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# Scientific Computation and Differential Equations

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New Zealand

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Institut Kajian Sains Fundamental Ibnu Sina

# Overview

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Within Scientific Computation, the approximate solution of differential equations has always been an area of special challenge.

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Today we will look briefly at the history of numerical methods for differential equations.

We will then look at some particular questions concerning the theory of general linear methods.

We will also look at some aspects of their practical implementation.

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# A short history of numerical ODEs

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We will make use of three standard types of initial value problems

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

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Problem (1) is used in traditional descriptions of numerical methods but in applications we need to use either (2) or (3).

These are actually equivalent and we will often use (3) instead of (2) because of its simplicity.

# The Euler method

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Euler proposed a simple numerical scheme in approximately 1770; this can be used for a system of first order equations.

# The Euler method

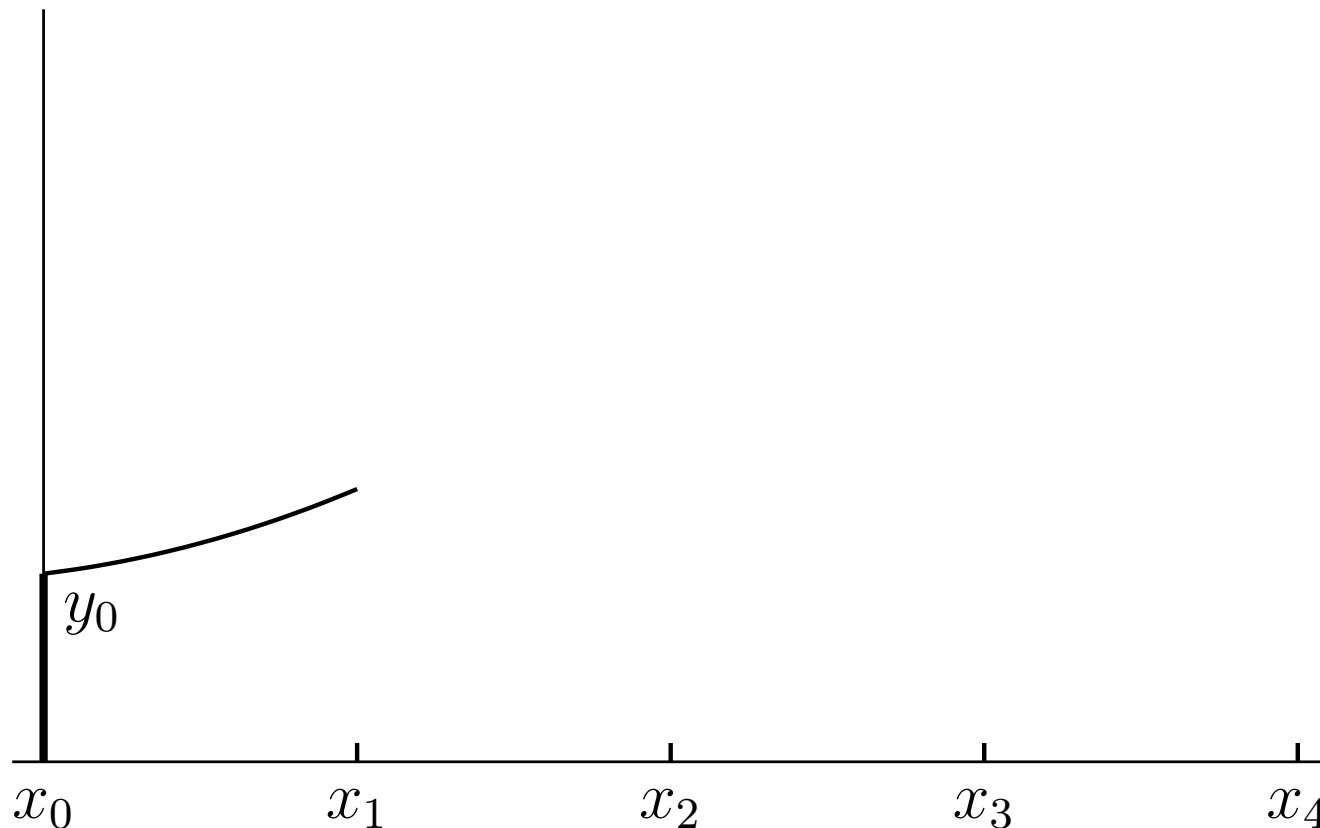
