

# *Numerical Analysis & Scientific Computing II*

## *Module 2*

# *Initial Value Problems*

*2.4 Implicit method*

*2.5 Stiffness*

***2.6 Linear Multistep Methods***



*Akash Anand*  
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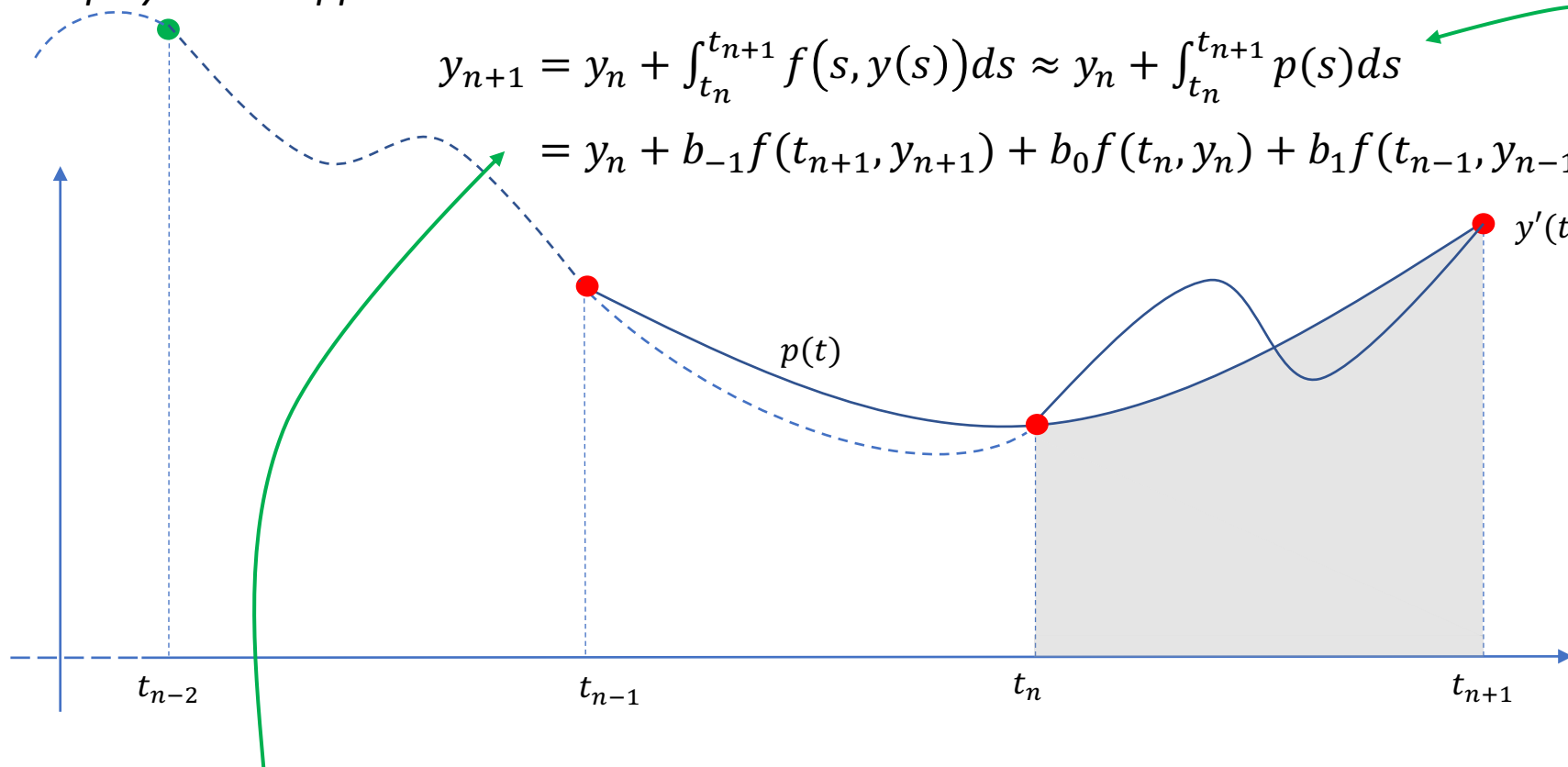
# Initial Value Problems: Linear Multistep Methods

Can we make the method higher order?

Following the idea that we used to derive trapezoidal method, we could use higher order polynomial approximations.

$$\begin{aligned} y_{n+1} &= y_n + \int_{t_n}^{t_{n+1}} f(s, y(s)) ds \approx y_n + \int_{t_n}^{t_{n+1}} p(s) ds \\ &= y_n + b_{-1}f(t_{n+1}, y_{n+1}) + b_0f(t_n, y_n) + b_1f(t_{n-1}, y_{n-1}) \end{aligned}$$

Adams—Moulton  
method

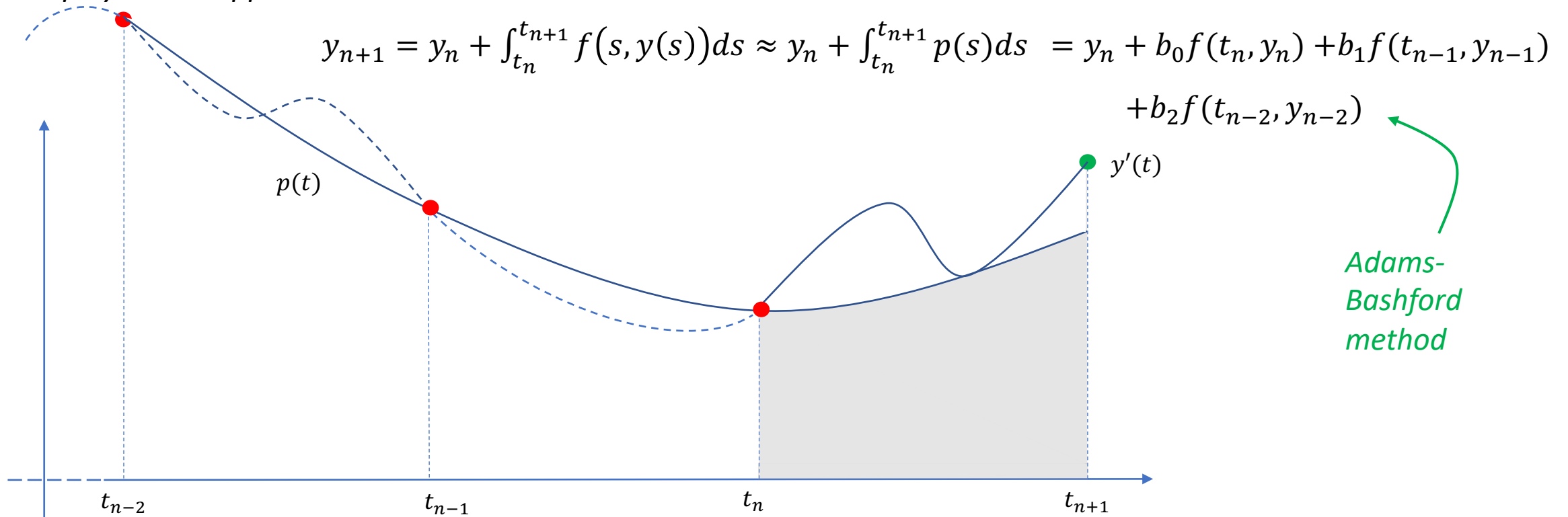


An implicit  
method

# Initial Value Problems: Linear Multistep Methods

Can we make the method higher order?

