Scientific Computation and Differential Equations

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The University of Auckland
New Zealand

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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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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

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

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

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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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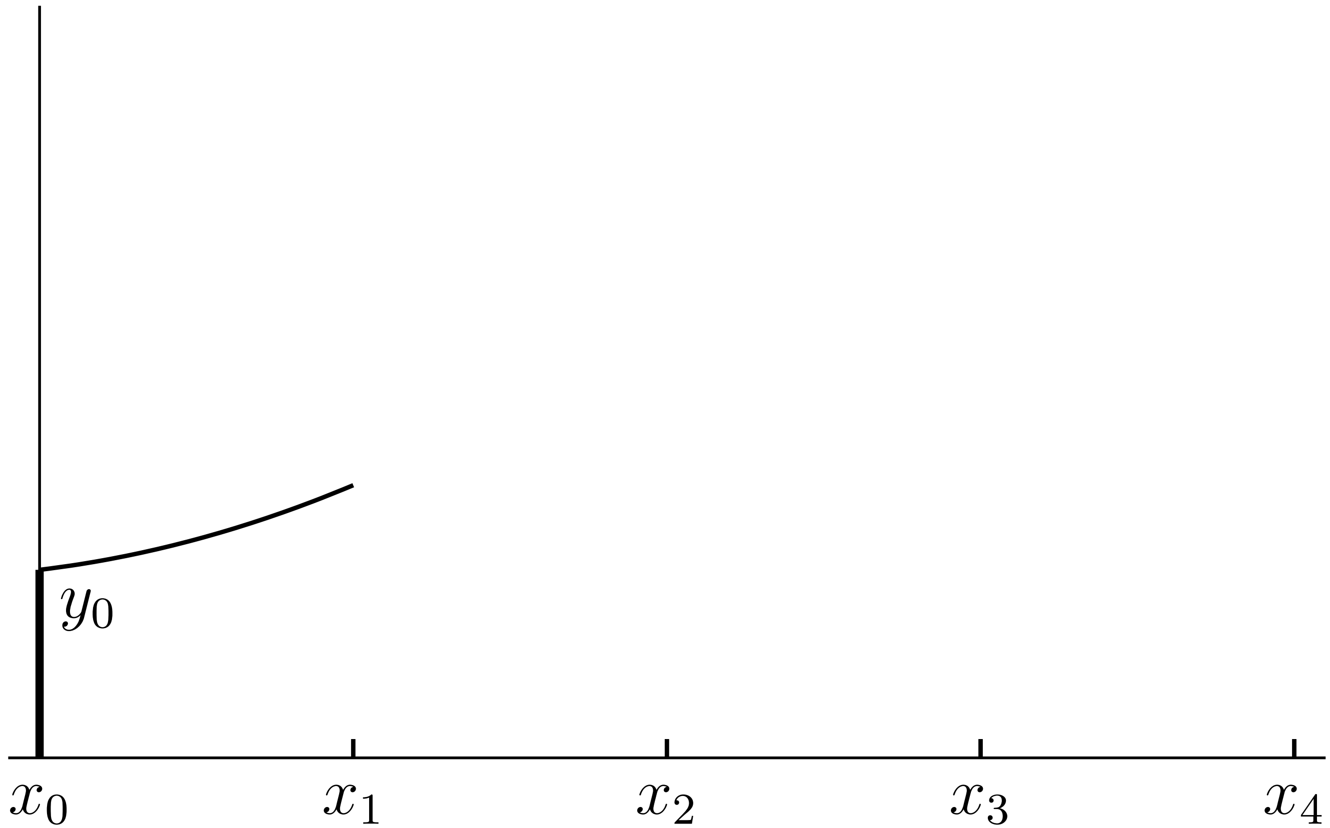

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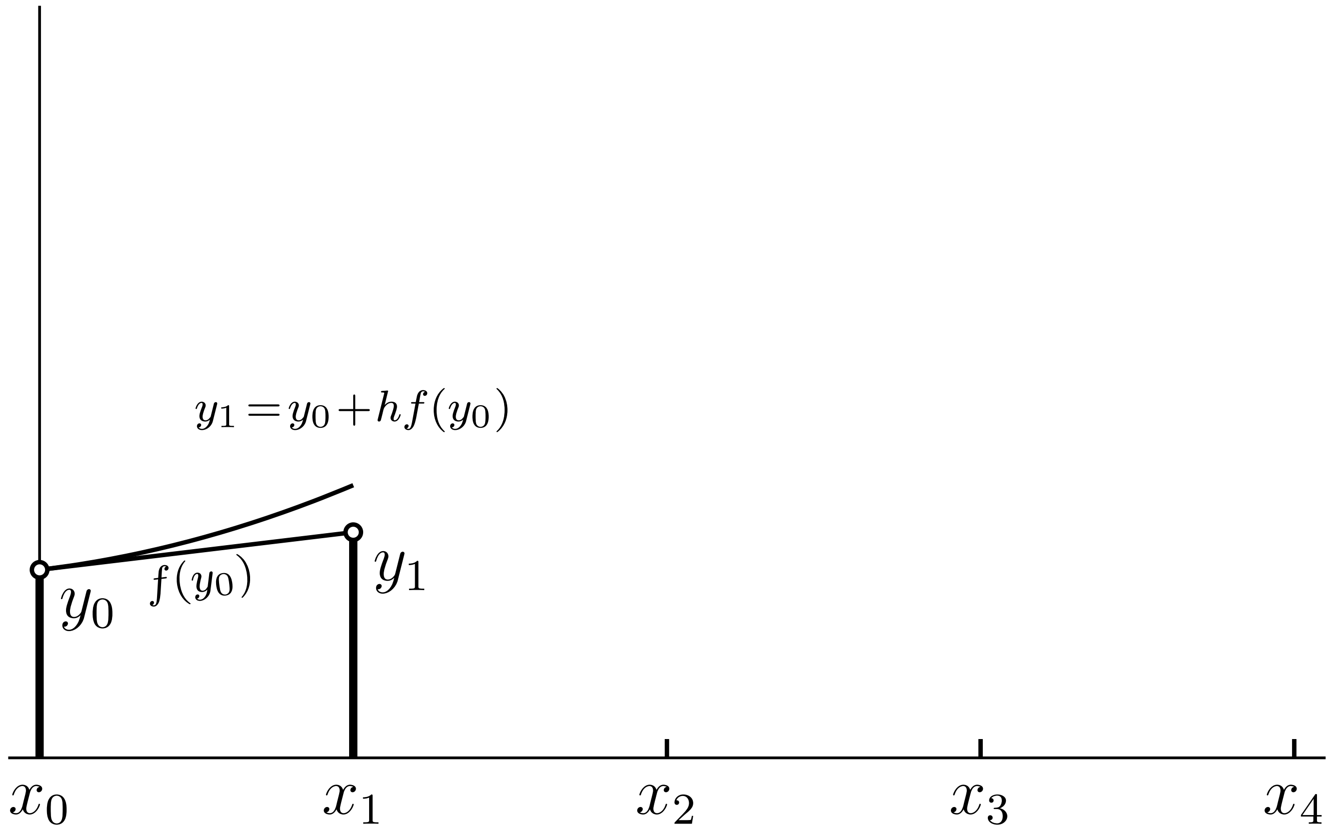

