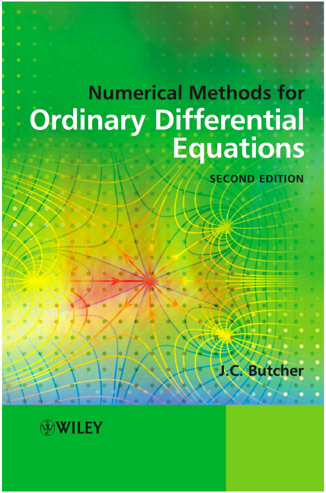
John Butcher's tutorials

Introduction to Runge–Kutta methods

$$\Phi(t) = \frac{1}{\gamma(t)}$$



Introduction

It will be convenient to consider only autonomous initial value problems

$$y'(x) = f(y(x)), \qquad y(x_0) = y_0,$$
$$f : \mathbb{R}^N \to \mathbb{R}^N.$$

The Euler method is the simplest way of obtaining numerical approximations at

$$x_1 = x_0 + h, \quad x_2 = x_1 + h, \ldots$$

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This method can be made more accurate by using either the mid-point quadrature formula

$$y_n = y_{n-1} + hf\big(y_{n-1} + \tfrac{1}{2}hf(y_{n-1})\big).$$

or the trapezoidal rule quadrature formula:

$$y_n = y_{n-1} + \tfrac{1}{2}hf(y_{n-1}) + \tfrac{1}{2}hf\big(y_{n-1} + hf(y_{n-1})\big).$$

These methods from Runge's 1895 paper are "second order" because the error in a single step behaves like $O(h^3)$.

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Shortly afterwards Kutta gave a detailed analysis of order 4 methods.

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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Formulation of Runge–Kutta methods

In carrying out a step we evaluate s stage values

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

and s stage derivatives

$$F_1, \quad F_2, \quad \dots, \quad F_s,$$

using the formula $F_i = f(Y_i)$.

Each Y_i is defined as a linear combination of the F_j added on to y_0:

$$Y_i = y_0 + h \sum_{j=1}^{s} a_{ij} F_j, \quad i = 1, 2, \dots, s,$$

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

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We represent the method by a tableau:

$$\begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \cdots & a_{1s} \\ c_2 & a_{21} & a_{22} & \cdots & a_{2s} \\ \vdots & \vdots & \vdots & & \vdots \\ c_s & a_{s1} & a_{s2} & \cdots & a_{ss} \\ \hline & b_1 & b_2 & \cdots & b_s \end{array}$$

or, if the method is explicit, by the simplified tableau

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

In each case, c_i $(i = 1, 2, \dots)$ is defined as $\sum_{j=1}^{s} a_{ij}$. The value of c_i indicates the point $X_i = x_0 + hc_i$ for which Y_i is a good approximation to $y(X_i)$.

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Examples:

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

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Taylor series of exact solution

We need formulae for the second, third, . . . , derivatives.

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y'(x) &= f(y(x)) \\
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This will become increasingly complicated as we evaluate higher derivatives.

Hence we look for a systematic pattern.

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

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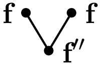
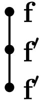


$$+\,\mathbf{f}'\mathbf{f}'\mathbf{f}$$



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.

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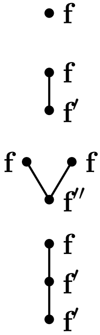

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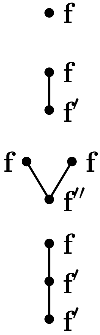

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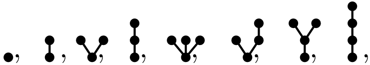
$T = \{$  $\ldots \}$

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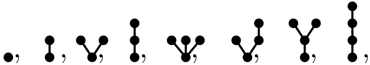
$$T = \Big\{$$  $$\ldots \Big\}$$

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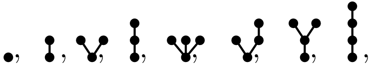
$T = \Big\{$  $\ldots \Big\}$

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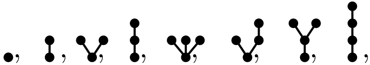
$T = \Big\{$  $\ldots \Big\}$

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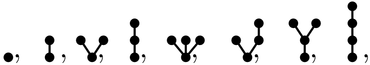
$T = \Big\{$  $\ldots \Big\}$

