SME 3023 Applied Numerical Methods

Ordinary Differential Equations

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Newton’s second law to compute velocity \( v \) of a falling mass \( m \) as a function of time \( t \) can be written as

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

(1)

where \( g \) is gravitational constant, and \( c \) is drag coefficient. Eq. (1) is composed of

- unknown function, \( v \), and
- its derivatives, \( dv/dt \)

Such equation is called differential equation or rate equation. Also, in Eq. (1)

- \( v \) is the dependent variable
- \( t \) is the independent variable

When function involves **ONE** independent variable, the equation is called the **ordinary differential equation**, e.g.

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

When function involves **TWO or MORE** independent variables, the equation is called the **partial differential equation**, e.g.

\[
\rho \frac{Du}{Dt} = - \frac{\partial p}{\partial x} + \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} + \rho f_x
\]
Sample Engineering Problems

- Newton’s second law of motion
  \[
  \frac{dv}{dt} = \frac{F}{m}
  \]
  (2)
  where \( v \) is velocity, \( F \) is force and \( m \) is mass
- Fourier’s heat law
  \[
  q = -k \frac{dT}{dx}
  \]
  (3)
  where \( q \) is heat flux, \( k \) is thermal conductivity and \( T \) is temperature
- Fick’s law of diffusion
  \[
  J = -D \frac{dc}{dx}
  \]
  (4)
  where \( J \) is mass flux, \( D \) is diffusion coefficient and \( c \) is concentration
- Faraday’s law (voltage drop across an inductor)
  \[
  \Delta V_t = L \frac{di}{dt}
  \]
  (5)
  where \( \Delta V_t \) is voltage drop, \( L \) is inductance and \( i \) is current
Differential equations are classified as to the order:

- **First order equation**—highest derivative is *first* derivative

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

- **Second order equation**—highest derivative is *second* derivative, for example equation describing position \( x \) of mass-spring system with damping

\[
m \frac{d^2x}{dt^2} + c \frac{dx}{dt} + kx = 0 \tag{6}
\]

where \( c \) is *gravitational constant* and \( k \) is *mass* and \( c \) is *drag coefficient*

- Similarly, \( n^{th} \) order differential equation would include \( n^{th} \) derivative.

- **Higher order differential equation** can be reduced to a system of first order equations. For Eq. (6) above, we do it by defining

\[
y = \frac{dx}{dt} \tag{7}
\]
Eq. (7) is differentiated to yield
\[ \frac{dy}{dt} = \frac{d^2x}{dt^2} \]  
(Eq. 8)

Eqs. (7) and (8) are then substituted into Eq. (6) to yield
\[ m \frac{dy}{dt} + cy + kx = 0 \]  
(Eq. 9)

Eq. (9) can be re-arranged into
\[ \frac{dy}{dt} = -\frac{cy + kx}{m} = 0 \]  
(Eq. 10)

Thus Eqs. (7) and (10) are two first order equations that are equivalent to the original second order equation, i.e. Eq. (6).
A linear ODE is one that fits the general form

\[ a_n(x)y^{(n)} + \ldots + a_1(x)y' + a_0(x)y = f(x) \]  

(11)

where \( y^{(n)} \) is the \( n \)th derivative of \( y \) w.r.t. \( x \), \( a \) is specified function of \( x \) and \( c \) is specified function of \( x \). Eq. (11) is linear because there are no products or nonlinear function of dependent variable \( y \) and its derivatives.

Motion of a swinging pendulum, Figure 1, is governed by

\[ \frac{d^2 \theta}{dt^2} + \frac{g}{l} \sin \theta = 0 \]  

(12)

Eq. (12) is nonlinear because of the term \( \sin \theta \).

Figure 1: Motion of swinging pendulum.
To obtain solution to Eq. (12) we \textit{linearize} it by assuming, for small values of $\theta$, \begin{equation}
\sin \theta \approx \theta \end{equation}

which, on substitution into Eq. (12), yields a linear form \begin{equation}
\frac{d^2 \theta}{dt^2} + \frac{g}{l} \theta = 0
\end{equation}

Why linear ODE are important? Because they can be solved analytically. In contrast, most nonlinear equations cannot be solved exactly!!
Non-computer Methods for Solving ODE

- Without computers, ODE are solved with *analytical* integration techniques in which Eq. (1) could be multiplied by $dt$ and then integrated to yield

\[
v = \int \left( g - \frac{c}{m}v \right) dt
\]

RHS of Eq. (15) is an *indefinite integral* because limits of integration are not specified.

