REVIEW NO. 3

O.D.E. CLASSIFICATION

- I.V.P.'s

$$A\frac{d^2y}{dt^2} + B\frac{dy}{dt} + Cy = g(t) \qquad y(0) = y_o \qquad \frac{dy}{dt}(0) = V_o$$

- B.V.P.'s

$$A\frac{d^2y}{dx^2} + B\frac{dy}{dx} + Cy = g(x) \qquad y(0) = y_o \qquad y(L) = y_L$$

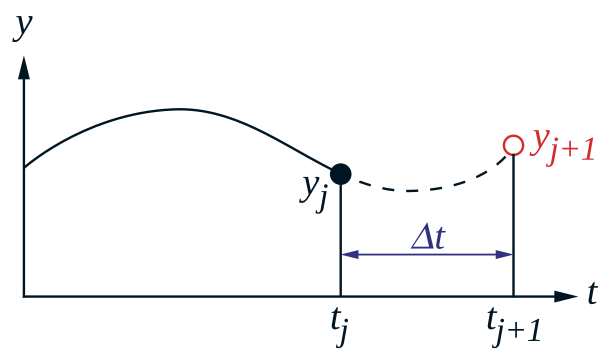
- Can always decompose an n^{th} order i.v.p. into n simultaneous 1^{st} order i.v.p.'s
  - e.g. - Converting the stated second order i.v.p. into two coupled first order i.v.p.'s

$$\frac{dy}{dt} = z \qquad y(0) = y_o$$

$$A\frac{dz}{dt} = -Bz - Cy + g(t) \qquad z(0) = V_o$$

I.V.P. SOLUTIONS - 1ST ORDER EQUATIONS - SINGLE STEP METHODS

- Solve $\frac{dy}{dt} = f(y, t), \quad y(0) = y_o$
- Runge-Kutta formulae are single step methods



Runge-Kutta Formulae

$$y_{j+1} = y_j + \Delta t(a_1 g_1 + a_2 g_2 + \ldots + a_n g_n)$$

$$g_1 = f(t_j, y_j) \quad \text{(slope at } (t_j, y_j))$$

$$g_2 = f(t_j + p_1 \Delta t, y_j + p_2 \Delta t g_1)$$

$$g_3 = f(t_j + p_3 \Delta t, y_j + p_4 \Delta t g_2)$$

Procedure for Deriving R.K. Methods

Step 1

- Taylor series expand for g_2, g_3 etc. about the point (t_j, y_j).

  We must use a 2-D Taylor series since the expansion is about (t_j, y_j)

  - e.g.

  $$g_2 = f(t_j + p_1 \Delta t, y_j + p_2 \Delta t g_1)$$

  - Letting $\Delta T \equiv p_1 \Delta t$ and $\Delta Y \equiv p_2 \Delta t g_1$

  $$g_2 = f(t_j, y_j) + \Delta T \frac{\partial f}{\partial t} + \Delta Y \frac{\partial f}{\partial y} + \frac{1}{2!}\left[\Delta T^2 \frac{\partial^2 f}{\partial t^2} + 2\Delta T \Delta Y \frac{\partial^2 f}{\partial y \partial t} + \Delta Y^2 \frac{\partial^2 f}{\partial y^2}\right] + \text{H.O.T.}$$

- Notes
  - The Taylor series expanded form of g_2 involves g_1, however expansion for g_1 is simply $f(t_j, y_j)$
  - The Taylor series expanded form of g_3 involves g_2 $\rightarrow$ must substitute in for Taylor series expanded form of g_2

Step 2

- Substitute in Taylor series expanded forms of $g_1, g_2, \ldots$ into the R.K. formula

Step 3

- Taylor series expand for y_{j+1} about y_j

$y(t)$ is a function of t only $\rightarrow$ apply a 1-D Taylor series

$$y_{j+1} = y_j + \Delta t \left.\frac{dy}{dt}\right|_j + \frac{\Delta t^2}{2} \left.\frac{d^2y}{dt^2}\right|_j + O(\Delta t)^3$$

