TMC: Ordinary Differential Equations

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Ordinary Differential Equations

Equations which are composed of an unknown function and its derivatives are called *differential equations*.

Differential equations play a fundamental role in engineering because many physical phenomena are best formulated mathematically in terms of their rate of change.

$$\frac{dv}{dt} = g - \frac{c}{m}v$$

v- dependent variable

t- independent variable

ODE & PDE

When a function involves one dependent variable, the equation is called an *ordinary differential equation (or ODE).* A *partial differential equation (or PDE)* involves two or more independent variables.

Differential equations are also classified as to their order.

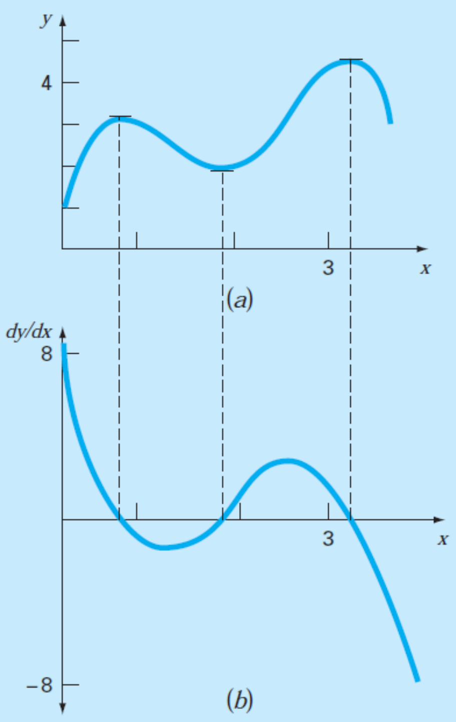
A first order equation includes a first derivative as its highest derivative.

A second order equation includes a second derivative.

Higher order equations can be reduced to a system of first order equations, by redefining a variable.

Mathematical Background

A solution of an ordinary differential equation is a specific function of the independent variable and parameters that satisfies the original differential equation.



To illustrate this concept, let us start with a given function

$$y = -0.5x^4 + 4x^3 - 10x^2 + 8.5^x + 1 \ (1)$$

which is a fourth-order polynomial. Now, if we differentiate Eq. (1), we obtain an ODE:

$$\frac{dy}{dx} = -2x^3 + 12x^2 - 20x + 8.5 \ (2)$$

This equation also describes the behavior of the polynomial, but in a manner different from Eq. (1). Rather than explicitly representing the values of y for each value of x, Eq. (2) gives the rate of change of y with respect to x (that is, the slope) at every value of x.

Mathematical Background

We can determine a differential equation given the original function, the object here is to determine the original function given the differential equation.

$$y = \int (-2x^3 + 12x^2 - 20x + 8.5)\, dx$$

Applying the integration rule

$$\int u^n\, du = \frac{u^{n+1}}{n+1} + C \qquad n \neq -1$$

to each term of the equation gives the solution

$$y = -0.5x^4 + 4x^3 - 10x^2 + 8.5x + C \text{ (3)}$$

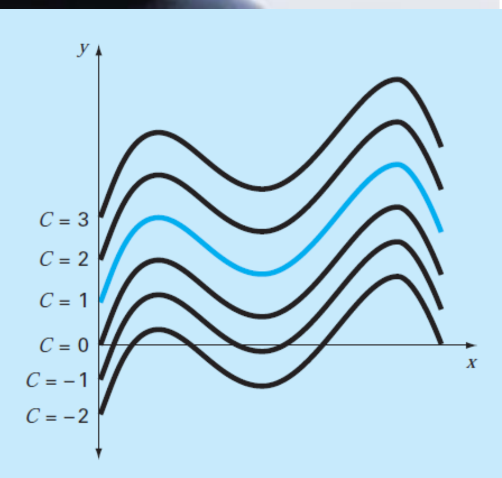
Where C is called a constant of integration.

Eq. (3) could be accompanied by *the initial condition* that at x = 0, y = 1. These values could be substituted into Eq. (3):

1 = −0.5(0)4 + 4(0)3 − 10(0)2 + 8.5(0) + C (4)

to determine C = 1. Therefore, the unique solution that satisfies both the differential equation and the specified initial condition is obtained by substituting C = 1 into Eq. (3) to yield

y = −0.5x4 + 4x3 − 10x2 + 8.5x + 1



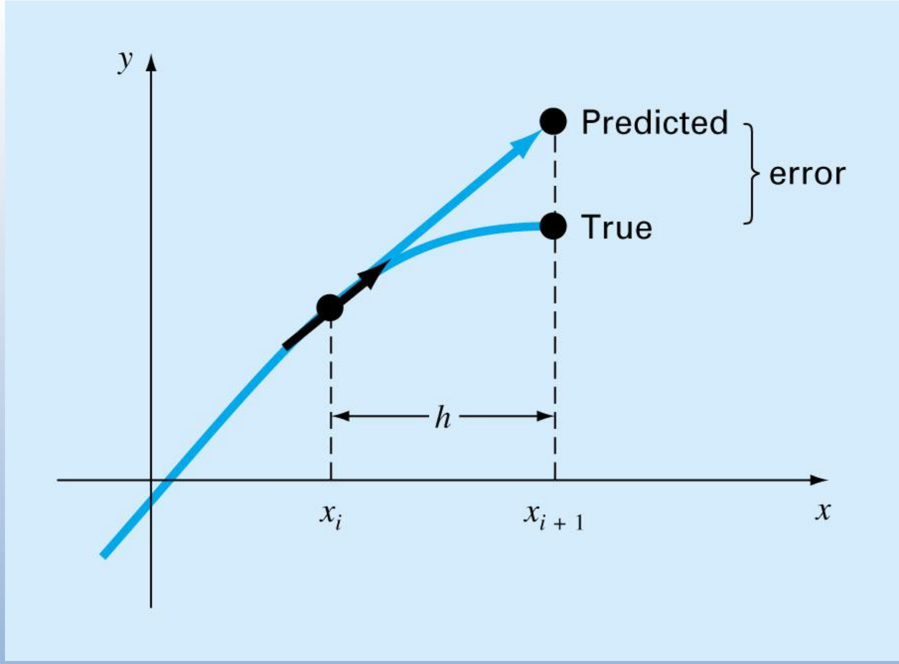
PART A

RUNGE-KUTTA METHODS

Runge-Kutta Methods

This section is devoted to solving ordinary differential equations of the form

$$\frac{dy}{dx} = f(x, y)$$



Euler's method

Euler's method

The *first derivative* provides a direct estimate of the slope at x_i

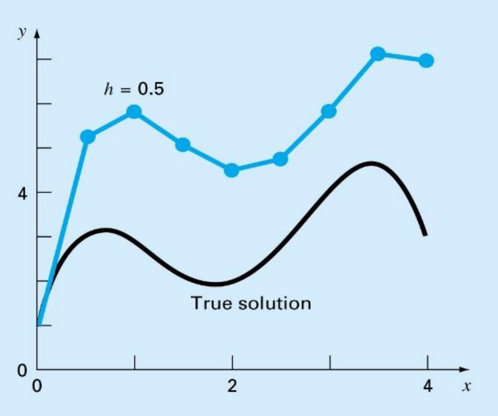
$$\phi = f(x_i, y_i)$$

where $f(x_i,y_i)$ is the differential equation evaluated at x_i and y_i. This estimate can be substituted into the equation:

$$y_{i+1} = y_i + f(x_i, y_i)h$$

A new value of y is predicted using the slope to extrapolate linearly over the step size h.