- Eq. (15) can be solved analytically, assuming $v = 0$ at $t = 0$, to yield

\[
v(t) = \frac{gm}{c} \left( 1 - e^{-\left(\frac{c}{m}\right)t} \right)
\]
A solution of an ODE is a *specific* function of independent variable and parameters that satisfy the original differential equation. Let say we were given a forth order polynomial

\[ y = -0.5x^4 + 4x^3 - 10x^2 + 8.5x + 1 \]  \hspace{1cm} (16)

Differentiating Eq. (16) gives us an ODE

\[ \frac{dy}{dx} = -2x^3 + 12x^2 - 20x + 8.5 \]  \hspace{1cm} (17)

Eq. (17) also describes the behaviour of a polynomial but in a different manner than Eq. (16)—i.e. it gives rate of change of \( y \) w.r.t. \( x \), which is a *slope*. 
But our objective here is to determine the original function (Eq. (16)) given the ODE (Eq. (17)). So we go back to Eq. (17) and solve analytically

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

which leads to

\[ y = -0.5x^4 + 4x^3 - 10x^2 + 8.5x + C \tag{18} \]

Eq. (18) is identical to Eq. (16) with one notable exception—1 in Eq. (16) being replaced by \( C \) in Eq. (18) and \( C \) is the constant of integration which is arbitrary.

Therefore, to specify the solution completely, an ODE is usually accompanied by auxiliary condition(s).

For first order ODE, this auxiliary condition, called initial value, is required to determine the constant of integration and obtain a unique solution.
In order to get back Eq. (16), Eq. (18) needs the initial value that \( x = 0, y = 1 \). Substituting the initial value into Eq. (18) yields

\[
1 = -0.5(0)^4 + 4(0)^3 - 10(0)^2 + 8.5x + C
\]

or

\[ C = 1 \]  \hspace{1cm} (20)

Hence,

\[
y = -0.5x^4 + 4x^3 - 10x^2 + 8.5x + 1
\]
Basis of numerical method devoted to solving ODE of the form

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

is

New value = Old value

\[+ \text{ (Slope } \times \text{ Step size)}\]

which can be mathematically expressed as

\[y_{i+1} = y_i + \phi h\] (21)

where \(\phi\) is the slope estimate. This method is known as one-step method, Figure 2.

Figure 2: One-step 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 differential equation evaluated at $x_i$ and $y_i$. Substituting this into Eq. (21) yields

$$y_{i+1} = y_i + f(x_i, y_i)h \quad \text{(22)}$$

Eq. (22) represents the Euler’s (or Cauchy-Euler) method.

Figure 3: Euler’s method.
Problem Statement:
Use Euler’s method to solve
\[
\frac{dy}{dx} = -2x^3 + 12x^2 - 20x + 8.5
\]
from \(x = 0\) to \(x = 4\) with step size of 0.5. Initial condition at \(x = 0\) is \(y = 1\).

Solution:
At \(x = 0.5\), Eq. (22), with initial condition \(y(0) = 1\), yield
\[
y(0.5) = y(0) + f(0, 1) \times 0.5
\]
\[
= 1.0 + [-2(0)^3 + 12(0)^2 - 20(0) + 8.5] \times 0.5 = 5.25
\]
True solution at \(x = 0.5\) is
\[
y = -0.5(0.5)^4 + 4(0.5)^3 - 10(0.5)^2 + 8.5(0.5) + 1 = 3.21875
\]
\[
\therefore E_x = 3.21875 - 5.25 = -2.03125 \quad \text{or} \quad R_x = -63.1\%
\]
Solution: continued...

At $x = 1.0$,

$$y(1.0) = y(0.5) + f(0.5, 5.25) \times (0.5)$$

$$= 5.25 + [-2(0.5)^3 + 12(0.5)^2 - 20(0.5) + 8.5] \times 0.5 = 5.875$$

True solution at $x = 1.0$ is

$$y = -0.5(1.0)^4 + 4(1.0)^3 - 10(1.0)^2 + 8.5(1.0) + 1 = 3.0$$

$\therefore \ E_x = 3.0 - 5.875 = -2.875 \text{ or } R_x = -95.8\%$

Computation is repeated and results tabulated

<table>
<thead>
<tr>
<th>$x$</th>
<th>$y_{true}$</th>
<th>$y_{Euler}$</th>
<th>Error (%)</th>
</tr>
</thead>
<tbody>
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<td>1.00000</td>
<td>0.0</td>
</tr>
<tr>
<td>0.5</td>
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<td>5.25000</td>
<td>-63.1</td>
</tr>
<tr>
<td>1.0</td>
<td>3.00000</td>
<td>5.87500</td>
<td>-95.8</td>
</tr>
<tr>
<td>1.5</td>
<td>2.21875</td>
<td>5.12500</td>
<td>131.0</td>
</tr>
<tr>
<td></td>
<td>:</td>
<td>:</td>
<td>:</td>
</tr>
<tr>
<td>4.0</td>
<td>3.00000</td>
<td>7.00000</td>
<td>-133.3</td>
</tr>
</tbody>
</table>
Solution: continued...
Using Matlab to solve the same involves the following steps:

1. Write the ODE into \texttt{dydx.m}
2. Optionally, write the known solution into \texttt{ytrue.m}
3. Matlab script to solve the ODE is written in \texttt{myeuler.m}

