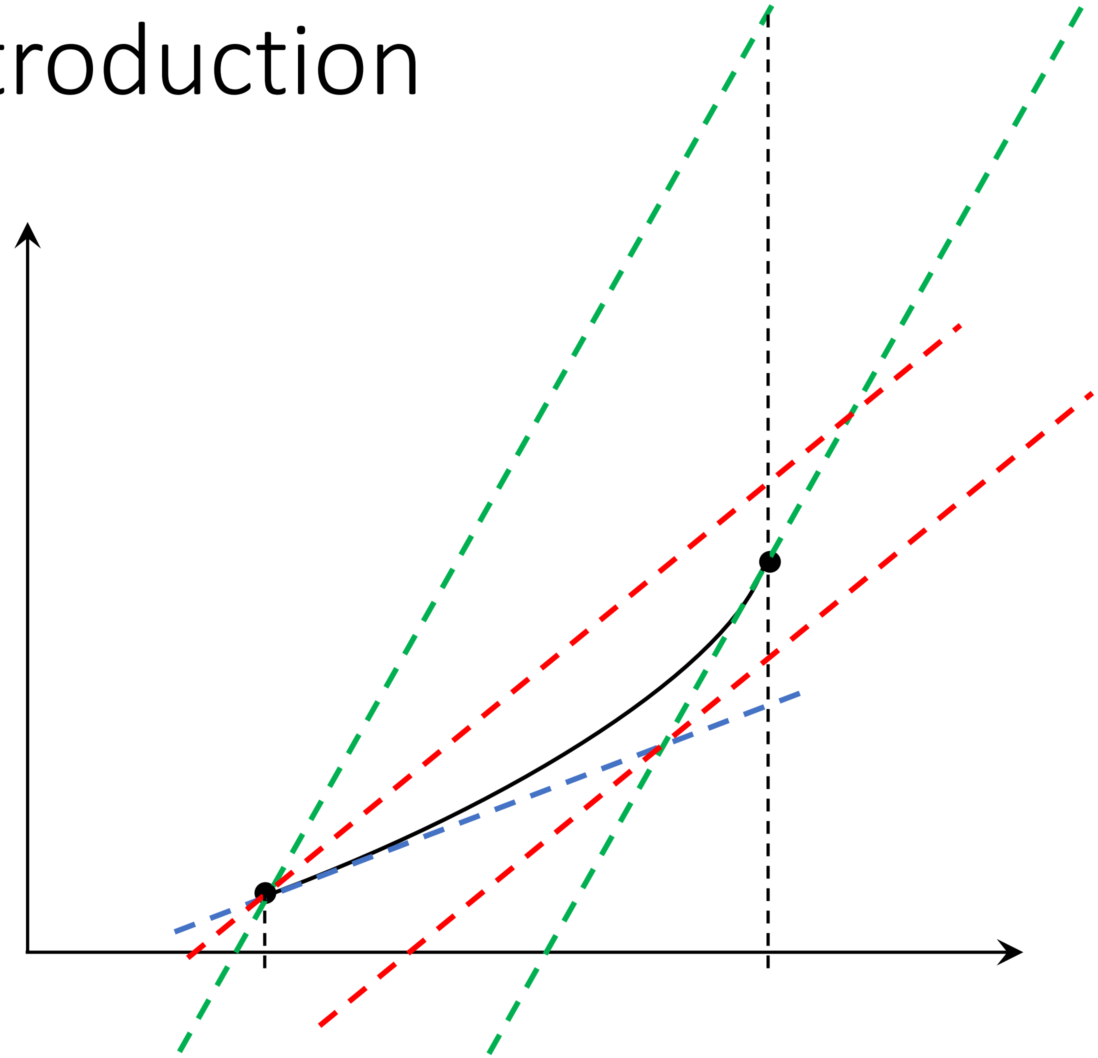
ODE: Introduction



✓ Blue: Euler Forward, Green: Euler Backward, Red: Trapezoidal

✓ Explicit vs. Implicit methods!