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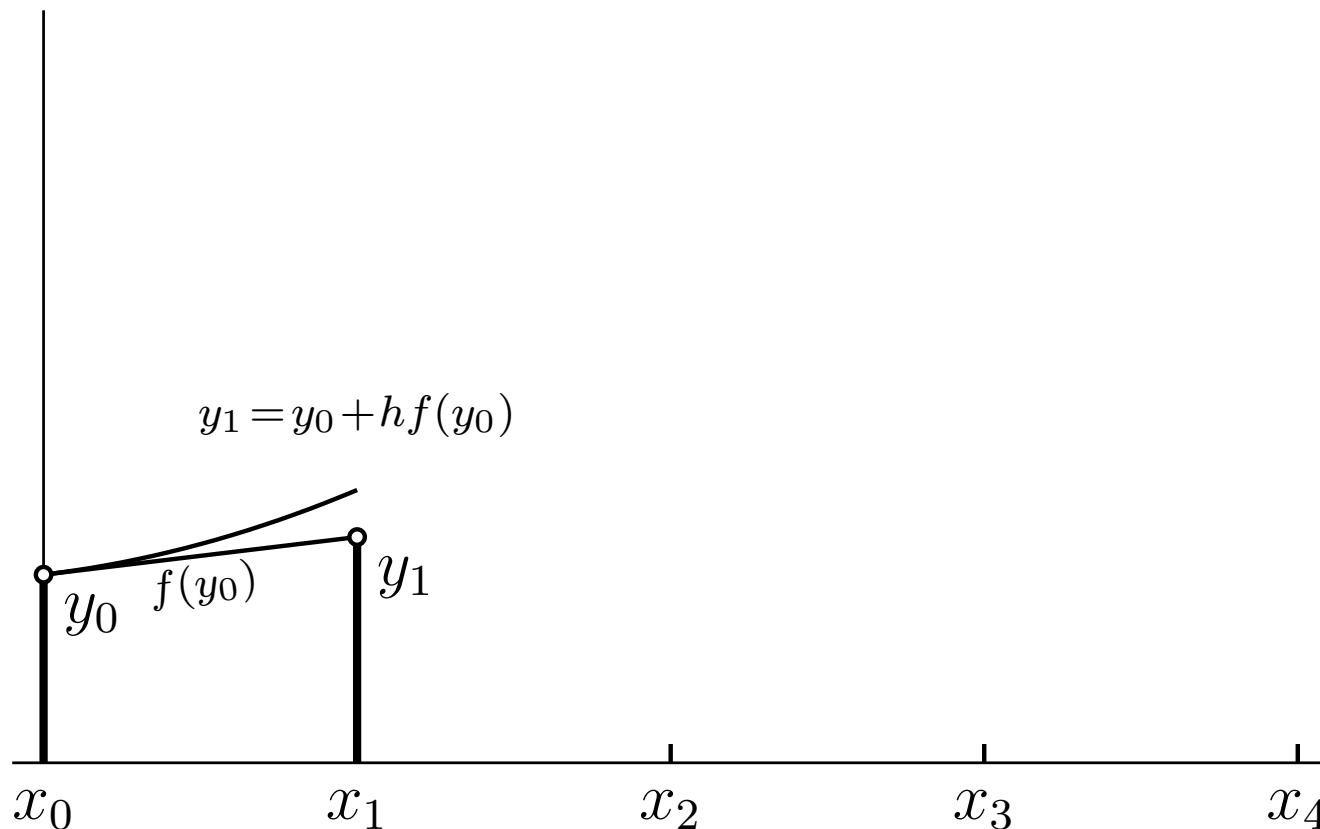
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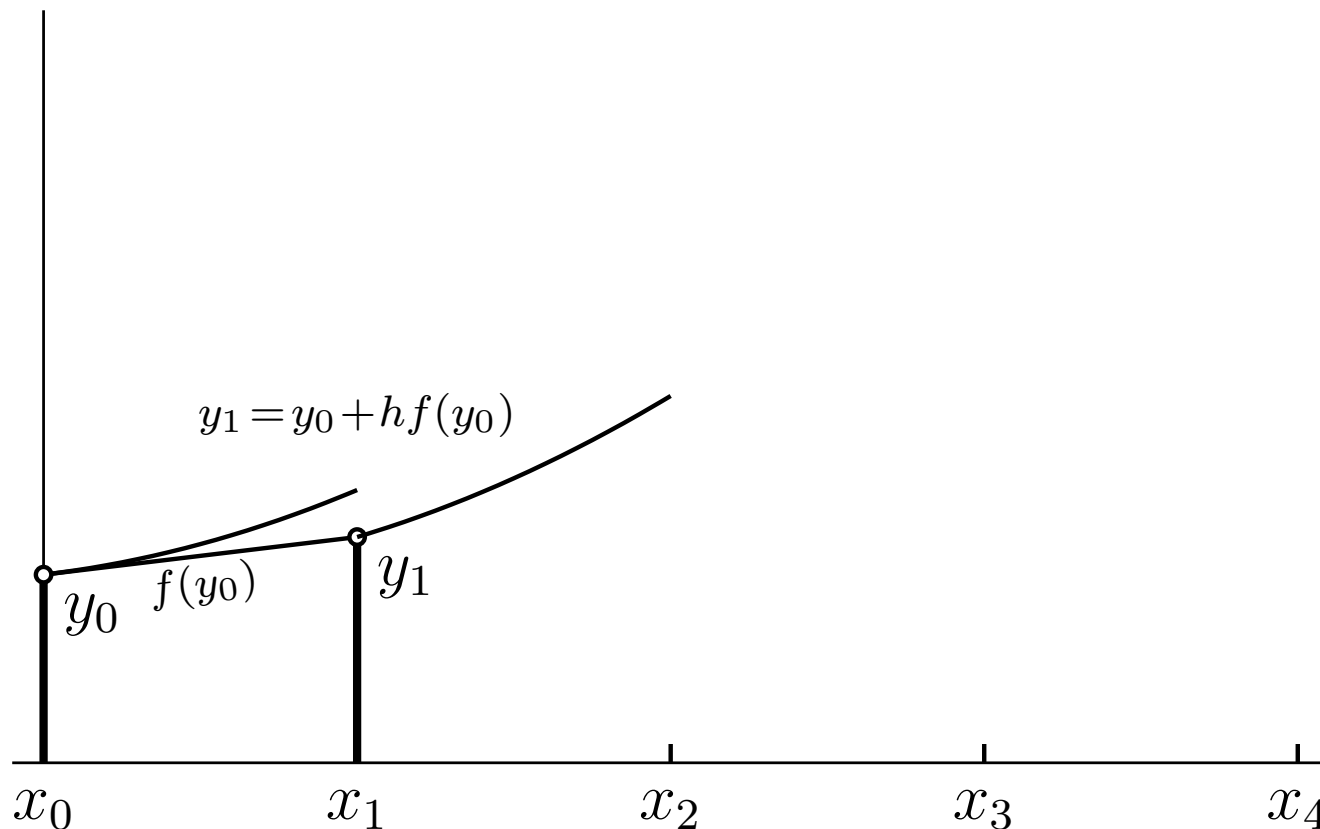
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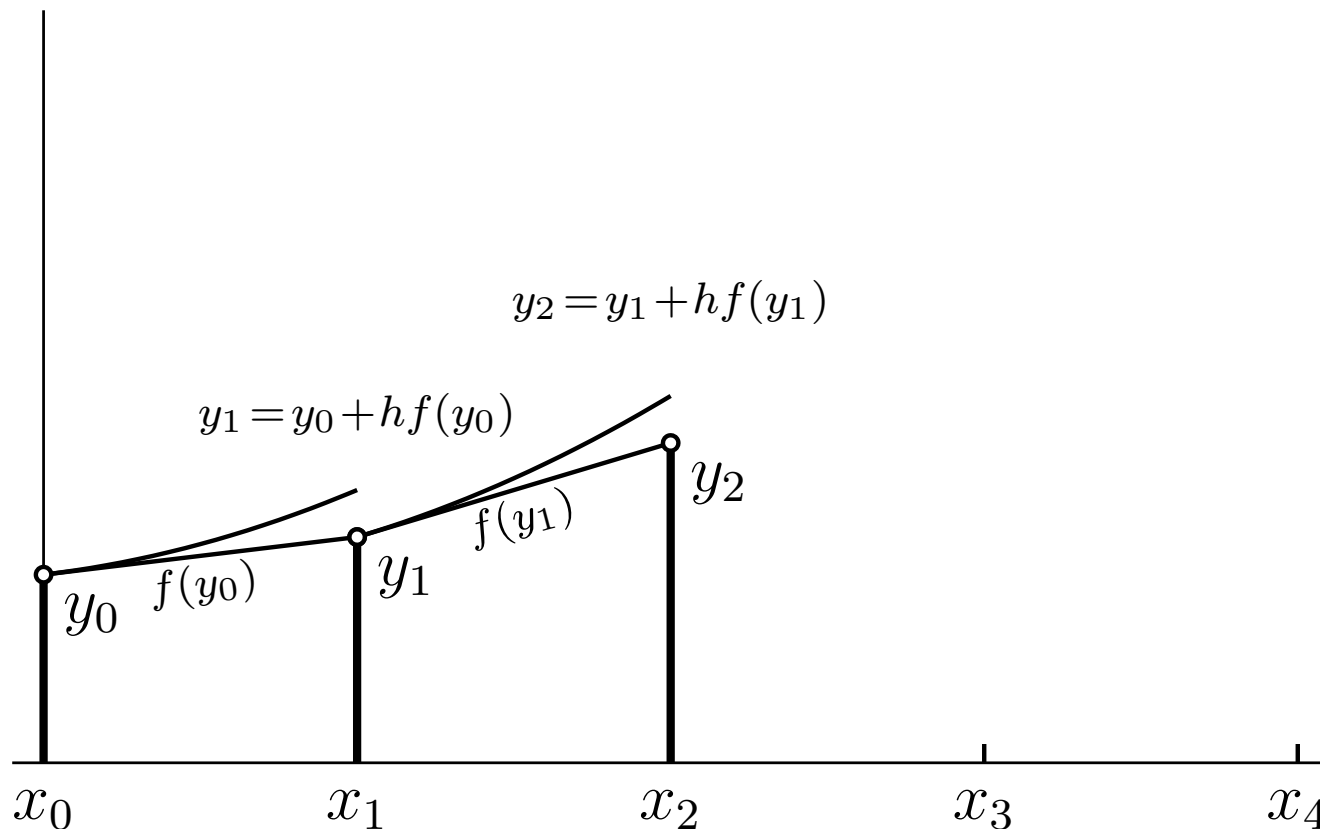
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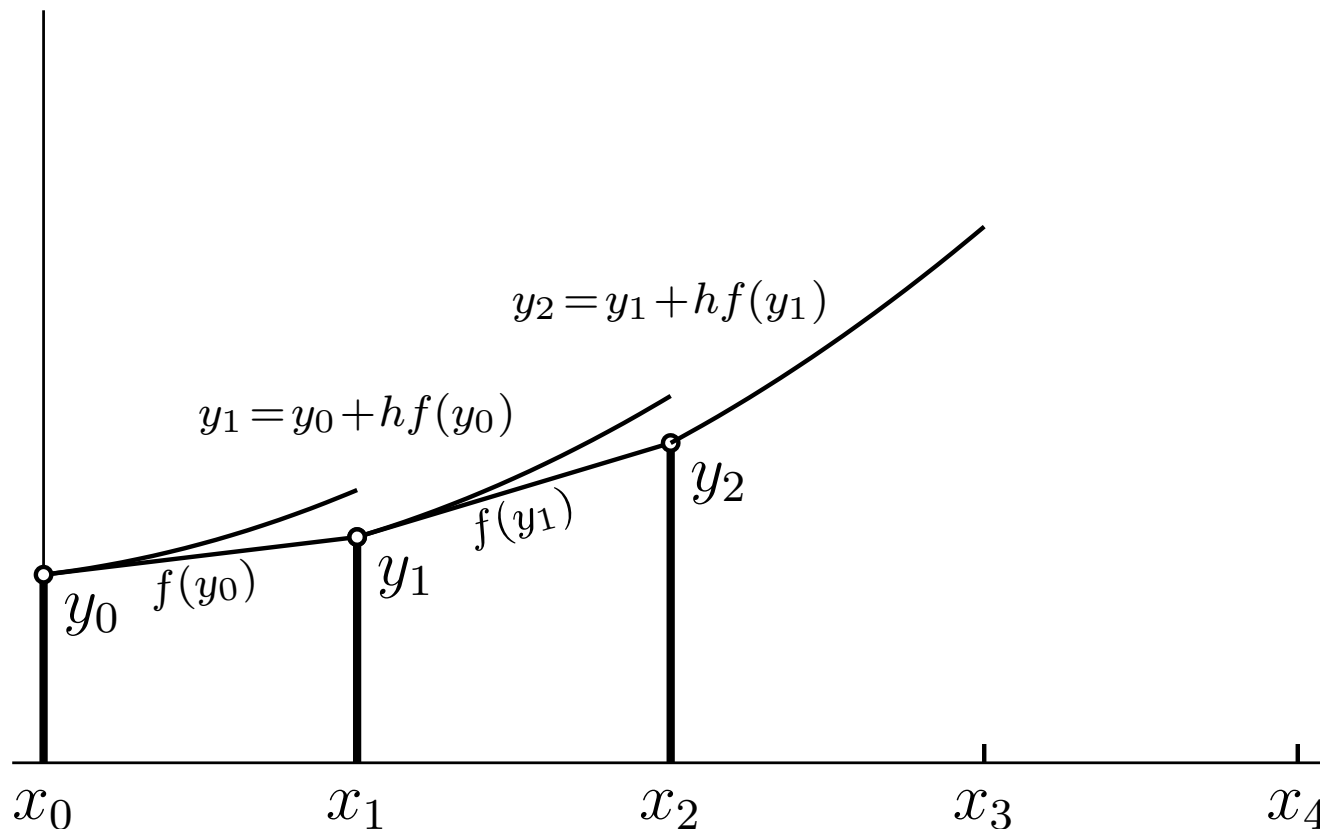
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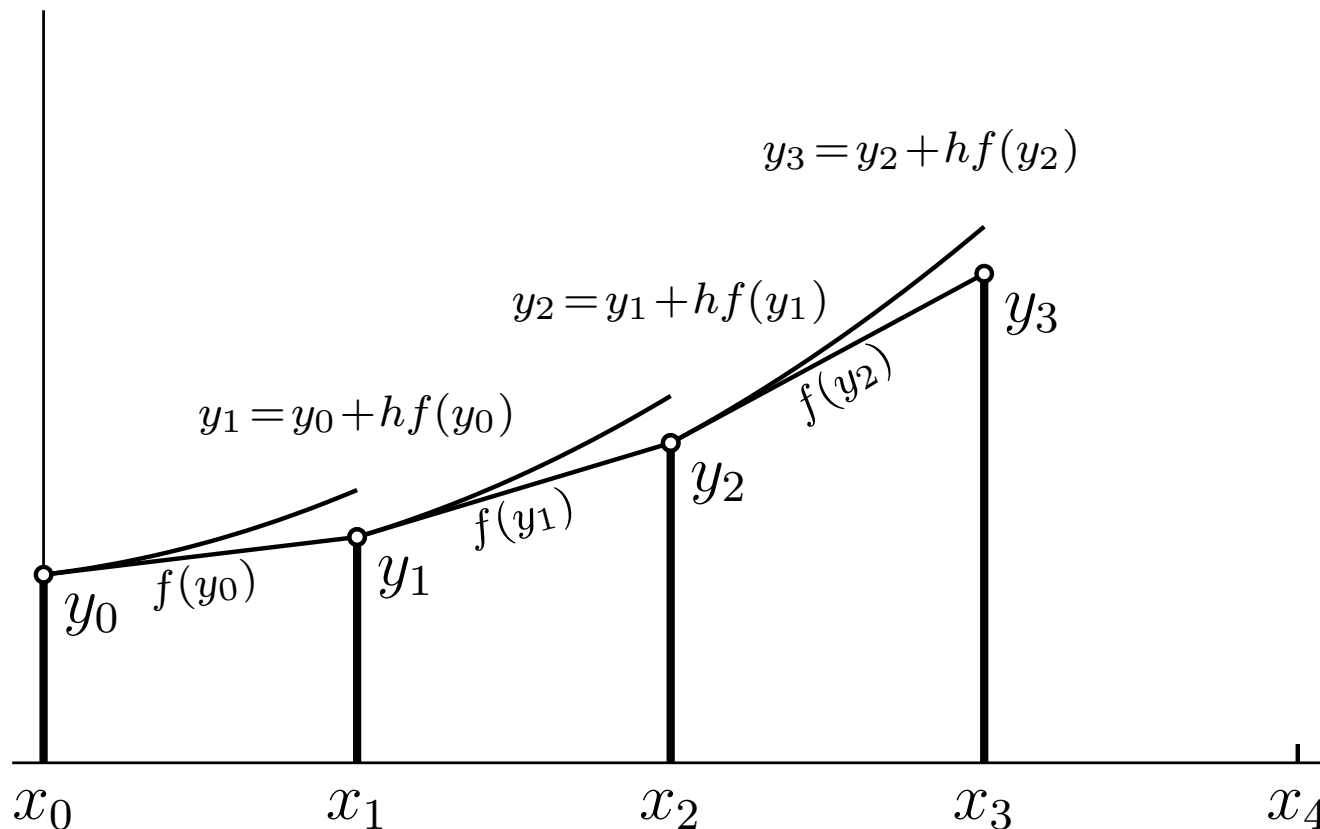
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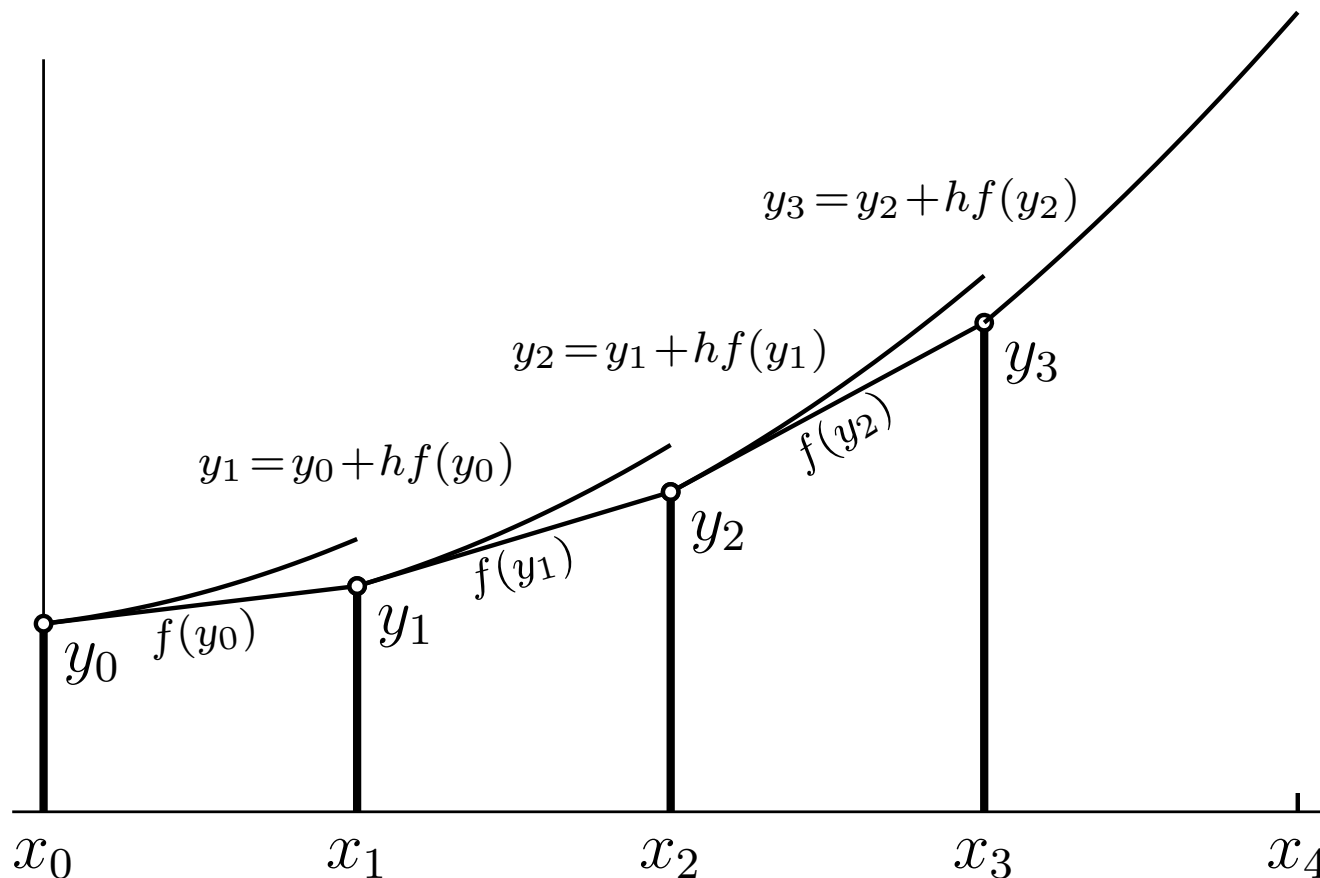
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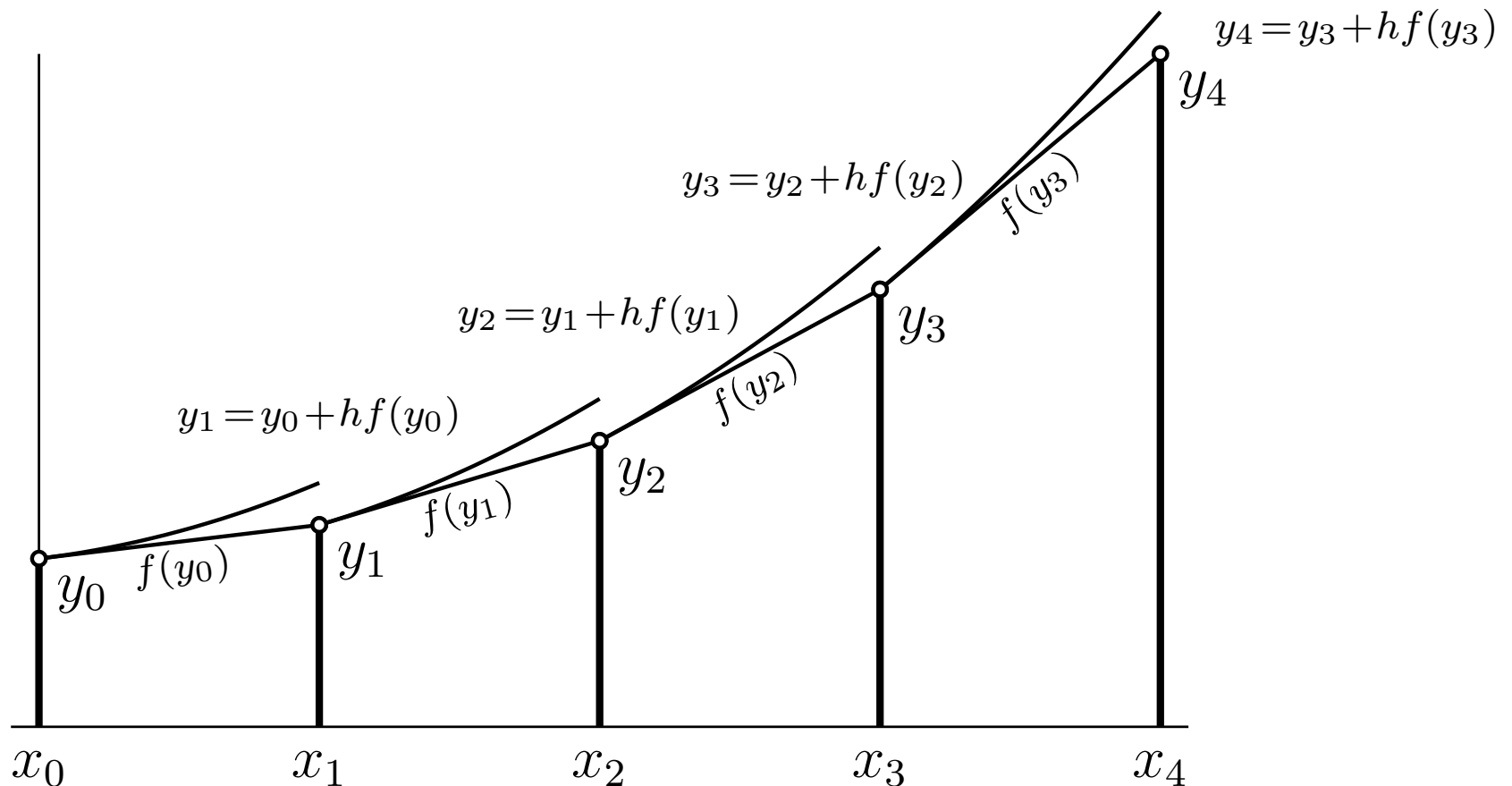
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3. Doing both of these
  - *General linear methods*

