Generalized Multi-Step Methods

Mathematical Problem:

$$\frac{dy}{dt} = f(y,t) \qquad y(t_0) = y_0 \qquad t \geq 0$$

All the multi-step (explicit and implicit) and BDF formulae derived so far can be expressed in a general form as follows:

$$\sum_{i=0}^{n+1} \alpha_i \, y_i = h \sum_{i=0}^{n+1} \beta_i \, f_i$$

This will require a set of initial conditions $\{y_0, y_1, y_2, \cdots y_n\}$

Next, we shall derive a group of methods that deviate from this general framework!

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Runge-Kutta (R-K) Methods

This is a group of Explicit methods that evaluates f at intermediate points within a time step h, i.e., between n and $(n + 1)$. In generalized form, the method may be expressed as:

$$\int_{y_n}^{y_{n+1}} dy = \int_{t_n}^{t_{n+1}} f(y,t)dt \quad \Longrightarrow \quad y_{n+1} = y_n + h\sum_{i=0}^{p} \omega_i\,\phi_i$$

where,

$$\phi_0 = f(y_n, t_n)$$
$$\phi_1 = f(y_n + h\alpha_0^1\phi_0, t_n + \beta_1 h)$$
$$\phi_2 = f(y_n + h\alpha_0^2\phi_0 + h\alpha_1^2\phi_1, t_n + \beta_2 h)$$
$$\phi_3 = f(y_n + h\alpha_0^3\phi_0 + h\alpha_1^3\phi_1 + h\alpha_2^3\phi_2, t_n + \beta_3 h)$$

....

$$\phi_i = f\left(y_n + h\sum_{j=1}^{i-1} \alpha_j^i\phi_j\,, t_n + \beta_i h \right)$$

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Runge-Kutta (R-K) Methods

Example: $p = 1$

$$y_{n+1} = y_n + \omega_0 h\phi_0 + \omega_1 h\phi_1$$

$$\phi_0 = f(y_n, t_n) \qquad \phi_1 = f(y_n + h\alpha_0\phi_0, t_n + \beta_1 h)$$

Objective: estimate $\omega_0, \omega_1, \alpha_0$ and β_1 to achieve maximum accuracy, i.e., highest possible order of truncation error

$$\frac{dy}{dt} = f(y,t) \quad \Longrightarrow \quad \frac{d^2y}{dt^2} = \frac{df}{dt} = \frac{\partial f}{\partial y}\frac{dy}{dt} + \frac{\partial f}{\partial t} = f\frac{\partial f}{\partial y} + \frac{\partial f}{\partial t}$$

$$LHS = y_{n+1} = y_n + h\frac{dy_n}{dt} + \frac{h^2}{2!}\frac{d^2y_n}{dt^2} + \frac{h^3}{3!}\frac{d^3y_n}{dt^3} + o(h^4)$$

$$= y_n + hf_n + \frac{h^2}{2!}\left(f_n\frac{\partial f}{\partial y}\bigg|_n + \frac{\partial f}{\partial t}\bigg|_n\right) + \frac{h^3}{3!}\frac{d^3y_n}{dt^3} + o(h^4)$$

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Runge-Kutta (R-K) Methods

$$y_{n+1} = y_n + \omega_0 h\phi_0 + \omega_1 h\phi_1$$
$$\phi_0 = f(y_n, t_n) \qquad \phi_1 = f(y_n + h\alpha_0\phi_0, t_n + \beta_1 h)$$

$$\phi_0 = f(y_n, t_n) = f_n$$
$$\phi_1 = f_n + \left(\alpha_0 h f_n \left.\frac{\partial f}{\partial y}\right|_n + \beta_1 h \left.\frac{\partial f}{\partial t}\right|_n \right) + \left(\alpha_0^2 h^2 f_n^2 \left.\frac{\partial^2 f}{\partial y^2}\right|_n + 2\alpha_0\beta_1 h^2 f_n \left.\frac{\partial f}{\partial y}\right|_n \left.\frac{\partial f}{\partial t}\right|_n + \beta_1^2 h^2 \left.\frac{\partial^2 f}{\partial t^2}\right|_n \right) + o(h^3)$$

$$RHS = y_n + (\omega_0 + \omega_1) h f_n + \omega_1 h^2 \left(\alpha_0 f_n \left.\frac{\partial f}{\partial y}\right|_n + \beta_1 \left.\frac{\partial f}{\partial t}\right|_n \right) + \omega_1 h^3 \left(\alpha_0 f_n^2 \left.\frac{\partial^2 f}{\partial y^2}\right|_n + 2\alpha_0\beta_1 f_n \left.\frac{\partial f}{\partial y}\right|_n \left.\frac{\partial f}{\partial t}\right|_n + \beta_1^2 \left.\frac{\partial^2 f}{\partial t^2}\right|_n \right) + o(h^4)$$

Runge-Kutta (R-K) Methods

$$y_{n+1} = y_n + \omega_0 h\phi_0 + \omega_1 h\phi_1$$

$$\phi_0 = f(y_n, t_n) \qquad \phi_1 = f(y_n + h\alpha_0\phi_0, t_n + \beta_1 h)$$

$$LHS = y_n + hf_n + \frac{h^2}{2!}\left(f_n \frac{\partial f}{\partial y}\bigg|_n + \frac{\partial f}{\partial t}\bigg|_n\right) + \frac{h^3}{3!}\frac{d^3 y_n}{dt^3} + o(h^4)$$

RHS

$$= y_n + (\omega_0 + \omega_1)hf_n + \omega_1 h^2\left(\alpha_0 f_n \frac{\partial f}{\partial y}\bigg|_n + \beta_1 \frac{\partial f}{\partial t}\bigg|_n\right) + \omega_1 h^3\left(\alpha_0 f_n^2 \frac{\partial^2 f}{\partial y^2}\bigg|_n\right.$$

$$\left. + 2\alpha_0\beta_1 f_n \frac{\partial f}{\partial y}\bigg|_n \frac{\partial f}{\partial t}\bigg|_n + \beta_1^2 \frac{\partial^2 f}{\partial t^2}\bigg|_n\right) + o(h^4)$$

$$\omega_0 + \omega_1 = 1 \qquad \omega_1\alpha_0 = \frac{1}{2} \qquad \omega_1\beta_1 = \frac{1}{2}$$

$\beta_1 = \alpha_0, \;\; \omega_0 = 1 - \dfrac{1}{2\alpha_0}, \qquad \omega_1 = \dfrac{1}{2\alpha_0} \;\rightarrow$ multiple **2^{nd} order** R – K

Runge-Kutta (R-K) Methods

$$y_{n+1} = y_n + \omega_0 h\phi_0 + \omega_1 h\phi_1$$

$$\phi_0 = f(y_n, t_n) \qquad \phi_1 = f(y_n + h\alpha_0\phi_0, t_n + \beta_1 h)$$

$$\beta_1 = \alpha_0, \quad \omega_0 = 1 - \frac{1}{2\alpha_0}, \qquad \omega_1 = \frac{1}{2\alpha_0}$$

Therefore, one can derive infinitely many 2nd order R-K method.

Most commonly used are the following three:

✓2nd Order Runge-Kutta (aka *Modified Euler*, *Midpoint* method):

$$\alpha_0 = \frac{1}{2} = \beta_1, \qquad \omega_0 = 0, \qquad \omega_1 = 1$$

$$y_{n+1} = y_n + h\phi_1$$

$$\phi_0 = f(y_n, t_n) \qquad \phi_1 = f\left(y_n + \frac{1}{2}h\phi_0, t_n + \frac{1}{2}h\right)$$

Runge-Kutta (R-K) Methods

✓2nd Order Runge-Kutta (aka *Ralston's* method):

$$\alpha_0 = \frac{3}{4} = \beta_1, \qquad \omega_0 = \frac{1}{3}, \qquad \omega_1 = \frac{2}{3}$$

$$y_{n+1} = y_n + h\left(\frac{\phi_0}{3} + \frac{2\phi_1}{3}\right)$$

$$\phi_0 = f(y_n, t_n) \qquad \phi_1 = f\left(y_n + \frac{3}{4}h\phi_0, t_n + \frac{3}{4}h\right)$$

✓2nd Order Runge-Kutta (aka *Improved Euler*, *Heun's* method):

$$\alpha_0 = 1 = \beta_1, \qquad \omega_0 = \frac{1}{2}, \qquad \omega_1 = \frac{1}{2}$$

$$y_{n+1} = y_n + h\left(\frac{\phi_0}{2} + \frac{\phi_1}{2}\right)$$

$$\phi_0 = f(y_n, t_n) \qquad \phi_1 = f(y_n + h\phi_0, t_n + h)$$

Runge-Kutta (R-K) Methods

Similarly, one can derive multiple 3rd and 4th order R-K methods. Two typically used algorithms for the 3rd and 4th order methods are as follow:

✓A 3rd Order Runge-Kutta Method:

$$y_{n+1} = y_n + h\left(\frac{1}{6}\phi_0 + \frac{2}{3}\phi_1 + \frac{1}{6}\phi_2\right)$$

$$\phi_0 = f(y_n, t_n)$$

$$\phi_1 = f\left(y_n + \frac{1}{2}h\phi_0, t_n + \frac{1}{2}h\right)$$

$$\phi_2 = f(y_n - h\phi_0 + 2h\phi_1, t_n + h)$$

Runge-Kutta (R-K) Methods

✓A 4th Order Runge-Kutta Method:

$$y_{n+1} = y_n + h\left(\frac{1}{6}\phi_0 + \frac{1}{3}(\phi_1 + \phi_2) + \frac{1}{6}\phi_3\right)$$

$$\phi_0 = f(y_n, t_n)$$

$$\phi_1 = f\left(y_n + \frac{1}{2}h\phi_0, t_n + \frac{1}{2}h\right)$$

$$\phi_2 = f\left(y_n + \frac{1}{2}h\phi_1, t_n + \frac{1}{2}h\right)$$

$$\phi_3 = f(y_n + h\phi_2, t_n + h)$$

Let us now see applications of all the methods!