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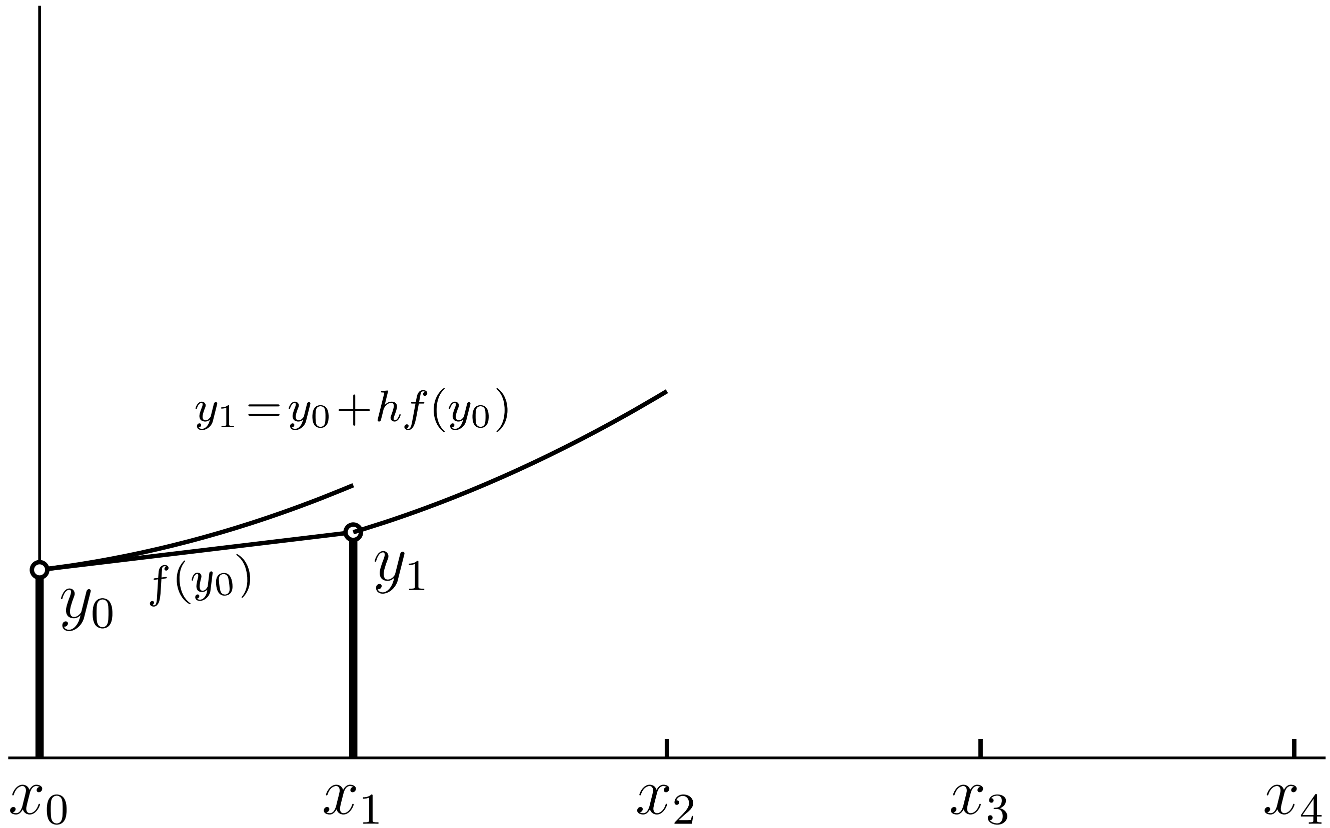

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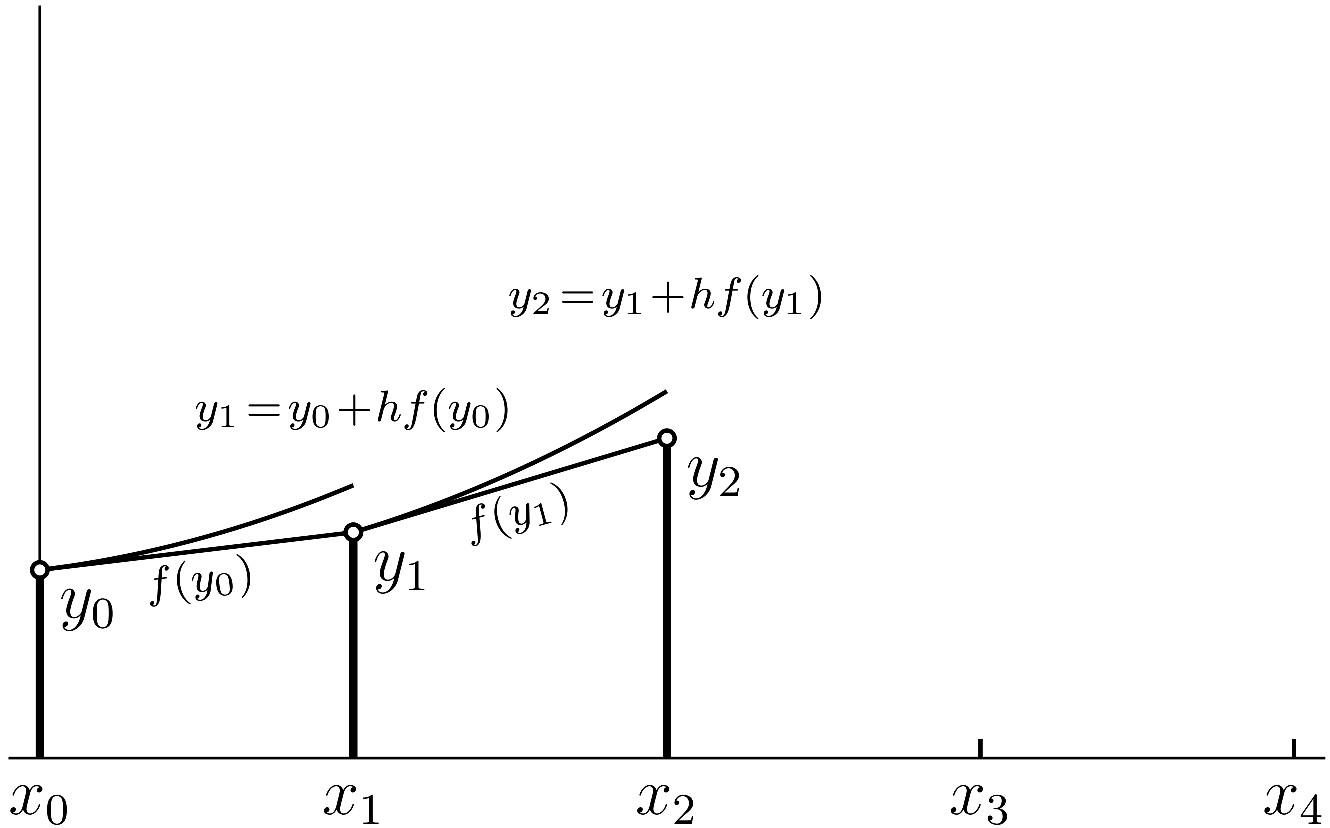