## Some important dates

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1883	Adams & Bashforth	Linear multistep methods
1895	Runge	Runge-Kutta method
1901	Kutta	
1925	Nyström	Special methods for second order
1926	Moulton	Adams-Moulton method
1952	Curtiss & Hirschfelder	Stiff problems

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Linear multistep methods base the approximation to  $y(x_n)$  on a linear combination of approximations to  $y(x_{n-i})$  and approximations to  $y'(x_{n-i})$ ,  $i = 1, 2, \dots, k$ .

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A linear multistep method can be written as

$$y_n = \sum_{i=1}^k \alpha_i y_{n-i} + h \sum_{i=0}^k \beta_i f_{n-i}$$

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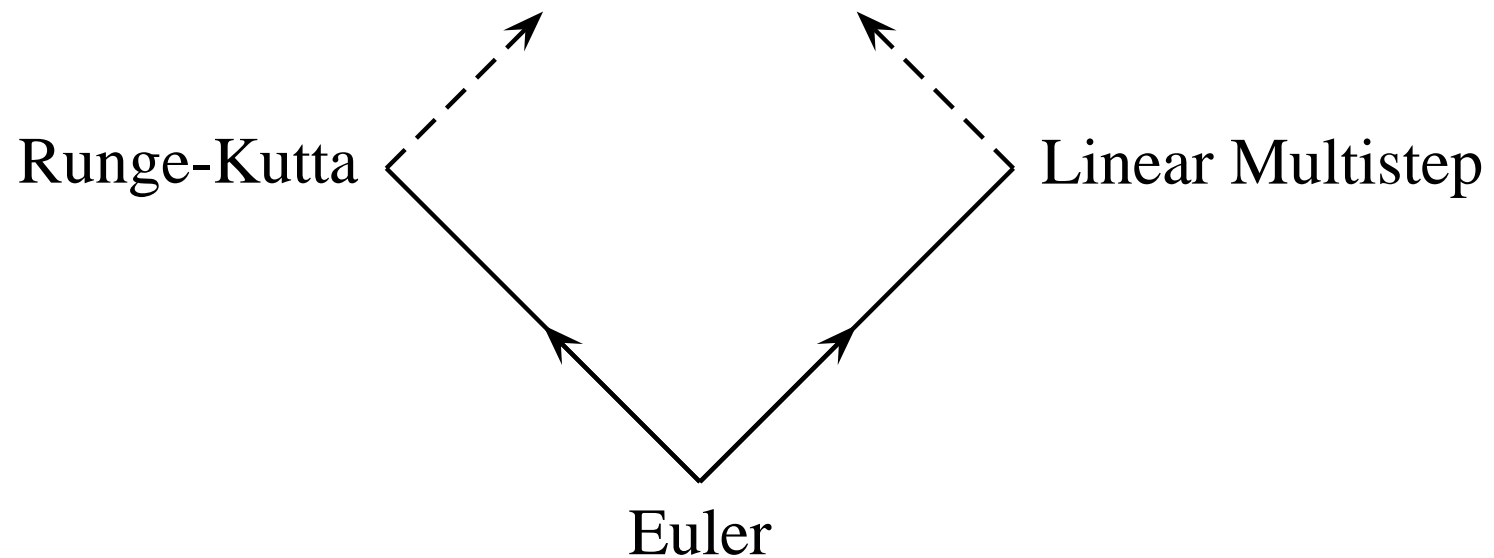
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It is natural to ask if there are useful methods which are multistage (as for Runge–Kutta methods) and multivalue (as for linear multistep methods).