Example #1



Use Euler's method to numerically integrate :

$$\frac{dy}{dx} = -2x^3 + 12x^2 - 20x + 8.5$$

from x = 0 to x = 4 with a step size of 0.5. The initial condition at x=0 is y=1.
Recall that the exact solution is given by:

$$y = -0.5x^4 + 4x^3 - 10x^2 + 8.5x + 1$$

We have

$$y(x_{i+1}) = y(x_i) + \frac{dy}{dx}h = y(x_i) + f(x_i, yi)h$$

where h=0.5

			Percent Relative Error	
x	**y_{true}**	**y_{Euler}**	**Global**	**Local**
0.0	1.00000	1.00000		
0.5	3.21875	5.25000	−63.1	−63.1
1.0	3.00000	5.87500	−95.8	−28.0
1.5	2.21875	5.12500	131.0	−1.41
2.0	2.00000	4.50000	−125.0	20.5
2.5	2.71875	4.75000	−74.7	17.3
3.0	4.00000	5.87500	46.9	4.0
3.5	4.71875	7.12500	−51.0	−11.3
4.0	3.00000	7.00000	−133.3	−53.0

Error Analysis for Euler's Method

Numerical solutions of ODEs involves two types of error:

Truncation error

Local truncation error

$$E_a = \frac{f'(x_i, y_i)}{2!} h^2$$

$$E_a = O(h^2)$$

Propagated truncation error

The sum of the two is the *total or global truncation error*

Round-off errors

Improvements of Euler's method

A fundamental source of error in Euler's method is that *the derivative at the beginning of the interval* is assumed to apply across the entire interval.

Two simple modifications are available to circumvent this shortcoming:

Heun's Method

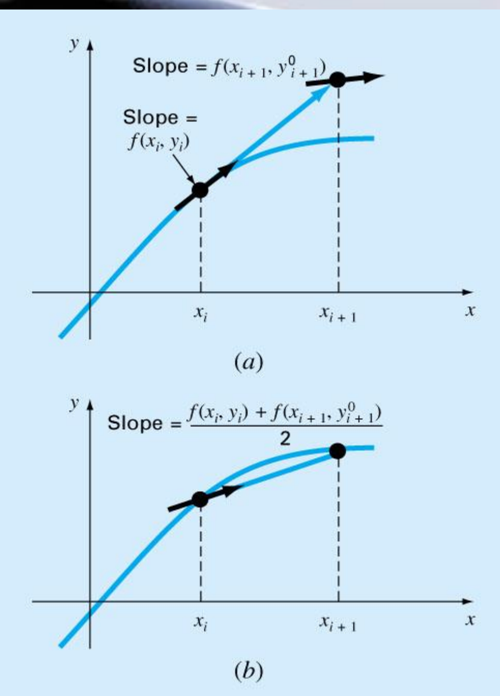
The Midpoint (or Improved Polygon) Method

Heun's Method

One method to *improve the estimate of the slope* involves the determination of two derivatives for the interval:

At the initial point

At the end point



The two derivatives are then averaged to obtain an improved estimate of the slope for the entire interval.

$$\text{Predictor}: \quad y^0_{i+1} = y_i + f(x_i, y_i)h$$

$$\text{Corrector}: \quad y_{i+1} = y_i + \frac{f(x_i, y_i) + f(x_{i+1}, y^0_{i+1})}{2}h$$

$$|\varepsilon_a| = \left| \frac{y^j_{i+1} - y^{j-1}_{i+1}}{y^j_{i+1}} \right| 100\% \qquad E_t = -\frac{f''(\xi)}{12}h^3$$

where y^{j-1}_{i+1} and y^j_{i+1} are the result from the prior and the present iteration of the corrector, respectively.

Example #2

Use Heun's method to integrate $y' = 4e^{0.8x} - 0.5y$ from x=0 to x=4 with a step size of 1. The initial condition at x=0 is y=2.

First, the slope at (x_0, y_0) is calculated as

$y'0 = 4e^{0} - 0.5(2) = 3$

This result is quite different from the actual average slope for the interval from 0 to 1.0, which is equal to 4.1946

Now, to improve the estimate for y_{i+1}, we use the value $y^0{}_1$ to predict the slope at the end of the interval

$y'1 = f(x_1, y^0{}_1) = 4e^{0.8(1)} - 0.5(5) = 6.402164$

which can be combined with the initial slope to yield an average slope over the interval from x = 0 to 1

$$y' = \frac{3 + 6.402164}{2} = 4.701082$$

which is closer to the true average slope of 4.1946. This result can then be substituted into the corrector equation to give the prediction at x = 1

$y_1 = 2 + 4.701082(1) = 6.701082$

which represents a percent relative error of −8.18%.

Now this estimate can be used to refine or correct the prediction of y_1 by substituting the new result back into the right-hand side of the corrector equation:

$$y_1 = 2 + \frac{[3 + 4e^{0.8(1)} - 0.5(6.701082)]}{2}1 = 6.275811$$

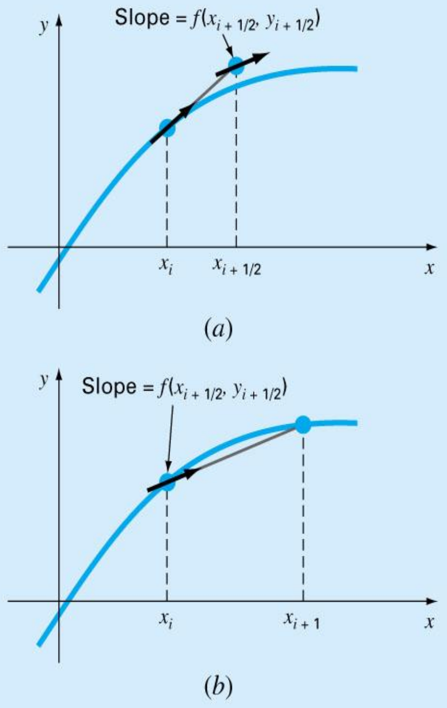
which represents an absolute percent relative error of 1.31 percent. This result, in turn, can be substituted back into the corrector equation to further correct:

$$y_1 = 2 + \frac{[3 + 4e^{0.8(1)} - 0.5(6.275811)]}{2}1 = 6.382129$$

which represents an $|\varepsilon_t|$ of 3.03%.

		Iterations of Heun's Method			
		1		15	
x	y_{true}	y_{Heun}	$\lvert\varepsilon_t\rvert$ (%)	y_{Heun}	$\lvert\varepsilon_t\rvert$ (%)
0	2.0000000	2.0000000	0.00	2.0000000	0.00
1	6.1946314	6.7010819	8.18	6.3608655	2.68
2	14.8439219	16.3197819	9.94	15.3022367	3.09
3	33.6771718	37.1992489	10.46	34.7432761	3.17
4	75.3389626	83.3377674	10.62	77.7350962	3.18

The Midpoint (or Improved Polygon) Method



Uses Euler’s method to predict a value of y at the midpoint of the interval:

$$y_{i+1} = y_i + f(x_{i+1/2}, y_{i+1/2})h$$

Runge-Kutta Methods (RK)

Runge-Kutta methods achieve the accuracy of a Taylor series approach without requiring the calculation of higher derivatives.

$$y_{i+1} = y_i + \phi(x_i, y_i, h)h$$

$$\phi = a_1 k_1 + a_2 k_2 + \cdots + a_n k_n$$

$$a's = \text{constants}$$

$$k_1 = f(x_i, y_i)$$

$$k_2 = f(x_i + p_1 h, y_i + q_{11} k_1 h)$$

$$k_3 = f(x_i + p_2 h, y_i + q_{21} k_1 h + q_{22} k_2 h)$$

$$\vdots$$

$$k_n = f(x_i + p_{n-1} h, y_i + q_{n-1} k_1 h + q_{n-1,2} k_2 h + \cdots + q_{n-1,n-1} k_{n-1} h)$$

Second-Order Runge-Kutta Methods

k's are recurrence functions. Because each *k* is a functional evaluation, this recurrence makes RK methods efficient for computer calculations.