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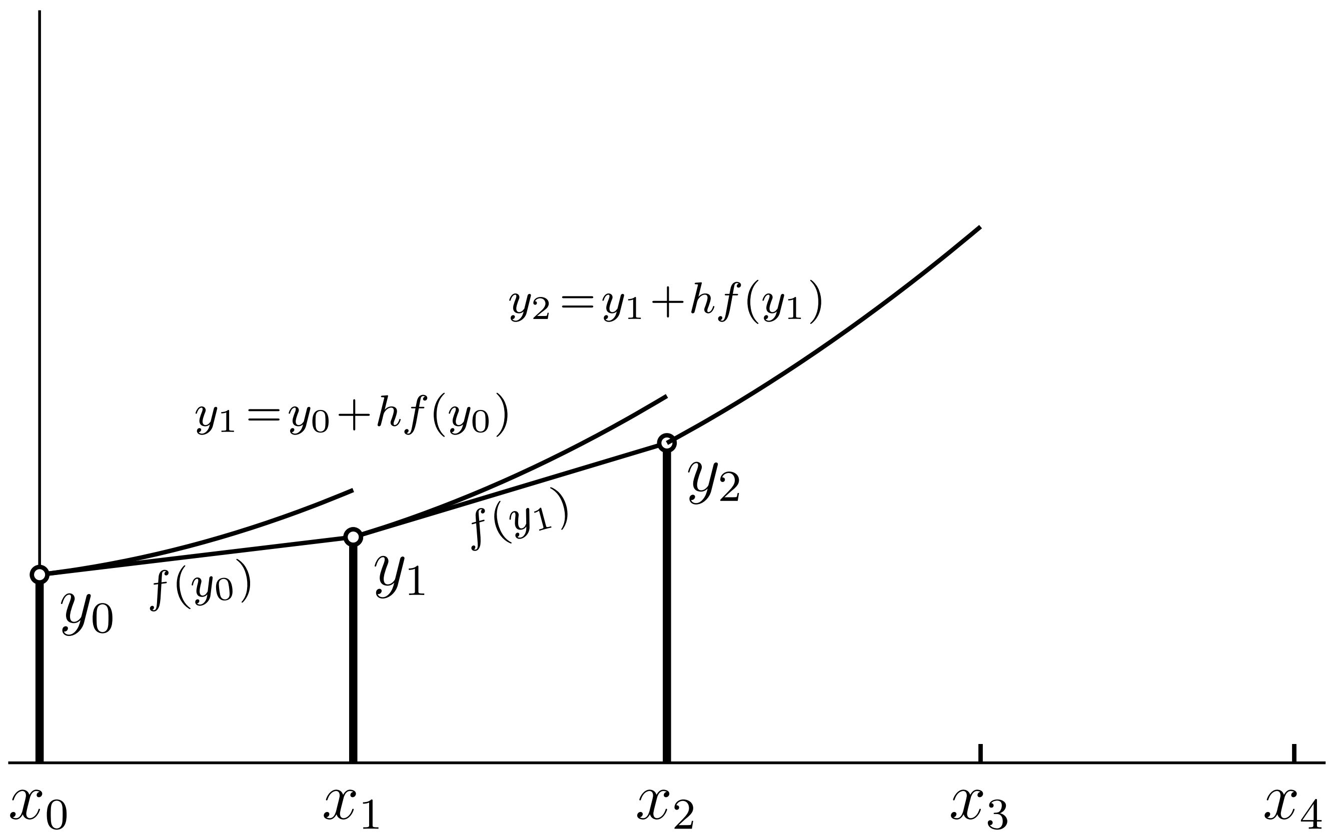

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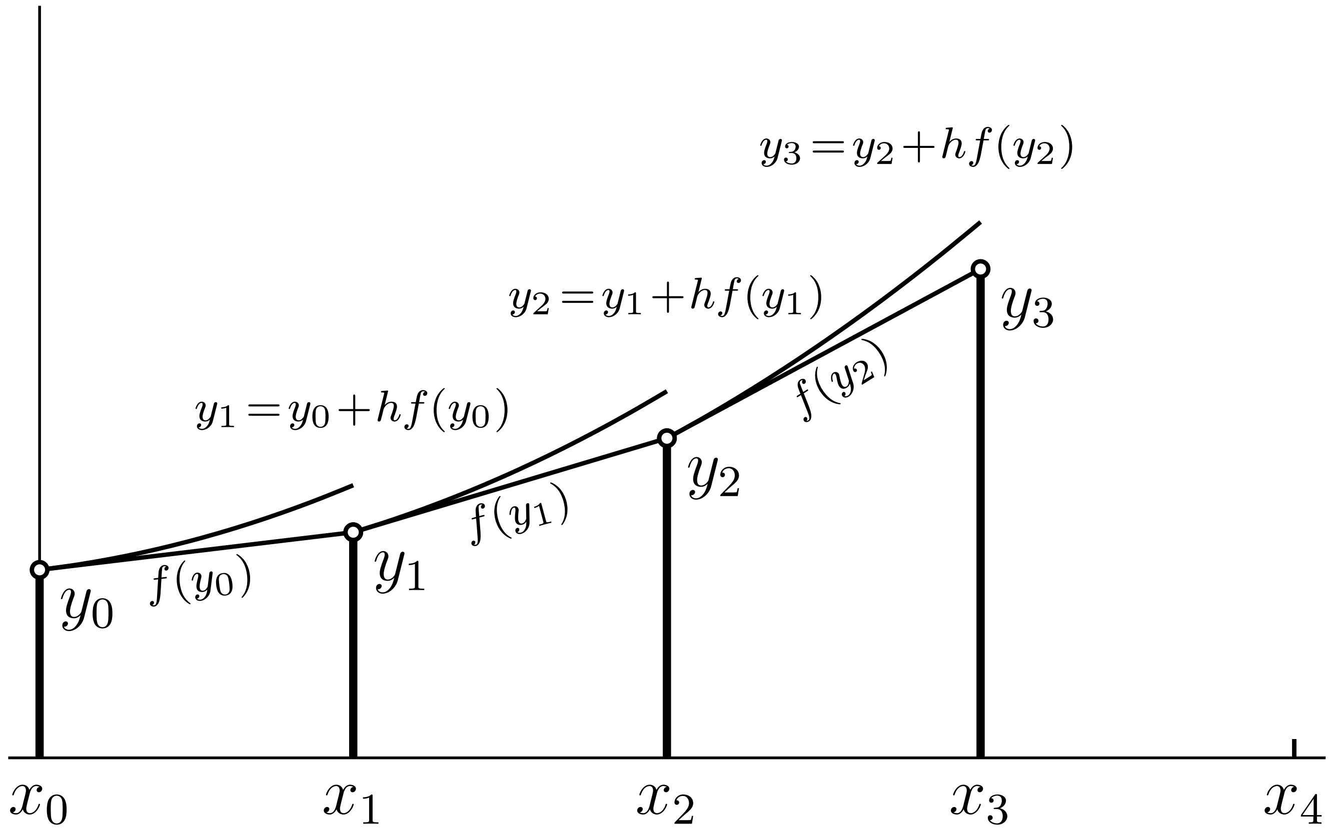