$$y_{n+1} = y_n + hf(y_n, t_n) \qquad\qquad y_{n+1} = y_n + hf(y_{n+1}, t_{n+1})$$

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)
- ✓ Consistency, Stability, Convergence
- ✓ Application to Systems of ODE
- ✓ Boundary Value Problems (BVPs)
  - ✓ Shooting Method
  - ✓ Direct Methods

Multi-Step Methods: Explicit

General form of multi-step or Adams-Bashforth methods:

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

$k = 0, 1, 2, \ldots., n$ and h is the uniform time step size

- ✓ Example: $k = 3$

$$y_{n+1} = y_n + h(\alpha_0 f_n + \alpha_1 f_{n-1} + \alpha_2 f_{n-2})$$

$$\frac{dy}{dt} = y' = f \quad \Longrightarrow \quad y_{n+1} = y_n + h\left(\alpha_0 {y'}_n + \alpha_1 {y'}_{n-1} + \alpha_2 {y'}_{n-2}\right)$$

Let’s expand all the terms in Taylor’s series and equate LHS with RHS!

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Multi-Step Methods: Explicit

$$y_{n+1} = y_n + h\left(\alpha_0 y'_n + \alpha_1 y'_{n-1} + \alpha_2 y'_{n-2}\right)$$

Expanding all the terms in Taylor's series:

$$LHS = y_{n+1} = y_n + hy'_n + \frac{h^2}{2!}y''_n + \frac{h^3}{3!}y'''_n + \frac{h^4}{4!}y_n^{IV} + o(h^5)$$

$$y'_{n-1} = y'_n - hy''_n + \frac{h^2}{2!}y'''_n - \frac{h^3}{3!}y_n^{IV} + o(h^4)$$

$$y'_{n-2} = y'_n - (2h)y''_n + \frac{(2h)^2}{2!}y'''_n - \frac{(2h)^3}{3!}y_n^{IV} + o(h^4)$$

Put these in the original equation!

RHS $= y_{n+1} \approx \tilde{y}_{n+1}$

$$= y_n + h\alpha_0 y'_n + h\alpha_1\left(y'_n - hy''_n + \frac{h^2}{2!}y'''_n - \frac{h^3}{3!}y_n^{IV} + o(h^4)\right)$$

$$+ h\alpha_2\left(y'_n - (2h)y''_n + \frac{(2h)^2}{2!}y'''_n - \frac{(2h)^3}{3!}y_n^{IV} + o(h^4)\right)$$

Multi-Step Methods: Explicit

$$y_{n+1} = y_n + h\left(\alpha_0 y'_n + \alpha_1 y'_{n-1} + \alpha_2 y'_{n-2}\right)$$

$$y_n + hy'_n + \frac{h^2}{2!}y''_n + \frac{h^3}{3!}y'''_n + \frac{h^4}{4!}y_n^{IV} + o(h^5) = y_n + h\alpha_0 y'_n +$$
$$h\alpha_1\left(y'_n - hy''_n + \frac{h^2}{2!}y'''_n - \frac{h^3}{3!}y_n^{IV} + o(h^4)\right) +$$
$$h\alpha_2\left(y'_n - (2h)y''_n + \frac{(2h)^2}{2!}y'''_n - \frac{(2h)^3}{3!}y_n^{IV} + o(h^4)\right)$$

Grouping Terms:

$$y_n + hy'_n + \frac{h^2}{2!}y''_n + \frac{h^3}{3!}y'''_n + \frac{h^4}{4!}y_n^{IV} + o(h^5) = y_n + h(\alpha_0 + \alpha_1 + \alpha_2)y'_n +$$
$$h^2(-\alpha_1 - 2\alpha_2)y''_n + h^3\left(\frac{\alpha_1}{2} + 2\alpha_2\right)y''' + h^4\left(-\frac{\alpha_1}{6} - \frac{4\alpha_2}{3}\right)y_n^{IV} + o(h^5)$$