Various types of RK methods can be devised by employing different number of terms in the increment function as specified by *n*.

First order RK method with *n=1* is in fact *Euler's method*.

The second-order version of RK method is

$$y_{i+1} = y_i + (a_1 k_1 + a_2 k_2)h$$

$$k_1 = f(x_i, y_i)$$

$$k_2 = f(x_i + p_1 h, y_i + q_{11} k_1 h)$$

Derivation of the Second-Order Runge-Kutta Methods

The second-order version of Eq. (25.28) is

$$y_{i+1} = y_i + (a_1 k_1 + a_2 k_2)h \tag{B25.1.1}$$

where

$$k_1 = f(x_i, y_i) \tag{B25.1.2}$$

and

$$k_2 = f(x_i + p_1 h, y_i + q_{11} k_1 h) \tag{B25.1.3}$$

To use Eq. (B25.1.1) we have to determine values for the constants a_1, a_2, p_1, and q_{11}. To do this, we recall that the second-order Taylor series for y_{i+1} in terms of y_i and $f(x_i, y_i)$ is written as [Eq. (25.11)]

$$y_{i+1} = y_i + f(x_i, y_i)h + \frac{f'(x_i, y_i)}{2!}h^2 \tag{B25.1.4}$$

where $f'(x_i, y_i)$ must be determined by chain-rule differentiation (Sec. 25.1.3):

$$f'(x_i, y_i) = \frac{\partial f(x, y)}{\partial x} + \frac{\partial f(x, y)}{\partial y}\frac{dy}{dx} \tag{B25.1.5}$$

Substituting Eq. (B25.1.5) into (B25.1.4) gives

$$y_{i+1} = y_i + f(x_i, y_i)h + \left(\frac{\partial f}{\partial x} + \frac{\partial f}{\partial y}\frac{dy}{dx}\right)\frac{h^2}{2!} \tag{B25.1.6}$$

The basic strategy underlying Runge-Kutta methods is to use algebraic manipulations to solve for values of a_1, a_2, p_1, and q_{11} that make Eqs. (B25.1.1) and (B25.1.6) equivalent.

To do this, we first use a Taylor series to expand Eq. (25.1.3). The Taylor series for a two-variable function is defined as [recall Eq. (4.26)]

$$g(x + r, y + s) = g(x, y) + r\frac{\partial g}{\partial x} + s\frac{\partial g}{\partial y} + \cdots$$

Applying this method to expand Eq. (B25.1.3) gives

$$f(x_i + p_1 h, y_i + q_{11} k_1 h) = f(x_i, y_i) + p_1 h\frac{\partial f}{\partial x} + q_{11} k_1 h\frac{\partial f}{\partial y} + O(h^2)$$

This result can be substituted along with Eq. (B25.1.2) into Eq. (B25.1.1) to yield

$$y_{i+1} = y_i + a_1 h f(x_i, y_i) + a_2 h f(x_i, y_i) + a_2 p_1 h^2 \frac{\partial f}{\partial x} + a_2 q_{11} h^2 f(x_i, y_i)\frac{\partial f}{\partial y} + O(h^3)$$

or, by collecting terms,

$$y_{i+1} = y_i + [a_1 f(x_i, y_i) + a_2 f(x_i, y_i)]h + \left[a_2 p_1 \frac{\partial f}{\partial x} + a_2 q_{11} f(x_i, y_i)\frac{\partial f}{\partial y}\right]h^2 + O(h^3) \tag{B25.1.7}$$

Now, comparing like terms in Eqs. (B25.1.6) and (B25.1.7), we determine that for the two equations to be equivalent, the following must hold:

$$a_1 + a_2 = 1$$

$$a_2 p_1 = \frac{1}{2}$$

$$a_2 q_{11} = \frac{1}{2}$$

These three simultaneous equations contain the four unknown constants. Because there is one more unknown than the number of equations, there is no unique set of constants that satisfy the equations. However, by assuming a value for one of the constants, we can determine the other three. Consequently, there is a family of second-order methods rather than a single version.

Derivation of the Second-Order Runge-Kutta Methods

We can solve for

$$a_1 = 1 - a_2$$

$$p_1 = q_{11} = \frac{1}{2a_2}$$

Because we can choose an infinite number of values for a_2, there are an infinite number of second-order RK methods.

Heun Method with a Single Corrector (a_2=1/2)

The Midpoint Method (a_2=1)

Ralston's Method (a_2=2/3)

Heun Method with a Single Corrector

$$a_2 = 1/2$$
$$a_1 = 1/2$$
$$p_1 = q_{11} = 1$$

So,

$$y_{i+1} = y_i + \left(\frac{1}{2}k_1 + \frac{1}{2}k_2\right)h$$

where

$$k_1 = f(xi\,, y_i)$$
$$k_2 = f(xi + h, y_i + k_1 h)$$

Note that k_1 *is the slope at the beginning of the interval* and k_2 *is the slope at the end of the interval*.

Consequently, this second-order Runge-Kutta method is actually *Heun's technique without iteration*.

The Midpoint Method

$$a_2 = 1$$
$$a_1 = 0$$
$$p_1 = q_{11} = 1/2$$

So,

$$y_{i+1} = y_i + k_2 h$$

where

$$k_1 = f(xi\,, y_i)$$
$$k_2 = f(xi + \frac{1}{2}h, y_i + \frac{1}{2}k_1 h)$$

Ralston’s Method

$$a_2 = 2/3$$
$$a_1 = 1/3$$
$$p_1 = q_{11} = 3/4$$

So,

$$y_{i+1} = y_i + \left(\frac{1}{3}k_1 + \frac{2}{3}k_2\right)h$$

where

$$k_1 = f(xi\,, y_i)$$
$$k_2 = f\left(xi + \frac{3}{4}h, y_i + \frac{3}{4}k_1 h\right)$$

Example #3

Use the midpoint method and Ralston’s method to numerically integrate

$$f(x, y) = -2x^3 + 12x^2 - 20x + 8.5$$

from x = 0 to x = 4 using a step size of 0.5. The initial condition at x = 0 is y = 1. Compare the results with the values obtained using another second-order RK algorithm, that is, the Heun method without corrector iteration