Following the idea that we used to derive trapezoidal method, we could use higher order polynomial approximations.



# Initial Value Problems: Linear Multistep Methods

We consider methods that take constant step size  $h$  and determine  $y_{n+1}$  using the values from several preceding steps:

$$y_{n+1} = \Phi(f, t_n, y_{n+1}, y_n, y_{n-1}, \dots, y_{n-k}, h).$$

Here  $y_{n+1}$  depends on  $k + 1$  previous values, so this is called a  $(k + 1)$ -step method.

For  $k \geq 1$ , that is, for a 2 or more step method, how do we start the time marching? Note that we need to know  $y_0, \dots, y_k$ , to compute  $y_{k+1}$  and we typically only know  $y_0$ !

... we use some other method such as a single step method.

Examples:

1.  $y_{n+1} = y_n + hf(t_n, y_n)$
  2.  $y_{n+1} = y_n + hf(t_{n+1}, y_{n+1})$
  3.  $y_{n+1} = y_n + h(f(t_n, y_n) + f(t_{n+1}, y_{n+1}))$
  4.  $y_{n+1} = y_n + b_0 f(t_n, y_n) + b_1 f(t_{n-1}, y_{n-1}) + b_2 f(t_{n-2}, y_{n-2})$
  5.  $y_{n+1} = y_n + h(f(t_n, y_n) + f(t_{n+1}, y_n + hf(t_n, y_n)))/2$
- Improved Euler Method*  
 ... an explicit one step method  
 ... an implicit one step method  
 ... an implicit one step method  
 ... an explicit **three** step method  
 ... an explicit one step method
- $\Phi$  is linear in  $y_n, f(t_n, y_n), f(t_{n+1}, y_{n+1}),$  etc.*
- non-linear  $\Phi$*

# Initial Value Problems: Linear Multistep Methods

We consider linear multistep methods with constant step size, which by definition, are methods of the form

$$y_{n+1} = -a_0 y_n - a_1 y_{n-1} - \cdots - a_k y_{n-k} + h[b_{-1} f_{n+1} + b_0 f_n + \cdots + b_k f_{n-k}]$$

where  $f_n$  denotes  $f(t_n, y_n)$  (for brevity) and  $a_j, b_j$  are constants which must be given and determine the specific method.

For explicit linear multistep method,  $b_{-1} = 0$ .

It is also convenient to define  $a_{-1} = 1$ , so that the method can be written more concisely as

$$\sum_{j=-1}^k a_j y_{n-j} = h \sum_{j=-1}^k b_j f_{n-j}.$$

## Theorem

Let  $h_0 = 1/(|b_{-1}|L)$  where  $L$  is the Lipschitz constant for  $f$ . Then for any  $h < h_0$  and any  $y_n, y_{n-1}, \dots, y_{n-k}$ , there is a unique  $y_{n+1}$  such that

$$\sum_{j=-1}^k a_j y_{n-j} = h \sum_{j=-1}^k b_j f(t_{n-j}, y_{n-j}).$$

# Initial Value Problems: Linear Multistep Methods

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$$\sum_{j=-1}^k a_j y_{n-j} = h \sum_{j=-1}^k b_j f(t_{n-j}, y_{n-j}).$$

## Proof.

Define

$$F(z) = - \sum_{j=0}^k a_j y_{n-j} + h \sum_{j=0}^k b_j f(t_{n-j}, y_{n-j}) + h b_{-1} f(t_{n+1}, z).$$

Now,  $F(z)$  is Lipschitz with Lipschitz constant less than or equal to  $h|b_{-1}|L$  (why?). By hypothesis ( $h < h_0$ ), the Lipschitz constant is strictly less than 1, that is,  $F(z)$  is a contraction. The contraction mapping theorem then guarantees a unique fixed point, say  $y_{n+1}$ . Thus, we have  $y_{n+1} = F(y_{n+1})$ , as desired.

## Remark

The contraction mapping theorem also implies that the solution can be computed by fixed point iteration as is often done in practice. Moreover, only a fixed (small) number of iterations are made (introducing an additional error).

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*2.4 Implicit method*

*2.5 Stiffness*

**2.6 Linear Multistep Methods**

**- Adams methods**



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# Initial Value Problems: Linear Multistep Methods