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Multi-Step Methods: Explicit

$$y_{n+1} = y_n + h(\alpha_0 f_n + \alpha_1 f_{n-1} + \alpha_2 f_{n-2})$$

$$y_n + hy'_n + \frac{h^2}{2!}y''_n + \frac{h^3}{3!}y'''_n + \frac{h^4}{4!}y_n^{IV} + o(h^5) = y_n + h(\alpha_0 + \alpha_1 + \alpha_2)y'_n + h^2(-\alpha_1 - 2\alpha_2)y''_n + h^3\left(\frac{\alpha_1}{2} + 2\alpha_2\right)y''' + h^4\left(-\frac{\alpha_1}{6} - \frac{4\alpha_2}{3}\right)y_n^{IV} + o(h^5)$$

Equating both sides:

$$\alpha_0 + \alpha_1 + \alpha_2 = 1; \qquad \alpha_1 + 2\alpha_2 = -\frac{1}{2}; \qquad \frac{\alpha_1}{2} + 2\alpha_2 = \frac{1}{6}$$

$$\alpha_0 = \frac{23}{12}, \alpha_1 = -\frac{4}{3} \text{ and } \alpha_2 = \frac{5}{12}$$

$$y_{n+1} = y_n + h\left(\frac{23}{12}f_n - \frac{4}{3}f_{n-1} + \frac{5}{12}f_{n-2}\right)$$

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Multi-Step Methods: Explicit

Effective approximation is:

$$y_{n+1} \approx \tilde{y}_{n+1} = y_n + h\left(\frac{23}{12}f_n - \frac{4}{3}f_{n-1} + \frac{5}{12}f_{n-2}\right)$$

$$\alpha_0 = \frac{23}{12}, \alpha_1 = -\frac{4}{3} \text{ and } \alpha_2 = \frac{5}{12}$$

We already have:

$$y_{n+1} = y_n + hy'_n + \frac{h^2}{2!}y''_n + \frac{h^3}{3!}y'''_n + \frac{h^4}{4!}y_n^{IV} + o(h^5)$$

$$\tilde{y}_{n+1} = y_n + h(\alpha_0 + \alpha_1 + \alpha_2)y'_n + h^2(-\alpha_1 - 2\alpha_2)y''_n + h^3\left(\frac{\alpha_1}{2} + 2\alpha_2\right)y'''$$

$$+h^4\left(-\frac{\alpha_1}{6} - \frac{4\alpha_2}{3}\right)y_n^{IV} + o(h^5) = y_n + hy'_n + \frac{h^2}{2}y''_n + \frac{h^3}{6}y'''_n - \frac{h^4}{3}y_n^{IV} + o(h^5)$$

$$y_n + hy'_n + \frac{h^2}{2}y''_n + \frac{h^3}{6}y'''_n = \tilde{y}_{n+1} + \frac{h^4}{3}y_n^{IV} + o(h^5)$$

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Multi-Step Methods: Explicit

Effective approximation is:

$$y_{n+1} \approx \tilde{y}_{n+1} = y_n + h\left(\frac{23}{12}f_n - \frac{4}{3}f_{n-1} + \frac{5}{12}f_{n-2}\right)$$

$$y_{n+1} = y_n + hy'_n + \frac{h^2}{2!}y''_n + \frac{h^3}{3!}y'''_n + \frac{h^4}{4!}y_n^{IV} + o(h^5)$$

$$y_n + hy'_n + \frac{h^2}{2}y''_n + \frac{h^3}{6}y'''_n = \tilde{y}_{n+1} + \frac{h^4}{3}y_n^{IV} + o(h^5)$$

$$y_{n+1} = \tilde{y}_{n+1} + \frac{h^4}{3}y_n^{IV} + o(h^5) + \frac{h^4}{4!}y_n^{IV} + o(h^5) = \tilde{y}_{n+1} + \frac{3h^4}{8}y_n^{IV} + o(h^5)$$

$$y_{n+1} = y_n + h\left(\frac{23}{12}f_n - \frac{4}{3}f_{n-1} + \frac{5}{12}f_{n-2}\right) + \frac{3h^4}{8}y_n^{IV} + o(h^5)$$

- ✓ Local truncation error (LTE) of this method is O(h^4)!
- ✓ The method is non-self starting, or cannot be started with the given initial condition $y = y_0$ at $t = t_0$ or 0.

