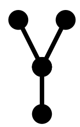
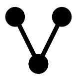
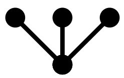
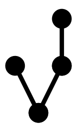
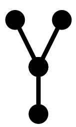
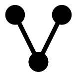
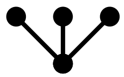
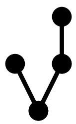
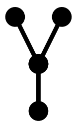
We will illustrate this operation in a table, where we also introduce the special member $E \in G$.

i	t_i
1	
2	
3	
4	
5	
6	
7	
8	

$r(t_i)$	i	t_i
1	1	
2	2	
3	3	
3	4	
4	5	
4	6	
4	7	
4	8	

$r(t_i)$	i	t_i	$\alpha(t_i)$	$\beta(t_i)$
1	1		α_1	β_1
2	2		α_2	β_2
3	3		α_3	β_3
3	4		α_4	β_4
4	5		α_5	β_5
4	6		α_6	β_6
4	7		α_7	β_7
4	8		α_8	β_8

$r(t_i)$	i	t_i	$\alpha(t_i)$	$\beta(t_i)$	$(\alpha\beta)(t_i)$
1	1		α_1	β_1	$\alpha_1 + \beta_1$
2	2		α_2	β_2	$\alpha_2 + \alpha_1\beta_1 + \beta_2$
3	3		α_3	β_3	$\alpha_3 + \alpha_1^2\beta_1 + 2\alpha_1\beta_2 + \beta_3$
3	4		α_4	β_4	$\alpha_4 + \alpha_2\beta_1 + \alpha_1\beta_2 + \beta_4$
4	5		α_5	β_5	$\alpha_5 + \alpha_1^3\beta_1 + 3\alpha_1^2\beta_2 + 3\alpha_1\beta_3 + \beta_5$
4	6		α_6	β_6	$\alpha_6 + \alpha_1\alpha_2\beta_1 + (\alpha_1^2 + \alpha_2)\beta_2$ $+ \alpha_1(\beta_3 + \beta_4) + \beta_6$
4	7		α_7	β_7	$\alpha_7 + \alpha_3\beta_1 + \alpha_1^2\beta_2 + 2\alpha_1\beta_4 + \beta_7$
4	8		α_8	β_8	$\alpha_8 + \alpha_4\beta_1 + \alpha_2\beta_2 + \alpha_1\beta_4 + \beta_8$

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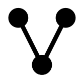
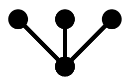
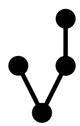
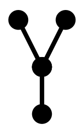
1	1		α_1	β_1	$\alpha_1 + \beta_1$	1
2	2		α_2	β_2	$\alpha_2 + \alpha_1\beta_1 + \beta_2$	$\frac{1}{2}$
3	3		α_3	β_3	$\alpha_3 + \alpha_1^2\beta_1 + 2\alpha_1\beta_2 + \beta_3$	$\frac{1}{3}$
3	4		α_4	β_4	$\alpha_4 + \alpha_2\beta_1 + \alpha_1\beta_2 + \beta_4$	$\frac{1}{6}$
4	5		α_5	β_5	$\alpha_5 + \alpha_1^3\beta_1 + 3\alpha_1^2\beta_2 + 3\alpha_1\beta_3 + \beta_5$	$\frac{1}{4}$
4	6		α_6	β_6	$\alpha_6 + \alpha_1\alpha_2\beta_1 + (\alpha_1^2 + \alpha_2)\beta_2$ $+ \alpha_1(\beta_3 + \beta_4) + \beta_6$	$\frac{1}{8}$
4	7		α_7	β_7	$\alpha_7 + \alpha_3\beta_1 + \alpha_1^2\beta_2 + 2\alpha_1\beta_4 + \beta_7$	$\frac{1}{12}$
4	8		α_8	β_8	$\alpha_8 + \alpha_4\beta_1 + \alpha_2\beta_2 + \alpha_1\beta_4 + \beta_8$	$\frac{1}{24}$

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Effective order p is defined by the existence of β such that

$$\beta \alpha G_p = E \beta G_p.$$

The computational interpretation of this idea is that we carry out a starting step corresponding to β

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Thus, the benefits of high order can be enjoyed by high effective order.

We analyse the conditions for effective order 4.

Without loss of generality assume $\beta(t_1) = 0$.

i	$(\beta\alpha)(t_i)$	$(E\beta)(t_i)$
1	α_1	1
2	$\beta_2 + \alpha_2$	$\frac{1}{2} + \beta_2$
3	$\beta_3 + \alpha_3$	$\frac{1}{3} + 2\beta_2 + \beta_3$
4	$\beta_4 + \beta_2\alpha_1 + \alpha_4$	$\frac{1}{6} + \beta_2 + \beta_4$
5	$\beta_5 + \alpha_5$	$\frac{1}{4} + 3\beta_2 + 3\beta_3 + \beta_5$
6	$\beta_6 + \beta_2\alpha_2 + \alpha_6$	$\frac{1}{8} + \frac{3}{2}\beta_2 + \beta_3 + \beta_4 + \beta_6$
7	$\beta_7 + \beta_3\alpha_1 + \alpha_7$	$\frac{1}{12} + \beta_2 + 2\beta_4 + \beta_7$
8	$\beta_8 + \beta_4\alpha_1 + \beta_2\alpha_2 + \alpha_8$	$\frac{1}{24} + \frac{1}{2}\beta_2 + \beta_4 + \beta_8$