## Examples

*Adams Bashford methods -*

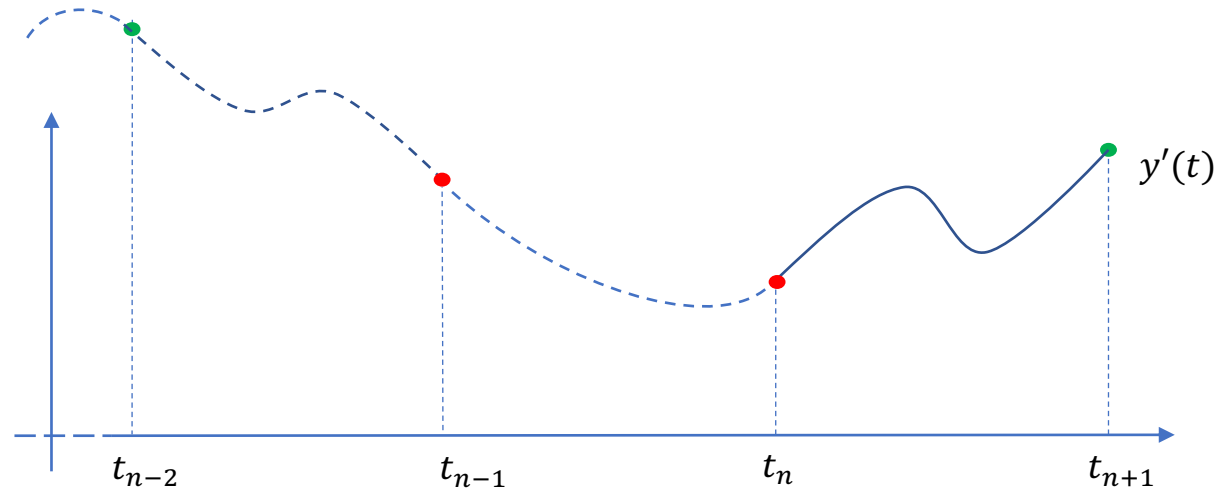


# Initial Value Problems: Linear Multistep Methods

## Examples

Adams Bashford methods -

-- 2-step method

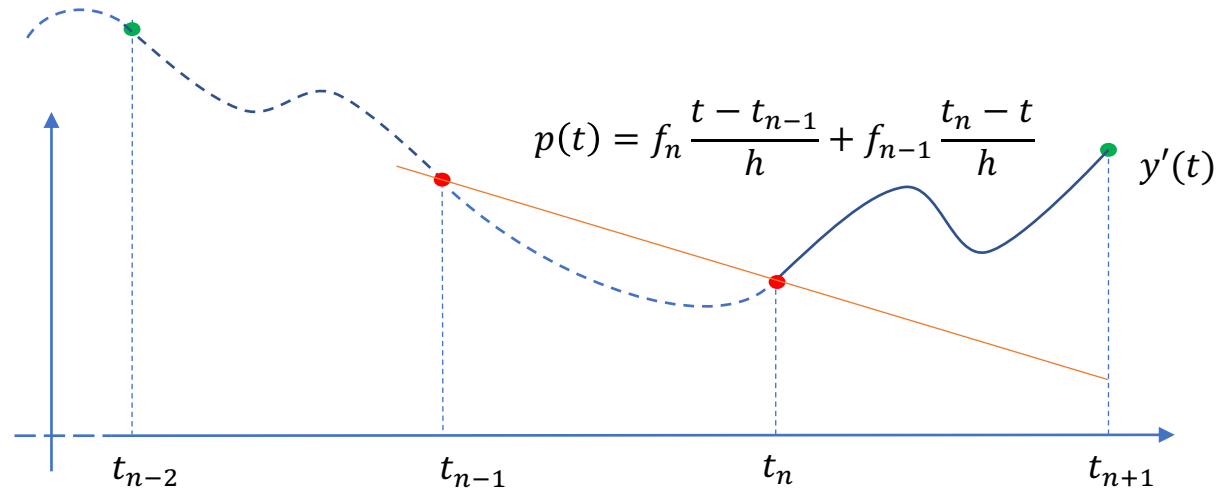


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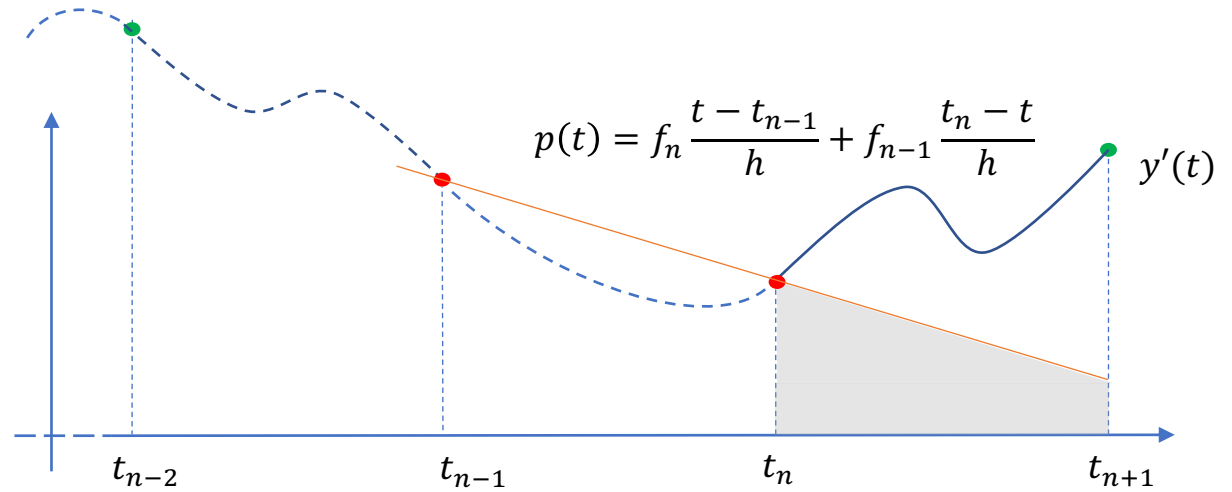


# Initial Value Problems: Linear Multistep Methods

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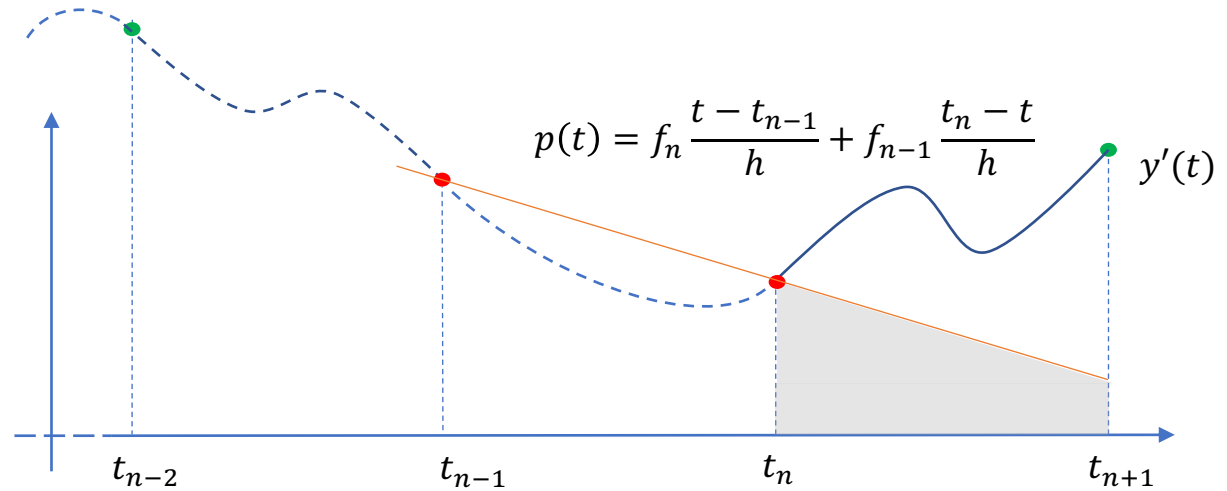
# Initial Value Problems: Linear Multistep Methods

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$$\int_{t_n}^{t_{n+1}} p(t) dt$$



# Initial Value Problems: Linear Multistep Methods

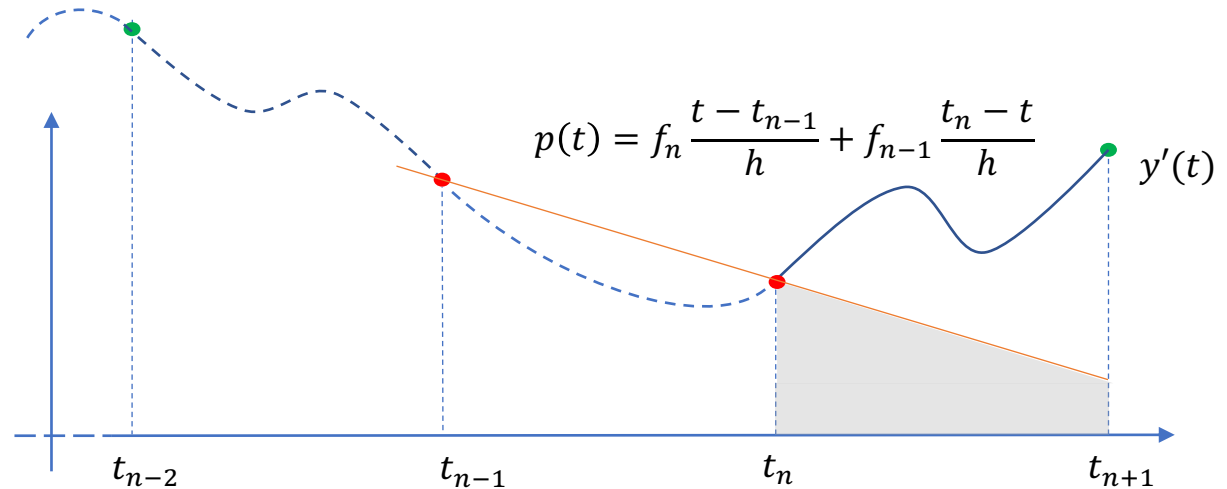
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-- 2-step method

$$\int_{t_n}^{t_{n+1}} p(t) dt =$$

$$\int_{t_n}^{t_{n+1}} \left( f_n \frac{t-t_{n-1}}{h} + f_{n-1} \frac{t_n-t}{h} \right) dt$$