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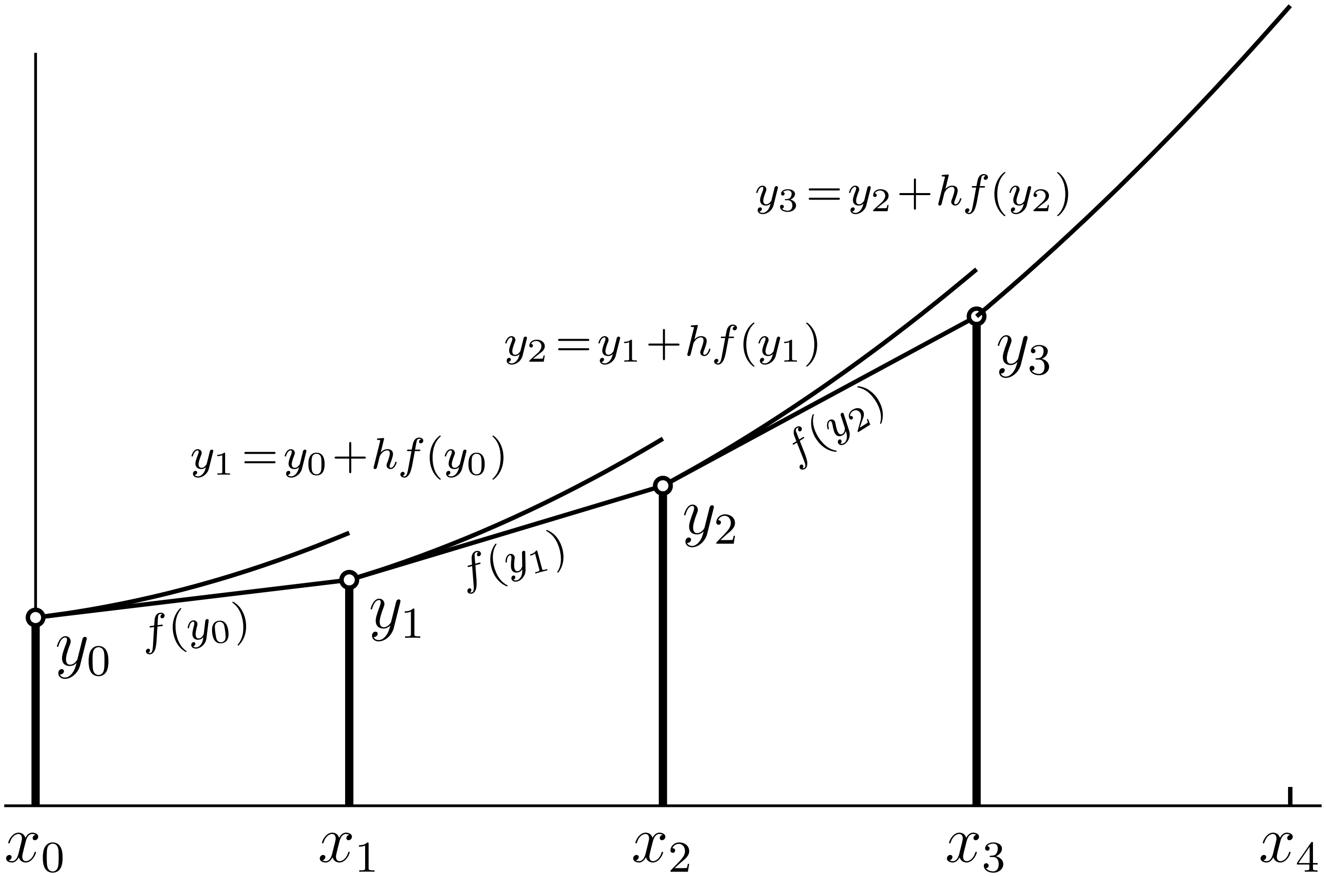