- However by definition

$$\frac{dy}{dt} = f(t, y)$$

- Must use chain rule to differentiate $f(t, y(t))$

$$\frac{d^2y}{dt^2} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial y}\frac{dy}{dt} \quad \Rightarrow \quad \frac{d^2y}{dt^2} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial y} f$$

- Substituting

$$y_{j+1} = y_j + \Delta t\ f_j + \frac{\Delta t^2}{2}\left(\left.\frac{\partial f}{\partial t}\right|_j + f_j \left.\frac{\partial f}{\partial y}\right|_j\right) + O(\Delta t^3)$$

Step 4

- Match term by term expressions for y_{j+1} obtained in steps 2 and 3
- Set up equations for coefficients and solve to a free variable

Step 5

- Select the free variable

Advantages of R.K. methods

- Self starting $\rightarrow \Delta t$ can be changed at any time very easily
- Easy to program
- Comparable accuracy to other similar order methods

Disadvantages of R.K. Methods

- More expensive to run in terms of CPU
- Difficult and/or expensive to get error estimates during time stepping

$$E_{j+1} = \frac{\hat{y}_{j+1} - y_{j+1}}{2^{-k} - 1}$$

where

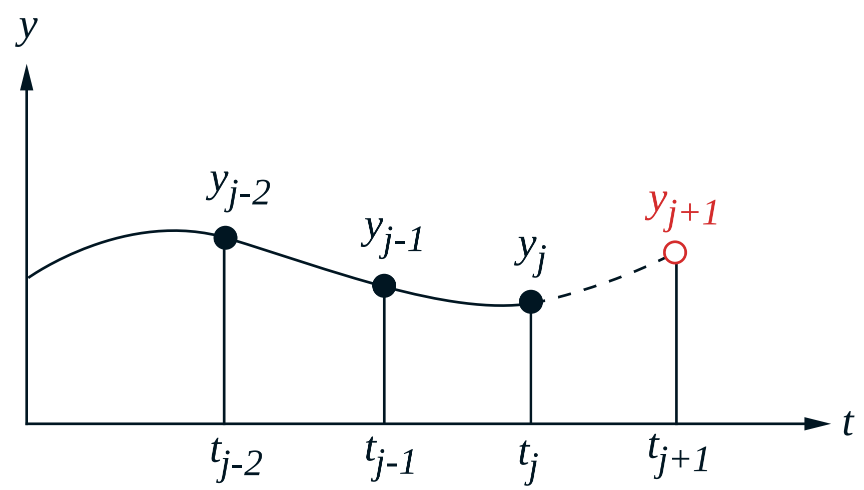
$\hat{y}_{j+1} \rightarrow$ solution found using $\frac{\Delta t}{2}$

$y_{j+1} \rightarrow$ solution found using Δt

k = order of the method

SOLUTIONS TO I.V.P.'S - MULTI-STEP METHODS

- Multi-step methods may involve more than one previous discrete point



- Open formulae, closed formulae and predictor-corrector methods are all multi-step methods

Open Formulae

- Solve $\frac{dy}{dt} = f(t, y) \quad y(0) = y_o$ such that unknown solution is computed explicitly (i.e. y_{j+1} is expressed in terms of only known values of y_j, y_{j-1}, y_{j-2}, etc.)

How to Derive Open Formulae

Step 1

- Take a forward Taylor series of y about t_j

$$y_{j+1} = y_j + \Delta t \frac{dy}{dt}\bigg|_j + \frac{\Delta t^2}{2!} \frac{d^2 y_j}{dt^2} + \frac{\Delta t^3}{3!} \frac{d^3 y_j}{dt^3} + \dots$$

- However $\frac{dy}{dt}\bigg|_j = f_j \quad \Rightarrow \quad \frac{d^2 y}{dt^2}\bigg|_j = \dot{f}_j \qquad$ etc.