Matlab codes

\texttt{dydx.m}

\begin{verbatim}
function df=dydx(x)
    df = -2*x.^3 + 12*x.^2 - 20*x + 8.5;
\end{verbatim}

\texttt{ytrue.m}

\begin{verbatim}
function y=ytrue(x)
    y = -0.5*x.^4 + 4*x.^3 - 10*x.^2 + 8.5*x + 1;
\end{verbatim}
**Solution:** continued...

```matlab
myeuler.m

x0 = 0.0; xn = 4.0; xstep=0.01;
x = [x0:xstep:xn]; n = length(x);
xt = linspace(x(1),x(n),100); yt = ytrue(x);
plot(x,yt,'r'); hold on
y(1) = 1.0;  % This is INITIAL VALUE
for i=2:n
    y(i) = y(i-1) + dydx(x(i-1))*xstep;
end
err = abs((yt-y)/yt)*100;
plot(x,y,'b')
[x' y' yt' err']
```
First order technique such as Euler’s method demands great computational effort to obtain acceptable error level.

Simplicity of Euler’s method makes it attractive, easy to program, suitable for quick analyses.
An attempt to improve Euler’s method

Determines two derivatives for the interval or steps

- at beginning of interval
- at end of interval

These two derivatives are then averaged to get an improved estimate of the slope.

Slope at beginning of interval

\[ y'_i = f(x_i, y_i) \]  \hspace{1cm} (23)

is used to extrapolate linearly to \( y^o_{i+1} \)

\[ y^o_{i+1} = y_i + f(x_i, y_i) \times h \]  \hspace{1cm} (24)

\( y^o_{i+1} \) is an intermediate prediction called predictor.

Figure 4: Heun’s method.
Slope at end of interval is estimated using the predictor in Eq. (24)

\[ y'_{i+1} = f(x_{i+1}, y_{i+1}) \]  

The two slopes—Eqs. (23) and (25)—are combined to obtain average slope for the interval

\[ \bar{y} = \frac{y'_{i} + y'_{i+1}}{2} = \frac{f(x_{i}, y_{i}) + f(x_{i+1}, y_{i+1})}{2} \]  

The average slope, Eq. (26), is then used to extrapolate linearly from \( y_i \) to \( y_{i+1} \) using Euler’s method

\[ y_{i+1} = y_i + \left[ \frac{f(x_{i}, y_{i}) + f(x_{i+1}, y_{i+1})}{2} \right] \times h \]  

Eq. (27) is known as the *corrector* equation

Heun’s method is the basis of many other *predictor-corrector* methods
Problem Statement:
Use Heun’s method to solve

\[
\frac{dy}{dx} = 4e^{0.8x} - 0.5y
\]

from \(x = 0\) to \(x = 4\) with step size of 1.0. Initial condition at \(x = 0\) is \(y = 2\).

Note: Analytical solution is

\[
y = \frac{4}{1.3} \left( e^{0.8x} - e^{-0.5x} \right) + 2e^{-0.5x}
\]
Solution:
Slope at initial point \((x_0, y_0)\)

\[
y'_0 = 4e^0 - 0.5(2) = 3
\]

Use predictor equation (Eq. (24)) to obtain estimate of \(y\) at 1.0

\[
y_1^o = 2 + 3(1) = 5
\]

Use value \(y_i^o\) to predict slope at end of interval

\[
y'_1 = f(x_1, y_i^o) = 4e^{0.8(1)} - 0.5(5) = 6.402164
\]

Average slope over the interval \(0 \leq x \leq 1\) \(x = 0\) and \(x = 1\) is

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

This average slope is then fed into the corrector equation (Eq. (27)) to give an estimate at \(x = 1\)

\[
y_1 = 2 + 4.701082(1) = 6.701082
\]
**Solution:** continued...

Computation is repeated and results tabulated

<table>
<thead>
<tr>
<th>$x$</th>
<th>$y_{\text{true}}$</th>
<th>$y_{\text{Heun}}$</th>
<th>Error (%)</th>
</tr>
</thead>
<tbody>
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<td>2.00000000</td>
<td>-0.00</td>
</tr>
<tr>
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<td>6.70108190</td>
<td>-8.18</td>
</tr>
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<td>2.0</td>
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<td>3.0</td>
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<tr>
<td>4.0</td>
<td>75.3389626</td>
<td>83.3377674</td>
<td>-10.62</td>
</tr>
</tbody>
</table>

Show the effect of reduced step size.
Solution: continued...
Using Matlab to solve the same involves the following steps:

1. Write the ODE into dydx1.m
2. Optionally, write the ‘known’ solution into ytrue1.m
3. Matlab script to solve the ODE is written in myheun.m

Matlab codes

**dydx1.m**

```matlab
def = dydx1(x,y)
def = 4*exp(0.8*x) - 0.5*y;
```

**ytrue1.m**

```matlab
function y=ytrue1(x)
y = (4/1.3)*(exp(0.8*x) - exp(-0.5*x)) + 2*exp(-0.5*x);
```
Example 2: Heun’s Method