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The 5 order conditions, written in terms of the Runge-Kutta tableau, are

$$\begin{aligned}
\sum b_i &= 1 \\
\sum b_i c_i &= \tfrac{1}{2} \\
\sum b_i a_{ij} c_j &= \tfrac{1}{6} \\
\sum b_i a_{ij} a_{jk} c_k &= \tfrac{1}{24} \\
\sum b_i c_i^2 (1 - c_i) + \sum b_i a_{ij} c_j (2c_i - c_j) &= \tfrac{1}{4}
\end{aligned}$$

Implicit Runge–Kutta methods

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For example the following method has order 5:

$$
\begin{array}{c|cccc}
0 & & & & \\
\frac{1}{4} & \frac{1}{8} & \frac{1}{8} & & \\
\frac{7}{10} & -\frac{1}{100} & \frac{14}{25} & \frac{3}{20} & \\
1 & \frac{2}{7} & 0 & \frac{5}{7} & \\
\hline
 & \frac{1}{14} & \frac{32}{81} & \frac{250}{567} & \frac{5}{54}
\end{array}
$$

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The following third order L-stable method illustrates what is possible for DIRK methods

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The following third order L-stable method illustrates what is possible for DIRK methods

$$\begin{array}{c|ccc}
\lambda & \lambda & & \\
\frac{1}{2}(1+\lambda) & \frac{1}{2}(1-\lambda) & \lambda & \\
1 & \frac{1}{4}(-6\lambda^2+16\lambda-1) & \frac{1}{4}(6\lambda^2-20\lambda+5) & \lambda \\
\hline
 & \frac{1}{4}(-6\lambda^2+16\lambda-1) & \frac{1}{4}(6\lambda^2-20\lambda+5) & \lambda
\end{array}$$

where $\lambda \approx 0.4358665215$ satisfies $\frac{1}{6}-\frac{3}{2}\lambda+3\lambda^2-\lambda^3 = 0$.

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How then is it possible to implement SIRK methods in a similarly efficient manner?

The answer lies in the inclusion of a transformation to Jordan canonical form into the computation.

Suppose the matrix T transforms A to canonical form as follows

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$$\overline{A} = \lambda(I - J) = \lambda \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 & 0 \\ -1 & 1 & 0 & \cdots & 0 & 0 \\ 0 & -1 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 1 \end{bmatrix}$$

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where e is the vector in $\mathbb{R}^n$ with every component equal to 1 and Y has subvectors Y_i, $i = 1, 2, \dots, s$

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The following table summarises the costs

LU factorisation	s^3N^3	
Backsolves	s^2N^2	

	without transformation	
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This is equivalent to

$$A^k c^0 = \frac{1}{k!}c^k, \qquad k = 1, 2, \ldots, s \qquad\qquad (*)$$

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$$(A - \lambda I)^s c^0 = 0$$

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Substitute from $(*)$ and it is found that

$$\sum_{i=0}^{s} \frac{1}{i!} \binom{s}{i} (-\lambda)^{s-i} c^i = 0.$$

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The question now is, how should λ be chosen?

Unfortunately, to obtain A-stability, at least for orders $p > 2$, λ has to be chosen so that some of the c_i are outside the interval $[0, 1]$.

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We will look at two approaches for overcoming this disadvantage.

However, we first look at the transformation matrix T for efficient implementation.

Define the matrix T as follows:

$$T = \begin{bmatrix} L_0(\xi_1) & L_1(\xi_1) & L_2(\xi_1) & \cdots & L_{s-1}(\xi_1) \\ L_0(\xi_2) & L_1(\xi_2) & L_2(\xi_2) & \cdots & L_{s-1}(\xi_2) \\ L_0(\xi_3) & L_1(\xi_3) & L_2(\xi_3) & \cdots & L_{s-1}(\xi_3) \\ \vdots & \vdots & \vdots & & \vdots \\ L_0(\xi_s) & L_1(\xi_s) & L_2(\xi_s) & \cdots & L_{s-1}(\xi_s) \end{bmatrix}$$

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It can be shown that for a SIRK method

$$T^{-1}AT = \lambda(I - J)$$

There are two ways in which SIRK methods can be generalized
In the first of these we add extra diagonally implicit stages so that the coefficient matrix looks like this:

$$\begin{bmatrix} \widehat{A} & 0 \\ W & \lambda I \end{bmatrix},$$

where the spectrum of the $p \times p$ submatrix $\widehat{A}$ is

$$\sigma(\widehat{A}) = \{\lambda\}$$

For $s - p = 1, 2, 3, \ldots$ we get improvements to the behaviour of the methods

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This seems to be as far as we can go in constructing efficient and accurate singly-implicit Runge-Kutta methods.