ESO 208A: Computational Methods in Engineering

Ordinary Differential Equation: Application, Startup, Predictor-Corrector

Saumyen Guha

Department of Civil Engineering
IIT Kanpur

Ordinary Differential Equation

- ✓ The methods for Initial Value Problems (IVPs):
  - ✓ Multi-step Methods
    - ✓ Explicit: Euler Forward, Adams-Bashforth
    - ✓ Implicit: Euler Backward, Trapezoidal and Adams-Moulton
  - ✓ Backward Difference Formulae (BDF)
  - ✓ Runge-Kutta Methods
- ✓ Applications, Startup, Combination Methods (Predictor-Corrector)
  - ✓ Tools: IVP methods, Richardson's extrapolation, judicious choice!
- ✓ Consistency, Stability, Convergence
- ✓ Application to Systems of ODE
- ✓ Boundary Value Problems (BVPs)
  - ✓ Shooting Method
  - ✓ Direct Methods

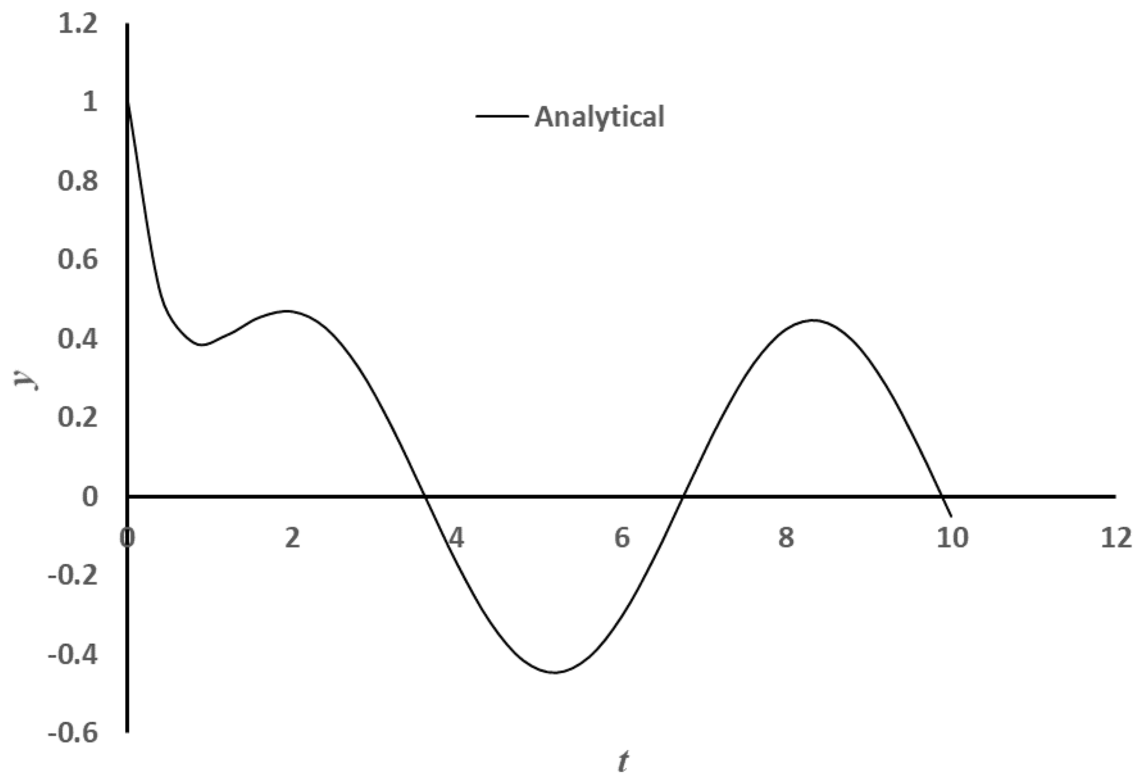
The Problem

- ✓ Let us apply all the methods to the following IVP:

$$\frac{dy}{dt} = -2y + \sin t \qquad\qquad y(0) = 1$$

- ✓ Analytical Solution

$$y = \frac{6}{5}e^{-2t} + \frac{1}{5}(2\sin t - \cos t)$$



Application: Multi-Step Methods (explicit)

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

Some commonly used explicit methods:

Name	***k***	***Method***	***GTE Order***
Euler Forward	0	$y_{n+1} = y_n + hf_n$	h
Adams-Bashforth	1	$y_{n+1} = y_n + h\left(\frac{3}{2}f_n - \frac{1}{2}f_{n-1}\right)$	h^2
	2	$y_{n+1} = y_n + h\left(\frac{23}{12}f_n - \frac{4}{3}f_{n-1} + \frac{5}{12}f_{n-2}\right)$	h^3
	3	$y_{n+1} = y_n + h\left(\frac{55}{24}f_n - \frac{59}{24}f_{n-1} + \frac{37}{24}f_{n-2} - \frac{3}{8}f_{n-3}\right)$	h^4

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Euler Forward

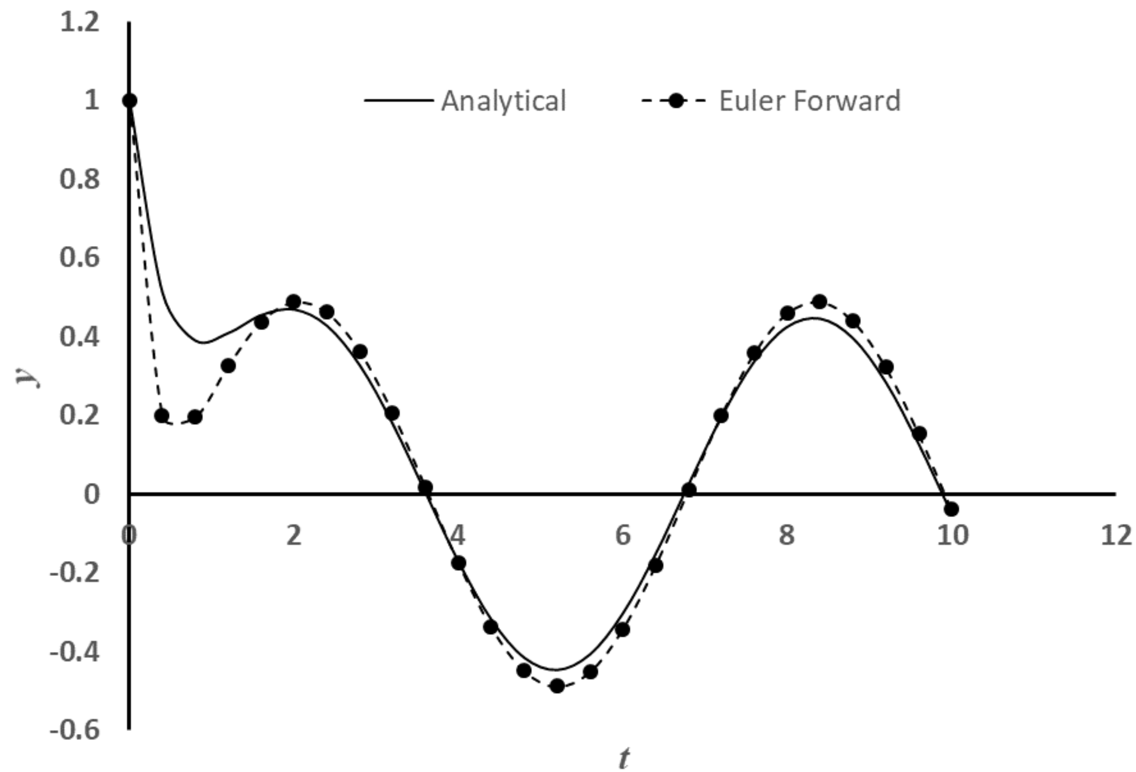
$$\frac{dy}{dt} = -2y + \sin t$$
$$y(0) = 1$$
$$y_{n+1} = y_n + h(-2y_n + \sin t_n)$$
$$= y_n(1 - 2h) + h \sin t_n$$
$$y_0 = y(0) = 1; \quad h = 0.4$$

$$y_1 = y(0.4)$$
$$= 1(1 - 2 \times 0.4) + 0.4 \sin 0$$
$$= 0.2$$

$$y_2 = y(0.8)$$
$$= 0.2(1 - 2 \times 0.4) + 0.4 \sin 0.4$$
$$= 0.1958$$

$$y_3 = y(1.2)$$
$$= 0.1958(1 - 2 \times 0.4)$$
$$+ 0.4 \sin 0.8 = 0.3261$$

Continuing like this for 25 time steps to t = 10



Adams-Bashforth (2^{nd} Order)