Why???

Multi-Step Methods: Explicit

$$y_{n+1} = y_n + h\left(\frac{23}{12} f_n - \frac{4}{3} f_{n-1} + \frac{5}{12} f_{n-2}\right) + \frac{3h^4}{8} y_n^{IV} + HOT$$

Let us assume that we have obtained y_1 at $t_1 = t_0 + h$ and y_2 at $t_2 = t_0 + 2h$ using another method and then applying this method for subsequent time steps:

$$y_3 = y_2 + h\left(\frac{23}{12} f_2 - \frac{4}{3} f_1 + \frac{5}{12} f_0\right) + \frac{3h^4}{8} y_2^{IV} + HOT$$

$$y_4 = y_3 + h\left(\frac{23}{12} f_3 - \frac{4}{3} f_2 + \frac{5}{12} f_1\right) + \frac{3h^4}{8} y_3^{IV} + HOT$$

$$= y_2 + h\left[\frac{23}{12}(f_2 + f_3) - \frac{4}{3}(f_1 + f_2) + \frac{5}{12}(f_0 + f_1)\right] + \frac{3h^4}{8}(y_2^{IV} + y_3^{IV})$$

$$+ HOT$$

This way, if we apply the method for n time steps,

$$y_{n+2} = y_2 + h\left[\frac{23}{12}\sum_{k=2}^{n+1} f_k - \frac{4}{3}\sum_{k=1}^{n} f_k + \frac{5}{12}\sum_{k=0}^{n-1} f_k\right] + \frac{3h^4}{8}\sum_{k=2}^{n+1} y_k^{IV} + HOT$$

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Multi-Step Methods: Explicit

$$y_{n+2} = y_2 + h\left[\frac{23}{12}\sum_{k=2}^{n+1} f_k - \frac{4}{3}\sum_{k=1}^{n} f_k + \frac{5}{12}\sum_{k=0}^{n-1} f_k\right] + \frac{3h^4}{8}\sum_{k=2}^{n+1} y_k^{IV} + HOT$$

Applying the first mean value theorem for integrals:

$$\sum_{k=2}^{n+1} y^{IV}(t_k) = ny^{IV}(\eta) = \frac{t_{n+1} - t_2}{h} f^{IV}(\eta); \qquad \eta \in [t_{n+1}, t_2]$$

Therefore,

$$y_{n+2} = y_2 + h\left[\frac{23}{12}\sum_{k=2}^{n+1} f_k - \frac{4}{3}\sum_{k=1}^{n} f_k + \frac{5}{12}\sum_{k=0}^{n-1} f_k\right] + \frac{3h^3}{8}(t_{n+1} - t_2) f^{IV}(\eta) + HOT$$

Global truncation error (GTE) of this method is O(h^3)!

A method is always referred to with it’s order of accuracy of GTE!

Therefore, this is ***3rd order Adams-Bashforth*** method!

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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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Multi-Step Methods: Implicit

General form of multi-step implicit methods:

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

$k = 0, 1, 2, \ldots., (n + 1)$ and h is the uniform time step size

$$y_{n+1} = y_n + h(\beta_0 f_{n+1} + \beta_1 f_n + \beta_2 f_{n-1})$$

✓ Example: $k = 2$

$$y_{n+1} = y_n + h(\beta_0 f_{n+1} + \beta_1 f_n + \beta_2 f_{n-1})$$

$$\frac{dy}{dt} = y' = f \qquad \Longrightarrow \qquad y_{n+1} = y_n + h(\beta_0 y'_{n+1} + \beta_1 y'_n + \beta_2 y'_{n-1})$$

Let's expand all the terms in Taylor's series and equate LHS with RHS!