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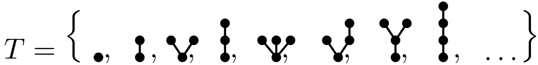

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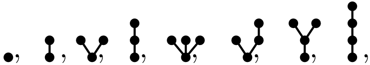
$T = \Big\{$  $\ldots \Big\}$

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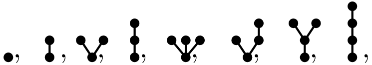
$T = \{$  $\ldots \}$

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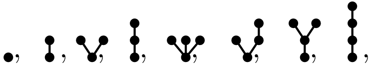
$T = \{$  $\ldots \}$

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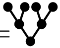
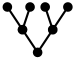
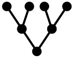
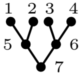
$F(t)(y_0)$	elementary differential

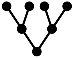
We will give examples of these functions based on $t =$ 

$t =$ 

$t =$ 

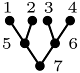
$r(t) = 7$

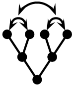


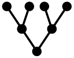
t = 

$r(t) = 7$

$\sigma(t) = 8$



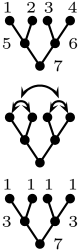


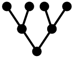
t = 

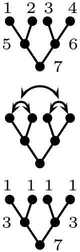
$r(t) = 7$

$\sigma(t) = 8$

$\gamma(t) = 63$



$t =$ 



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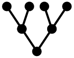
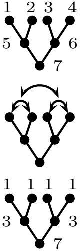
$$\alpha(t) = \frac{r(t)!}{\sigma(t)\gamma(t)} = 10$$

$t =$ 



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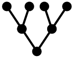
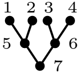
$t =$ 



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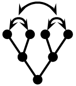
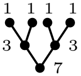


$\sigma(t) = 8$

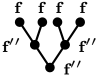


$\gamma(t) = 63$

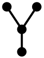
$$\alpha(t) = \frac{r(t)!}{\sigma(t)\gamma(t)} = 10$$

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

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



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

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

Using the known formula for $\alpha(t)$, we can write this as

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

Our aim will now be to find a corresponding formula for the result computed by one step of a Runge–Kutta method.

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

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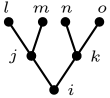

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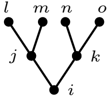

$$\Phi(t) = \sum_{i,j,k,l,m,n,o=1}^{s} b_i a_{ij} a_{ik} a_{jl} a_{jm} a_{kn} a_{ko}$$

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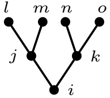
$t =$ 

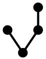
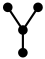
$$\Phi(t) = \sum_{i,j,k,l,m,n,o=1}^{s} b_i a_{ij} a_{ik} a_{jl} a_{jm} a_{kn} a_{ko}$$

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
$\Phi(t)$	$\sum b_i c_i^3$	$\sum b_i c_i a_{ij} c_j$	$\sum b_i a_{ij} c_j^2$	$\sum b_i a_{ij} a_{jk} c_k$

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

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

Using the known formula for $\beta(t)$, we can write this as

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

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Order conditions

To match the Taylor series

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

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

up to h^p terms we need to ensure that

$$\Phi(t) = \frac{1}{\gamma(t)},$$

for all trees such that

$$r(t) \leq p.$$

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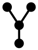
The order conditions will be illustrated in the case of explicit 4 stage methods with order 4.

t	$\Phi(t) = \frac{1}{\gamma(t)}$
	$b_1 + b_2 + b_3 + b_4 = 1$
	$b_2c_2 + b_3c_3 + b_4c_4 = \frac{1}{2}$
	$b_2c_2^2 + b_3c_3^2 + b_4c_4^2 = \frac{1}{3}$
	$b_3a_{32}c_2 + b_4a_{42}c_2 + b_4a_{43}c_3 = \frac{1}{6}$
	$b_2c_2^3 + b_3c_3^3 + b_4c_4^3 = \frac{1}{4}$
	$b_3c_3a_{32}c_2 + b_4c_4a_{42}c_2 + b_4c_4a_{43}c_3 = \frac{1}{8}$
	$b_3a_{32}c_2^2 + b_4a_{42}c_2^2 + b_4a_{43}c_3^2 = \frac{1}{12}$
	$b_4a_{43}a_{32}c_2 = \frac{1}{24}$