$y_0 = y(0) = 1; \;\; h = 0.4;$

From Euler Forward:
$y_1 = y(0.4) = 0.2$

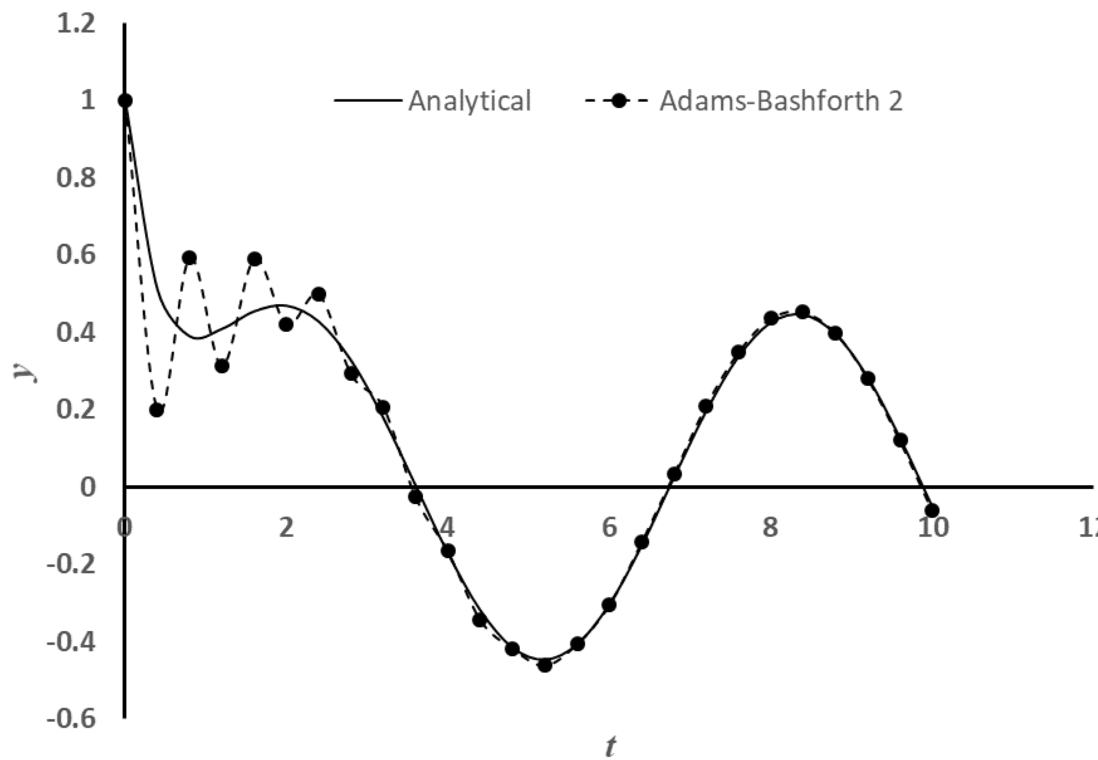
$$\frac{dy}{dt} = -2y + \sin t \qquad y(0) = 1$$

$$y_{n+1} = y_n + h\left[\frac{3}{2}(-2y_n + \sin t_n) - \frac{1}{2}(-2y_{n-1} + \sin t_{n-1})\right]$$

$$y_2 = y(0.8) = 0.2 + 0.4\left[\frac{3}{2}(-2 \times 0.2 + \sin 0.4) - \frac{1}{2}(-2 \times 1 + \sin 0)\right] = 0.5937$$

$$y_3 = y(1.2) = 0.5937 + 0.4\left[\frac{3}{2}(-2 \times 0.5937 + \sin 0.8) - \frac{1}{2}(-2 \times 0.2 + \sin 0.4)\right] = 0.3138$$

Continuing like this up to t = 10



Adams-Bashforth (3rd Order)

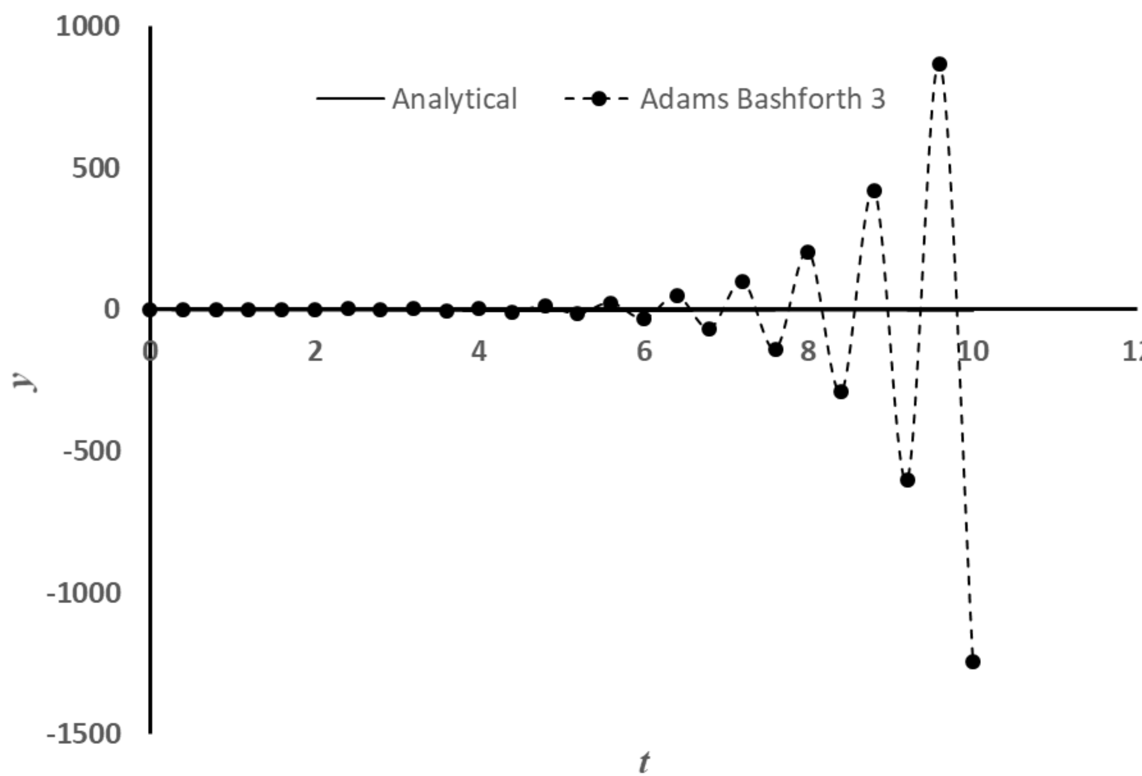
$$y_0 = y(0) = 1;\ \ h = 0.4;$$
$$y_1 = y(0.4) = 0.2\ (EF)$$
$$y_2 = y(0.8) = 0.5937\ (AB2)$$

$$y_3 = y(1.2) = 0.5937 + 0.4\left[\frac{23}{12}(-2\times 0.5937 + \sin 0.8) - \frac{4}{3}(-2\times 0.2 + \sin 0.4) + \frac{5}{12}(-2\times 1 + \sin 0)\right] = -0.9433\times 10^{-1}$$

$$y_4 = y(1.6) = -0.9433\times 10^{-1} + 0.4\left[\frac{23}{12}(-2\times -0.9433\times 10^{-1} + \sin 1.2) - \frac{4}{3}(-2\times 0.5937 + \sin 0.8) + \frac{5}{12}(-2\times 0.2 + \sin 0.4)\right] = 1.014$$

$$y_{n+1} = y_n + h\left[\frac{23}{12}(-2y_n + \sin t_n) - \frac{4}{3}(-2y_{n-1} + \sin t_{n-1}) + \frac{5}{12}(-2y_{n-2} + \sin t_{n-2})\right]$$

Continuing like this up to $t = 10$



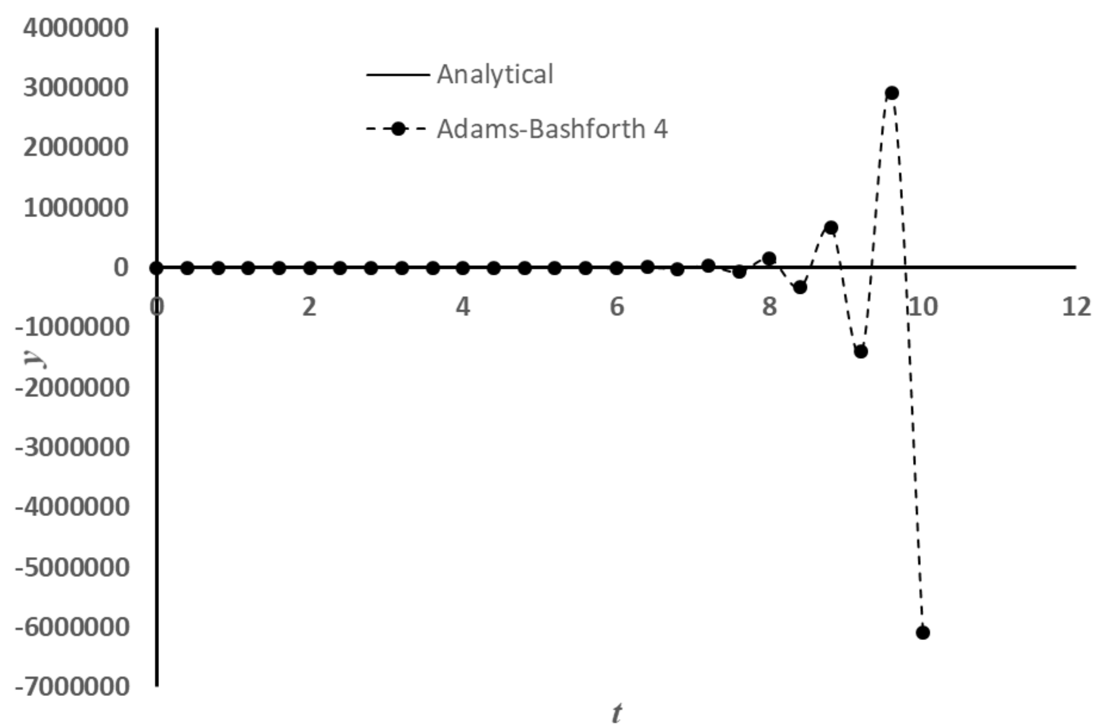
Adams-Bashforth (4th Order)

$$y_0 = y(0) = 1; \quad h = 0.4;$$
$$y_1 = y(0.4) = 0.2\ (EF)$$
$$y_2 = y(0.8) = 0.5937\ (AB2)$$
$$y_3 = y(1.2) = -0.09433\ (AB3)$$