Solution: continued...

myheun.m

x0=0.0; xn=4.0; xstep=0.25; x=[x0:xstep:xn]; n=length(x);
yt = ytrue1(x);
plot(x,yt,’r’); hold on
x(1)=0.0; y(1)=2.0; % INITIAL CONDITION
for i=2:n
    islope = dydx1(x(i-1),y(i-1));
    predictor = y(i-1) + islope*xstep;
    eslope = dydx1(x(i),predictor);
    avslope = (islope + eslope)/2;
    y(i) = y(i-1) + avslope*xstep;
end
err = abs((yt-y)/yt)*100;
plot(x,y,’b’)
[x’ y’ yt’ err’]
ODE - Initial Value Problem
Runge-Kutta (RK) Methods

- Advantage—achieve accuracy of a Taylor series approach without requiring calculation of higher derivatives. Generalized form

\[ y_{i+1} = y_i + \phi(x_i, y_i, h) \times h \tag{28} \]

where \( \phi(x_i, y_i, h) \) is an *increment function* which is a representative slope over the interval and given by

\[ \phi = a_1 k_1 + a_2 k_2 + \ldots + a_n k_n \tag{29} \]

- \( k \)'s in Eq. (29) are *recurrence relationships* i.e. \( k_1 \) appears in \( k_2 \) which appears in \( k_3 \) and so forth

\[
\begin{align*}
    k_1 &= f(x_i, y_i) \tag{30} \\
    k_2 &= f(x_i + p_1 h, y_i + q_{11} k_1 h) \tag{31} \\
    k_3 &= f(x_i + p_2 h, y_i + q_{21} k_1 h + q_{22} k_2 h) \tag{32} \\
    \ldots \\
    k_n &= f(x_i + p_{n-1} h, y_i + q_{n-1,1} k_1 h + q_{n-2,2} k_2 h + \ldots + q_{n-1,n-1} k_{n-1} h) \tag{33}
\end{align*}
\]
Various types of RK methods can be devised by employing different numbers of terms in the increment function as specified by $n$.

Once $n$ is chosen, values for $a$’s, $p$’s and $q$’s are evaluated by setting Eq. (28) equal to terms in a Taylor series expansion.

First order RK method, when $n = 1$, is actually Euler’s method.

Second order RK method, when $n = 2$, is exact if solution to ODE is quadratic.
For \( n = 1 \), we can write, using Eq. (28), the first order RK (RK1) method as

\[
y_{i+1} = y_i + (a_1 k_1)h 
\]

(34)

where

\[
k_1 = f(x_i, y_i)
\]

With \( a_1 = 1 \), the first order RK method

\[
y_{i+1} = y_i + f(x_i, y_i)h
\]

(35)

can be seen to be the same as Euler’s method.
For \( n = 2 \), we can write, using Eq. (28), the second order RK (RK2) method as

\[
y_{i+1} = y_i + (a_1 k_1 + a_2 k_2) h
\]  

(36)

where

\[
k_1 = f(x_i, y_i)
\]

(37)

\[
k_2 = f(x_i + p_1 h, y_i + q_1 k_1 h)
\]

(38)

To use Eq. (36), values for \( a_1, a_2, p_1 \) and \( q_1 \) must first be determined.

Recall second order Taylor series for \( y_{i+1} \) in terms of \( y_i \) and \( f(x_i, y_i) \)

\[
y_{i+1} = y_i + f(x_i, y_i) h + f'(x_i, y_i) \frac{h^2}{2!}
\]

(39)

where \( f'(x_i, y_i) \), by *chain-rule differentiation*, yields

\[
f'(x_i, y_i) = \frac{\partial f(x, y)}{\partial x} + \frac{\partial f(x, y)}{\partial y} \frac{dy}{dx}
\]

(40)
ODE - Initial Value Problem
Runge-Kutta Order 2 (RK2) Methods

- Substituting Eq. (40) into Eq. (39) yields

\[ y_{i+1} = y_i + f(x_i, y_i)h + \left( \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y} \frac{dy}{dx} \right) \frac{h^2}{2!} \] (41)

- Taylor series for two-variable function is

\[ g(x + r, y + s) = g(x, y) + r \frac{\partial g}{\partial x} + s \frac{\partial g}{\partial y} + \ldots \]

and apply this to expand Eq. (38)

\[ f(x_i + p_1h, y_i + q_{11}k_1h) = f(x_i, y_i) + p_1h \frac{\partial f}{\partial x} + q_{11}k_1h \frac{\partial f}{\partial y} + O(h^2) \] (42)
Eqs. (42) and (37) are then substituted into Eq. (36) to yield

\[ y_{i+1} = y_i + a_1 hf(x_i, y_i) + a_2 hf(x_i, y_i) + a_2 p_1 h^2 \frac{\partial f}{\partial x} + \\
+ a_2 q_{11} h^2 f(x_i, y_i) \frac{\partial f}{\partial y} + O(h^3) \]  \quad (43)

and collecting terms we get

\[ y_{i+1} = y_i + \left[ a_1 f(x_i, y_i) + a_2 f(x_i, y_i) \right] h + \\
+ \left[ a_2 p_1 \frac{\partial f}{\partial x} + a_2 q_{11} f(x_i, y_i) \frac{\partial f}{\partial y} \right] h^2 + O(h^3) \] \quad (44)
Comparing like terms in Eqs. (41) and (44), the following must hold

\[ a_1 + a_2 = 1 \]
\[ a_2 p_1 = \frac{1}{2} \]
\[ a_2 q_{11} = \frac{1}{2} \]