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Multi-Step Methods: Implicit

$$y_{n+1} = y_n + h(\beta_0 y'_{n+1} + \beta_1 y'_n + \beta_2 y'_{n-1})$$

Expanding all the terms in Taylor's series:

$$LHS = y_{n+1} = y_n + hy'_n + \frac{h^2}{2!}y''_n + \frac{h^3}{3!}y'''_n + \frac{h^4}{4!}y^{IV}_n + o(h^5)$$

$$y'_{n-1} = y'_n - hy''_n + \frac{h^2}{2!}y'''_n - \frac{h^3}{3!}y^{IV}_n + o(h^4)$$

$$y'_{n+1} = y'_n + hy''_n + \frac{h^2}{2!}y'''_n + \frac{h^3}{3!}y^{IV}_n + o(h^4)$$

Put these in the original equation!

$$\text{RHS} = y_{n+1} \approx \tilde{y}_{n+1}$$

$$= y_n + h\beta_0\left(y'_n + hy''_n + \frac{h^2}{2!}y'''_n + \frac{h^3}{3!}y^{IV}_n + o(h^4)\right) + h\beta_1 y'_n$$

$$+ h\beta_2\left(y'_n - hy''_n + \frac{h^2}{2!}y'''_n - \frac{h^3}{3!}y^{IV}_n + o(h^4)\right)$$

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Multi-Step Methods: Implicit

$$LHS = y_{n+1} = y_n + hy_n' + \frac{h^2}{2!}y_n'' + \frac{h^3}{3!}y_n''' + \frac{h^4}{4!}y_n^{IV} + o(h^5)$$

$$\mathrm{RHS} = y_{n+1} \approx \tilde{y}_{n+1}$$

$$= y_n + h\beta_0\left(y_n' + hy_n'' + \frac{h^2}{2!}y_n''' + \frac{h^3}{3!}y_n^{IV} + o(h^4)\right) + h\beta_1 y_n'$$

$$+ h\beta_2\left(y_n' - hy_n'' + \frac{h^2}{2!}y_n''' - \frac{h^3}{3!}y_n^{IV} + o(h^4)\right)$$

$$= y_n + h(\beta_0 + \beta_1 + \beta_2)y'_n + h^2(\beta_0 - \beta_2)y_n'' + h^3\left(\frac{\beta_0}{2} + \frac{\beta_2}{2}\right)y_n'''$$

$$+ h^4\left(\frac{\beta_0}{6} - \frac{\beta_2}{6}\right)y_n^{IV} + o(h^5)$$

Comparing two sides:

$$\beta_0 + \beta_1 + \beta_2 = 1; \qquad \beta_0 - \beta_2 = \frac{1}{2}; \qquad \beta_0 + \beta_2 = \frac{1}{3}$$

Multi-Step Methods: Implicit

$$\beta_0 + \beta_1 + \beta_2 = 1; \qquad \beta_0 - \beta_2 = \frac{1}{2}; \qquad \beta_0 + \beta_2 = \frac{1}{3}$$

$$\beta_0 = \frac{5}{12}, \qquad \beta_1 = \frac{2}{3}, \qquad \beta_2 = -\frac{1}{12}$$

The method is:

$$y_{n+1} = y_n + h\left(\frac{5}{12} f_{n+1} + \frac{2}{3} f_n - \frac{1}{12} f_{n-1}\right)$$

$$\text{LHS} = y_{n+1} = y_n + h y_n' + \frac{h^2}{2!} y_n'' + \frac{h^3}{3!} y_n''' + \frac{h^4}{4!} y_n^{IV} + o(h^5)$$

$$\text{RHS} = \tilde{y}_{n+1} = y_n + h y'_n + \frac{h^2}{2} y_n'' + \frac{h^3}{6} y_n''' + \frac{h^4}{12} y_n^{IV} + o(h^5)$$

$$y_{n+1} = \tilde{y}_{n+1} - \frac{h^4}{12} y_n^{IV} + \frac{h^4}{4!} y_n^{IV} + o(h^5) = \tilde{y}_{n+1} - \frac{h^4}{24} y_n^{IV} o(h^5)$$

The LTE of the method is O(h^4) and GTE is O(h^3).

This is the **3rd order *Adams-Moulton* method**!