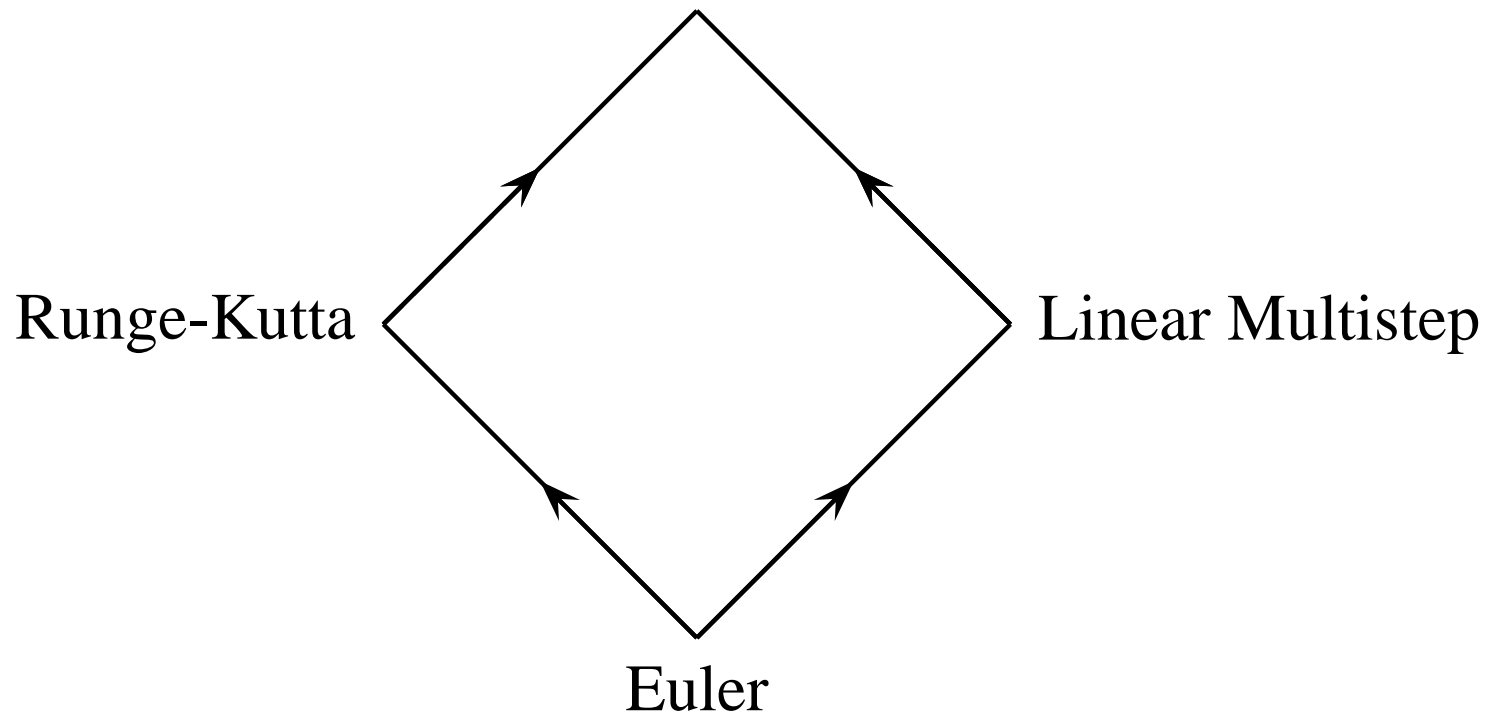
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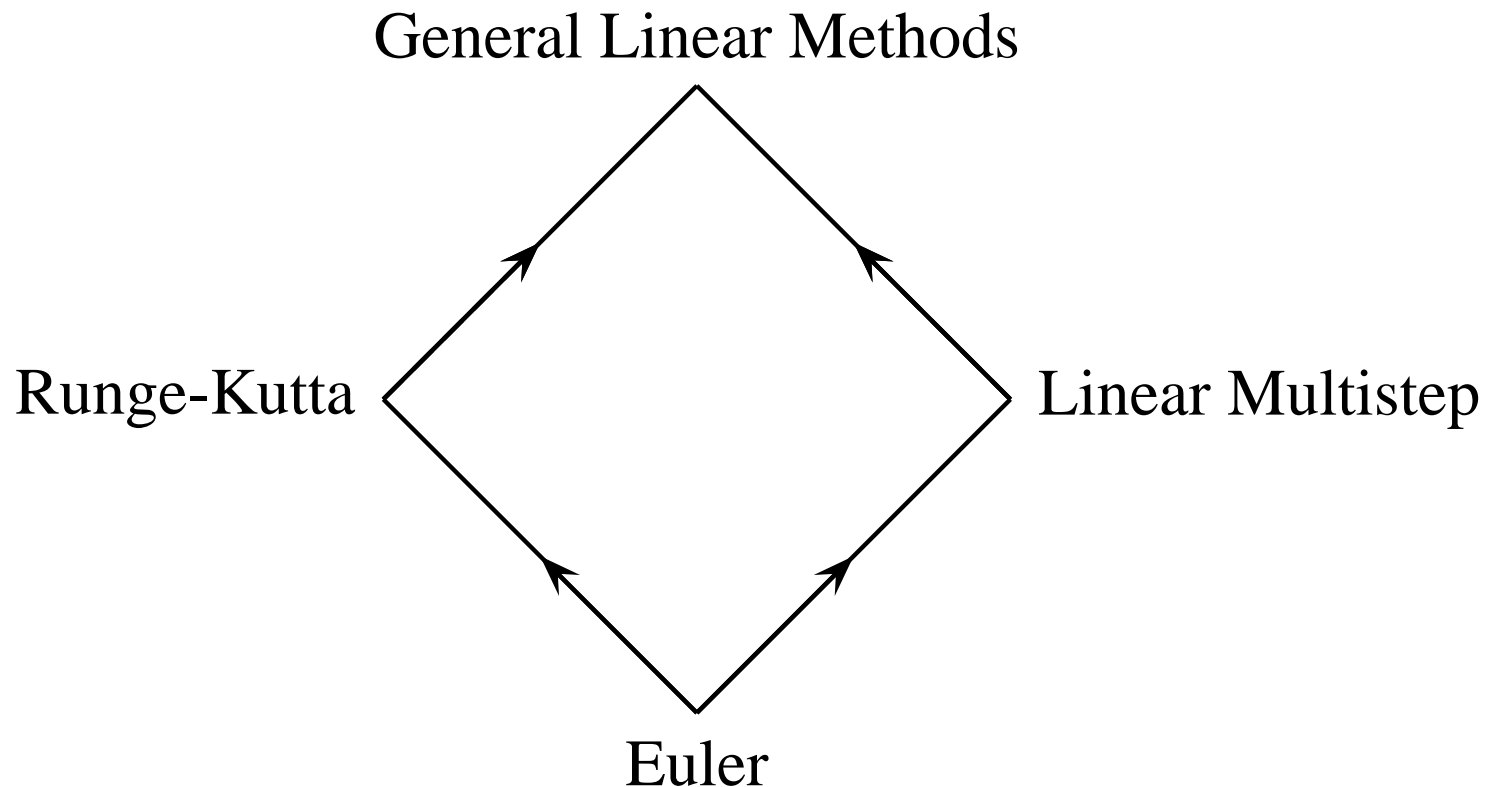
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# General linear methods

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We will consider methods characterised by an  $(s + r) \times (s + r)$  partitioned matrix of the form

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The  $r$  values input to step  $n - 1$  will be denoted by  $y_i^{[n-1]}$ ,  $i = 1, 2, \dots, r$  with corresponding output values  $y_i^{[n]}$  and the stage values by  $Y_i$ ,  $i = 1, 2, \dots, s$ .