For the midpoint method,

$k_1 = -2(0)3 + 12(0)2 - 20(0) + 8.5 = 8.5$

$k_2 = -2(0.25)3 + 12(0.25)2 - 20(0.25) + 8.5 = 4.21875$

$y(0.5) = 1 + 4.21875(0.5) = 3.109375 \qquad \varepsilon_t = 3.4\%$

For Ralston’s method,

$k_1 = -2(0)3 + 12(0)2 - 20(0) + 8.5 = 8.5$

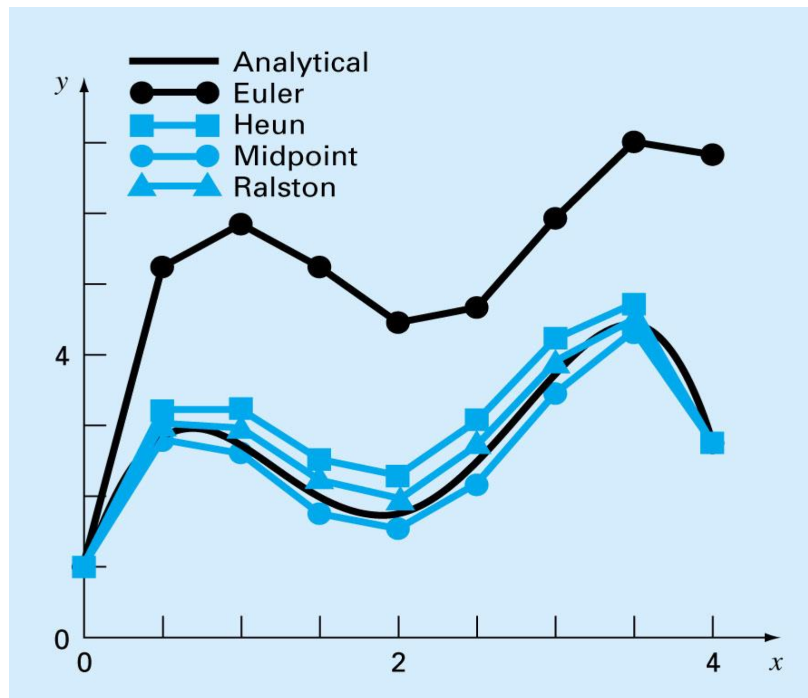
$k_2 = -2(0.375)3 + 12(0.375)2 - 20(0.375) + 8.5 = 2.58203125$

The average slope is computed by

$$\phi = \frac{1}{3}(8.5) + \frac{2}{3}(2.58203125) = 4.5546875$$

$y(0.5) = 1 + 4.5546875(0.5) = 3.27734375 \qquad \varepsilon_t = -1.82\%$

x	y_{true}	Heun		Midpoint		Second-Order Ralston RK	
		y	$\lvert\varepsilon_t\rvert$ (%)	y	$\lvert\varepsilon_t\rvert$ (%)	y	$\lvert\varepsilon_t\rvert$ (%)
0.0	1.00000	1.00000	0	1.00000	0	1.00000	0
0.5	3.21875	3.43750	6.8	3.109375	3.4	3.277344	1.8
1.0	3.00000	3.37500	12.5	2.81250	6.3	3.101563	3.4
1.5	2.21875	2.68750	21.1	1.984375	10.6	2.347656	5.8
2.0	2.00000	2.50000	25.0	1.75	12.5	2.140625	7.0
2.5	2.71875	3.18750	17.2	2.484375	8.6	2.855469	5.0
3.0	4.00000	4.37500	9.4	3.81250	4.7	4.117188	2.9
3.5	4.71875	4.93750	4.6	4.609375	2.3	4.800781	1.7
4.0	3.00000	3.00000	0	3	0	3.031250	1.0



Third-Order Runge-Kutta Methods

$$y_{i\,+\,1} = y_i + (k_1 + 4k_2 + k_3)h$$

where

$$k_1 = f(xi, yi)$$

$$k_2 = f\left(x_i + \frac{1}{2}h, yi + \frac{1}{2}k_1h\right)$$

$$k_3 = f(x_i + h, yi - k_1h + 2k_2h)$$

Fourth-Order Runge-Kutta Methods

$$y_{i+1} = y_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)h$$

where

$$k_1 = f(xi, yi)$$

$$k_2 = f\left(x_i + \frac{1}{2}h, yi + \frac{1}{2}k_1 h\right)$$

$$k_3 = f\left(x_i + \frac{1}{2}h, yi + \frac{1}{2}k_2 h\right)$$

$$k_4 = f(x_i + h, yi + k_3 h)$$

Example #4

(a) Use the classical fourth-order RK method to integrate

$$f(x, y) = -2x^3 + 12x^2 - 20x + 8.5$$

using a step size of h = 0.5 and an initial condition of y = 1 at x = 0.

(b) Similarly, integrate

$$f(x, y) = 4e^{0.8x} - 0.5y$$

using h = 0.5 with y(0) = 2 from x = 0 to 0.5.

(a) For the classical fourth-order RK method,

$k_1 = 8.5,$

$k_2 = 4.21875$

$k_3 = 4.21875$

$k_4 = 1.25$

$$y(0.5) = 1 + \left\{\frac{1}{6}[8.5 + 2(4.21875) + 2(4.21875) + 1.25]\right\} 0.5$$

$$= 3.21875$$

(b) For this case,

$k_1 = f(0, 2) = 4e0.8(0) - 0.5(2) = 3$

$y(0.25) = 2 + 3(0.25) = 2.75$

$k_2 = f(0.25, 2.75) = 4e0.8(0.25) - 0.5(2.75) = 3.510611$

$y(0.25) = 2 + 3.510611(0.25) = 2.877653$

$k_3 = f(0.25, 2.877653) = 4e0.8(0.25) - 0.5(2.877653) = 3.446785$

$y(0.5) = 2 + 3.071785(0.5) = 3.723392$

$k_4 = f(0.5, 3.723392) = 4e0.8(0.5) - 0.5(3.723392) = 4.105603$

$$\phi = \frac{1}{6}[3 + 2(3.510611) + 2(3.446785) + 4.105603] = 3.503399$$

$y(0.5) = 2 + 3.503399(0.5) = 3.751699$

which compares favorably with the true solution of 3.751521.