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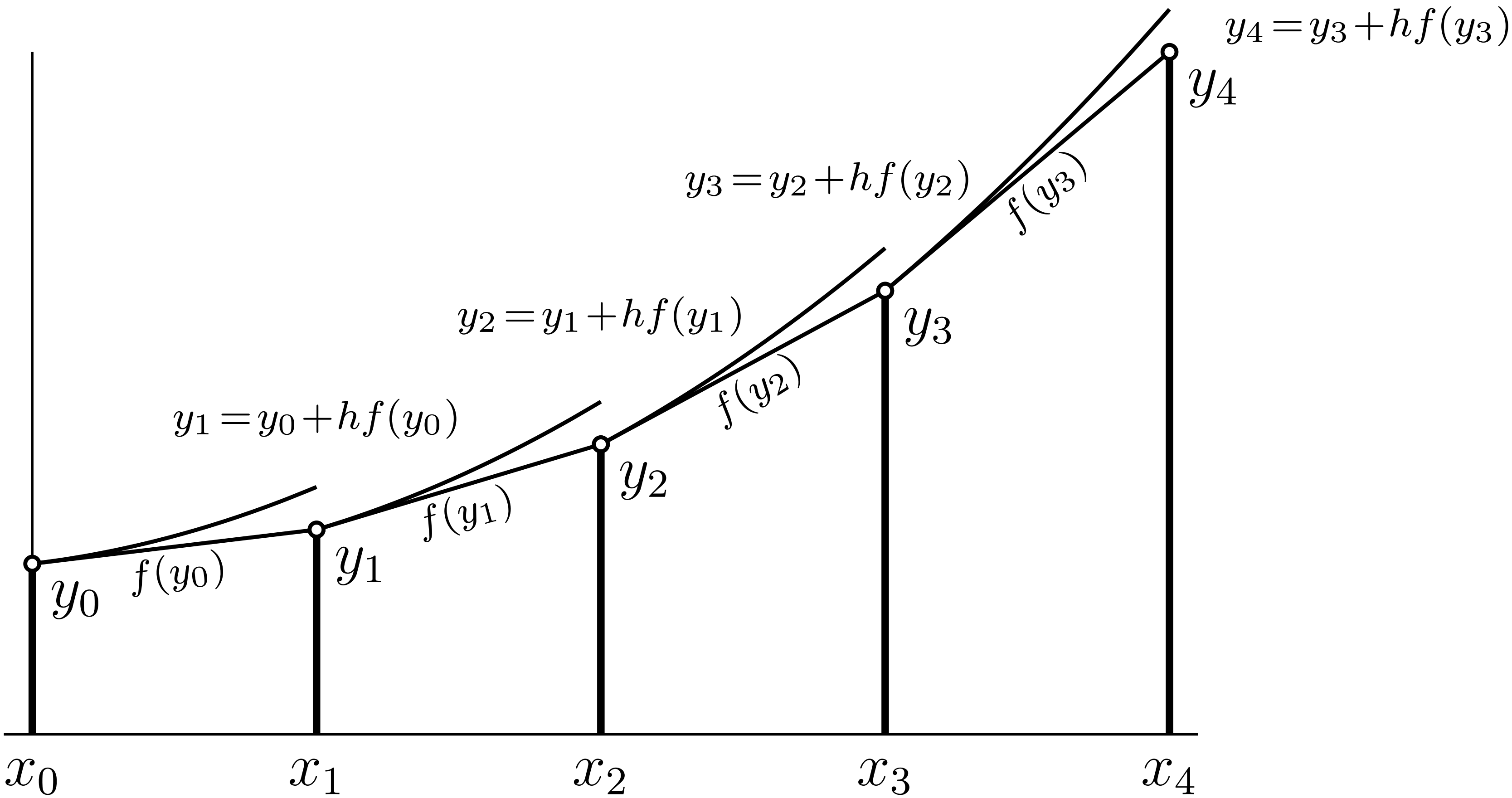

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   – *General linear methods*

Some important dates

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

Linear multistep methods

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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 $y'(x_{n-i})$, $i = 1, 2, \ldots, k$.

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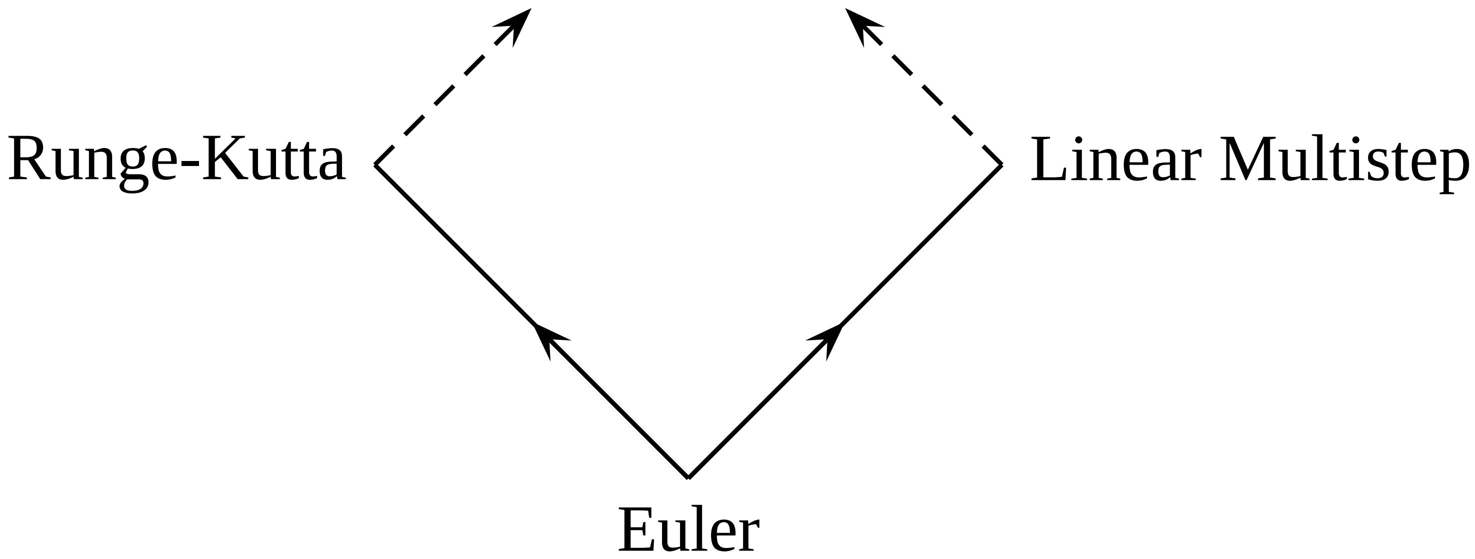
It is natural to ask if there are useful methods which are multistage (as for Runge–Kutta methods) and multivalue (as for linear multistep methods).

In other words, we ask if there is any value in completing this diagram:



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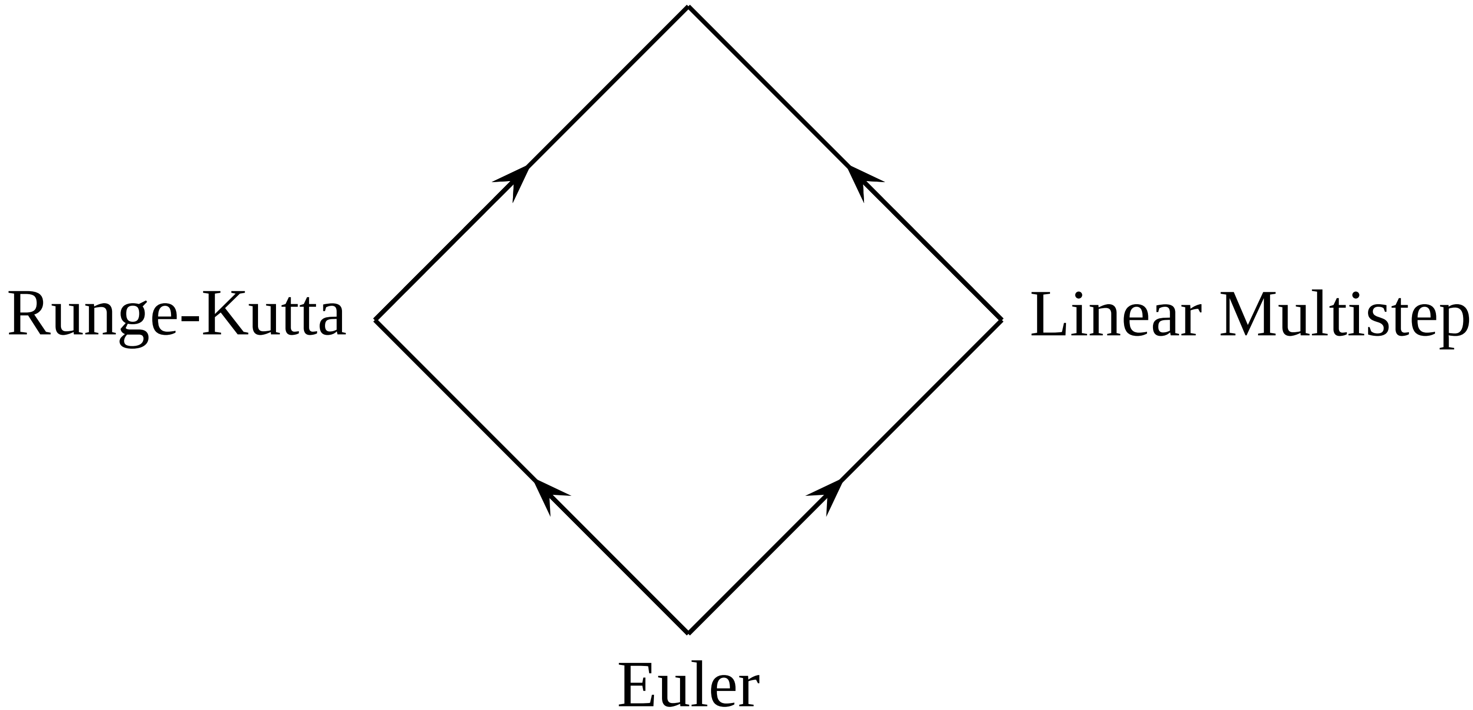