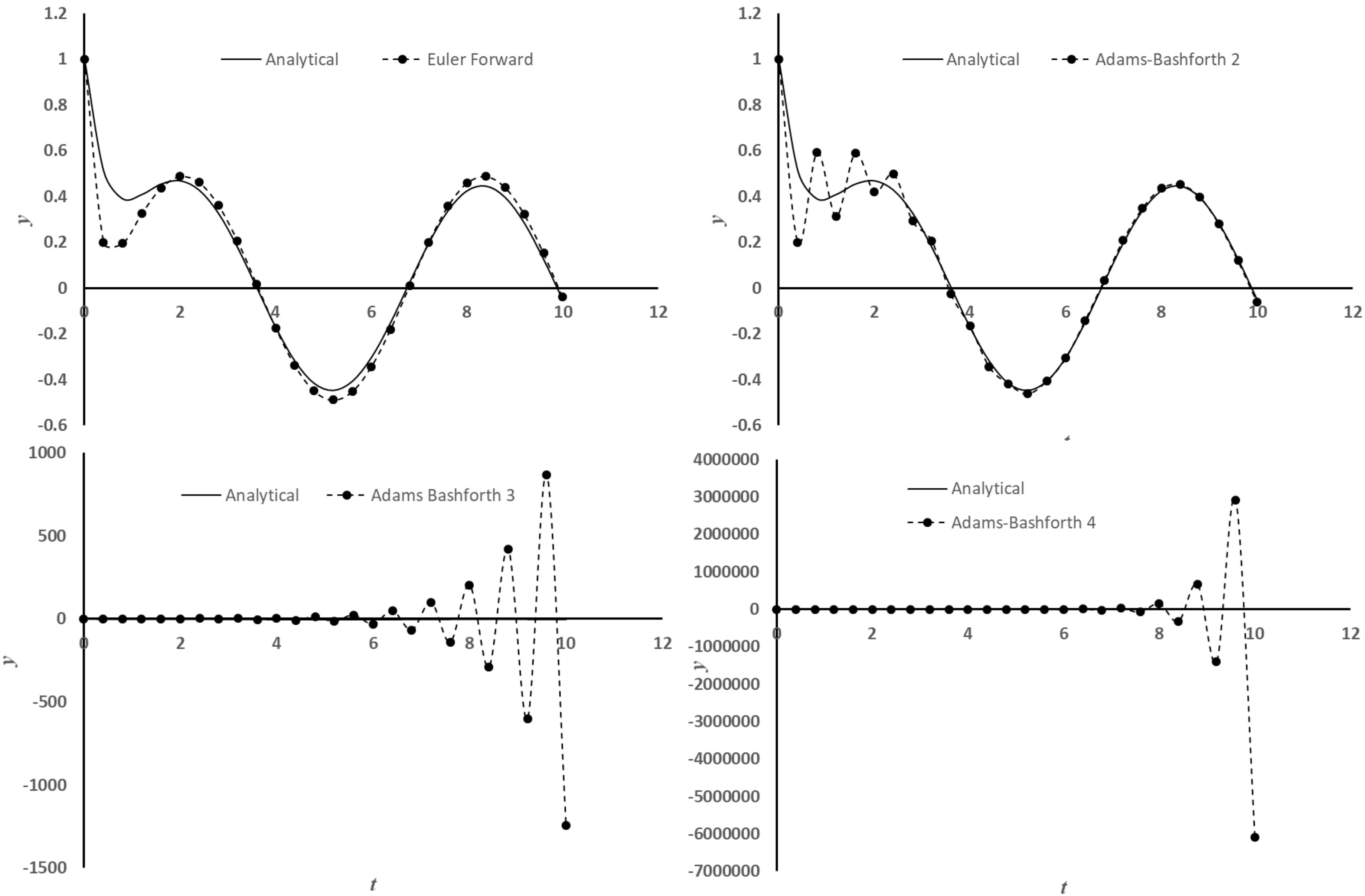
$$y_{n+1} = y_n + h\left[\frac{55}{24}(-2y_n + \sin t_n) - \frac{59}{24}(-2y_{n-1} + \sin t_{n-1}) + \frac{37}{24}(-2y_{n-2} + \sin t_{n-2}) - \frac{3}{8}(-2y_{n-3} + \sin t_{n-3})\right]$$

Continuing like this up to t = 10

$$y_4 = y(1.6) = -0.9433 \times 10^{-1} + 0.4\left[\frac{55}{24}(-2 \times -0.9433 \times 10^{-1} + \sin 1.2) - \frac{59}{24}(-2 \times 0.5937 + \sin 0.8) + \frac{37}{24}(-2 \times 0.2 + \sin 0.4) - \frac{3}{8}(-2 \times 1 + \sin 0)\right] = 1.689$$



Euler Forward, Adams-Bashforth (2nd, 3rd and 4th Order)



Observations: explicit multi-step methods

A few things to note for multi-step explicit methods: Euler Forward, Adams-Bashforth

- ✓ All methods above the **first** order cannot start by themselves:
  - ✓ how to solve the start-up problem?
- ✓ Some strange oscillation showing up in some of the methods (uncontrolled growth, instability):
  - ✓ Is there a system to this?
  - ✓ Can it be predicted? How to know when this will happen?
  - ✓ Can it be avoided? If yes, then how?

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Application: Multi-Step Methods (implicit)

$$y_{n+1} \approx \tilde{y}_{n+1} = y_n + h \sum_{i=0}^{k} \beta_i f_{n+1-i}$$

Some commonly used implicit methods:

Name	***k***	***Method***	***GTE Order***
Euler Backward	0	$y_{n+1} = y_n + hf_{n+1}$	h
Trapezoidal	1	$y_{n+1} = y_n + h\left(\frac{1}{2}f_{n+1} + \frac{1}{2}f_n\right)$	h^2
Adams-Moulton	2	$y_{n+1} = y_n + h\left(\frac{5}{12}f_{n+1} + \frac{2}{3}f_n - \frac{1}{12}f_{n-1}\right)$	h^3
	3	$y_{n+1} = y_n + h\left(\frac{3}{8}f_{n+1} + \frac{19}{24}f_n - \frac{5}{24}f_{n-1} + \frac{1}{24}f_{n-2}\right)$	h^4