- Substituting

$$y_{j+1} = y_j + \Delta t\left(f_j + \frac{\Delta t}{2!} \dot{f}_j + \frac{(\Delta t)^2}{3!} \ddot{f}_j + \dots\right)$$

Step 2

- Substitute in for various derivatives of f_j using backward differences (carrying a ***sufficient*** number of truncation terms or using a high enough accurate approximation)

- For example in deriving the second order Adams Open Formula, we approximate $\dot{f}_j$ as:

$$\dot{f}_j = \frac{f_j - f_{j-1}}{\Delta t} + \frac{\Delta t}{2}\ddot{f}_j + O(\Delta t)^2$$

- Substituting into the result of Step 1

$$y_{j+1} = y_j + \Delta t\left\{f_j + \frac{\Delta t}{2}\left[\frac{f_j - f_{j-1}}{\Delta t} + \frac{\Delta t}{2}\ddot{f}_j + O(\Delta t)^2\right] + \frac{(\Delta t)^2}{3!}\ddot{f}_j\right\}$$

- This results in the 2nd order Adams Open Formula

$$\boldsymbol{y_{j+1} = y_j + \Delta t\left[\frac{3}{2}f_j - \frac{1}{2}f_{j-1}\right] + O(\Delta t)^3}$$

Advantages of Open formulae

- f only needs to be evaluated at ***known*** values, therefore no iteration is required
- More efficient per time step than R.K.

Disadvantages of Open formulae

- Stability
- Accuracy
- Difficult to change time step

Closed Formulae

- Solve $\frac{dy}{dt} = f(t, y) \quad y(0) = y_o$ such that the unknown solution is computed implicitly (i.e. y_{j+1} is expressed in terms of both unknown y_{j+1} and known values of y_j, y_{j-1}, y_{j-2}, etc.)

How to Derive Closed Formulae

Step 1

- Use a backward Taylor series expansion for $y(t)$ about $y(t + \Delta t)$

$$y_j = y_{j+1} - \Delta t \frac{dy}{dt}\bigg|_{j+1} + \frac{\Delta t^2}{2!}\frac{d^2y}{dt^2}\bigg|_{j+1} - \frac{\Delta t^3}{3!}\frac{d^3y}{dt^3}\bigg|_{j+1} + H.O.T.$$

- Re-arrange and substitute $\frac{dy}{dt}\bigg|_{j+1} = f_{j+1}$, $\frac{d^2y}{dt^2}\bigg|_{j+1} = \dot{f}_{j+1}$ etc.

$$y_{j+1} = y_j + \Delta t\left[f_{j+1} - \frac{\Delta t}{2}\dot{f}_{j+1} + \frac{\Delta t^2}{3!}\ddot{f}_{j+1} + \dots\right]$$

Step 2

- Substitute for derivatives of f_{j+1} using backward differences
- For example to derive a second order closed formula

$$\dot{f}_{j+1} = \frac{f_{j+1} - f_j}{\Delta t} + O(\Delta t)$$

- Substituting into the result of Step 1 we obtain trapezoidal rule

$$y_{j+1} = y_j + \frac{\Delta t}{2}[f_{j+1} + f_j] + O(\Delta t)^3$$

Advantages of Closed Formulae

- Better accuracy than open formulae of the same order
- Stability properties are good

Disadvantages of Closed Formulae

- Need to iterate $\rightarrow$ this may be expensive

Predictor-Corrector Methods

Predictor → Open Formula

- e.g.

$$y_{j+1}^{(0)} = y_j + \Delta t\left[\frac{3}{2} f_j - \frac{1}{2} f_{j-1}\right]$$

Corrector → Closed Formula

- e.g.

