

# Numerical Methods

## DS288 and UMC201

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# Single step method

Consider the initial value problem

$$\frac{dy}{dx} = f(x, y), \quad y(y_0) = y_0, \quad x \in [a, b] \quad (1)$$

Classified mainly into two types. Singlestep methods and Multistep methods.

- Singlestep method: The solution at any point is obtained using the solution at only the previous point. A general singlestep method can be written as

$$y_{n+1} = y_n + h\phi(x_{n+1}, x_n, y_{n+1}, y_n, h) \quad (2)$$

here  $\phi$  is a function of the arguments  $x_n, x_{n+1}, y_n, y_{n+1}, h$  and also depends on  $f$ . We often write it as  $\phi(t, u, h)$ . This function  $\phi$  is called the **increment function**. If  $y_{n+1}$  can be obtained simply by evaluating the right hand side of (2), then the method is called an **explicit method**. In this case, the method is of the form

$$y_{n+1} = y_n + h\phi(x_n, y_n, h). \quad (3)$$

If the right hand side of (2) depends on  $y_{n+1}$  also, then it is called an **implicit method**. The general form in this case is given in (2).



# Local Truncation Error or Discretization Error

The true (exact) value  $y(x_n)$  satisfies the equation

$$y(x_{n+1}) = y(x_n) + h\phi(x_{n+1}, x_n, y(x_{n+1}), y(x_n), h) + T_{n+1} \quad (4)$$

where  $T_{n+1}$  is called the local truncation error or discretization error of the method. Therefore, the truncation error is given by

$$T_{n+1} = y(x_{n+1}) - y(x_n) - h\phi(x_{n+1}, x_n, y(x_{n+1}), y(x_n), h) \quad (5)$$



# Multistep Methods



# Multistep method

An  $m$ -step method for initial-value problem.

$$y' = f(x, y), \quad a \leq x \leq b, \quad y(a) = \alpha,$$

- To find  $w_{i+1}$  at  $x_{i+1}$ , consider  $m > 1$  an integer with the following equations

$$\begin{aligned} w_{i+1} = & a_{m-1}w_i + a_{m-2}w_{i-1} + \cdots + a_0w_{i+1-m} \\ & + h[b_m f(x_{i+1}, w_{i+1}) + b_{m-1}f(x_i, w_i) + \cdots + b_0f(x_{i+1-m}, w_{i+1-m})] \end{aligned}$$

- for  $i = m - 1, m, \dots, N - 1$ , where  $h = (b - a)/N$ ,  $a_0, a_1, \dots, a_{m-1}$ .
- Further,  $b_0, b_1, \dots, b_m$  are constants and starting values  $w_0 = \alpha, \quad w_1 = \alpha_1, \quad w_2 = \alpha_2 \cdots, \quad w_{m-1} = \alpha_{m-1}$  are specified.
- If  $b_m = 0$  it is an explicit or open method.
- If  $b_m \neq 0$  it is an implicit or closed method.



# Multistep method

## Example

$$w_0 = \alpha, w_1 = \alpha_1, w_2 = \alpha_2, w_3 = \alpha_3$$

$$w_{i+1} = w_i + \frac{h}{24} [55f(x_i, w_i) - 59f(x_{i-1}, w_{i-1}) + 37f(x_{i-2}, w_{i-2}) - 9f(x_{i-3}, w_{i-3})]$$

for each  $i = 3, 4, 5, \dots, N-1$ , defined an explicit four-step method, called **fourth-order Adams-Bashforth technique**

## Example

$$w_0 = \alpha, w_1 = \alpha_1, w_2 = \alpha_2,$$

$$w_{i+1} = w_i + \frac{h}{24} [9f(x_{i+1}, w_{i+1}) + 19f(x_i, w_i) - 5f(x_{i-1}, w_{i-1}) + f(x_{i-2}, w_{i-2})]$$

for each  $i = 2, 3, 4, 5, \dots, N-1$ , defined an implicit four-step method, called **fourth-order Adams-Moulton technique**