# Initial Value Problems: Linear Multistep Methods

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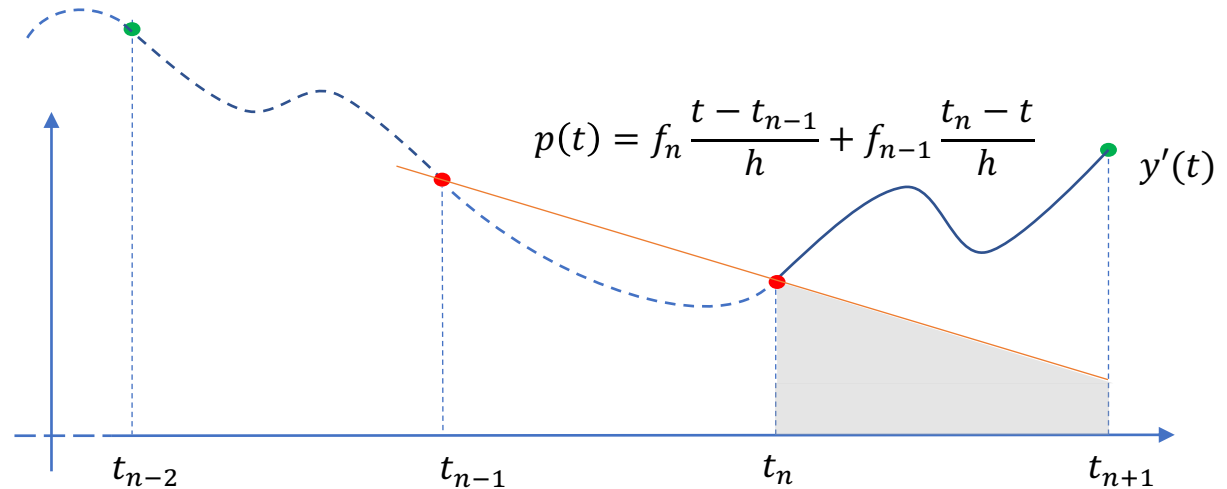
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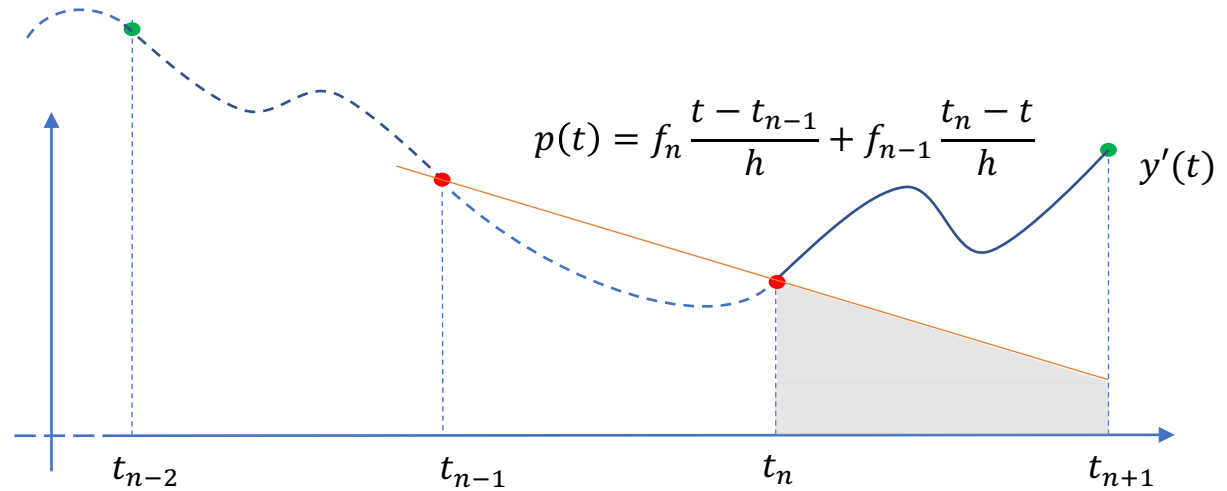
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Thus,

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



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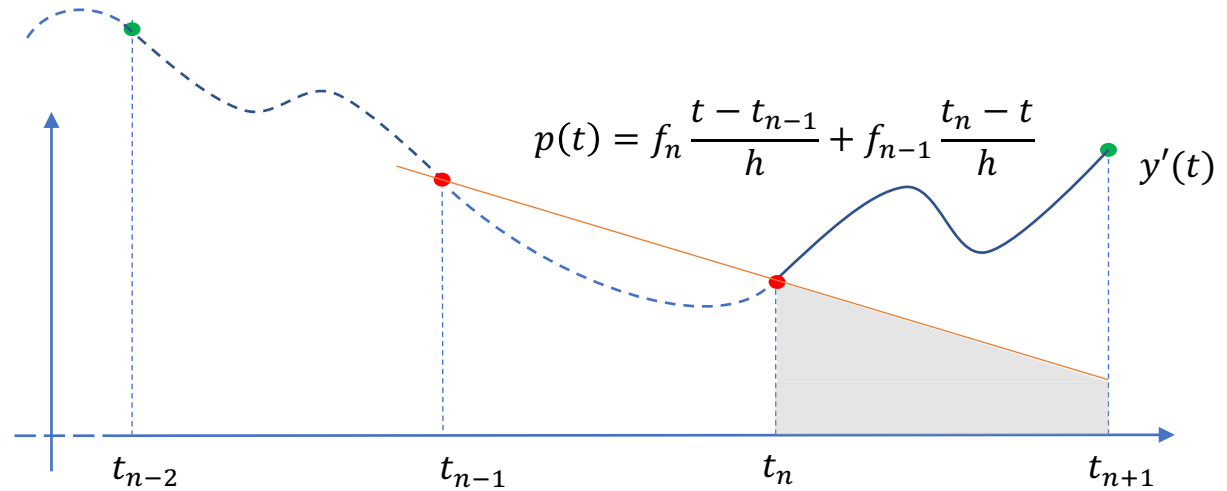
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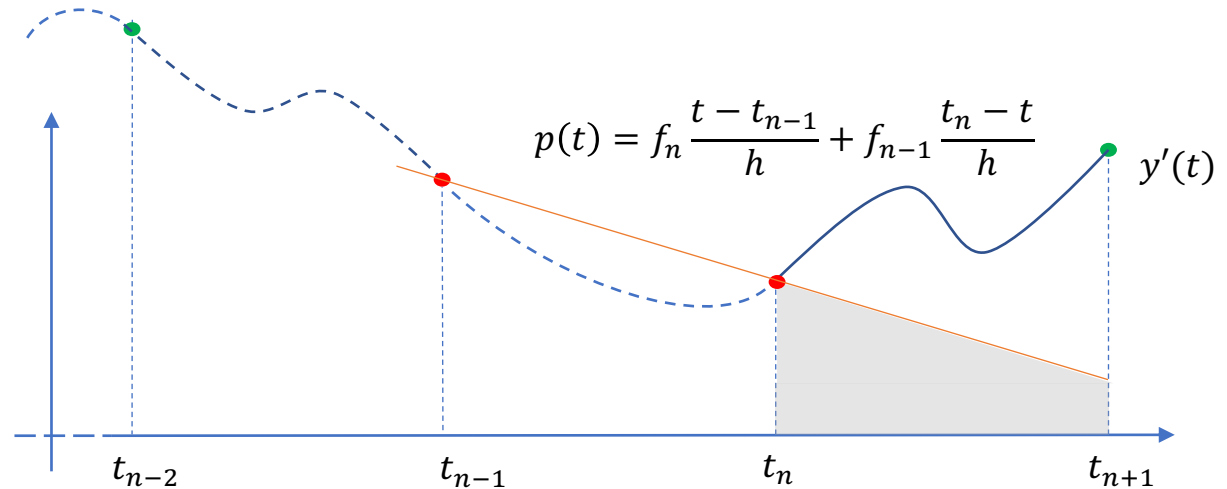
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-- General (k+1) step method

$$p(t) = \sum_{j=0}^k l_j^{(k)}(t) f_{n-j}, \quad \text{where} \quad l_j^{(k)}(t) = \prod_{i=0, i \neq j}^k (t - t_{n-i}) / (t_{n-j} - t_{n-i})$$