$$y_{j+1}^{(k+1)} = y_j + \frac{\Delta t}{2}[f_{j+1}^{(k)} + f_j]$$

  - first iteration → use predictor value
  - then iterate until convergence

Starter

- Applies a R.K. formula to start the computation

Modifier

- Improves first iteration value for the Corrector based on estimated truncation error

Advantages of Predictor-Corrector Methods

- Very efficient
    - Less work per time step as compared to R.K. methods
    - Only few iterations needed when compared to closed formulae
- Good stability (stability of the corrector)
- Very accurate (more so than open formulae)
- Easy to estimate errors

SIMULTANEOUS FIRST ORDER I.V.P.'S

- Use ***same*** methods except apply to all equations simultaneously (must account for coupling)

- Overall ***accuracy*** of time stepping is $\rightarrow$ one order less than per time step truncation error

B.V.P. SOLUTIONS

- Matrix methods
  - Simply discretize o.d.e. at all nodes using F.D. based formulae
  - Implement b.c.'s
  - Solve system
- Shooting methods
  - Convert b.v.p. into an i.v.p. with one or more unknown b.c.'s

COURSE SUMMARY

Survey of Many Numerical Methods

Numerical Interpolation

- Describe a function by passing a polynomial through a set of functional values and/or functional derivative values
- Example Uses:
  - Find functional values at locations other than the nodes
  - Basis of the finite element method

Numerical Differentiation

- Find discrete approximations to differentiation. Derivatives are approximated by sums and differences of functional values at discrete points (nodes) in space/time
- Uses:
  - Solve o.d.e.'s and p.d.e.'s using F.D. methods
  - Estimate errors in numerical approximations

Numerical Integration

- Find integrals based on discrete functional values at a given set of integration points
- Uses:
    - Integrate results such as flows etc.
    - Use for finite element methods (integral methods)

O.D.E./I.V.P.'s → Time Dependent Problems

- Can reduce any order o.d.e./i.v.p. into a system of 1st order o.d.e./i.v.p.'s
- Time march → go from one time level to the next
    - One step methods → Runge-Kutta
    - Multi-step methods → Open, Closed and Predictor-Corrector Methods

O.D.E./B.V.P.'s → Spatially Dependent Problems

- Solve by substituting in F.D. approximations for the terms
- Generate enough algebraic equations to solve for the unknowns

P.D.E. Solutions

- Time discretization: apply one of the methods for o.d.e./i.v.p.'s (R.K., open, closed, P-C) or simply substitute in for the time derivatives using F.D. approximations.
- Spatial discretization: substitute in for the spatial derivatives using F.D. approximations evaluated at the appropriate time level(s).
- "Time March" $\rightarrow$ go from one time level to the next while solving all spatial locations.
- **Always write the same number of discrete equations as there are (interior and boundary) unknowns.**

Solutions of Simultaneous Linear Algebraic Equations

- Solve a system of simultaneous equations efficiently
- Uses:
  - Both F.D. and F.E. solutions to o.d.e.'s and p.d.e.'s typically generate systems of simultaneous equations.

Course Concepts

- Many of these methods are inter-related/used together
  - In their derivation
  - In their use
- **All methods are based on representing continuous functions at discrete points in space/time**
- As engineers we wish to solve complicated problems often described by mathematical equations
  - Solve o.d.e.'s/p.d.e.'s
  - Numerical methods allow us to solve mathematical problems for which closed form solutions are not available

- We must be very careful in the application of numerical methods
  - **Numerical models/codes are never a black box!**
  - **Numerical models/codes must be applied understanding both the numerics and physics incorporated into the model/code!**
  - **Numerical models/codes can give results which look nice but are totally wrong!!!**
  - Must try to ***assess errors***!!!
  - Error analysis is very important!
  - **A solution without an error estimate is NOT A GOOD SOLUTION**
- We have learned many tools used in numerical analysis
  - Built a foundation with which to understand numerical models/codes
  - Take advanced numerical courses
  - Extensive literature on numerical analysis