1. We now have 3 simultaneous equations containing 4 unknown constants—hence, there’s no unique solution.
2. However, assuming a value for one of the constants, we can determine the other 3!
3. Consequently, there is a family of second order RK methods rather than a single version!
The second order RK method version of Eq. (28) is

\[ y_{i+1} = y_i + (a_1 k_1 + a_2 k_2)h \]  

where

\[ k_1 = f(x_i, y_i) \]  

\[ k_1 = f(x_i + p_1 h, y_i + q_{11} k_1 h) \]  

\[ a_1 + a_2 = 1 \]  

\[ a_2 p_1 = \frac{1}{2} \]  

\[ a_2 q_{11} = \frac{1}{2} \]  

Suppose we specify a value for \( a_2 \), then Eqs. (48)–(50) can be solved simultaneously for

\[ a_1 = 1 - a_2 \]  

\[ p_1 = q_{11} = \frac{1}{2a_2} \]
Heun’s Method with a Single Corrector: $a_2 = \frac{1}{2}$

If $a_2 = \frac{1}{2}$, Eqs. (51) and (52) can be solved for $a_1 = \frac{1}{2}$ and $p_1 = q_{11} = 1$. These parameters, when substituted into Eq. (45) yield

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

(53)

where

$$k_1 = f(x_i, y_i): \text{slope at begining of interval}$$

(54)

$$k_2 = f(x_i + h, y_i + k_1h): \text{slope at end of interval}$$

(55)
The Midpoint Method: $a_2 = 1$

If $a_2 = 1$, then $a_1 = 0$ and $p_1 = q_{11} = \frac{1}{2}$ and Eq. (45) becomes

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

(56)

where

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

(57)

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

(58)
**Ralston’s Method:** $a_2 = \frac{2}{3}$

Choosing $a_2 = \frac{2}{3}$ provides a minimum bound on the truncation error for second order RK algorithms. It leads to $a_1 = \frac{1}{3}$ and $p_1 = q_{11} = \frac{3}{4}$, and yields

$$y_{i+1} = y_i + \left(\frac{1}{3}k_1 + \frac{2}{3}k_2\right)h \quad (59)$$

where

$$k_1 = f(x_i, y_i) \quad (60)$$
$$k_2 = f(x_i + \frac{3}{4}h, y_i + \frac{3}{4}k_1h) \quad (61)$$
For $n = 3$, we can write, using Eq. (28), the third order RK (RK3) method as

$$y_{i+1} = y_i + (a_1 k_1 + a_2 k_2 + a_3 k_3)h$$  \hspace{1cm} (62)

where

$$k_1 = f(x_i, y_i)$$  \hspace{1cm} (63)
$$k_2 = f(x_i + p_1 h, y_i + q_{11} k_1 h)$$  \hspace{1cm} (64)
$$k_3 = f(x_i + p_2 h, y_i + q_{21} k_1 h + q_{22} k_2 h)$$  \hspace{1cm} (65)

To use Eq. (62), values for $a_1$, $a_2$, $a_3$, $p_1$, $p_2$, $q_{11}$, $q_{21}$ and $q_{22}$ must first be determined.
One of the more popular version of Eq. (62) is

\[ y_{i+1} = y_i + \frac{1}{6}(k_1 + 4k_2 + k_3)h \]  

where

\[ k_1 = f(x_i, y_i) \]
\[ k_2 = f(x_i + \frac{1}{2}h, y_i + \frac{1}{2}hk_1) \]
\[ k_3 = f(x_i + h, y_i - hk_1 + 2hk_2) \]

Note: See Section 9.7.3 on page 658 of Rao (2002) for details.
RK4 methods are by far the most popular, with the classical fourth order RK method being the most commonly used:

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

(67)

where

\[ k_1 = f(x_i, y_i) \]
\[ k_2 = f(x_i + \frac{1}{2}h, y_i + \frac{1}{2}hk_1) \]
\[ k_3 = f(x_i + \frac{1}{2}h, y_i + \frac{1}{2}hk_2) \]
\[ k_4 = f(x_i + h, y_i + hk_3) \]

Note: See Section 25.3.3 on page 707 of Chapra and Canale (2006) for details.
Problem Statement:
Use the classical RK4 method to solve