# Initial Value Problems: Linear Multistep Methods

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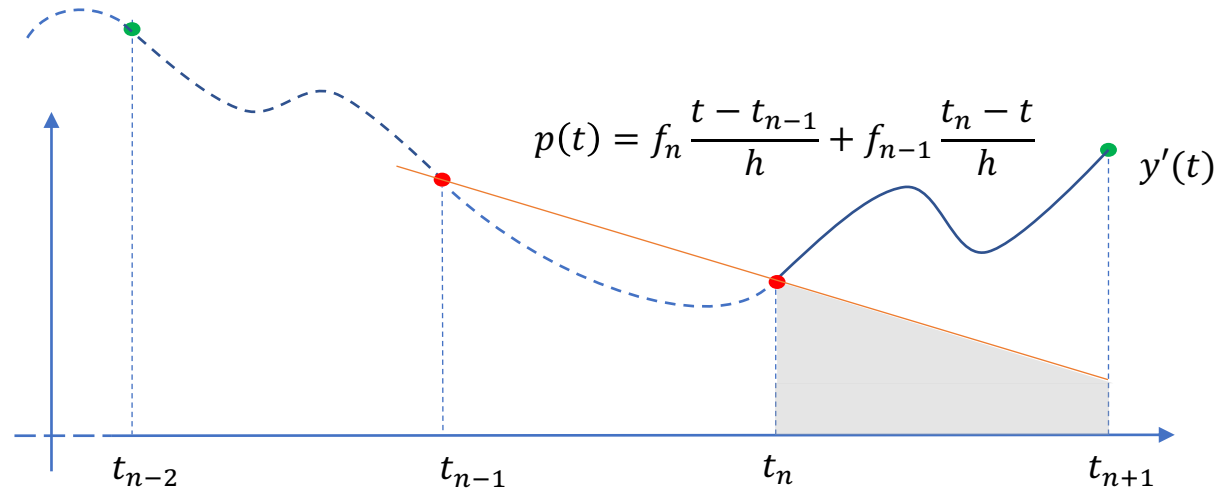
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Thus,

$$y_{n+1} = y_n + \sum_{j=0}^k b_j f_{n-j}, \quad \text{with}$$

$$b_j = \int_{t_n}^{t_{n+1}} l_j^{(k)}(t) dt.$$



# Initial Value Problems: Linear Multistep Methods



## Examples

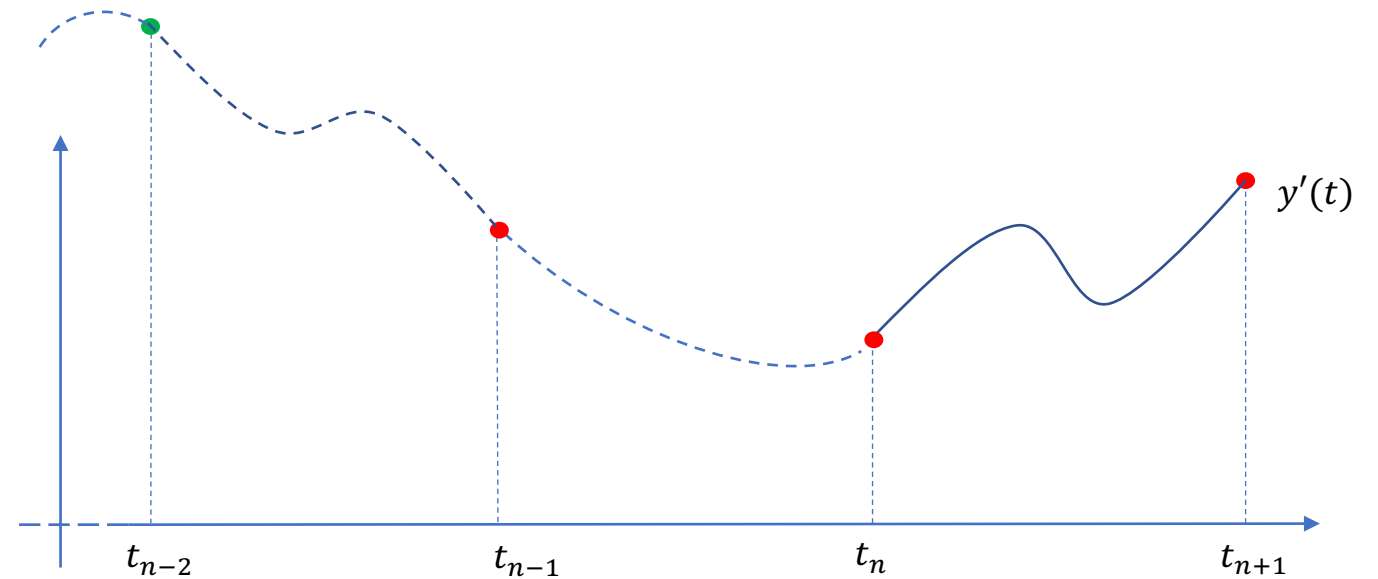
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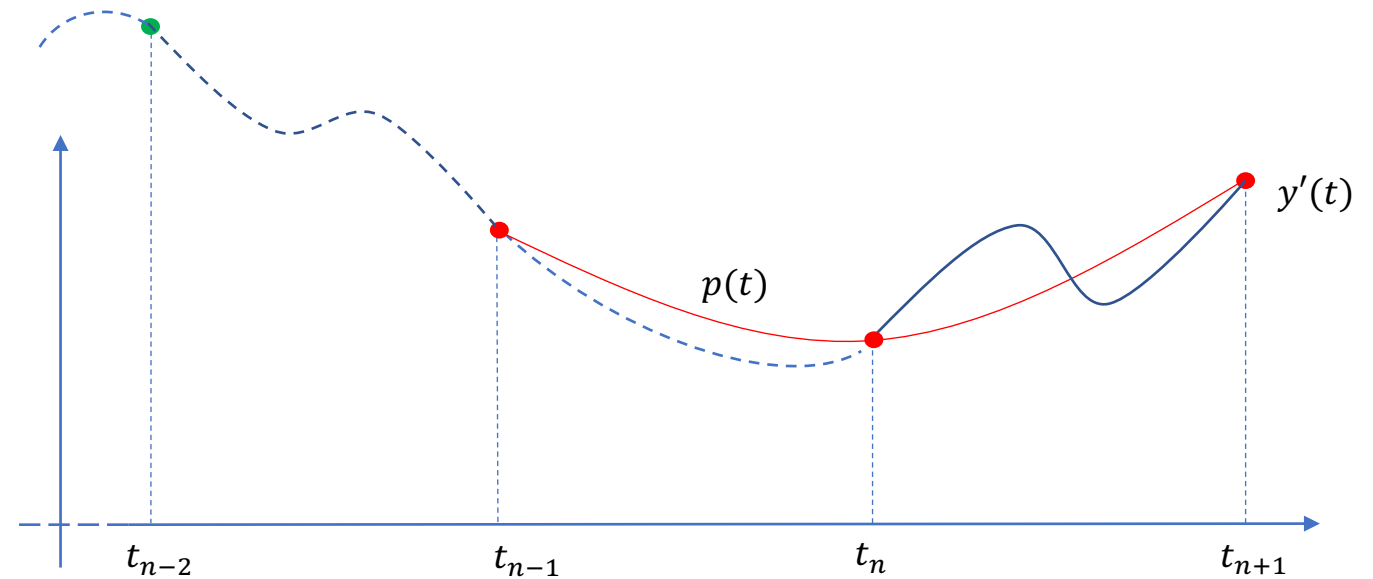
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## Examples