# Derivation of multistep method

Consider the following initial value problem

$$y' = f(t, y), \quad a \leq t \leq b, \quad y(a) = \alpha, \quad (6)$$

if integrated over the interval  $[t_i, t_{i+1}]$ , has the property that

$$y(t_{i+1}) - y(t_i) = \int_{t_i}^{t_{i+1}} y'(t) dt = \int_{t_i}^{t_{i+1}} f(t, y(t)) dt. \quad (7)$$

Consequently,

$$y(t_{i+1}) = y(t_i) + \int_{t_i}^{t_{i+1}} f(t, y(t)) dt. \quad (8)$$

However we cannot integrate  $f(t, y(t))$  without knowing  $y(t)$ , the solution to the problem, so we instead integrate an interpolating polynomial  $P(t)$  to  $f(t, y(t))$ , one that is determined by some of the previously obtained data points  $(t_0, w_0)$ ,  $(t_1, w_1)$ ,  $\dots$ ,  $(t_i, w_i)$ . When we assume, in addition, that  $y(t_i) \approx w_i$ , Eq. (8) becomes

$$y(t_{i+1}) \approx w_i + \int_{t_i}^{t_{i+1}} P(t) dt. \quad (5.28)$$



# Derivation of multistep method

To derive an Adams-Bashforth explicit  $m$ -step technique, we form the backward-difference polynomial  $P_{m-1}(t)$  through

$$(t_i, f(t_i, y(t_i))), \quad (t_{i-1}, f(t_{i-1}, y(t_{i-1}))), \dots, \quad (t_{i+1-m}, f(t_{i+1-m}, y(t_{i+1-m}))).$$

Since  $P_{m-1}(t)$  is an interpolatory polynomial of degree  $m-1$ , some number  $\xi_i$  in  $(t_{i+1-m}, t_i)$  exists with

$$f(t, y(t)) = P_{m-1}(t) + \frac{f^{(m)}(\xi_i, y(\xi_i))}{m!} (t - t_i)(t - t_{i-1}) \cdots (t - t_{i+1-m}).$$

Introducing the variable substitution  $t = t_i + sh$ , with  $dt = h ds$ , into  $P_{m-1}(t)$  and the error term implies that



# Derivation of multistep method

$$\begin{aligned}\int_{t_i}^{t_{i+1}} f(t, y(t)) dt &= \int_{t_i}^{t_{i+1}} \sum_{k=0}^{m-1} (-1)^k \binom{-s}{k} \nabla^k f(t_i, y(t_i)) dt \\ &\quad + \int_{t_i}^{t_{i+1}} \frac{f^{(m)}(\xi_i, y(\xi_i))}{m!} (t - t_i)(t - t_{i-1}) \cdots (t - t_{i+1-m}) dt \\ &= \sum_{k=0}^{m-1} \nabla^k f(t_i, y(t_i)) h (-1)^k \int_0^1 \binom{-s}{k} ds \\ &\quad + \frac{h^{m+1}}{m!} \int_0^1 s(s+1) \cdots (s+m-1) f^{(m)}(\xi_i, y(\xi_i)) ds.\end{aligned}$$

# Derivation of multistep method

For example, when  $k = 3$ ,

$$\begin{aligned} (-1)^3 \int_0^1 \binom{-s}{3} ds &= - \int_0^1 \frac{(-s)(-s-1)(-s-2)}{1 \cdot 2 \cdot 3} ds \\ &= \frac{1}{6} \int_0^1 (s^3 + 3s^2 + 2s) ds = \frac{1}{6} \left[ \frac{s^4}{4} + s^3 + s^2 \right]_0^1 = \frac{1}{6} \left( \frac{9}{4} \right) = \frac{3}{8}. \end{aligned}$$

$k$	0	1	2	3	4	5
$\int_0^1 \binom{-s}{k} ds$	1	$\frac{1}{2}$	$\frac{5}{12}$	$\frac{3}{8}$	$\frac{251}{720}$	$\frac{95}{288}$