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

using step size of \( h = 0.5 \) and initial condition of \( y = 1 \) at \( x = 0 \).
ODE - Initial Value Problem
Example 3: Runge-Kutta Order 4 (RK4) Methods

Solution:

At \( x = 0.0 \)

\[
\begin{align*}
  k_1 &= -2(0.0)^3 + 12(0.0)^2 - 20(0.0) + 8.5 = 8.5000 \\
  k_2 &= -2(0.0 + 0.5 \times 0.5)^3 + 12(0.0 + 0.5 \times 0.5)^2 - 20(0.0 + 0.5 \times 0.5) + 8.5 = 4.2188 \\
  k_3 &= -2(0.0 + 0.5 \times 0.5)^3 + 12(0.0 + 0.5 \times 0.5)^2 - 20(0.0 + 0.5 \times 0.5) + 8.5 = 4.2188 \\
  k_4 &= -2(0.0 + 0.5)^3 + 12(0.0 + 0.5)^2 - 20(0.0 + 0.5) + 8.5 = 1.2500
\end{align*}
\]

Hence, estimate at \( x = 0.5 \) is

\[
\begin{align*}
  y_{i+1} &= y_i + \frac{1}{6} (k_1 + 2k_2 + 2k_3 + k_4)h \\
  y(0.5) &= 1 + \left(\frac{1}{6} [8.5 + 2(4.21875) + 2(4.21875) + 1.25]\right)0.5 = 3.2188
\end{align*}
\]
Solution: continued...

At $x = 0.5$

\[ k_1 = -2(0.5)^3 + 12(0.5)^2 - 20(0.5) + 8.5 = 1.25000 \]
\[ k_2 = -2(0.5 + 0.5 \times 0.5)^3 + 12(0.0 + 0.5 \times 0.5)^2 - 20(0.0 + 0.5 \times 0.5) + 8.5 = -0.5938 \]
\[ k_3 = -2(0.0 + 0.5 \times 0.5)^3 + 12(0.0 + 0.5 \times 0.5)^2 - 20(0.0 + 0.5 \times 0.5) + 8.5 = -0.5938 \]
\[ k_4 = -2(0.5 + 0.5)^3 + 12(0.5 + 0.5)^2 - 20(0.5 + 0.5) + 8.5 = -1.50000 \]

Hence, estimate at $x = 1.0$ is

\[ y_{i+1} = y_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)h \]
\[ y(1.0) = 1 + \left( \frac{1}{6} \left[ 1.2500 + 2(-0.5938) + 2(-0.5938) - 1.5000 \right] \right) 0.5 = 3.0000 \]
Problem Statement:
Use the classical RK4 method to solve

\[ f(x, y) = \frac{dy}{dx} = 4e^{0.8x} - 0.5y \]

from \( x = 0 \) to \( x = 0.5 \) with step size of 0.5 and initial condition of \( y(0) = 2 \).

Solution:
Using Matlab to solve the above involves the following steps:

1. Write the ODE into \texttt{dydx1.m}
2. Optionally, write the ‘known’ solution into \texttt{ytrue1.m}
3. Matlab script to solve the ODE is written in \texttt{myrk4xy.m}
Solution: continued...
Matlab codes

dydx1.m

function df=dydx1(x,y)
df = 4*exp(0.8*x) - 0.5*y;

ytrue1.m

function y=ytrue1(x)
y = (4/1.3)*(exp(0.8*x) - exp(-0.5*x)) + 2*exp(-0.5*x);
Solution: continued...

myrk4xy.m

```matlab
x0 = 0.0; xn = 0.5; h=0.05;
x = [x0:h:xn]; n = length(x);
yt = ytrue1(x);
plot(x,yt,’r’); hold on
x(1) = 0.0; y(1) = 0.5; % INITIAL CONDITION
for i=2:n
    k1 = dydx1(x(i-1),y(i-1));
    k2 = dydx1(x(i-1)+0.5*h,y(i-1)+0.5*k1*h);
    k3 = dydx1(x(i-1)+0.5*h,y(i-1)+0.5*k2*h);
    k4 = dydx1(x(i-1)+h,y(i-1)+k3*h);
    phi = (k1+2*k2+2*k3+k4)/6;
    y(i) = y(i-1) + phi*h;
end
err = abs((yt-y)/yt)*100;
plot(x,y,’o’)
display([’x y yt err’])
[x’ y’ yt’ err’]
```
**Problem Statement:**
Use built-in Matlab function `ode23` to numerically solve first order ODE

\[ f(x, y) = \frac{dy}{dx} = xy^2 + y \]

Initial condition of at \( x = 0 \) is \( y = 1 \).