Euler Backward

$$\frac{dy}{dt} = -2y + \sin t \qquad y(0) = 1$$

$$y_{n+1} = y_n + h(-2y_{n+1} + \sin t_{n+1})$$

$$y_{n+1} = \frac{y_n + h \sin t_{n+1}}{(1 + 2h)}$$

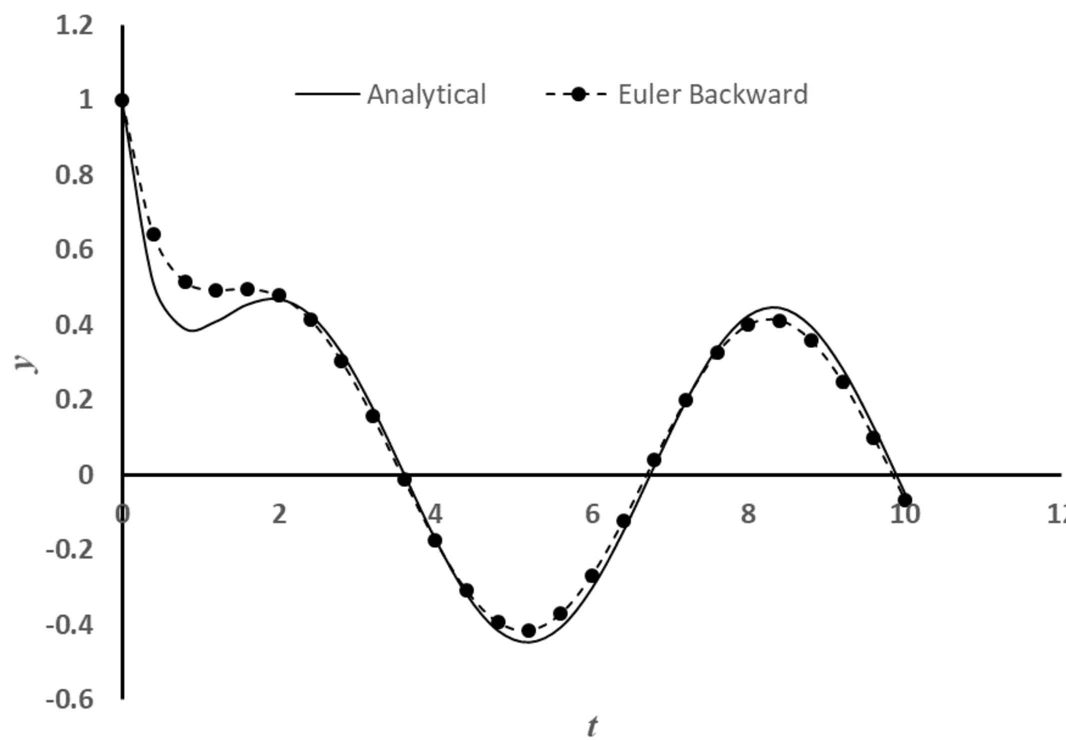
$$y_0 = y(0) = 1; \quad h = 0.4$$

$$y_1 = y(0.4) = \frac{1 + 0.4 \sin 0.4}{(1 + 2 \times 0.4)}$$
$$= 0.6421$$

$$y_2 = y(0.8)$$
$$= \frac{0.6421 + 0.4 \sin 0.8}{(1 + 2 \times 0.4)} = 0.5161$$

$$y_3 = y(1.2)$$
$$= \frac{0.5161 + 0.4 \sin 1.2}{(1 + 2 \times 0.4)} = 0.4939$$

Continuing like this for 25 time steps to t = 10



Trapezoidal Method

$$y_{n+1} = y_n + \frac{h}{2}[(-2y_{n+1} + \sin t_{n+1}) + (-2y_n + \sin t_n)]$$

$$y_{n+1} = \frac{y_n(1-h) + \frac{h}{2}(\sin t_{n+1} + \sin t_n)}{(1+h)}$$

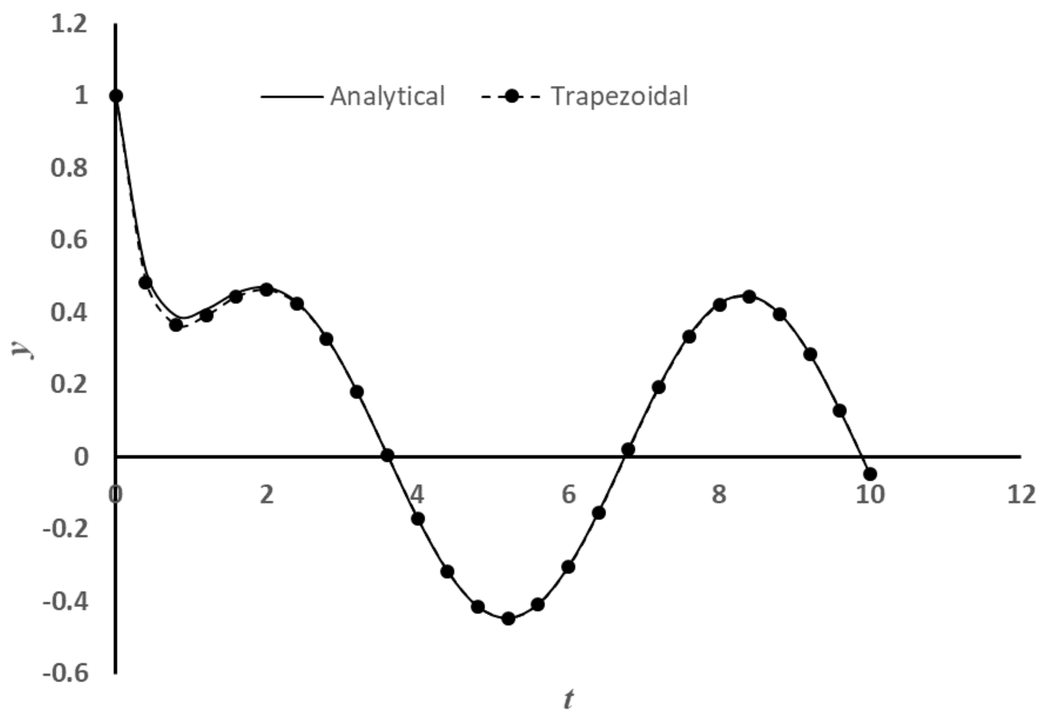
$y_0 = y(0) = 1; \quad h = 0.4$

$$y_1 = y(0.4) = \frac{1(1-0.4) + 0.2(\sin 0 + \sin 0.4)}{(1+0.4)} = 0.4842$$

$$y_2 = y(0.8) = \frac{0.4842(1-0.4) + 0.2(\sin 0.4 + \sin 0.8)}{(1+0.4)} = 0.3656$$

$$y_3 = y(1.2) = \frac{0.3656(1-0.4) + 0.2(\sin 0.8 + \sin 1.2)}{(1+0.4)} = 0.3923$$

Continuing like this up to t = 10



Adams-Moulton (3rd Order)

$$y_{n+1} = y_n + h\left[\frac{5}{12}(-2y_{n+1} + \sin t_{n+1}) + \frac{2}{3}(-2y_n + \sin t_n) - \frac{1}{12}(-2y_{n-1} + \sin t_{n-1})\right]$$

$$y_{n+1} = \frac{y_n + h\left[\frac{5}{12}\sin t_{n+1} + \frac{2}{3}(-2y_n + \sin t_n) - \frac{1}{12}(-2y_{n-1} + \sin t_{n-1})\right]}{\left(1 + \frac{5}{6}h\right)}$$

$$y_0 = y(0) = 1; \quad y_1 = y(0.4) = 0.6421\ (EB); \quad h = 0.4$$

$$y_2 = y(0.8) = \frac{0.6421 + 0.4\left[\frac{5}{12}\sin 0.8 + \frac{2}{3}(-2 \times 0.6421 + \sin 0.4) - \frac{1}{12}(-2 \times 1 + \sin 0)\right]}{\left(1 + \frac{5}{6} \times 0.4\right)}$$

$$= 0.4423$$

$$y_3 = y(1.2) = \frac{0.4423 + 0.4\left[\frac{5}{12}\sin 1.2 + \frac{2}{3}(-2 \times 0.4423 + \sin 0.8) - \frac{1}{12}(-2 \times 0.6421 + \sin 0.4)\right]}{\left(1 + \frac{5}{6} \times 0.4\right)}$$

$$= 0.4371$$

Adams-Moulton (4th Order)

$$y_{n+1} = y_n + h\left[\frac{3}{8}(-2y_{n+1} + \sin t_{n+1}) + \frac{19}{24}(-2y_n + \sin t_n) - \frac{5}{24}(-2y_{n-1} + \sin t_{n-1}) + \frac{1}{24}(-2y_{n-2} + \sin t_{n-2})\right]$$

$$y_{n+1} = \frac{y_n + h\left[\frac{3}{8}\sin t_{n+1} + \frac{19}{24}(-2y_n + \sin t_n) - \frac{5}{24}(-2y_{n-1} + \sin t_{n-1}) + \frac{1}{24}(-2y_{n-2} + \sin t_{n-2})\right]}{\left(1 + \frac{3}{4}h\right)}$$

$$y_0 = y(0) = 1; \quad y_1 = y(0.4) = 0.6421\ (EB); \quad y_2 = y(0.8) = 0.4423\ (AM3); \quad h = 0.4$$

$$y_3 = y(1.2) = \frac{1}{\left(1 + \frac{3}{4}\times 0.4\right)}\left\{0.4423 + 0.4\left[\frac{3}{8}\sin 1.2 + \frac{19}{24}(-2\times 0.4423 + \sin 0.8) - \frac{5}{24}(-2\times 0.6421 + \sin 0.4) - \frac{5}{24}(-2\times 1 + \sin 0)\right]\right\} = 0.4387$$

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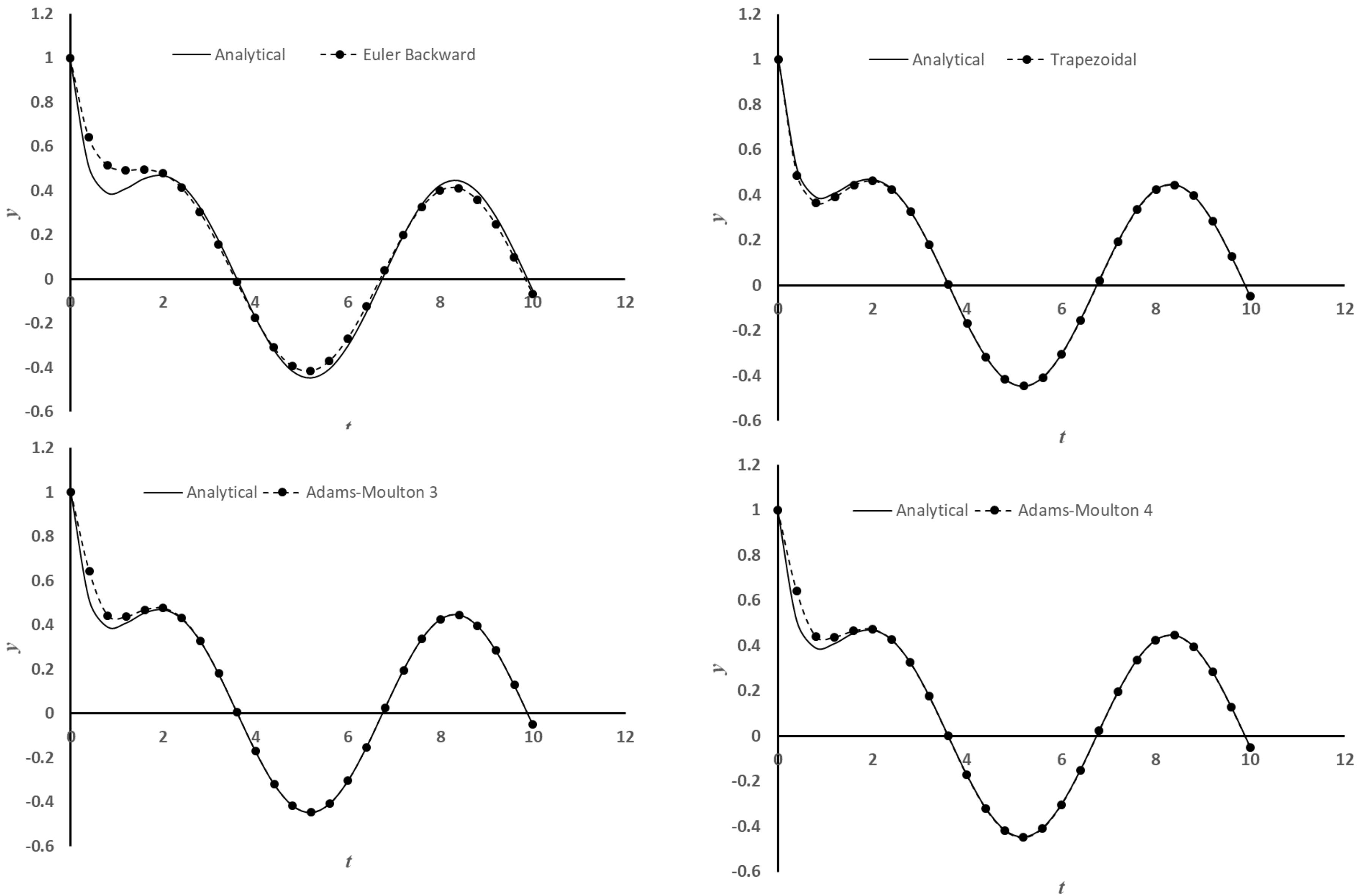
Euler Backward, Trapezoidal, Adams-Moulton (3rd and 4th Order)



Observations: implicit multi-step methods

A few things to note for multi-step implicit methods: Euler Backward, Trapezoidal, Adams-Moulton

- ✓ All methods above the **second** order cannot start by themselves. Accuracy of the higher order method is affected if the starting values are used from the lower order methods.
  - ✓ how to solve the start-up problem?
- ✓ All implicit multi-step methods may involve solution of non-linear equations (if f contains a non-linear function of the dependent variable y)
  - ✓ Is there a way to avoid this solution of non-linear equations?
- ✓ No numerical oscillations (instability) observed in any of the implicit methods:
  - ✓ Why the same order explicit multi-step methods show oscillation but implicit ones don't?
  - ✓ Do they show oscillation under any conditions or are they oscillation-proof under all conditions?