Butcher’s sixth-order RK method

$$y_{i+1} = y_i + \frac{1}{90}(7k_1 + 32k_3 + 12k_4 + 32k_5 + 7k_6)h$$

where

$$k_1 = f(x_i, y_i)$$

$$k_2 = f\left(x_i + \frac{1}{4}h,\ y_i + \frac{1}{4}k_1 h\right)$$

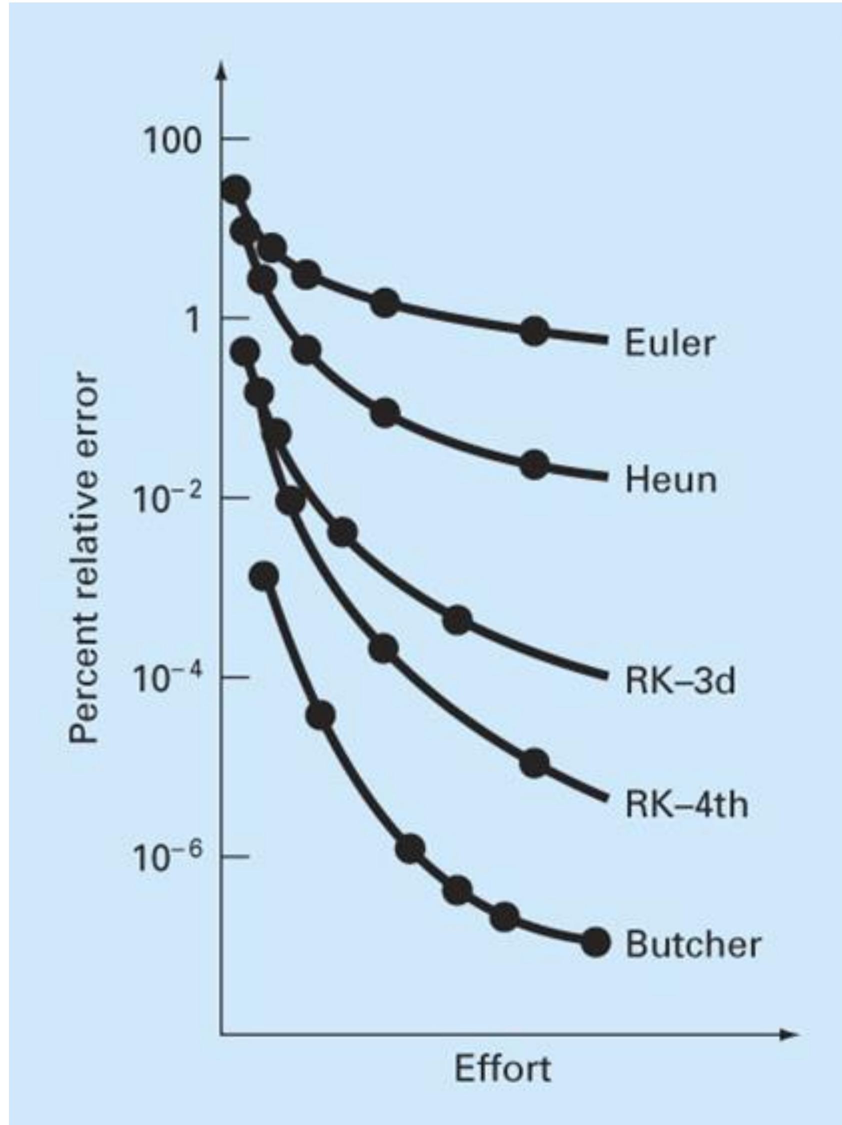
$$k_3 = f\left(x_i + \frac{1}{4}h,\ y_i + \frac{1}{8}k_1 h + \frac{1}{8}k_2 h\right)$$

$$k_4 = f\left(x_i + \frac{1}{2}h,\ y_i - \frac{1}{2}k_2 h + k_3 h\right)$$

$$k_5 = f\left(x_i + \frac{3}{4}h,\ y_i + \frac{3}{16}k_1 h + \frac{9}{16}k_4 h\right)$$

$$k_6 = f\left(x_i + h,\ y_i - \frac{3}{7}k_1 h + \frac{2}{7}k_2 h + \frac{12}{7}k_3 h - \frac{12}{7}k_4 h + \frac{8}{7}k_5 h\right)$$

Comparison of Runge-Kutta Methods



Systems of Equations

Many practical problems in engineering and science require the solution of a system of simultaneous ordinary differential equations rather than a single equation:

$$
\begin{aligned}
\frac{dy_1}{dx} &= f_1(x, y_1, y_2, \ldots, y_n) \\
\frac{dy_2}{dx} &= f_2(x, y_1, y_2, \ldots, y_n) \\
&\vdots \\
\frac{dy_n}{dx} &= f_n(x, y_1, y_2, \ldots, y_n)
\end{aligned}
$$

Solution requires that n initial conditions be known at the starting value of x.

Example #5

Solve the following set of differential equations using Euler's method, assuming that at x = 0, y1 = 4, and y2 = 6. Integrate to x = 2 with a step size of 0.5.

$$\frac{dy_1}{dx} = -0.5y_1 \qquad \frac{dy_2}{dx} = 4 - 0.3y_2 - 0.1y_1$$

Euler's method is implemented for each variable as

$$y1(0.5) = 4 + [-0.5(4)]0.5 = 3$$

$$y2(0.5) = 6 + [4 - 0.3(6) - 0.1(4)]0.5 = 6.9$$

x	y_1	y_2
0	4	6
0.5	3	6.9
1.0	2.25	7.715
1.5	1.6875	8.44525
2.0	1.265625	9.094087

Example #6

Use the fourth-order RK method to solve the following set of differential equations, assuming that at x = 0, y1 = 4, and y2 = 6. Integrate to x = 2 with a step size of 0.5.

$$\frac{dy_1}{dx} = -0.5y_1 \qquad \frac{dy_2}{dx} = 4 - 0.3y_2 - 0.1y_1$$

First, we must solve for all the slopes at the beginning of the interval:

$k_{1,1} = f_1(0, 4, 6) = -0.5(4) = -2$

$k_{1,2} = f_2(0, 4, 6) = 4 - 0.3(6) - 0.1(4) = 1.8$

where $k_{i,j}$ is the i^{th} value of k for the j^{th} dependent variable. Next, we must calculate the first values of y_1 and y_2 at the midpoint:

$$y_1 + k_{1,1}\frac{h}{2} = 4 + (-2)\frac{0.5}{2} = 3.5$$

$$y_2 + k_{1,2}\frac{h}{2} = 6 + (1.8)\frac{0.5}{2} = 6.45$$

which can be used to compute the first set of midpoint slopes,

$k_{2,1} = f_1(0.25, 3.5, 6.45) = -1.75$

$k_{2,2} = f_2(0.25, 3.5, 6.45) = 1.715$

These are used to determine the second set of midpoint predictions,

$$y_1 + k_{2,1}\frac{h}{2} = 4 + (-1.75)\frac{0.5}{2} = 3.5625$$

$$y_2 + k_{2,2}\frac{h}{2} = 6 + (1.715)\frac{0.5}{2} = 6.42875$$

which can be used to compute the second set of midpoint slopes,

$$k_{3,1} = f_1(0.25, 3.5625, 6.42875) = -1.78125$$
$$k_{3,2} = f_2(0.25, 3.5625, 6.42875) = 1.715125$$

These are used to determine the predictions at the end of the interval

$$y_1 + k_{3,1}h = 4 + (-1.78125)(0.5) = 3.109375$$
$$y_2 + k_{3,2}h = 6 + (1.715125)(0.5) = 6.857563$$

which can be used to compute the endpoint slopes,

$$k_{4,1} = f_1(0.5, 3.109375, 6.857563) = -1.554688$$
$$k_{4,2} = f_2(0.5, 3.109375, 6.857563) = 1.631794$$

The values of k can then be used to compute

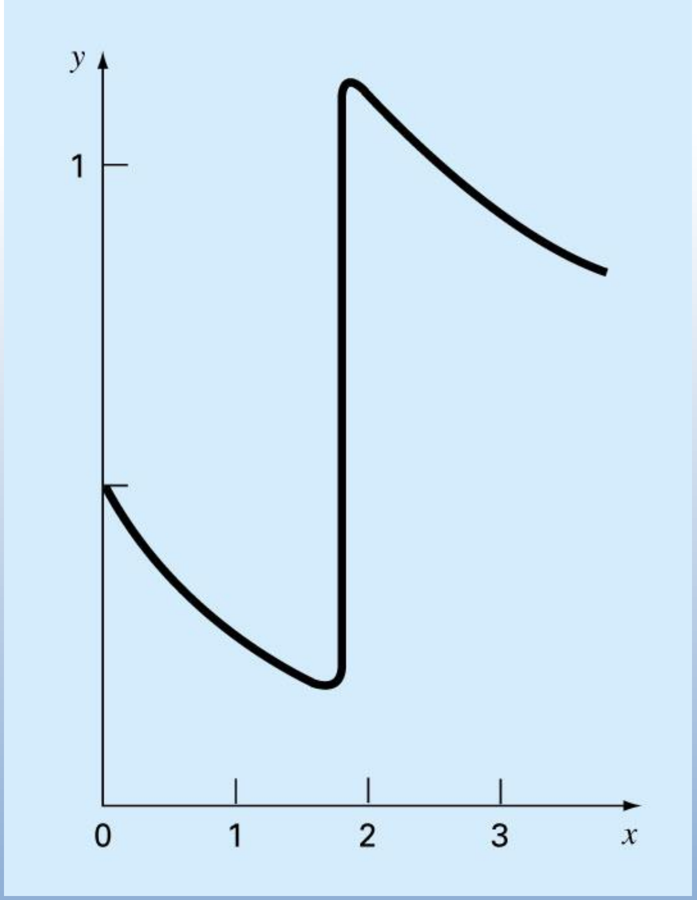
$$y_1(0.5) = 4 + \frac{1}{6}[-2 + 2(-1.75 - 1.78125) - 1.554688]0.5 = 3.115234$$