Adams Moulton methods -

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$$\begin{aligned} p(t) = & f_{n+1} \frac{(t - t_n)(t - t_{n-1})}{2h^2} \\ & - f_n \frac{(t - t_{n+1})(t - t_{n-1})}{h^2} \\ & + f_{n-1} \frac{(t - t_{n+1})(t - t_n)}{2h^2} \end{aligned}$$



# Initial Value Problems: Linear Multistep Methods

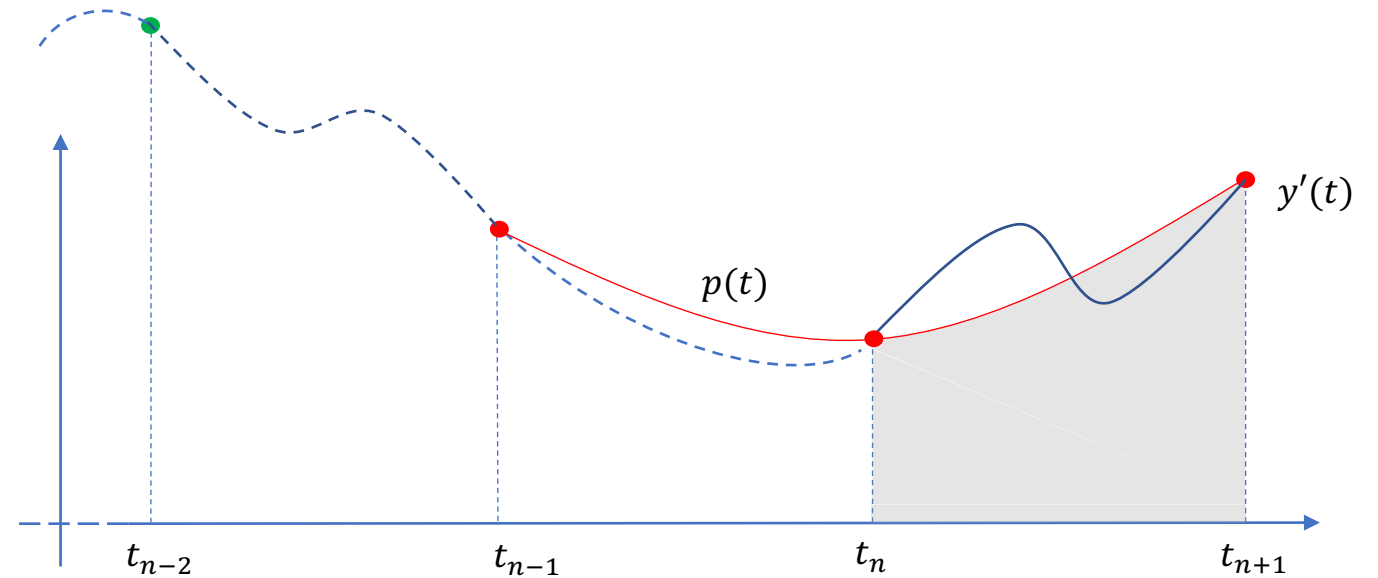
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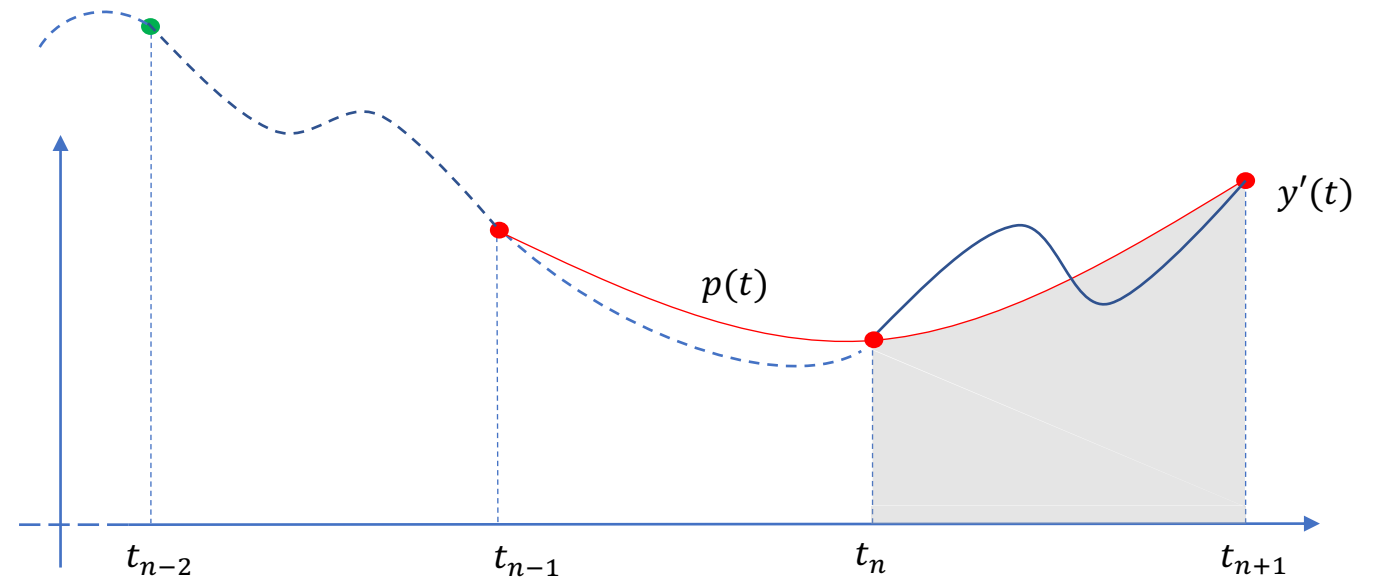
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$$\int_{t_n}^{t_{n+1}} p(t) dt = f_{n+1} \left( \frac{5h}{12} \right) - f_n \left( -\frac{2h}{3} \right) + f_{n-1} \left( -\frac{h}{12} \right)$$