**Solution:**
Using Matlab to solve the same involves the following steps:

1. Write the ODE into `myode1.m`
2. Matlab script to solve `myode1.m` is written in `solvemyode1.m`
**Solution:** (continued...)  
Matlab codes

```matlab
myode1.m

function df=myode1(x,y)
yprime = x*y.^2 + y;
```

```matlab
solvemyode1.m

xr = [0,0.5]; % set x-range
y0 = 1; % initial conditions
[x,y] = ode23('myode1',xr,y0)
plot(x,y)
```
**Problem Statement:**
Use built-in Matlab function *ode45* to solve the first order ODE

\[
f(t, y) = \frac{dy}{dt} = -y + t + 1
\]

Initial condition of at \(x = 0\) is \(y = 1\).

**Solution:**
Using Matlab to solve the above involves the following steps:

1. Write the ODE into *iv1.m*
2. Matlab script to solve *iv1.m* is written in *solveiv1.m*
Solution: (continued...) Matlab codes

**iv1.m**

```matlab
function ydot=iv1(t,y)
ydot = -y+t+1;
```

**solveiv1.m**

```matlab
tspan = [0,1.0];  % set time span
y0 = 1;          % initial condition
[t,y] = ode45('iv1',tspan,y0)
plot(t,y)
```
We will show this kind of problem through an example:

\[
\frac{d^2x}{dt^2} + 3\frac{dx}{dt} + x = 5
\]

This is \( n^{th} \) order problem where, in this case \( n = 2 \). It can be re-written as a system of \( n \) first order ODE. This can be done in the following steps:

1. Let \( x_1 = x \), then

\[
\frac{d^2x_1}{dt^2} + 3\frac{dx_1}{dt} + x_1 = 5
\]

or, re-written as

\[
\frac{d^2x_1}{dt^2} = -3\frac{dx_1}{dt} - x_1 + 5 \quad (68)
\]
Next, let

\[ \frac{dx_1}{dt} = x_2 \]  \hspace{1cm} (69)

This is the first equation of the system.

Differentiate \( x_2 \) and substitute it into Eq. (69)

\[ \frac{dx_2}{dt} = \frac{d^2 x_1}{dt^2} = -3 \frac{dx_1}{dt} - x_1 + 5 = -3x_2 - x_1 + 5 \]  \hspace{1cm} (70)

This is the second equation of the system.

System of ODE represented by the first order Eqs. (69) and (70) can be then be written into a user-defined function in Matlab—see Matlab codes \texttt{iv0.m}.
ODE - Initial Value Problem

Problems of Order $n$

Matlab codes

iv0.m

function ydot=iv0(t,y)
y1dot = y(2);
y2dot = -3*y(2) - y(1) + 5;
ydot = [y1dot;y2dot];
**Problem Statement:**
Use built-in Matlab function(s) to solve the classic van de Pol equation

\[ \ddot{x} - \mu (1 - x^2) \dot{x} + x = 0 \]

where \( \mu \) is a parameter greater than zero.

**Solution:**
Choose

\[ y_1 = x \quad \implies \quad \dot{y}_1 = \frac{dx}{dt} = y_2 \]

\[ y_2 = \frac{dx}{dt} \quad \implies \quad \dot{y}_2 = \frac{d^2x}{dt^2} = \mu (1 - y_1^2)y_2 - y_1 \]
Solution: (continued...) Using Matlab to solve the above involves the following steps:

1. Write the system of first order ODE into \texttt{vdpol.m}
2. Matlab script to solve \texttt{vdpol.m} is written in \texttt{solvevdpol.m}

Matlab codes:

\texttt{vdpol.m}

```matlab
function ydot=vdpol(t,y)
mu = 2;       \% set to a value greater than zero
y1dot = y(2);
y2dot = mu*(1-y(1)^2)*y(2)-y(1)
ydot = [y1dot; y2dot];
```

\texttt{solvevdpol.m}

```matlab
tspan=[0 20];       \% time span
yo = [2; 0];        \% initial condition
[t,y] = ode45(’vdpol’,tspan,yo);  \% solve the ODE-IVP
plot(t,y(:,1),t,y(:,2),’--’)
xlabel(’time’)
ylabel(’ydot and y2dot’)
title(’van der Pol Solution’)
```
Problem Statement:
Use built-in Matlab function(s) to solve the following third order ODE

\[ \frac{d^3 y}{dt^3} + 3 \frac{d^2 y}{dt^2} + 5 \frac{dy}{dt} + 7y = 6 \]

This is \( n^{th} \) order problem with \( n = 3 \). It can be re-written as a system of 3 first order ODE.
Solution:

Let \( x_1 = y \), then

\[
\frac{d^3x_1}{dt^3} + 3 \frac{d^2x_1}{dt^2} + 5 \frac{dx_1}{dt} + 7x_1 = 6
\]

or, re-written as

\[
\frac{d^3x_1}{dt^3} = -3 \frac{d^2x_1}{dt^2} - 5 \frac{dx_1}{dt} - 7x_1 + 6
\]  

(71)
Solution: continued...

Let

\[ x_2 = \frac{dx_1}{dt} \]  \hspace{1cm} (72)

This is the first equation of the system. Differentiate \( x_2 \), twice

\[ \frac{dx_2}{dt} = \frac{d^2x_1}{dt^2} \]  \hspace{1cm} (73a)

\[ \frac{d^2x_2}{dt^2} = \frac{d^3x_1}{dt^3} \]  \hspace{1cm} (73b)
Solution: continued...