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Application: Backward Difference Formulae (BDF)

$$\sum_{i=0}^{k} \gamma_i \, y_{n+1-i} = hf_{n+1}$$

1st Order BDF is Euler Backward. Let's apply the rest.

k	***Method***	***GTE Order***
1	$y_{n+1} - y_n = hf_{n+1}$	h
2	$\frac{3}{2}y_{n+1} - 2y_n + \frac{1}{2}y_{n-1} = hf_{n+1}$	h^2
3	$\frac{11}{6}y_{n+1} - 3y_n + \frac{3}{2}y_{n-1} - \frac{1}{3}y_{n-2} = hf_{n+1}$	h^3
4	$\frac{25}{12}y_{n+1} - 4y_n + 3y_{n-1} - \frac{4}{3}y_{n-2} + \frac{1}{4}y_{n-3} = hf_{n+1}$	h^4
5	$\frac{137}{60}y_{n+1} - 5y_n + 5y_{n-1} - \frac{10}{3}y_{n-2} + \frac{5}{4}y_{n-3} - \frac{1}{5}y_{n-4} = hf_{n+1}$	h^5
6	$\frac{49}{20}y_{n+1} - 6y_n + \frac{15}{2}y_{n-1} - \frac{20}{3}y_{n-2} + \frac{15}{4}y_{n-3} - \frac{6}{5}y_{n-4} + \frac{1}{6}y_{n-5} = hf_{n+1}$	h^6

BDF (1st and 2nd Order)

$$\frac{dy}{dt} = -2y + \sin t \qquad\qquad y(0) = 1$$

✓ 1st Order (Euler Backward)

$$y_{n+1} - y_n = h(-2y_{n+1} + \sin t_{n+1}) \quad y_{n+1} = \frac{y_n + h\sin t_{n+1}}{(1+2h)}$$

✓ 2nd Order

$$\frac{3}{2}y_{n+1} - 2y_n + \frac{1}{2}y_{n-1} = h(-2y_{n+1} + \sin t_{n+1}) \quad \Longrightarrow \quad y_{n+1} = \frac{2y_n - \frac{1}{2}y_{n-1} + h\sin t_{n+1}}{\left(\frac{3}{2} + 2h\right)}$$

$$h = 0.4; \qquad y_0 = y(0) = 1; \qquad y_1 = y(0.4) = 0.6421\ (EB)$$

$$y_2 = y(0.8) = \frac{2 \times 0.6421 - \frac{1}{2} \times 1 + 0.4\sin 0.8}{\left(\frac{3}{2} + 2 \times 0.4\right)} = 0.4657$$

$$y_3 = y(1.2) = \frac{2 \times 0.4657 - \frac{1}{2} \times 0.6421 + 0.4\sin 1.2}{\left(\frac{3}{2} + 2 \times 0.4\right)} = 0.4275$$

BDF (3^{rd} and 4^{th} Order)

✓ 3^{rd} Order

$$\frac{11}{6}y_{n+1} - 3y_n + \frac{3}{2}y_{n-1} - \frac{1}{3}y_{n-2} = h(-2y_{n+1} + \sin t_{n+1})$$

$$y_{n+1} = \frac{3y_n - \frac{3}{2}y_{n-1} + \frac{1}{3}y_{n-2} + h\sin t_{n+1}}{\left(\frac{11}{6} + 2h\right)}$$

$h = 0.4;\quad y_0 = y(0) = 1;\quad y_1 = y(0.4) = 0.6421\ (EB);\quad y_2 = y(0.8) = 0.4657\ (BDF2)$

$$y_3 = y(1.2) = \frac{3 \times 0.4657 - \frac{3}{2} \times 0.6421 + \frac{1}{3} \times 1 + 0.4\sin 1.2}{\left(\frac{11}{6} + 2 \times 0.4\right)} = 0.4330$$

✓ 4^{th} Order

$$y_{n+1} = \frac{4y_n - 3y_{n-1} + \frac{4}{3}y_{n-2} - \frac{1}{4}y_{n-3} + h\sin t_{n+1}}{\left(\frac{25}{12} + 2h\right)}$$

$h = 0.4;\quad y_0 = y(0) = 1;\quad y_1 = y(0.4) = 0.6421\ (EB);$
$y_2 = y(0.8) = 0.4657\ (BDF2);\quad y_3 = y(1.2) = 0.4330\ (BDF3)$

$$y_4 = y(1.6) = \frac{4 \times 0.4330 - 3 \times 0.4657 + \frac{4}{3} \times 0.6421 - \frac{1}{4} \times 1 + 0.4\sin 1.6}{\left(\frac{25}{12} + 2 \times 0.4\right)} = 0.4650$$

BDF (5^{th} and 6^{th} Order)

✓ 5^{th} Order

$$y_{n+1} = \frac{5y_n - 5y_{n-1} + \frac{10}{3}y_{n-2} - \frac{5}{4}y_{n-3} + \frac{1}{5}y_{n-4} + h\sin t_{n+1}}{\left(\frac{137}{60} + 2h\right)}$$

$h = 0.4;$ $y_0 = y(0) = 1;$ $y_1 = y(0.4) = 0.6421\ (EB);$

$y_2 = y(0.8) = 0.4657\ (BDF2);$ $y_3 = y(1.2) = 0.4330\ (BDF3);$ $y_4 = y(1.6) = 0.4650\ (BDF4)$

$$y_5 = y(2.0) = \frac{5 \times 0.4650 - 5 \times 0.4330 + \frac{10}{3} \times 0.4657 - \frac{5}{4} \times 0.6421 + \frac{1}{5} \times 1 + 0.4\sin 2}{\left(\frac{137}{60} + 2 \times 0.4\right)} = 0.4779$$

✓ 6^{th} Order

$$y_{n+1} = \frac{6y_n - \frac{15}{2}y_{n-1} + \frac{20}{3}y_{n-2} - \frac{15}{4}y_{n-3} + \frac{6}{5}y_{n-4} - \frac{1}{6}y_{n-5} + h\sin t_{n+1}}{\left(\frac{49}{20} + 2h\right)}$$

$h = 0.4;$ $y_0 = y(0) = 1;$ $y_1 = y(0.4) = 0.6421\ (EB);$ $y_2 = y(0.8) = 0.4657\ (BDF2);$

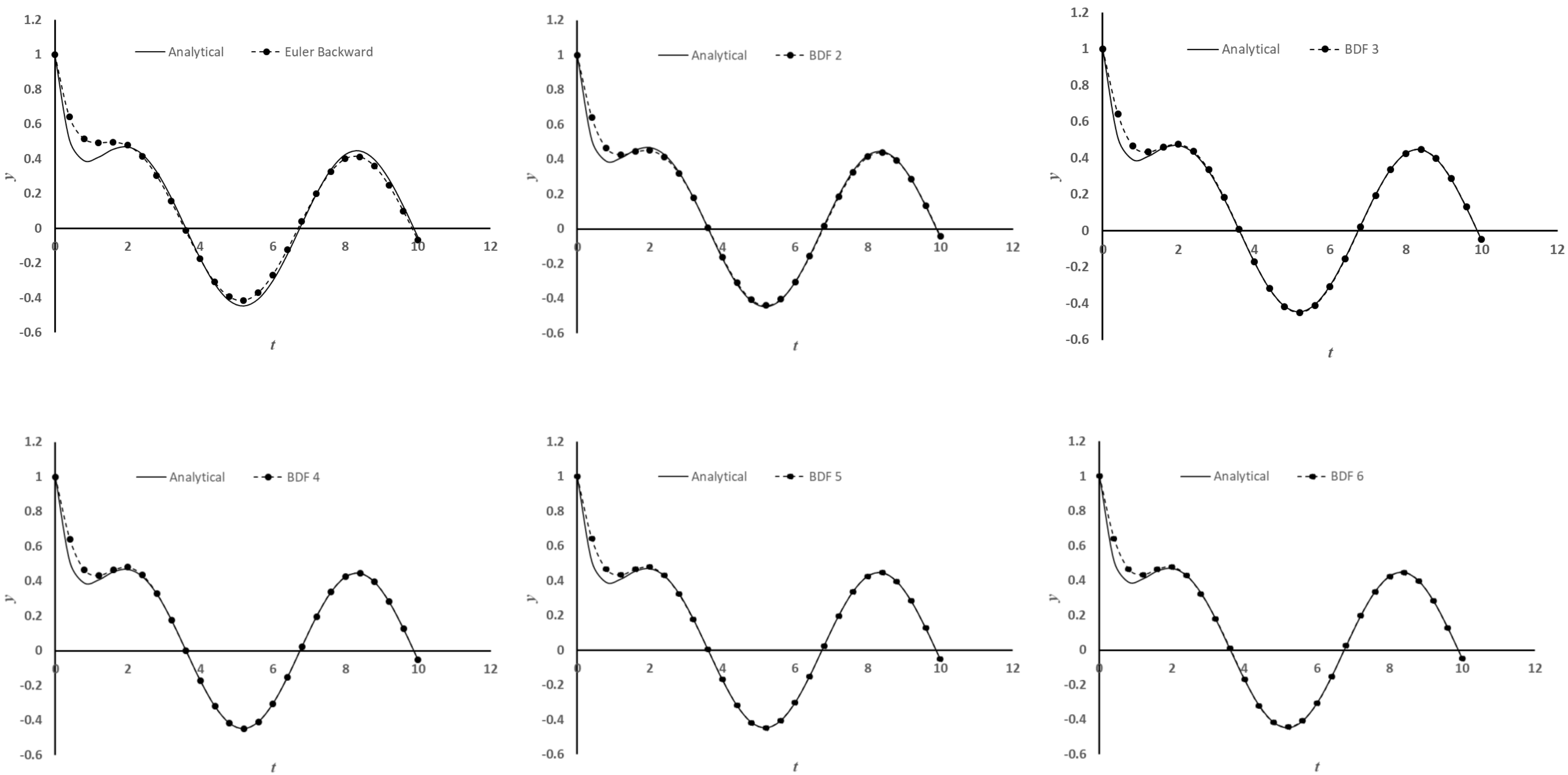
$y_3 = y(1.2) = 0.4330\ (BDF3);$ $y_4 = y(1.6) = 0.4650\ (BDF4);$ $y_5 = y(2.0) = 0.4779\ (BDF5)$