$$y_2(0.5) = 6 + \frac{1}{6}[1.8 + 2(1.715 + 1.715125) + 1.631794]0.5 = 6.857670$$

x	y_1	y_2
0	4	6
0.5	3.115234	6.857670
1.0	2.426171	7.632106
1.5	1.889523	8.326886
2.0	1.471577	8.946865

Adaptive Runge-Kutta Methods

For an ODE with an abrupt changing solution, a constant step size can represent a serious limitation.



Adaptive RK or Step-Halving Method

$$\Delta = y2 - y1$$
$$y2 \leftarrow y2 + \frac{\Delta}{15}$$

where y_1 designates the single-step prediction and y_2 designates the prediction using the two half steps.

This estimate is fifth-order accurate

Example #7

Use the adaptive fourth-order RK method to integrate $y' = 4e^{0.8x} - 0.5y$ from x = 0 to 2 using h = 2 and an initial condition of y(0) = 2. Recall that the true solutions is $y(2) = 14.84392$.

Solution. The single prediction with a step of h is computed as

$$y(2) = 2 + \frac{1}{6}[3 + 2(6.40216 + 4.70108) + 14.11105]2 = 15.10584$$

The two half-step predictions are

$$y(1) = 2 + \frac{1}{6}[3 + 2(4.21730 + 3.91297) + 5.945681]1 = 6.20104$$

and

$$y(2) = 6.20104 + \frac{1}{6}[5.80164 + 2(8.72954 + 7.99756) + 12.71283]1 = 14.86249$$

Therefore, the approximate error is

$$E_a = \frac{14.86249 - 15.10584}{15} = -0.01622$$

which compares favorably with the true error of

$$E_t = 14.84392 - 14.86249 = -0.01857$$

The error estimate can also be used to correct the prediction

$$y(2) = 14.86249 - 0.01622 = 14.84627$$

which has an $E_t = -0.00235$.

Runge-Kutta Fehlberg

For the present case, we use the following fourth-order estimate

$$y_{i+1} = y_i + \left(\frac{37}{378}k_1 + \frac{250}{621}k_3 + \frac{125}{594}k_4 + \frac{512}{1771}k_6\right)h$$

along with the fifth-order formula:

$$y_{i+1} = y_i + \left(\frac{2825}{27{,}648}k_1 + \frac{18{,}575}{48{,}384}k_3 + \frac{13{,}525}{55{,}296}k_4 + \frac{277}{14{,}336}k_5 + \frac{1}{4}k_6\right)h$$

where

$$\begin{aligned}
k_1 &= f(x_i, y_i) \\
k_2 &= f\left(x_i + \frac{1}{5}h,\ y_i + \frac{1}{5}k_1 h\right) \\
k_3 &= f\left(x_i + \frac{3}{10}h,\ y_i + \frac{3}{40}k_1 h + \frac{9}{40}k_2 h\right) \\
k_4 &= f\left(x_i + \frac{3}{5}h,\ y_i + \frac{3}{10}k_1 h - \frac{9}{10}k_2 h + \frac{6}{5}k_3 h\right) \\
k_5 &= f\left(x_i + h,\ y_i - \frac{11}{54}k_1 h + \frac{5}{2}k_2 h - \frac{70}{27}k_3 h + \frac{35}{27}k_4 h\right) \\
k_6 &= f\left(x_i + \frac{7}{8}h,\ y_i + \frac{1631}{55{,}296}k_1 h + \frac{175}{512}k_2 h + \frac{575}{13{,}824}k_3 h + \frac{44{,}275}{110{,}592}k_4 h \right. \\
&\qquad \left. + \frac{253}{4096}k_5 h\right)
\end{aligned}$$

Example #7

Use the Runge-Kutta Fehlberg approach to integrate $y' = 4e^{0.8x} - 0.5y$ from x = 0 to 2 using h = 2 and an initial condition of y(0) = 2. Recall that the true solutions is $y(2) = 14.84392$.

Solution. The calculation of the k's can be summarized in the following table:

	x	y	f(x, y)
k_1	0	2	3
k_2	0.4	3.2	3.908511
k_3	0.6	4.20883	4.359883
k_4	1.2	7.228398	6.832587
k_5	2	15.42765	12.09831
k_6	1.75	12.17686	10.13237

These can then be used to compute the fourth-order prediction

$$y_1 = 2 + \left(\frac{37}{378}3 + \frac{250}{621}4.359883 + \frac{125}{594}6.832587 + \frac{512}{1771}10.13237\right)2 = 14.83192$$

along with a fifth-order formula:

$$y_1 = 2 + \left(\frac{2825}{27{,}648}3 + \frac{18{,}575}{48{,}384}4.359883 + \frac{13{,}525}{55{,}296}6.832587 + \frac{277}{14{,}336}12.09831 + \frac{1}{4}10.13237\right)2 = 14.83677$$

The error estimate is obtained by subtracting these two equations to give

$$E_a = 14.83677 - 14.83192 = 0.004842$$

Step-Size Control

The strategy is to *increase the step size if the error is too small* and *decrease it if the error is too large*. Press et al. (1992) have suggested the following criterion to accomplish this:

$$h_{new} = h_{present} \left| \frac{\Delta_{new}}{\Delta_{present}} \right|^{\alpha}$$

$\Delta_{present}$= computed present accuracy

Δ_{new}= desired accuracy

α= a constant power that is equal to 0.2 when step size increased and 0.25 when step size is decreased

PART B

STIFFNESS AND MULTISTEP METHODS

Stiffness and Multistep Methods

Two areas are covered:

Stiff ODEs will be described - ODEs that have both fast and slow components to their solution.

Implicit solution technique and *multistep methods* will be described.

Stiffness

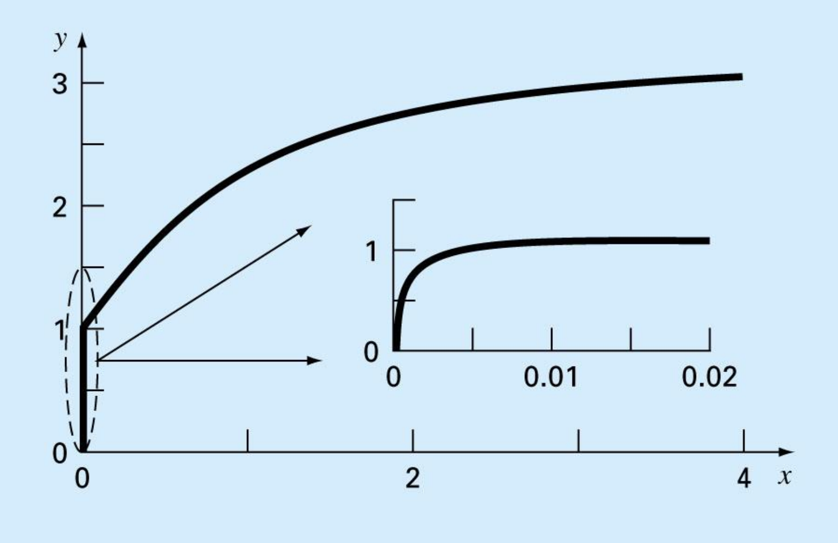
A *stiff system* is the one involving rapidly changing components together with slowly changing ones.