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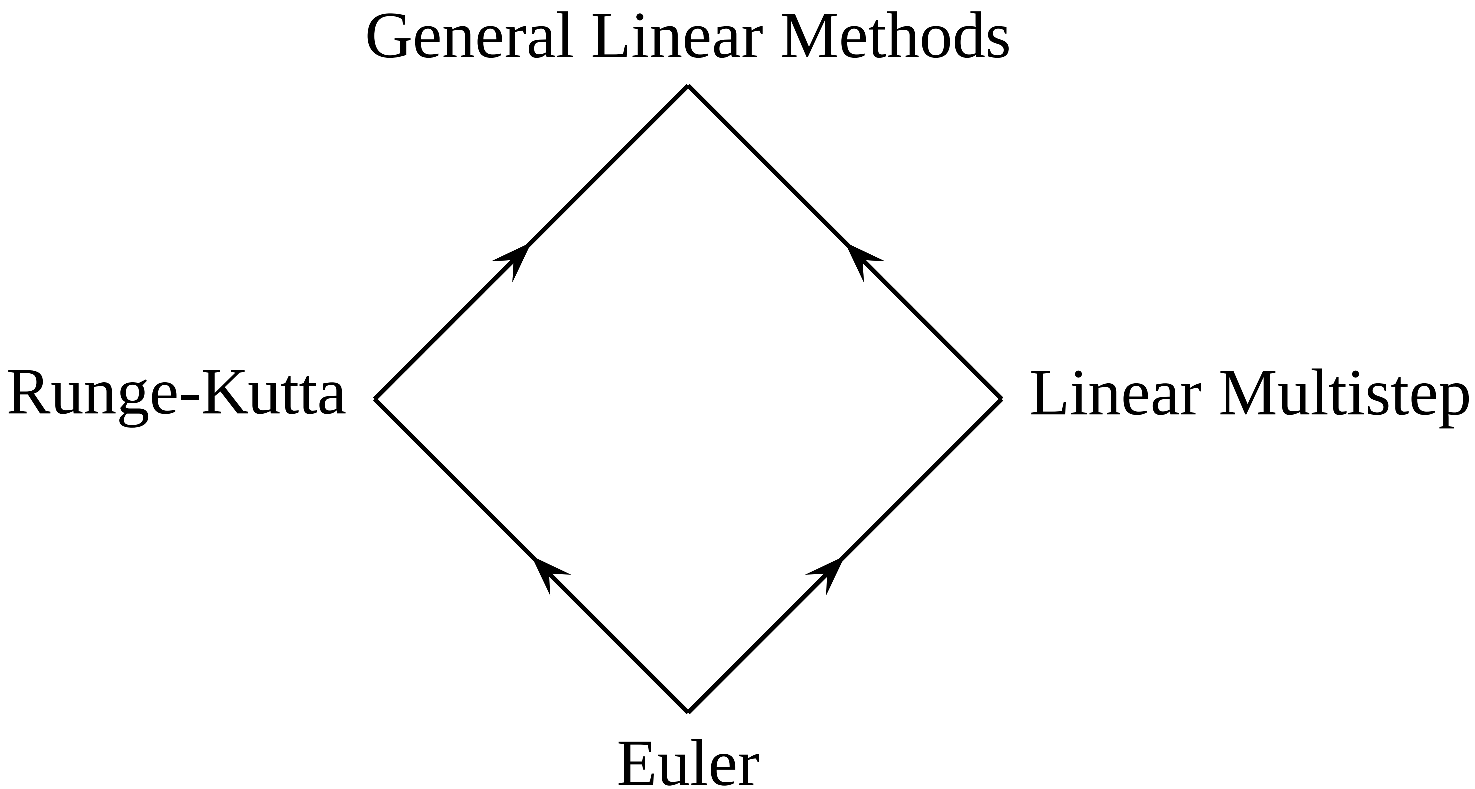

General linear methods

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

$$\begin{array}{cc} & \begin{array}{cc} \overset{s}{\longleftrightarrow} & \overset{r}{\longleftrightarrow} \end{array} \\ \begin{array}{c} s \updownarrow \\ r \updownarrow \end{array} & \left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right] \end{array}.$$

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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 $F_i=f(Y_i)$.

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

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

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To compute the output values, use the formula

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

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

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

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

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

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

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

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Because the derivative at

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

was evaluated in the previous step, we can try re-using this value.

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

was evaluated in the previous step, we can try re-using this value.

This will save one function evaluation.

A ‘re-use’ method

This gives the re-use method

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Why should this method not be preferred to a standard Runge–Kutta method?

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- Stepsize change is complicated and difficult
- 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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$$
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\hline
0 & \frac{2}{3} & \frac{1}{6} & 0 & 1 & \frac{1}{6} & 0 \\
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with

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

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- It has the same stability region as for a genuine Runge–Kutta method
- 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

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

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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'.

A modified linear multistep method

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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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$$\begin{aligned} y_n &= \tfrac{32}{31}y_{n-1} - \tfrac{1}{31}y_{n-2} \\ &\quad + h\Big(\tfrac{64}{93}f(y^*_{n-\frac{1}{2}}) + \tfrac{5}{31}f(y^*_n) + \tfrac{4}{31}f(y_{n-1}) - \tfrac{1}{93}f(y_{n-2})\Big). \end{aligned}$$

Order of general linear methods

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We want to understand order in a similar general way.