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 Forward	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

Backward Difference Formulae (BDF)

Explicit multi-step methods:

$$\frac{dy}{dt} = f(y,t) \qquad \Longrightarrow \qquad \frac{y_{n+1} - y_n}{h} = \sum_{i=0}^{k} \alpha_i f_{n-i}$$

$k = 0, 1, 2, \ldots., n$ and h is the uniform time step size

Implicit multi-step methods:

$$\frac{dy}{dt} = f(y,t) \qquad \Longrightarrow \qquad \frac{y_{n+1} - y_n}{h} = \sum_{i=0}^{k} \beta_i f_{n+1-i}$$

$k = 0, 1, 2, \ldots., (n + 1)$ and h is the uniform time step size

All variations were in the evaluations of *f*.

What happens if we keep the *f* evaluation at only one point and use multi-point approximation of the derivative d*y*/d*t*?

Backward Difference Formulae (BDF)

Backward Difference Formulae or BDFs:

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

$k = 0, 1, 2, \ldots., (n + 1)$ and h is the uniform time step size

✓ Example: $k = 2$

$$\gamma_0 y_{n+1} + \gamma_1 y_n + \gamma_2 y_{n+1} = hf_{n+1}$$

$$\frac{dy}{dt} = y' = f \qquad \Longrightarrow \gamma_0 y_{n+1} + \gamma_1 y_n + \gamma_2 y_{n-1} = hy'_{n+1}$$

Let's expand all the terms in Taylor's series and equate LHS with RHS!

Backward Difference Formulae (BDF)

$$\gamma_0 y_{n+1} + \gamma_1 y_n + \gamma_2 y_{n-1} = h y'_{n+1}$$

$$y_{n+1} = y_n + h y'_n + \frac{h^2}{2!} y''_n + \frac{h^3}{3!} y'''_n + \frac{h^4}{4!} y^{IV}_n + o(h^5)$$

$$y_{n-1} = y_n - h y'_n + \frac{h^2}{2!} y''_n - \frac{h^3}{3!} y'''_n + \frac{h^4}{4!} y^{IV}_n + o(h^5)$$

$$y'_{n+1} = y'_n + h y''_n + \frac{h^2}{2!} y'''_n + \frac{h^3}{3!} y^{IV}_n + o(h^4)$$

$$LHS =$$

$$= (\gamma_0 + \gamma_1 + \gamma_2) y_n + h(\gamma_0 - \gamma_2) y'_n + \frac{h^2}{2!} (\gamma_0 + \gamma_2) y''_n$$

$$+ \frac{h^3}{3!} (\gamma_0 - \gamma_2) y'''_n + \frac{h^4}{4!} (\gamma_0 + \gamma_2) y^{IV}_n + o(h^5)$$

$$RHS = h y'_n + h^2 y''_n + \frac{h^3}{2!} y'''_n + \frac{h^4}{3!} y^{IV}_n + o(h^5)$$

$\gamma_0 + \gamma_1 + \gamma_2 = 0$ $\qquad$ $\gamma_0 - \gamma_2 = 1$ $\qquad$ $\gamma_0 + \gamma_2 = 2$

Backward Difference Formulae (BDF)

$$\gamma_0 y_{n+1} + \gamma_1 y_n + \gamma_2 y_{n-1} = hf_{n+1}$$

$\gamma_0 + \gamma_1 + \gamma_2 = 0$ $\qquad \gamma_0 - \gamma_2 = 1$ $\qquad \gamma_0 + \gamma_2 = 2$

$$\gamma_0 = \frac{3}{2} \qquad \gamma_1 = -2 \qquad \gamma_2 = \frac{1}{2}$$

$$3y_{n+1} - 4y_n + y_{n-1} = 2hf_{n+1}$$

Comparing LHS and RHS, the truncation error term is:

$$TE = -\frac{h^4}{4!}(\gamma_0 + \gamma_2)y_n^{IV} + \frac{h^4}{3!}y_n^{IV} + o(h^5) = \frac{h^4}{12}y_n^{IV} + o(h^5)$$

The *LTE* of the method is $O(h^4)$ and the *GTE* is $O(h^3)$.

This is the **3rd order *BDF***!

Backward Difference Formulae (BDF)

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

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