Both individual and systems of ODEs can be stiff:

$$\frac{dy}{dt} = -1000y + 3000 - 2000e^{-t}$$

If y(0)=0, the analytical solution is developed as:

$$y = 3 - 0.998e^{-1000t} - 2.002^{e-t}$$



Insight into the step size required for stability of such a solution can be gained by examining the homogeneous part of the ODE:

$$\frac{dy}{dt} = -ay$$

$$y = y_0 e^{-at}$$

The solution starts at $y(0)=y_0$ and asymptotically approaches zero.

If Euler's method is used to solve the problem numerically:

$$y_{i+1} = y_i + \frac{dy_i}{dt} h$$

$$y_{i+1} = y_i - a y_i h \qquad \text{or} \qquad y_{i+1} = y_i (1 - ah)$$

The stability of this formula depends on the step size *h*:

$$|1 - ah| \prec 1$$

$$h \succ 2/a \quad \Rightarrow \quad |y_i| \to \infty \quad \text{as} \quad i \to \infty$$

Implicit Euler's method

Backward or *implicit Euler's* method

$$y_{i+1} = y_i + \frac{dy_{i+1}}{dt} h$$

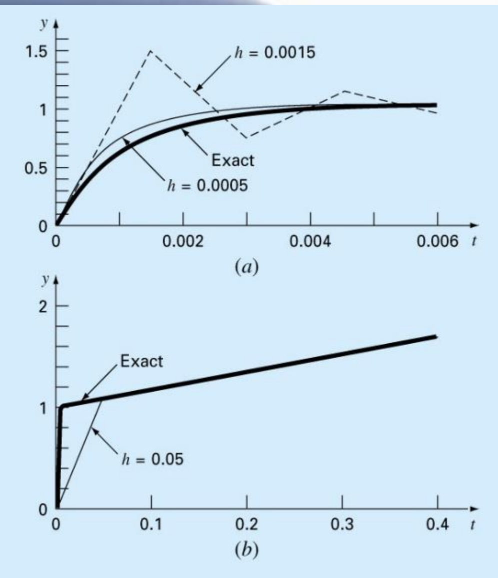
$$y_{i+1} = y_i - a y_{i+1} h$$

$$y_{i+1} = \frac{y_i}{1 + ah}$$

The approach is called *unconditionally stable*. Regardless of the step size:

$$|y_i| \to 0 \quad as \quad i \to \infty$$

Example #8



Use both the explicit and implicit Euler methods to solve

$$\frac{dy}{dt} = -1000y + 3000 - 2000e^{-t}$$

where y(0) = 0.

(a) Use the explicit Euler with step sizes of 0.0005 and 0.0015 to solve for y between t = 0 and 0.006.

(b) Use the implicit Euler with a step size of 0.05 to solve for y between 0 and 0.4.

(a) For this problem, the explicit Euler's method is

$$y_{i+1} = y_i + (-1000yi + 3000 - 2000e^{-ti})h$$

The result for h = 0.0005 is displayed in Fig. a along with the analytical solution.

(b) The implicit Euler's method is

$$y_{i+1} = y_i + (-1000yi_{+1} + 3000 - 2000e^{-ti+1})h$$

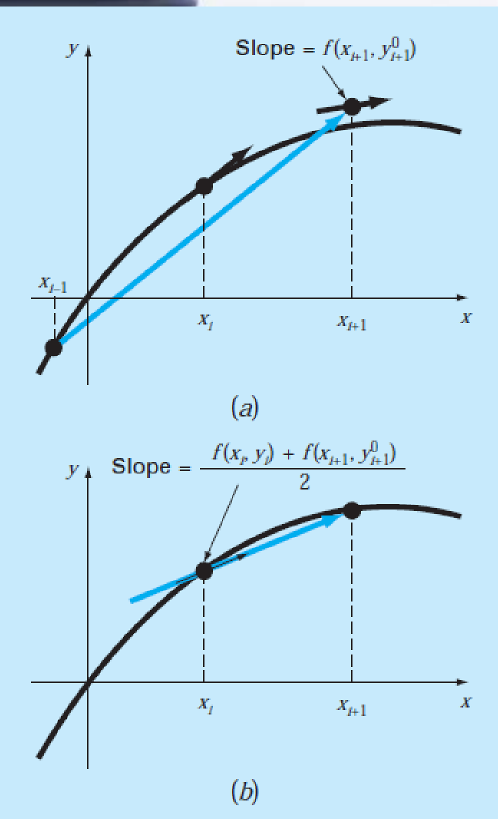
Now because the ODE is linear, we can rearrange this equation so that yi+1 is isolated on the left-hand side,

$$y_{i+1} = \frac{y_i + 3000h - 2000he^{ti+1}}{1 + 1000h}$$

The result for h = 0.05 is displayed in Fig. b along with the analytical solution.

The Non-Self-Starting Heun Method

Huen method uses *Euler's method* as a *predictor* and *trapezoidal rule* as a *corrector*.



$$\text{Predictor:} \quad y_{i+1}^0 = y_{i-1}^m + f(x_i, y_i^m)\,2h$$

$$\text{Corrector:} \quad y_{i+1}^j = y_i^m + \frac{f(x_i, y_i^m) + f(x_{i+1}, y_{i+1}^{j-1})}{2}h$$

$$(\text{for } j = 1, 2, \ldots, m)$$

$$|\varepsilon_a| = \left| \frac{y_{i+1}^j - y_{i+1}^{j-1}}{y_{i+1}^j} \right| 100\%$$

Example #9

Use the non-self-starting Heun method to integrate $y' = 4e^{0.8x} - 0.5y$ from x = 0 to x = 4 using a step size of 1.0, the initial condition at x = 0 is y = 2. However, because we are now dealing with a multistep method, we require the additional information that y is equal to −0.3929953 at x=−1.

The predictor equation is used to extrapolate linearly from x=−1 to x = 1.

$$y_1^0 = -0.3929953 + [4e^{0.8(0)} - 0.5(2)]2 = 5.607005$$

The corrector equation is then used to compute the value:

$$y_1^1 = 2 + \frac{4e^{0.8(0)} - 0.5(2) + 4e^{0.8(1)} - 0.5(5.607005)}{2} 1 = 6.549331$$

which represents a percent relative error of −5.73% (true value = 6.194631).

Now, the corrector equation can be applied iteratively to improve the solution:

$$y_1^2 = 2 + \frac{3 + 4e^{0.8(1)} - 0.5(6.549331)}{2} 1 = 6.313749$$

which represents an ε_t of −1.92%. An approximate estimate of the error can also be determined

$$|\varepsilon_a| = \left| \frac{6.313749 - 6.549331}{6.313749} \right| 100\% = 3.7\%$$

For the second step, the predictor is

$$y_2^0 = 2 + [4e^{0.8(1)} - 0.5(6.360865)]2 = 13.44346$$

$$\varepsilon t = 9.43\%$$

The first corrector yields 15.76693 (ε_t = 6.8%)

The Non-Self-Starting Heun Method

Predictor:

$$y_{i+1}^{0} = y_{i-1}^{m} + f(x_i,\ y_i^{m})2h$$

(Save result as $y_{i+1,u}^{0} = y_{i+1}^{0}$ where the subscript u designates that the variable is unmodified.)