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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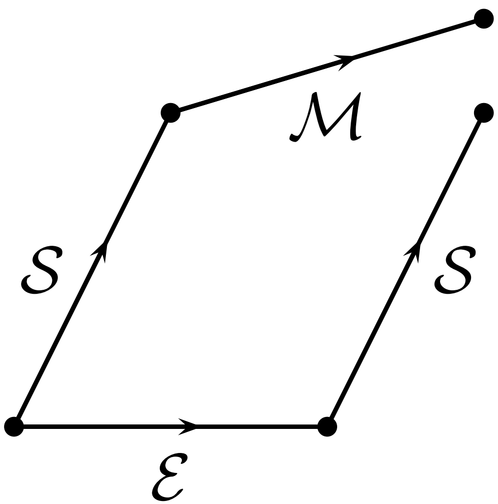
The order of accuracy of a multivalue method is defined in terms of the diagram



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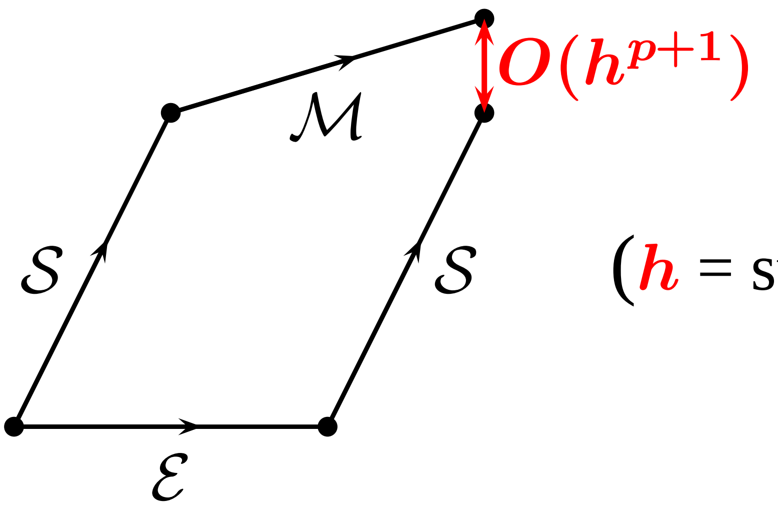

(h = stepsize)

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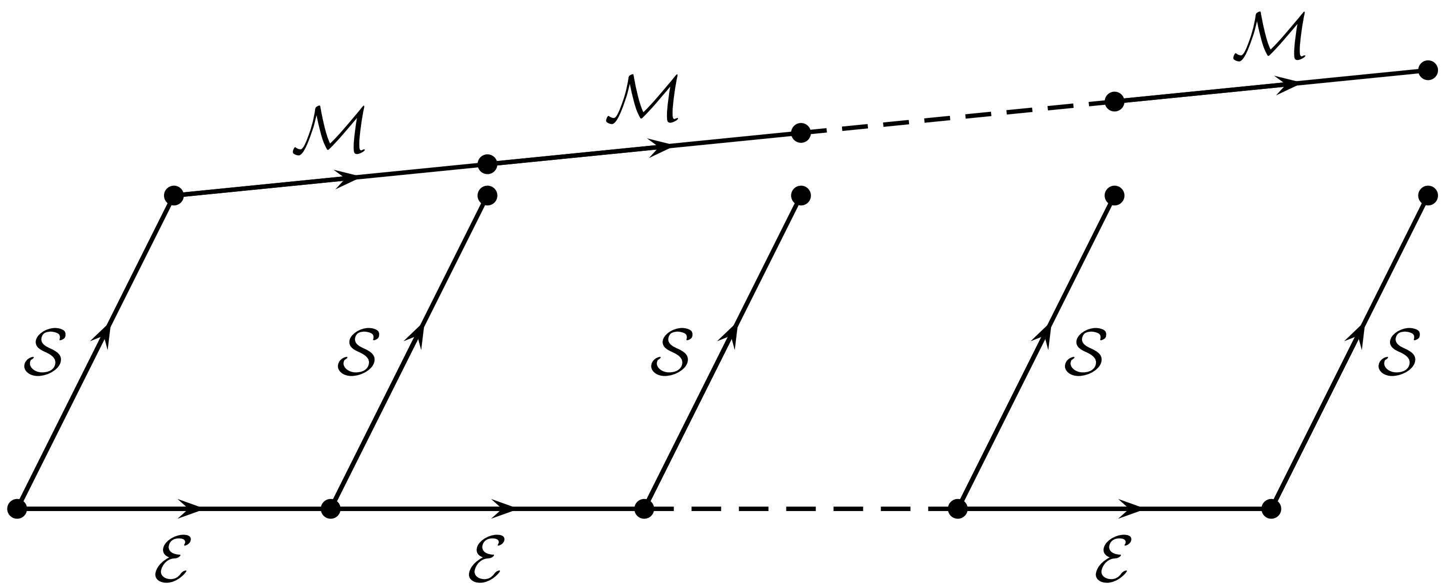

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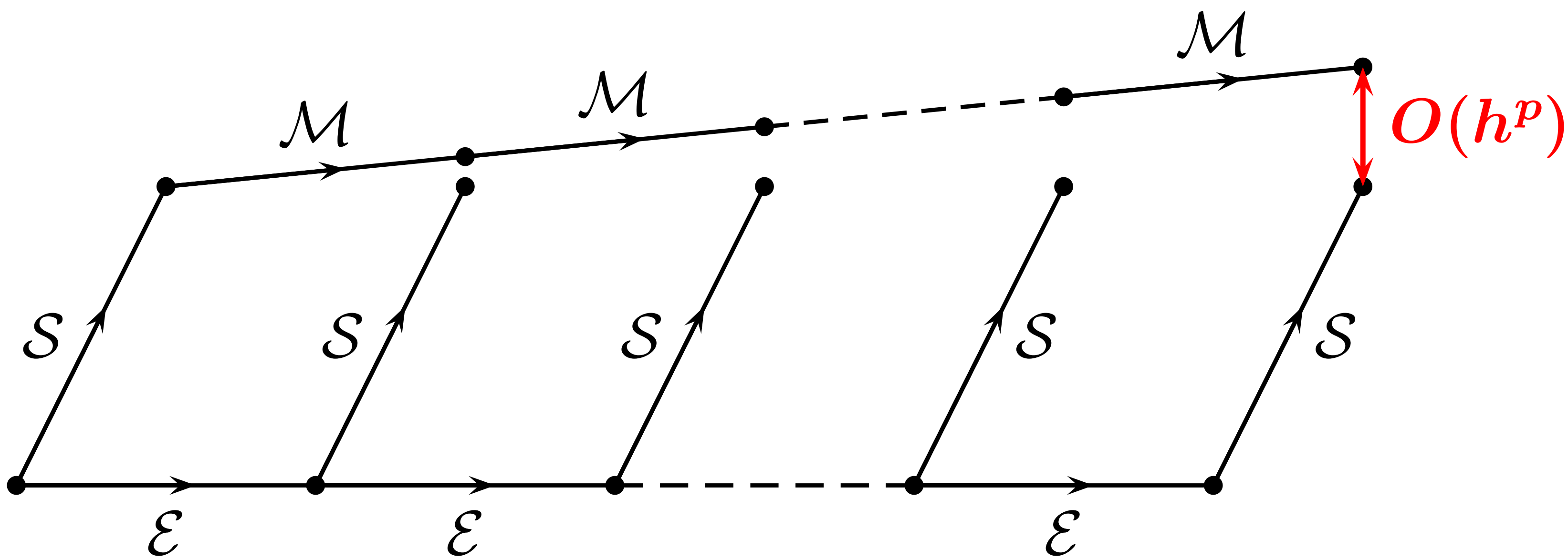