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The stage derivatives will be denoted by  $F_i = f(Y_i)$ .

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The formula for computing the stages (and simultaneously the stage derivatives) are:

$$Y_i = h \sum_{j=1}^s a_{ij} F_j + \sum_{j=1}^r u_{ij} y_j^{[n-1]}, \quad F_i = f(Y_i),$$

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To compute the output values, use the formula

$$y_i^{[n]} = h \sum_{j=1}^s b_{ij} F_j + \sum_{j=1}^r v_{ij} y_j^{[n-1]}, \quad i = 1, 2, \dots, r.$$

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For convenience, write

$$y^{[n-1]} = \begin{bmatrix} y_1^{[n-1]} \\ y_2^{[n-1]} \\ \vdots \\ y_r^{[n-1]} \end{bmatrix}, \quad y^{[n]} = \begin{bmatrix} y_1^{[n]} \\ y_2^{[n]} \\ \vdots \\ y_r^{[n]} \end{bmatrix}, \quad Y = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_s \end{bmatrix}, \quad F = \begin{bmatrix} F_1 \\ F_2 \\ \vdots \\ F_s \end{bmatrix},$$

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so that we can write the calculations in a step more simply as

$$\begin{bmatrix} Y \\ y^{[n]} \end{bmatrix} = \begin{bmatrix} A & U \\ B & V \end{bmatrix} \begin{bmatrix} hF \\ y^{[n-1]} \end{bmatrix}.$$

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- A Runge–Kutta method
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- An Adams-Bashforth/Adams-Moulton method
- A modified linear multistep method

# A Runge–Kutta method

One of the famous families of fourth order methods of Kutta, written as a general linear method, is

$$\begin{bmatrix} A & U \\ B & V \end{bmatrix} = \left[ \begin{array}{cccc|c} 0 & 0 & 0 & 0 & 1 \\ \theta & 0 & 0 & 0 & 1 \\ \frac{1}{2} & -\frac{1}{8\theta} & \frac{1}{8\theta} & 0 & 1 \\ \frac{1}{2\theta} & -1 & -\frac{1}{2\theta} & 2 & 1 \\ \hline \frac{1}{6} & 0 & \frac{2}{3} & \frac{1}{6} & 1 \end{array} \right]$$

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In a step from  $x_{n-1}$  to  $x_n = x_{n-1} + h$ , the stages give approximations at

$$x_{n-1}, \quad x_{n-1} + \theta h, \quad x_{n-1} + \frac{1}{2}h \quad \text{and} \quad x_{n-1} + h.$$

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We will look at the special case  $\theta = -\frac{1}{2}$ .

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In the special  $\theta = -\frac{1}{2}$  case

$$\begin{bmatrix} A & U \\ B & V \end{bmatrix} = \left[ \begin{array}{cccc|c} 0 & 0 & 0 & 0 & 1 \\ -\frac{1}{2} & 0 & 0 & 0 & 1 \\ \frac{3}{4} & -\frac{1}{4} & 0 & 0 & 1 \\ -2 & 1 & 2 & 0 & 1 \\ \hline \frac{1}{6} & 0 & \frac{2}{3} & \frac{1}{6} & 1 \end{array} \right]$$

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Because the derivative at

$$x_{n-1} + \theta h = x_{n-1} - \frac{1}{2}h = x_{n-2} + \frac{1}{2}h,$$

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This will save one function evaluation.

## A 're-use' method

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This gives the re-use method

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- The stability region is smaller

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We then get methods like the following:

# An ARK method

$$\left[ \begin{array}{cccc|ccc} 0 & 0 & 0 & 0 & 1 & 1 & \frac{1}{2} \\ \frac{1}{16} & 0 & 0 & 0 & 1 & \frac{7}{16} & \frac{1}{16} \\ -\frac{1}{4} & 2 & 0 & 0 & 1 & -\frac{3}{4} & -\frac{1}{4} \\ 0 & \frac{2}{3} & \frac{1}{6} & 0 & 1 & \frac{1}{6} & 0 \\ \hline 0 & \frac{2}{3} & \frac{1}{6} & 0 & 1 & \frac{1}{6} & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ -\frac{1}{3} & 0 & -\frac{2}{3} & 2 & 0 & -1 & 0 \end{array} \right],$$

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$$Y_1 \approx Y_3 \approx Y_4 \approx y(x_n), \quad Y_2 \approx y(x_{n-1} + \frac{1}{2}h).$$

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- Unlike standard Runge–Kutta methods, the stage order is 2.

*This means that the stage values are computed to the same accuracy as an order 2 Runge-Kutta method.*

- Although it is a multi-value method, both starting the method and changing stepsize are essentially cost-free operations.

## An Adams-Bashforth/Adams-Moulton method

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For example, the ‘PECE’ method of order 3 computes a predictor  $y_n^*$  and a corrector  $y_n$  by the formulae

$$y_n^* = y_{n-1} + h \left( \frac{23}{12} f(y_{n-1}) - \frac{4}{3} f(y_{n-2}) + \frac{5}{12} f(y_{n-3}) \right),$$

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It might be asked: Is it possible to obtain improved order by using values of  $y_{n-2}$ ,  $y_{n-3}$  in the formulae?

The answer is that not much can be gained because we are limited by the famous ‘Dahlquist barrier’.

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This new method, with predictors at the off-step point and also at the end of the step, is

$$y_{n-\frac{1}{2}}^* = y_{n-2} + h \left( \frac{9}{8} f(y_{n-1}) + \frac{3}{8} f(y_{n-2}) \right),$$

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The key ideas are

- Use a general starting method to represent the input to a step.
- Require the output to be similarly related to the starting method applied one time-step later.

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We will refer to the calculation which produces  $y^{[n-1]}$  from  $y(x_{n-1})$  as a “starting method”.