Predictor Modifier:

$$y_{i+1}^{0} \leftarrow y_{i+1,u}^{0} + \frac{4}{5}(y_{i,u}^{m} - y_{i,u}^{0})$$

Corrector:

$$y_{i+1}^{j} = y_i^{m} + \frac{f(x_i,\ y_i^{m}) + f(x_{i+1},\ y_{i+1}^{j-1})}{2}h \qquad \text{(for } j = 1 \text{ to maximum iterations } m\text{)}$$

Error Check:

$$|\varepsilon_a| = \left|\frac{y_{i+1}^{j} - y_{i+1}^{j-1}}{y_{i+1}^{j}}\right| 100\%$$

(If $|\varepsilon_a| >$ error criterion, set $j = j + 1$ and repeat corrector; if $\varepsilon_a \le$ error criterion, save result as $y_{i+1,u}^{m} = y_{i+1}^{m}$.)

Corrector Error Estimate:

$$E_c = -\frac{1}{5}(y_{i+1,u}^{m} - y_{i+1,u}^{0})$$

(If computation is to continue, set $i = i + 1$ and return to predictor.)

Step-Size Control

Constant Step Size.

A value for *h* must be chosen prior to computation.

It must be small enough to yield a sufficiently small truncation error.

It should also be as large as possible to minimize run time cost and round-off error.

Variable Step Size.

If the corrector error is greater than some specified error, the step size is decreased.

A step size is chosen so that the convergence criterion of the corrector is satisfied in two iterations.

A more efficient strategy is to increase and decrease by doubling and halving the step size.

Integration Formulas

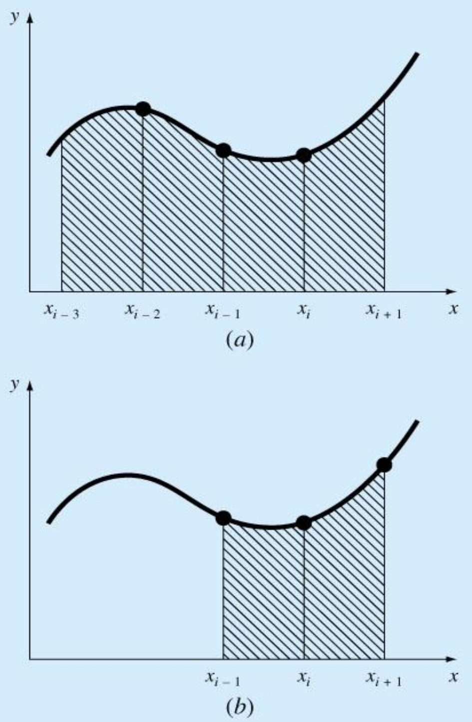
The non-self-starting Heun method is characteristic of most multistep methods.

It employs an open integration formula (the midpoint method) to make an initial estimate. This predictor step requires a previous data point.

Then, a closed integration formula (the trapezoidal rule) is applied iteratively to improve the solution.

It should be obvious that a strategy *for improving multistep methods would be to use higher-order integration formulas* as predictors and correctors.

Newton-Cotes Formulas.



Open Formulas.

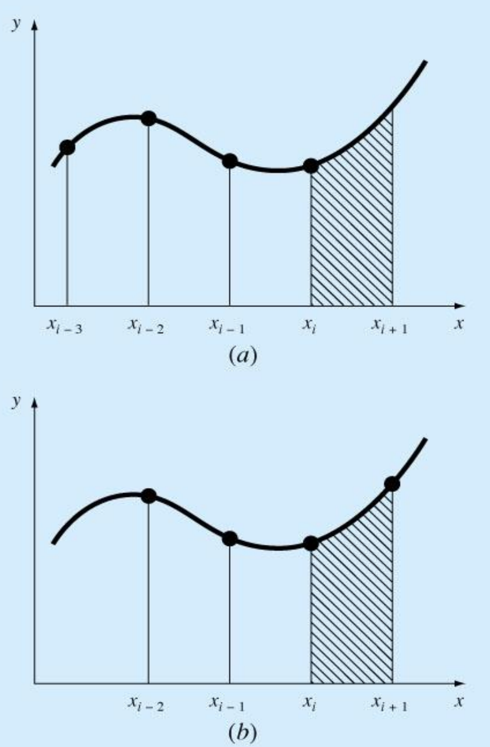
$$y_{i+1} = y_{i-n} + \int_{x_{i-n}}^{x_{i+1}} f_n(x)dx$$

Closed Formulas.

$$y_{i+1} = y_{i-n+1} + \int_{x_{i-n+1}}^{x_{i+1}} f_n(x)dx$$

$f_n(x)$ is an n^{th} order interpolating polynomial.

Adams Formulas (Adams-Bashforth)



Open Formulas.

The Adams formulas can be derived in a variety of ways. One way is to write *a forward Taylor series* expansion around x_i. A second order open Adams formula:

$$y_{i+1} = y_i + h\left(\frac{3}{2} f_i - \frac{1}{2} f_{i-1}\right) + \frac{5}{12} h^3 f_i'' + O(h^4)$$

Closed Formulas.

A backward Taylor series around xi+1 can be written:

$$y_{i+1} = y_i + h\sum_{k=0}^{n-1} \beta_k f_{i+1-k} + O(h^{n+1})$$

Higher-Order multistep Methods

Milne's Method.

Uses the three point Newton-Cotes open formula as a predictor and three point Newton-Cotes closed formula as a corrector.

$$y_{i+1}^{0} = y_{i-3}^{m} + \frac{4h}{3}\left(2\, f_i^{m} - \, f_{i-1}^{m} + 2\, f_{i-2}^{m}\right)$$

$$y_{i+1}^{j} = y_{i-1}^{m} + \frac{h}{3}\left(\, f_{i-1}^{m} + 4\, f_i^{m} + \, f_{i+1}^{j-1}\right)$$

$$E_p = \frac{28}{29}\left(y_i^{m} - y_i^{0}\right)$$

$$E_c \cong -\frac{1}{29}\left(y_{i+1}^{m} - y_{i+1}^{0}\right)$$

Higher-Order multistep Methods

Fourth-Order Adams Method.

Based on the Adams integration formulas. Uses the fourth-order Adams-Bashforth formula as the predictor and fourth-order Adams-Moulton formula as the corrector.

$$y_{i+1}^{0} = y_i^m + h\left(\frac{55}{24} f_i^m - \frac{59}{24} f_{i-1}^m + \frac{37}{24} f_{i-2}^m - \frac{9}{24} f_{i-3}^m\right)$$

$$y_{i+1}^{j} = y_i^m + h\left(\frac{9}{24} f_{i+1}^{j-1} + \frac{19}{24} f_i^m - \frac{5}{24} f_{i-1}^m + \frac{1}{24} f_{i-2}^m\right)$$

$$E_p = \frac{251}{270}(y_i^m - y_i^0)$$

$$E_c = -\frac{19}{270}(y_{i+1}^m - y_{i+1}^0)$$

Any Questions?

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