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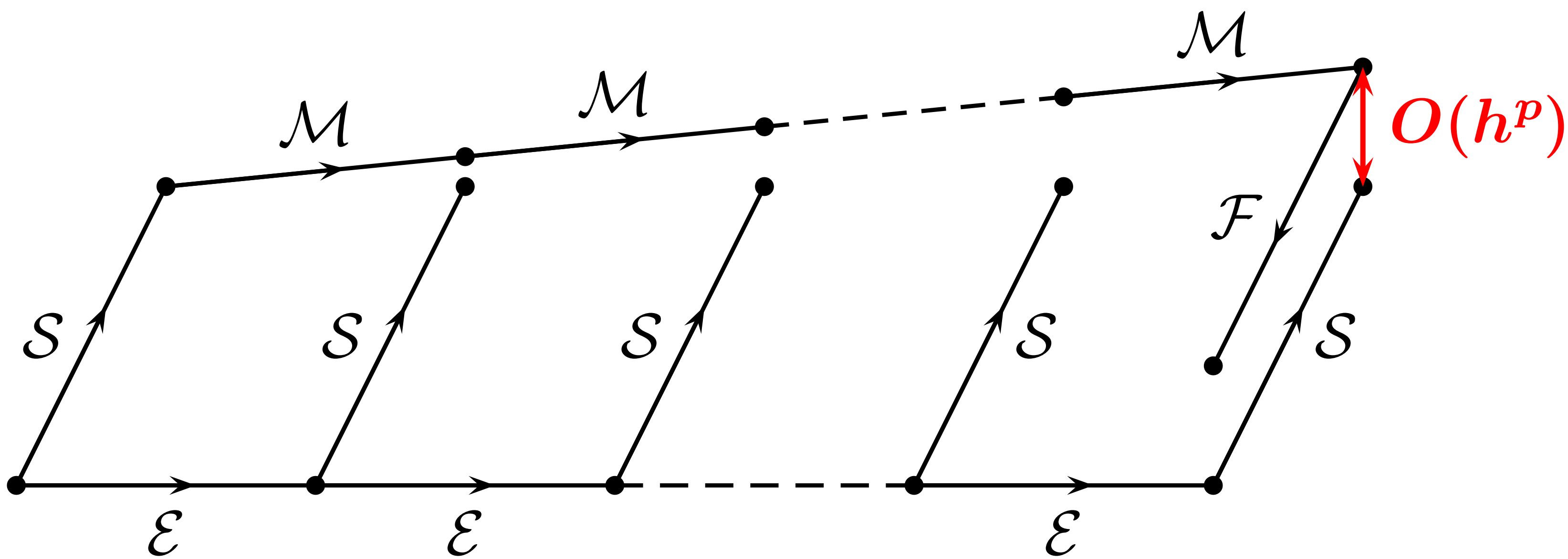

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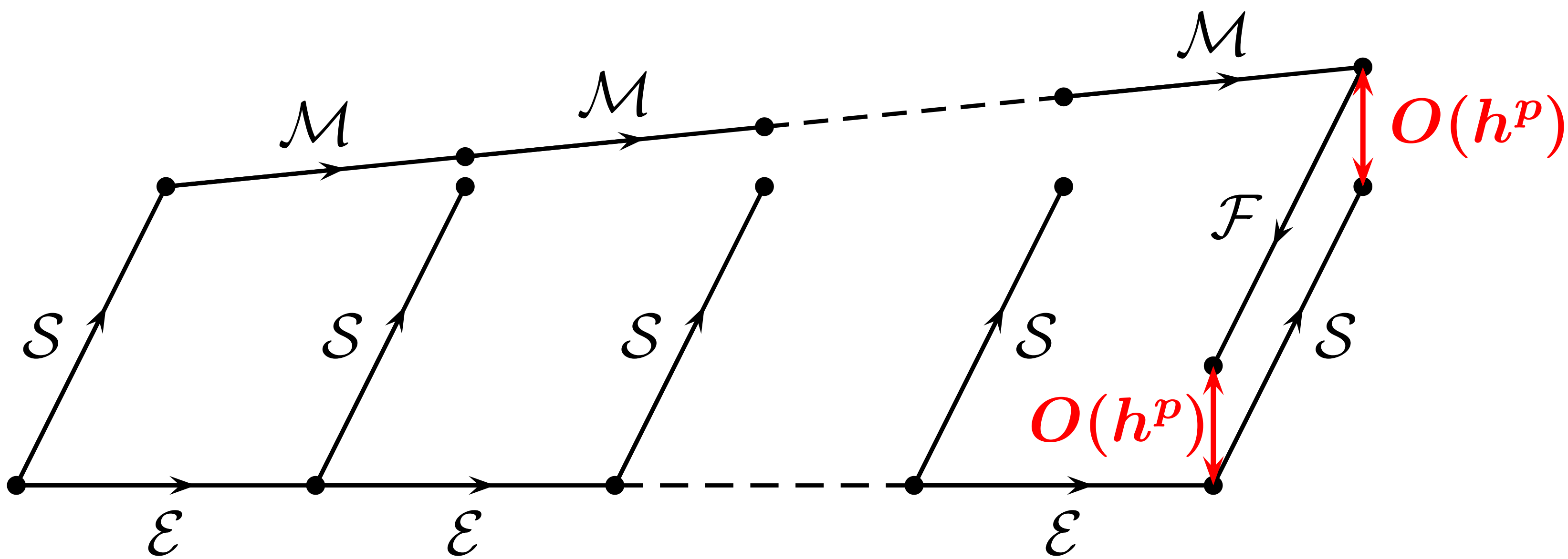

Methods with the IRK Stability property

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$$M(z) = V + zB(I - zA)^{-1}U.$$

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

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- For an A-stable method,

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

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

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

$$\det(wI - M(z)) = w^{r-1}(w - R(z)).$$

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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

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

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- Change the stepsize with little cost and with little impact on stability

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