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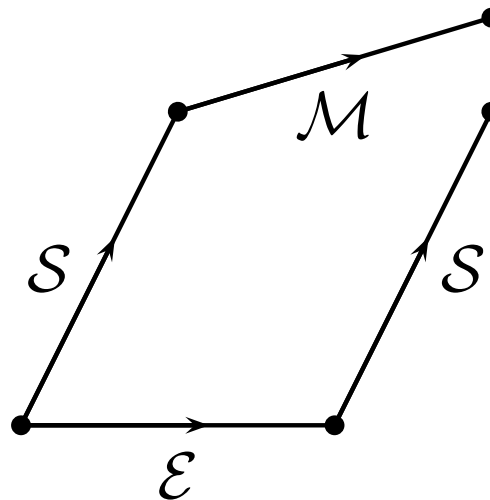
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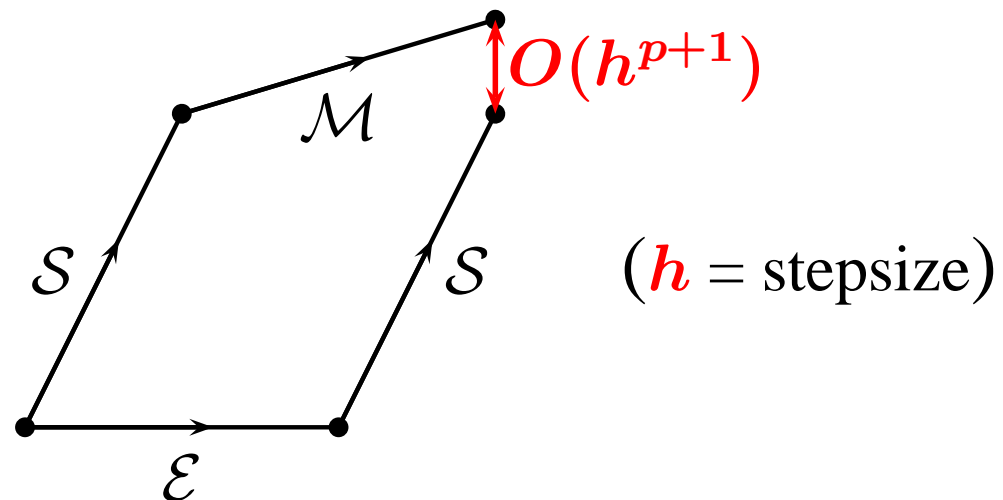
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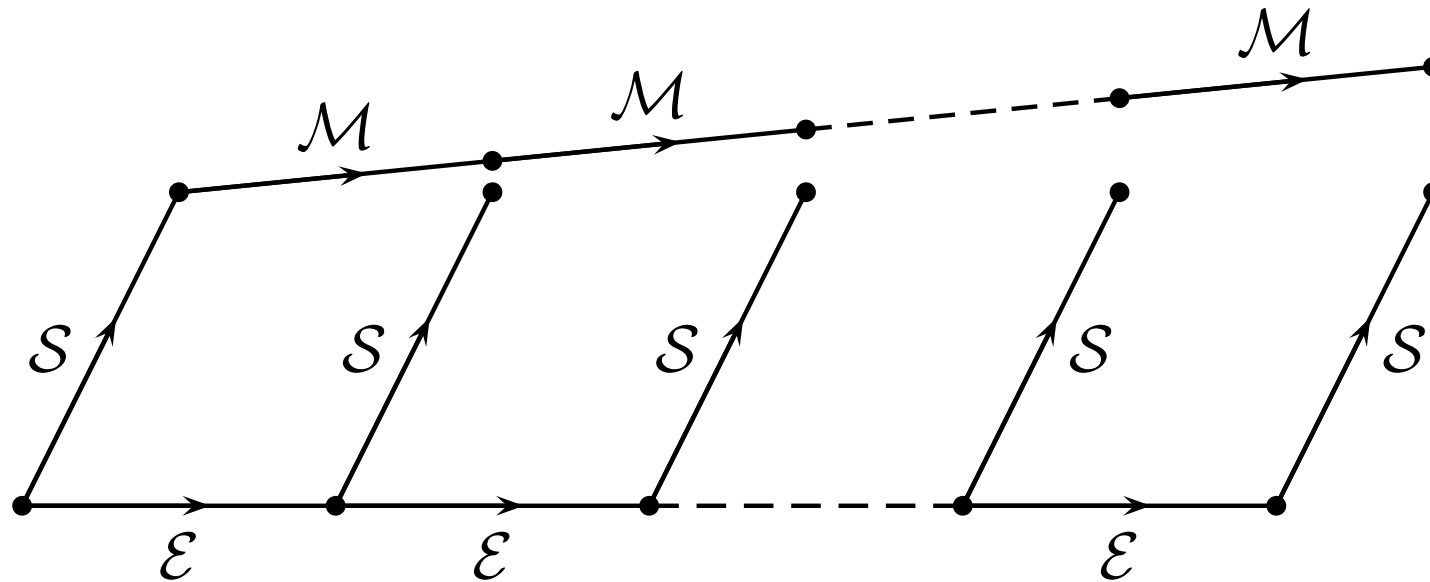


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By duplicating this diagram over many steps, global error estimates can be found.

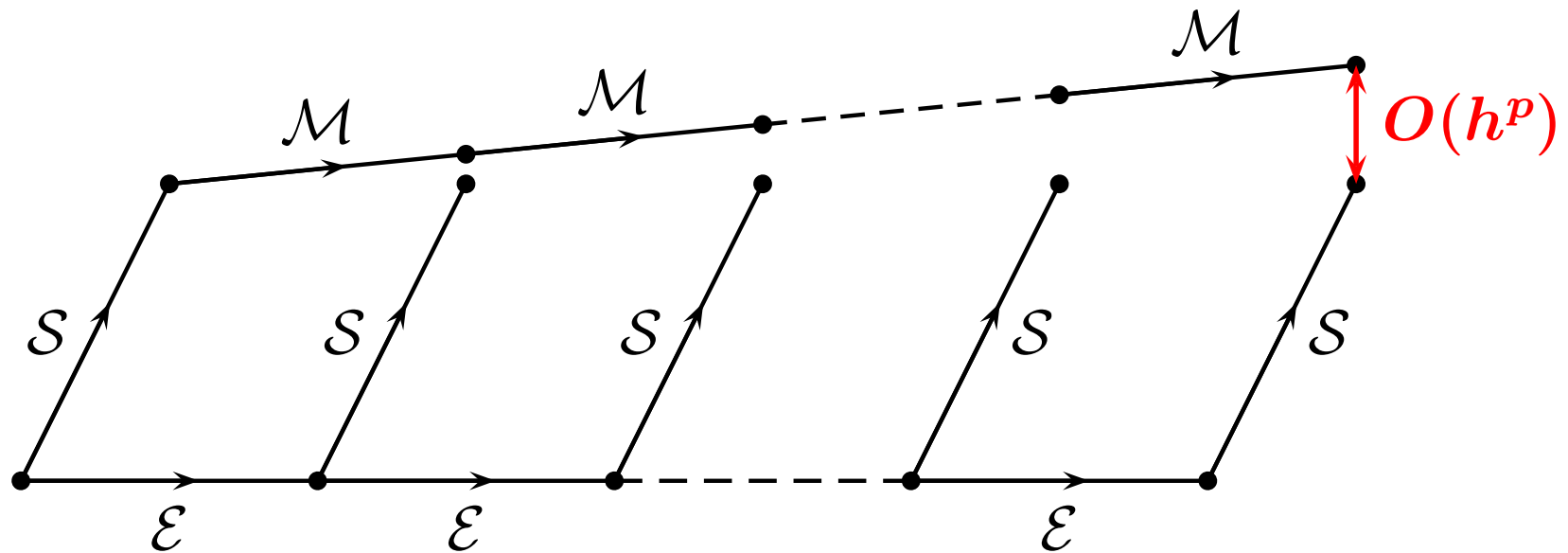
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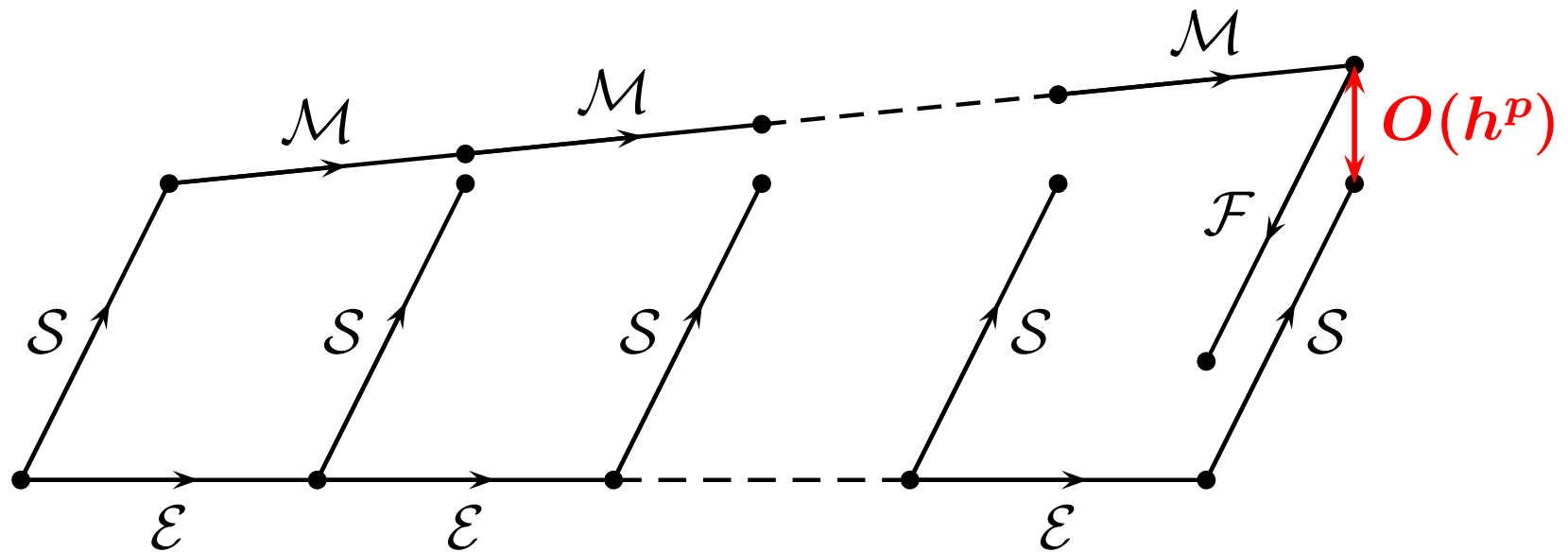
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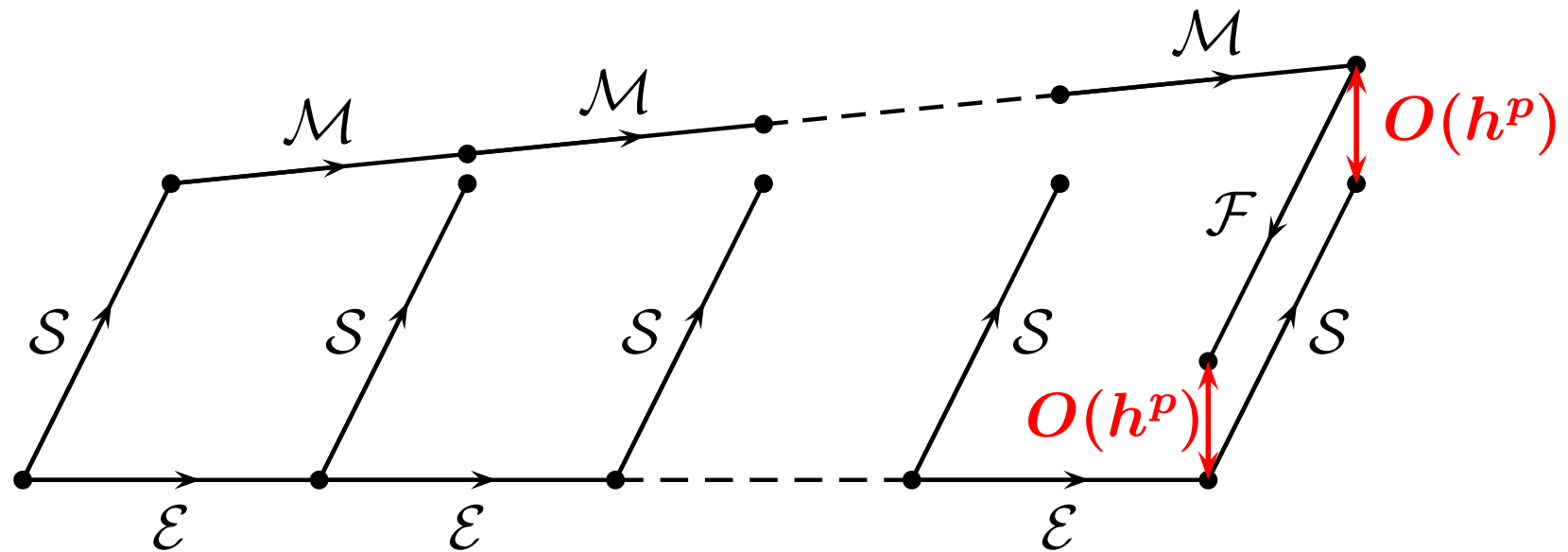