$y_5 = y(2.4)$

$$= \frac{6 \times 0.4779 - \frac{15}{2} \times 0.4650 + \frac{20}{3} \times 0.4330 - \frac{15}{4} \times 0.4657 + \frac{6}{5} \times 0.6421 - \frac{1}{6} \times 1 + 0.4\sin 2.4}{\left(\frac{49}{20} + 2 \times 0.4\right)}$$

$= 0.4290$

BDF (1^{st} to 6^{th} Order)



Observations: BDF methods

A few things to note for the BDF:

- ✓ All methods above the **first** order cannot start by themselves. Accuracy of the higher order method is affected if the starting values are used from the lower order methods.
  - ✓ how to solve the start-up problem?
- ✓ All BDF may involve solution of non-linear equations (if *f* contains a non-linear function of the dependent variable *y*)
  - ✓ Is there a way to avoid this solution of non-linear equations?
- ✓ No numerical oscillations (instability) observed in any of the BDFs:
  - ✓ Why the same order explicit multi-step methods show oscillation but BDFs do not?
  - ✓ Do they show oscillation under any conditions or are they oscillation-proof under all conditions?

'

Applications: Runge-Kutta (R-K) Methods

✓ 2nd Order Runge-Kutta (aka *Ralston's* method):

$$y_{n+1} = y_n + h\left(\frac{\phi_0}{3} + \frac{2\phi_1}{3}\right)$$

$$\phi_0 = f(y_n, t_n) \qquad \phi_1 = f\left(y_n + \frac{3}{4}h\phi_0, t_n + \frac{3}{4}h\right)$$

✓ A 4th Order Runge-Kutta Method:

$$y_{n+1} = y_n + h\left(\frac{1}{6}\phi_0 + \frac{1}{3}(\phi_1 + \phi_2) + \frac{1}{6}\phi_3\right)$$

$$\phi_0 = f(y_n, t_n) \qquad \phi_1 = f\left(y_n + \frac{1}{2}h\phi_0, t_n + \frac{1}{2}h\right)$$

$$\phi_2 = f\left(y_n + \frac{1}{2}h\phi_1, t_n + \frac{1}{2}h\right) \qquad \phi_3 = f(y_n + h\phi_2, t_n + h)$$

Runge-Kutta (R-K) Method (2nd Order)

$$\frac{dy}{dt} = -2y + \sin t \qquad y(0) = 1$$

$$y_{n+1} = y_n + h\left(\frac{\phi_0}{3} + \frac{2\phi_1}{3}\right);\ \phi_0 = f(y_n, t_n);\ \phi_1 = f\left(y_n + \frac{3}{4}h\phi_0, t_n + \frac{3}{4}h\right)$$

$$\phi_0 = -2y_n + \sin t_n\,;\ \ \phi_1 = -2\left(y_n + \frac{3}{4}h\phi_0\right) + \sin\left(t_n + \frac{3}{4}h\right)$$

$$h = 0.4; \qquad y_0 = y(0) = 1$$

$$\phi_0 = -2\times 1 + \sin 0 = -2; \phi_1 = -2\left(1 + \frac{3}{4}\times 0.4(-2)\right) + \sin\left(0 + \frac{3}{4}\times 0.4\right)$$

$$= -0.5045; \qquad y_1 = 1 + 0.4\left(\frac{-2}{3} + \frac{2(-0.5045)}{3}\right) = 0.5988$$

$$\phi_0 = -2\times 0.5988 + \sin 0.4 = -0.8082$$

$$\phi_1 = -2\left(0.5988 + \frac{3}{4}\times 0.4(-0.8082)\right) + \sin\left(0.4 + \frac{3}{4}\times 0.4\right) = -0.06848$$

$$y_2 = 0.5988 + 0.4\left(\frac{-0.8082}{3} + \frac{2(-0.06848)}{3}\right) = 0.4728$$

Runge-Kutta (R-K) Method (4th Order)

$$\frac{dy}{dt} = -2y + \sin t \qquad y(0) = 1$$

$$y_{n+1} = y_n + h\left(\frac{1}{6}\phi_0 + \frac{1}{3}(\phi_1 + \phi_2) + \frac{1}{6}\phi_3\right) \qquad \phi_0 = f(y_n, t_n)$$

$$\phi_1 = f\left(y_n + \frac{1}{2}h\phi_0, t_n + \frac{1}{2}h\right); \; \phi_2 = f\left(y_n + \frac{1}{2}h\phi_1, t_n + \frac{1}{2}h\right); \; \phi_3 = f(y_n + h\phi_2, t_n + h)$$

$$\phi_0 = -2y_n + \sin t_n\,; \qquad \phi_1 = -2\left(y_n + \frac{1}{2}h\phi_0\right) + \sin\left(t_n + \frac{h}{2}\right)$$

$$\phi_2 = -2\left(y_n + \frac{1}{2}h\phi_1\right) + \sin\left(t_n + \frac{h}{2}\right); \qquad \phi_3 = -2(y_n + h\phi_2) + \sin(t_n + h)$$

$$h = 0.4; \qquad y_0 = y(0) = 1$$

$$\phi_0 = -2 \times 1 + \sin 0 = -2; \quad \phi_1 = -2\left(1 + \frac{0.4}{2}(-2)\right) + \sin\left(0 + \frac{0.4}{2}\right) = -1.10013$$

$$\phi_2 = -2\left(1 + \frac{0.4}{2}(-1.10013)\right) + \sin\left(0 + \frac{0.4}{2}\right) = -1.4008$$

$$\phi_3 = -2\big(1 + 0.4(-1.4008)\big) + \sin(0 + 0.4) = -0.4899$$

$$y_1 = y(0.4) = 1 + 0.4\left(\frac{-2}{6} + \frac{(-1.10013 - 1.4008)}{3} + \frac{-0.4899}{6}\right) = 0.5137$$

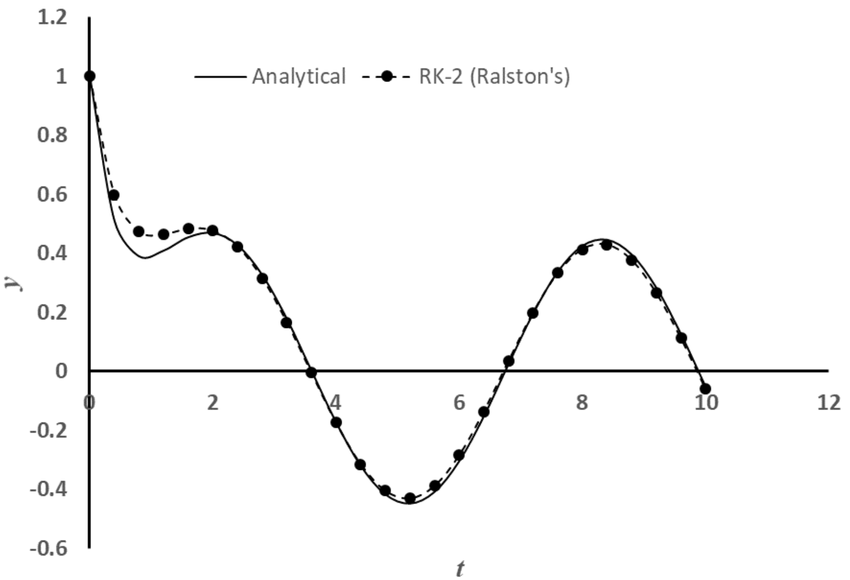
Runge-Kutta (R-K) Method (4th Order)