# Initial Value Problems: Linear Multistep Methods

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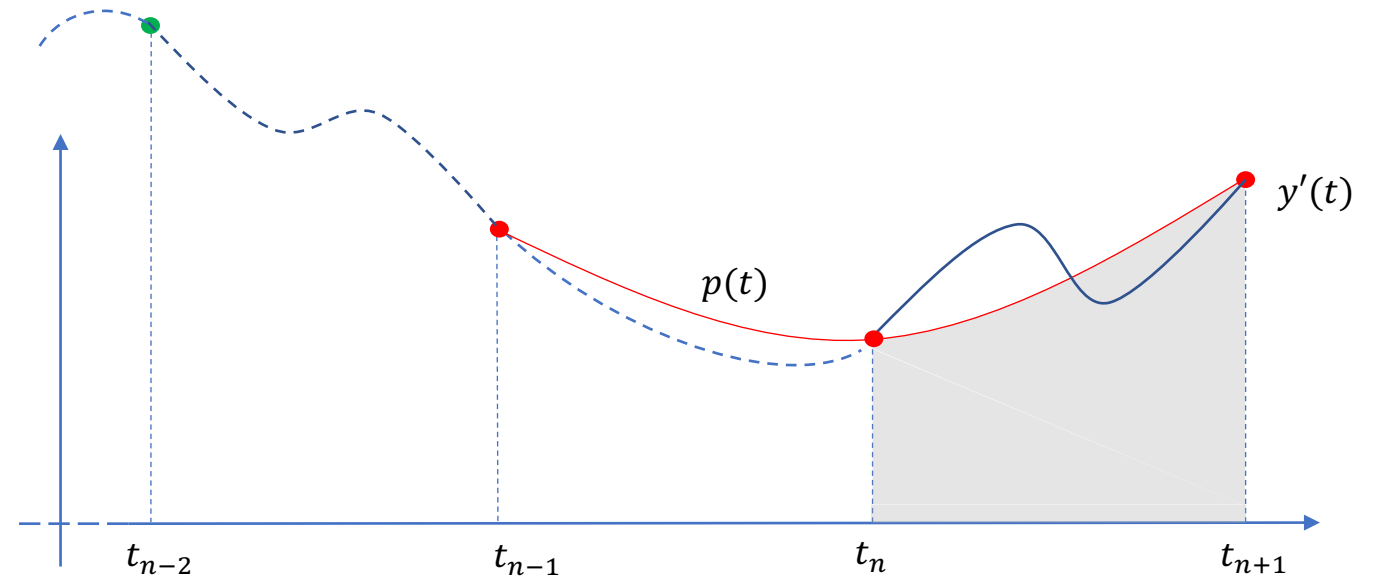
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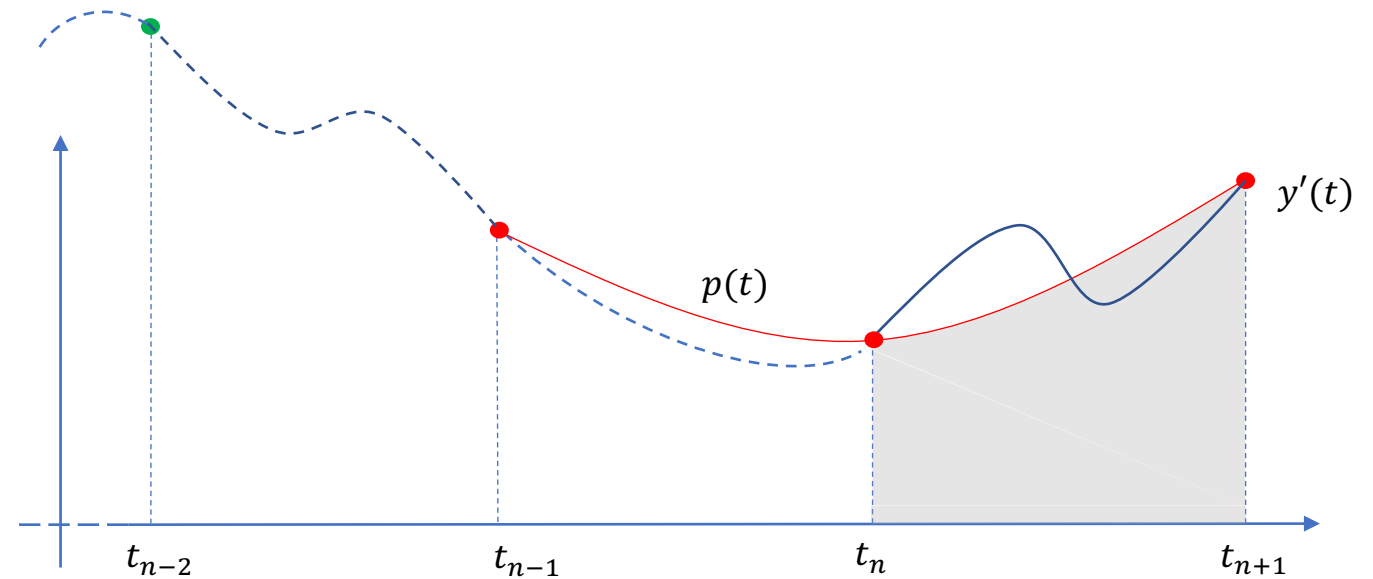
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## *Module 2*

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*2.4 Implicit method*

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**2.6 Linear Multistep Methods**

**- Consistency and Order**



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# Initial Value Problems: Linear Multistep Methods

## Consistency and Order

For the linear multistep method

$$\sum_{j=-1}^k a_j y_{n-j} = h \sum_{j=-1}^k b_j f(t_{n-j}, y_{n-j})$$

define the local error as

$$\ell_{n+1}(y, h) = h \sum_{j=-1}^k b_j y'(t_n - jh) - \sum_{j=-1}^k a_j y(t_n - jh)$$

for any  $y \in C^1$ , and  $h > 0$ .

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The linear multistep method is **consistent** if

$$\lim_{h \rightarrow 0} \max_{k \leq n < N} \left\| \frac{\ell_{n+1}(y, h)}{h} \right\| = 0$$

for all  $y \in C^1$ .

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The method has **order  $p$**  if for all  $y \in C^{p+1}$  there exists constants  $C, h_0 > 0$  such that

$$\max_{k \leq n < N} \left\| \frac{\ell_{n+1}(y, h)}{h} \right\| \leq Ch^p$$

whenever  $h < h_0$ .

# Initial Value Problems: Linear Multistep Methods



## Note

*It is not true that every method of order  $p$  converges with order  $p$ . It may not even converge at all!*

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## Theorem

*A linear multistep is consistent if and only if*

$$\sum_{j=-1}^k a_j = 0, \quad \sum_{j=-1}^k j a_j + \sum_{j=-1}^k b_j = 0.$$

*The method is of order  $p$  if and only if*

$$\sum_{j=-1}^k (-j)^m a_j - m \sum_{j=-1}^k (-j)^{m-1} b_j = 0, \quad m = 0, 1, \dots, p.$$

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## Proof.

*Using Taylor's theorem, we have  $y(t_n - jh) = y(t_n) - jhy'(\xi_j)$  for some  $\xi_j \in (t_n - kh, t_n + h)$ ,  $j = -1, \dots, k$ .*

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# Initial Value Problems: Linear Multistep Methods

## Note

*It is not true that every method of order  $p$  converges with order  $p$ . It may not even converge at all!*

## Theorem

*A linear multistep is consistent if and only if*

$$\sum_{j=-1}^k a_j = 0, \quad \sum_{j=-1}^k ja_j + \sum_{j=-1}^k b_j = 0.$$

Consistency conditions

*The method is of order  $p$  if and only if*

$$\sum_{j=-1}^k (-j)^m a_j - m \sum_{j=-1}^k (-j)^{m-1} b_j = 0, \quad m = 0, 1, \dots, p.$$

Order conditions

## Proof.

Using Taylor's theorem, we have  $y(t_n - jh) = y(t_n) - jhy'(\xi_j)$  for some  $\xi_j \in (t_n - kh, t_n + h)$ ,  $j = -1, \dots, k$ .