# Derivation of multistep method

As a consequence,

$$\begin{aligned} \int_{t_i}^{t_{i+1}} f(t, y(t)) dt &= h \left[ f(t_i, y(t_i)) + \frac{1}{2} \nabla f(t_i, y(t_i)) + \frac{5}{12} \nabla^2 f(t_i, y(t_i)) + \cdots \right] \\ &+ \frac{h^{m+1}}{m!} \int_0^1 s(s+1) \cdots (s+m-1) f^{(m)}(\xi_s, y(\xi_s)) ds. \end{aligned} \quad (9)$$

Because  $s(s+1) \cdots (s+m-1)$  does not change sign on  $[0, 1]$ , the Weighted Mean Value Theorem for Integrals can be used to deduce that for some number  $\mu_i$ , where  $t_{i+1-m} < \mu_i < t_{i+1}$ , the error term in Eq. (9) becomes

$$\begin{aligned} &\frac{h^{m+1}}{m!} \int_0^1 s(s+1) \cdots (s+m-1) f^{(m)}(\xi_s, y(\xi_s)) ds \\ &= \frac{h^{m+1} f^{(m)}(\mu_i, y(\mu_i))}{m!} \int_0^1 s(s+1) \cdots (s+m-1) ds. \end{aligned}$$



# Derivation of multistep method

Hence the error in Eq. (9) simplifies to

$$h^{m+1} f^{(m)}(\mu_i, y(\mu_i)) (-1)^m \int_0^1 \binom{-s}{m} ds. \quad (10)$$

But  $y(t_{i+1}) - y(t_i) = \int_{t_i}^{t_{i+1}} f(t, y(t)) dt$ , so Eq. (8) can be written as

$$y(t_{i+1}) = y(t_i) + h \left[ f(t_i, y(t_i)) + \frac{1}{2} \nabla f(t_i, y(t_i)) + \frac{5}{12} \nabla^2 f(t_i, y(t_i)) + \cdots \right] \quad (11)$$

$$+ h^{m+1} f^{(m)}(\mu_i, y(\mu_i)) (-1)^m \int_0^1 \binom{-s}{m} ds. \quad (12)$$



# Three-step Adams-Bashforth method

## Example

Using Eq. (12) with  $m = 3$ , derive three-step Adams-Bashforth technique.

$$\begin{aligned}y(t_{i+1}) &\approx y(t_i) + h \left[ f(t_i, y(t_i)) + \frac{1}{2} \nabla f(t_i, y(t_i)) + \frac{5}{12} \nabla^2 f(t_i, y(t_i)) \right] \\&= y(t_i) + h \left\{ f(t_i, y(t_i)) + \frac{1}{2} [f(t_i, y(t_i)) - f(t_{i-1}, y(t_{i-1}))] \right. \\&\quad \left. + \frac{5}{12} [f(t_i, y(t_i)) - 2f(t_{i-1}, y(t_{i-1})) + f(t_{i-2}, y(t_{i-2}))] \right\} \\&= y(t_i) + \frac{h}{12} [23f(t_i, y(t_i)) - 16f(t_{i-1}, y(t_{i-1})) + 5f(t_{i-2}, y(t_{i-2}))].\end{aligned}$$

The three-step Adams-Bashforth method is, consequently,

$$w_0 = \alpha, \quad w_1 = \alpha_1, \quad w_2 = \alpha_2,$$

$$w_{i+1} = w_i + \frac{h}{12} [23f(t_i, w_i) - 16f(t_{i-1}, w_{i-1}) + 5f(t_{i-2}, w_{i-2})],$$

for  $i = 2, 3, \dots, N-1$ .