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In the special case of a Runge–Kutta method,  $M(z)$  is a scalar  $R(z)$ .

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- An L-stable method is A-stable and, in addition,

$$R(\infty) = 0.$$

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A general linear method is said to have

“Runge–Kutta stability”

if the stability matrix for the method  $M(z)$  has characteristic polynomial of the form

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This means that the method has exactly the same stability region as a Runge–Kutta method whose stability function is  $R(z)$ .

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We will give just two examples.

The following third order method is explicit and suitable for the solution of non-stiff problems

$$\begin{bmatrix} AU \\ BV \end{bmatrix} = \left[ \begin{array}{cccc|cccc} 0 & 0 & 0 & 0 & 1 & \frac{1}{4} & \frac{1}{32} & \frac{1}{384} \\ -\frac{176}{1885} & 0 & 0 & 0 & 1 & \frac{2237}{3770} & \frac{2237}{15080} & \frac{2149}{90480} \\ -\frac{335624}{311025} & \frac{29}{55} & 0 & 0 & 1 & \frac{1619591}{1244100} & \frac{260027}{904800} & \frac{1517801}{39811200} \\ -\frac{67843}{6435} & \frac{395}{33} & -5 & 0 & 1 & \frac{29428}{6435} & \frac{527}{585} & \frac{41819}{102960} \\ \hline -\frac{67843}{6435} & \frac{395}{33} & -5 & 0 & 1 & \frac{29428}{6435} & \frac{527}{585} & \frac{41819}{102960} \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ \frac{82}{33} & -\frac{274}{11} & \frac{170}{9} & -\frac{4}{3} & 0 & \frac{482}{99} & 0 & -\frac{161}{264} \\ -8 & -12 & \frac{40}{3} & -2 & 0 & \frac{26}{3} & 0 & 0 \end{array} \right]$$

The following fourth order method is implicit, L-stable, and suitable for the solution of stiff problems

$\frac{1}{4}$	0	0	0	0	1	$\frac{3}{4}$	$\frac{1}{2}$	$\frac{1}{4}$	0
$\frac{513}{54272}$	$\frac{1}{4}$	0	0	0	1	$\frac{27649}{54272}$	$\frac{5601}{27136}$	$\frac{1539}{54272}$	$\frac{459}{6784}$
$\frac{3706119}{69088256}$	$\frac{488}{3819}$	$\frac{1}{4}$	0	0	1	$\frac{15366379}{207264768}$	$\frac{756057}{34544128}$	$\frac{1620299}{69088256}$	$\frac{4854}{454528}$
$\frac{32161061}{197549232}$	$\frac{111814}{232959}$	$\frac{134}{183}$	$\frac{1}{4}$	0	1	$\frac{32609017}{197549232}$	$\frac{929753}{32924872}$	$\frac{4008881}{32924872}$	$\frac{174981}{3465776}$
$\frac{135425}{2948496}$	$\frac{641}{10431}$	$\frac{73}{183}$	$\frac{1}{2}$	$\frac{1}{4}$	1	$\frac{367313}{8845488}$	$\frac{22727}{1474248}$	$\frac{40979}{982832}$	$\frac{323}{25864}$
$\frac{135425}{2948496}$	$\frac{641}{10431}$	$\frac{73}{183}$	$\frac{1}{2}$	$\frac{1}{4}$	1	$\frac{367313}{8845488}$	$\frac{22727}{1474248}$	$\frac{40979}{982832}$	$\frac{323}{25864}$
0	0	0	0	1	0	0	0	0	0
$\frac{2255}{2318}$	$\frac{47125}{20862}$	$\frac{447}{122}$	$\frac{11}{4}$	$\frac{4}{3}$	0	$\frac{28745}{20862}$	$\frac{1937}{13908}$	$\frac{351}{18544}$	$\frac{65}{976}$
$\frac{12620}{10431}$	$\frac{96388}{31293}$	$\frac{3364}{549}$	$\frac{10}{3}$	$\frac{4}{3}$	0	$\frac{70634}{31293}$	$\frac{2050}{10431}$	$\frac{187}{2318}$	$\frac{113}{366}$
$\frac{414}{1159}$	$\frac{29954}{31293}$	$\frac{130}{61}$	$-1$	$\frac{1}{3}$	0	$\frac{27052}{31293}$	$\frac{113}{10431}$	$\frac{491}{4636}$	$\frac{161}{732}$

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- Estimate the local truncation error of an alternative method of higher order
- Change the stepsize with little cost and with little impact on stability

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