Note that  $\xi_j \rightarrow t_n$  as  $h \rightarrow 0$ . Now,

$$\ell_{n+1}(y, h) = h \sum_{j=-1}^k b_j y'(t_n - jh) - \sum_{j=-1}^k a_j y(t_n - jh) = h \sum_{j=-1}^k b_j y'(t_n - jh) - \sum_{j=-1}^k a_j [y(t_n) - jhy'(\xi_j)]$$

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where

$$C_0 = \sum_{j=-1}^k a_j, \quad C_1 = \sum_{j=-1}^k ja_j + \sum_{j=-1}^k b_j,$$

$$R = h \sum_{j=-1}^k b_j [y'(t_n - jh) - y'(t_n)] + h \sum_{j=-1}^k ja_j [y'(\xi_j) - y'(t_n)]$$

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By uniform continuity of  $y'$ , we see that  $R/h \rightarrow 0$  as  $h \rightarrow 0$ .

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By uniform continuity of  $y'$ , we see that  $R/h \rightarrow 0$  as  $h \rightarrow 0$ . Therefore,  $\ell_{n+1}(y, h)/h \rightarrow 0$  if and only if  $C_0 = 0$  and  $C_1 = 0$ , that is consistency conditions are satisfied.

# Initial Value Problems: Linear Multistep Methods

**Proof.** ...

Similarly, if  $y \in C^{p+1}$  we have

$$y(t_n - jh) = \sum_{m=0}^p \frac{(-j)^m}{m!} h^m y^{(m)}(t_n) + \frac{(-j)^{p+1}}{(p+1)!} h^{p+1} y^{(p+1)}(\xi_j)$$
$$y'(t_n - jh) = \sum_{m=1}^p \frac{(-j)^{m-1}}{(m-1)!} h^{m-1} y^{(m)}(t_n) + \frac{(-j)^p}{p!} h^p y^{(p+1)}(\zeta_j)$$

for some  $\xi_j, \zeta_j \in (t_n - kh, t_n + h), j = -1, \dots, k$ .

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for some  $\xi_j, \zeta_j \in (t_n - kh, t_n + h), j = -1, \dots, k$ . This yields

$$\ell_{n+1}(y, h) = \sum_{m=0}^p h^m y^{(m)}(t_n) C_m + R$$

where

$$C_m = \frac{1}{m!} \left[ m \sum_{j=-1}^k (-j)^{m-1} b_j - \sum_{j=-1}^k (-j)^m a_j \right], \quad R = h^{p+1} \sum_{j=-1}^k \left[ b_j \frac{(-j)^p}{p!} y^{(p+1)}(\zeta_j) - a_j \frac{(-j)^{p+1}}{(p+1)!} y^{(p+1)}(\xi_j) \right].$$

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Since  $R = O(h^{p+1})$ ,  $\ell_{n+1}(y, h)/h = O(h^p)$  if and only if all the  $C_m$  vanish.

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## Theorem

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$$\sum_{j=-1}^k a_j = 0, \quad \sum_{j=-1}^k j a_j + \sum_{j=-1}^k b_j = 0.$$

The method is of order  $p$  if and only if

$$\sum_{j=-1}^k (-j)^m a_j - m \sum_{j=-1}^k (-j)^{m-1} b_j = 0, \quad m = 0, 1, \dots, p.$$

## Remarks

1. This theorem is an example of how a complicated analytic condition may sometimes reduce to a simple algebraic criterion.

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## Remarks

1. This theorem is an example of how a complicated analytic condition may sometimes reduce to a simple algebraic criterion.
2. Such algebraic criteria for multistep methods can be expressed in terms of characteristic polynomials of the method:

$$\rho(z) = \sum_{j=-1}^k a_j z^{k-j}, \quad \sigma(z) = \sum_{j=-1}^k b_j z^{k-j}.$$

For example, the consistency conditions are  $\rho(1) = 0$  and  $\rho'(1) = \sigma(1)$ .

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Construct the 2-step method of highest order!

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For a 2-step method, there are 5 undetermined coefficients:  $a_0, a_1, b_{-1}, b_0, b_1$ .



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$$1 + a_0 + a_1 = 0,$$

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$$\underline{1 + a_0 + a_1 = 0, \quad 1 - a_1 - b_{-1} - b_0 - b_1 = 0,} \quad \text{see } a_0, \text{ for } j=0, m=0$$

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This system of linear equation has a unique solution

$$a_0 = 0, a_1 = -1, b_{-1} = \frac{1}{3}, b_0 = \frac{4}{3}, b_1 = \frac{1}{3}.$$

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This scheme is known as Milne-Simpson method and it is the unique fourth order 2-step method.

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There are 4 undetermined coefficients:  $a_0, a_1, b_0, b_1$ .

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Construct the explicit 2-step method of highest order!

There are 4 undetermined coefficients:  $a_0, a_1, b_0, b_1$ . The first four order conditions are

$$\begin{aligned} 1 + a_0 + a_1 &= 0, & 1 - a_1 - b_0 - b_1 &= 0, \\ 1 + a_1 + 2b_1 &= 0, & 1 - a_1 - 3b_1 &= 0, \end{aligned}$$

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which gives

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Thus, the unique explicit 2-step method of order 3 is  $y_{n+1} + 4y_n - 5y_{n-1} = h(4f_n + 2f_{n-1})$ .

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Does this method converge?

# *Numerical Analysis & Scientific Computing II*

## *Lesson 2*

# *Initial Value Problems*

*2.4 Implicit method*

*2.5 Stiffness*

**2.6 Linear Multistep Methods**

**- Convergence**



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Does this method converge?

## Convergence

A linear multistep method is **convergent** if whenever the initial values  $y_n$  are chosen such that  $\max_{0 \leq n \leq k} \|e_n\| \rightarrow 0$ , as  $h \rightarrow 0$ , then  $\max_{0 \leq n \leq N} \|e_n\| \rightarrow 0$ .

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## Example

Does

$$y_{n+1} + 4y_n - 5y_{n-1} = h(4f_n + 2f_{n-1}).$$

this method converge?



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$$v_n = \begin{bmatrix} y_{n+1} \\ y_n \end{bmatrix}$$

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Using,  $v_n = A^n v_0$  and  $y_0 = 0$ , we get

$$y_n = (1 - (-5)^n)y_1/6$$

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# *Numerical Analysis & Scientific Computing II*

## *Module 2*

# *Initial Value Problems*

*2.4 Implicit method*

*2.5 Stiffness*

**2.6 Linear Multistep Methods**

**- Stability**



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MATH, IIT KANPUR





# Initial Value Problems: Linear Multistep Methods

## Stability

A linear  $k + 1$  step method is **stable** if for any initial value problem with Lipschitz continuous  $f$  and of  $\varepsilon > 0$ , there exists  $\delta, h_0 > 0$  such that if  $h \leq h_0$  and two choices of starting values  $y_j$  and  $\hat{y}_j$  are chosen satisfying

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If  $y' = 0$ , then the general linear multistep method becomes

$$y_{n+1} + \sum_{j=0}^k a_j y_{n-j} = 0, \quad n = k, k+1, \dots$$

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Thus, for  $\rho(t) = \prod_{j=1}^J (t - \lambda_j)^{M_j}$  where  $\sum_{j=1}^J M_j = k+1$ , the general solution is  $y_n = \sum_{j=1}^J \sum_{m=0}^{M_j-1} c_{jm} n^m \lambda_j^n$ .