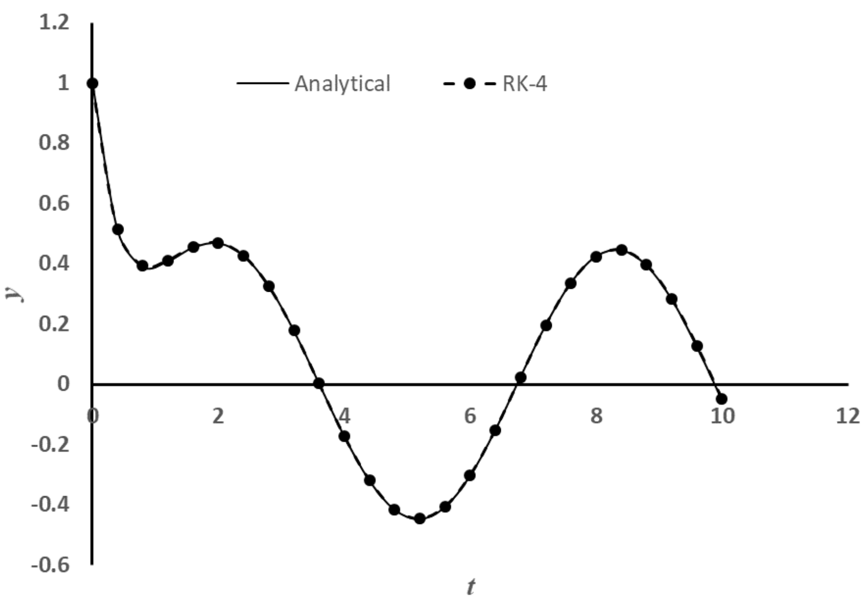
$h = 0.4; \qquad y_1 = y(0.4) = 0.5137$

$$\phi_0 = -2 \times 0.5137 + \sin 0.4 = -0.6380$$
$$\phi_1 = -2\left(0.5137 + \frac{0.4}{2}(-0.6380)\right) + \sin\left(0.4 + \frac{0.4}{2}\right) = -0.2076$$
$$\phi_2 = -2\left(0.5137 + \frac{0.4}{2}(-0.2076)\right) + \sin\left(0.4 + \frac{0.4}{2}\right) = -0.3798$$
$$\phi_3 = -2\big(0.5137 + 0.4(-0.3798)\big) + \sin(0.4 + 0.4) = -0.00627$$

$$y_3 = y(0.8) = 1 + 0.4\left(\frac{-0.6380}{6} + \frac{(-0.2076 - 0.3798)}{3} + \frac{-0.00627}{6}\right) = 0.3925$$

Runge-Kutta Methods (2^{nd} and 4^{th} Order)





A few things to note for the R-K:

- ✓ All order methods are explicit!
- ✓ None of them involve solution of non-linear equations
- ✓ None of them have start-up problems!
- ✓ At every time steps, number of FLOPs are larger for the R-K methods!
- ✓ No numerical oscillations (instability) observed in any of the R-Ks:
  - ✓ Why the same order explicit multi-step methods show oscillation but R-Ks do not?
  - ✓ Do they show oscillation under any conditions or are they oscillation-proof under all conditions?

Applications: Summary of Concerns

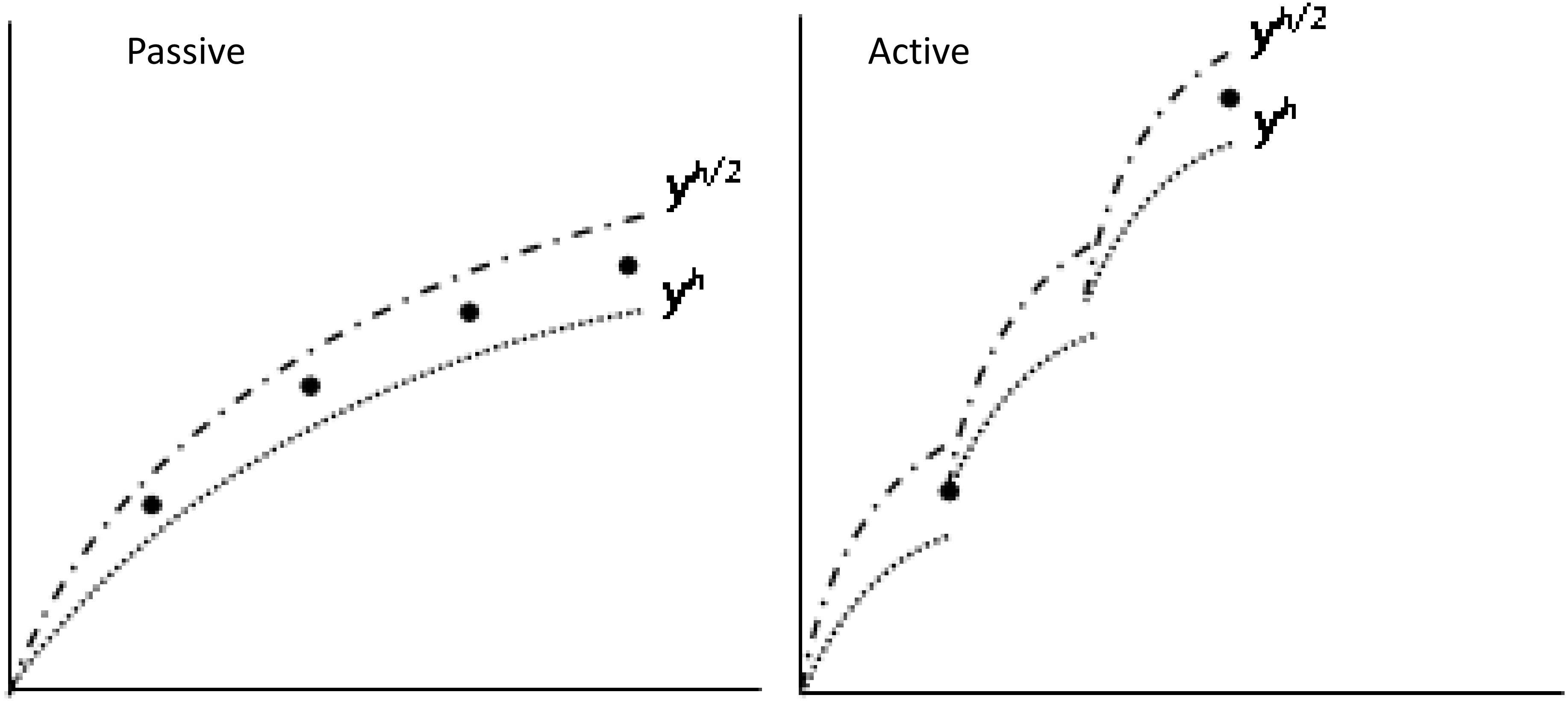
- ✓ Accuracy of the higher order multi-step and BDF methods are affected if the starting values are used from the lower order methods.
  - ✓ How to start these non-self starting algorithms?
- ✓ All implicit methods (multi-step and BDF) may involve solution of non-linear equations (if f contains a non-linear function of the dependent variable y)
  - ✓ Is there a way to avoid this solution of non-linear equations?
- ✓ Numerical oscillations (instability) observed in some methods and not in some!
  - ✓ Is there a way to predict and therefore, choose correct parameters for algorithm so that the numerical oscillations can be avoided?

How to start the non-self starting algorithms?

Three commonly used options:

- ✓ Passive Richardson’s Extrapolation
- ✓ Active Richardson’s Extrapolation
  - ✓ With same lower order method
  - ✓ With progressively higher order methods
- ✓ Using the same order Runge-Kutta method!

Active vs. Passive Richardson’s Extrapolation



Application: Passive Richardson's extrapolation

Let us apply passive Richardson's extrapolation with Euler-Forward method for starting 4th order Adams-Bashforth, Adams-Moulton and BDF methods for the same problem:

$$\frac{dy}{dt} = -2y + \sin t \qquad\qquad y(0) = 1$$

Euler Forward:

$$y_{n+1} = y_n + h(-2y_n + \sin t_n) = y_n(1 - 2h) + h \sin t_n$$

For startup, we require the following:

- 4th order Adams-Bashforth: $y(0)$, $y(0.4)$, $y(0.8)$ and $y(1.2)$
- 4th order Adams-Moulton: $y(0)$, $y(0.4)$ and $y(0.8)$
- 4th order BDF: $y(0)$, $y(0.4)$, $y(0.8)$ and $y(1.2)$

We shall apply the Euler Forward method with h = 0.4, 0.2, 0.1 and 0.05 between t = 0 - 1.2

Time	EF(h = 0.4)	Time	EF(h = 0.2)	Time	EF(h = 0.1)	Time	EF(h = 0.05)
0	1	0	1	0	1	0	1
0.4	**0.2**	0.2	0.6	0.1	0.8	0.05	0.9
0.8	**0.195767**	**0.4**	**0.399734**	0.2	0.649983	0.1	0.812499
1.2	**0.326096**	0.6	0.317724	0.3	0.539854	0.15	0.736241
		0.8	**0.303563**	**0.4**	**0.461435**	0.2	0.670089
		1	0.325609	0.5	0.40809	0.25	0.613013
		1.2	**0.36366**	0.6	0.374414	0.3	0.564082
				0.7	0.355996	0.35	0.52245
				0.8	**0.349218**	**0.4**	**0.48735**
				0.9	0.35111	0.45	0.458086
				1	0.359221	0.5	0.434025
				1.1	0.371524	0.55	0.414594
				1.2	**0.38634**	0.6	0.399269
						0.65	0.387574
						0.7	0.379076
						0.75	0.373379
						0.8	**0.370123**
						0.85	0.368979
						0.9	0.369645
						0.95	0.371847
						1	0.375333
						1.05	0.379873
						1.1	0.385257
						1.15	0.391292
						1.2	**0.397801**

Passive Richardson's Extrapolation with Euler Forward: 4th order method start-up

t	EF(0.4)	EF(0.2)	EF(0.1)	EF(0.05)
0	1	1	1	1
0.4	0.2	0.399734	0.4614349	0.487349766
0.8	0.195767	0.303563	0.3492184	0.370123455
1.2	0.326096	0.36366	0.3863398	0.397800748

t	EF(0.4,0.2)	EF(0.2,0.1)	EF(0.1,0.05)	EF(0.4,0.2,0.1)	EF(0.2,0.1,0.05)	EF(h^4)
0	1	1	1	1	1	**1**
0.4	0.599468	0.523136	0.513265	0.497692	0.509974186	**0.511729**
0.8	0.411358	0.394874	0.391029	0.389379	0.389746793	**0.389799**
1.2	0.401223	0.40902	0.409262	0.411619	0.409342235	**0.409017**

With these four initial values, any 4th order multi-step or BDF methods can start!