Let

\[ \frac{dx_2}{dt} = x_3 \]

This is the second equation of the system. But from Eq. (73a)

\[ \frac{dx_2}{dt} = \frac{d^2x_1}{dt^2} \]

Thus

\[ x_3 = \frac{d^2x_1}{dt^2} \quad (74) \]
Solution: continued... 

Differentiate $x_3$

$$\frac{dx_3}{dt} = \frac{d^3 x_1}{dt^3}$$  \hspace{1cm} (75)

Substituting Eqs. (75), (74) and (72) into Eq. (71) and making substitution $dx_3/dt = d^3 x_1/dt^3$, etc. yields

$$\frac{dx_3}{dt} = -3x_3 - 5x_2 - 7x_1 + 6$$  \hspace{1cm} (76)

This is the third equation of the system.
Solution: continued...

Thus, the third order ODE

\[
\frac{d^3 y}{dt^3} + 3 \frac{d^2 y}{dt^2} + 5 \frac{dy}{dt} + 7y = 6
\]

can be re-written as a system of 3 first order ODE:

\[
\frac{dx_1}{dt} = x_2; \quad \frac{dx_2}{dt} = x_3; \quad \frac{dx_3}{dt} = -3x_3 - 5x_2 - 7x_1 + 6
\]
ODE - Initial Value Problem
Example 8: Problems of Order $n = 3$

Solution: continued...

Using Matlab to solve the above involves the following steps:

1. Write a Matlab user-defined function called, say `iv3.m`
2. Matlab script to solve `iv3.m` is written in `solveiv3.m`

Matlab codes:

```matlab
iv3.m
function ydot=iv3(t,x)
x1dot = x(2);
x2dot = x(3);
x3dot = -3*x(3) - 5*x(2) - 7*x(1) + 6;
xdot = [x1dot;x2dot;x3dot];
```

```matlab
solveiv3.m
tspan=[0 20]; % time span
xo = [2; 0]; % initial condition
[t,x] = ode45('iv3',tspan,xo); % solve the ODE-IVP
plot(t,x(:,1),t,x(:,2),t,x(:,3),'-');
xlabel('time')
ylabel('x1dot and x2dot x3dot')
title('ODE of Order 3')
```
Differences between ODE-IVP and ODE-BVP are:

<table>
<thead>
<tr>
<th>ODE - Initial Value Problem (ODE-IVP)</th>
<th>ODE - Boundary Value Problem (ODE-BVP)</th>
</tr>
</thead>
<tbody>
<tr>
<td>conditions are specified at the <strong>same</strong> value of the independent variable</td>
<td>conditions are specified at the <strong>different</strong> values of the independent variable</td>
</tr>
<tr>
<td>for $n^{th}$ order ODE, $n$ conditions are required.</td>
<td>because these conditions are often specified at the extreme points or boundaries of a system, they are referred to as ODE-BVP.</td>
</tr>
</tbody>
</table>

ODE-BVP may be classified into
- linear or nonlinear,
- separated or mixed,
- specified at two points or more.

Two general approaches to numerical solution of ODE-BVP are
- shooting method,
- finite-difference method
Take conservation of energy to develop a heat balance for a long, thin rod. Mathematical model is represented by

\[
\frac{d^2 T}{dx^2} + h(T_a - T) = 0 \tag{77}
\]

where

- \( h \): heat transfer coefficient
- \( T_a \): temperature of surrounding air

To solve Eq. (77), appropriate boundary conditions (BC) must be specified. They are

\[
T(0) = T_1 \quad \text{and} \quad T(L) = T_2
\]

With these two BC, Eq. (77) can be solved analytically using calculus. If \( L = 10 \) m, \( T_a = 20^\circ C \), \( T_1 = 40^\circ C \), \( T_2 = 200^\circ C \) and \( h = 0.01 \), the analytical solution is

\[
T = 73.4523e^{0.1x} - 53.4523e^{-0.1x} + 20 \tag{78}
\]
Problem Statement:
To show both solution approaches for ODE-BVP, we will solve Eq. (77)

\[ \frac{d^2 T}{dx^2} + h(T_a - T) = 0 \]

for a 10 m rod with \( h = 0.001 \), \( T_a = 20 \) and BC: \( T(0) = 40 \) and \( T(10) = 200 \)
Solution:
Shooting methods is

1. based on converting BVP into equivalent IVP.
Here, the second order ODE of Eq. (77) is transformed into two first order ODE

\[
\frac{dT}{dx} = z; \quad \frac{dz}{dx} = h(T - T_a)
\]

We need initial value for \( z \) to solve this system of ODE, using, for example, RK4.

2. A trial-and-error approach is then implemented to solve IVP.
Finite difference methods is ... (coming soon to classroom near you!)
Bibliography