# Truncation error

## Definition

If  $y(t)$  is the solution to the initial-value problem then

$$y' = f(t, y), \quad a \leq t \leq b, \quad y(a) = \alpha \quad \text{and}$$

$$w_{i+1} = a_{m-1}w_i + a_{m-2}w_{i-1} + \cdots + a_0w_{i+1-m} \\ + h[b_m f(t_{i+1}, w_{i+1}) + b_{m-1}f(t_i, w_i) + \cdots + b_0f(t_{i+1-m}, w_{i+1-m})]$$

is the  $(i + 1)$ th step, the **local truncation error** at this step is given by:

$$\tau_{i+1}(h) = \frac{y(t_{i+1}) - a_{m-1}y(t_i) - \cdots - a_0y(t_{i+1-m})}{h} \quad (13) \\ - [b_m f(t_{i+1}, y(t_{i+1})) + \cdots + b_0f(t_{i+1-m}, y(t_{i+1-m}))]$$

for each  $i = m - 1, m, \cdots, N - 1$ .



# Adams-Bashforth Explicit Methods

## Adams-Bashforth two-step explicit method

$$\begin{aligned}w_0 &= \alpha, \quad w_1 = \alpha_1, \quad \text{and for } i = 1, 2, \dots, N-1 \\w_{i+1} &= w_i + \frac{h}{2} [3f(t_i, w_i) - 5f(t_{i-1}, w_{i-1})]\end{aligned}$$

Truncation error:  $\tau_{i+1}(h) = \frac{5}{12}y'''(\mu_i)h^2$  for some  $\mu_i \in (t_{i-1}, t_{i+1})$

## Adams-Bashforth three-step explicit method

$$\begin{aligned}w_0 &= \alpha, \quad w_1 = \alpha_1, \quad w_2 = \alpha_2 \quad \text{and for } i = 2, 3, \dots, N-1 \\w_{i+1} &= w_i + \frac{h}{12} [23f(t_i, w_i) - 16f(t_{i-1}, w_{i-1}) + 5f(t_{i-2}, w_{i-2})]\end{aligned}$$

Truncation error:  $\tau_{i+1}(h) = \frac{3}{8}y^{(4)}(\mu_i)h^3$  for some  $\mu_i \in (t_{i-2}, t_{i+1})$

# Adams-Bashforth Explicit Methods

## Adams-Bashforth four-step explicit method

$$w_0 = \alpha, w_1 = \alpha_1, w_2 = \alpha_2, w_3 = \alpha_3 \text{ and for } i = 3, 4, \dots, N-1$$

$$w_{i+1} = w_i + \frac{h}{24} [55f(t_i, w_i) - 59f(t_{i-1}, w_{i-1}) + 37f(t_{i-2}, w_{i-2}) - 9f(t_{i-3}, w_{i-3})]$$

$$\text{Truncation error: } \tau_{i+1}(h) = \frac{251}{720} y^{(5)}(\mu_i) h^4 \text{ for some } \mu_i \in (t_{i-3}, t_{i+1})$$

## Adams-Bashforth five-step explicit method

$$w_0 = \alpha, w_1 = \alpha_1, w_2 = \alpha_2, w_3 = \alpha_3, w_4 = \alpha_4 \text{ and for } i = 4, 5, \dots, N-1$$

$$w_{i+1} = w_i + \frac{h}{720} [1901f(t_i, w_i) - 2774f(t_{i-1}, w_{i-1}) \\ + 2616f(t_{i-2}, w_{i-2}) - 1274f(t_{i-3}, w_{i-3}) + 251f(t_{i-4}, w_{i-4})]$$

$$\text{Truncation error: } \tau_{i+1}(h) = \frac{95}{288} y^{(6)}(\mu_i) h^5 \text{ for some } \mu_i \in (t_{i-4}, t_{i+1})$$

# Adams-Moulton Implicit Methods

## Adams-Moulton two-step implicit method

$$\begin{aligned}w_0 &= \alpha, \quad w_1 = \alpha_1, \quad \text{and for } i = 1, 2, \dots, N-1 \\w_{i+1} &= w_i + \frac{h}{2} [5f(t_{i+1}, w_{i+1}) + 8f(t_i, w_i) - f(t_{i-1}, w_{i-1})]\end{aligned}$$

Truncation error:  $\tau_{i+1}(h) = -\frac{1}{24}y^{(4)}(\mu_i)h^3$  for some  $\mu_i \in (t_{i-1}, t_{i+1})$

## Adams-Moulton three-step implicit method

$$\begin{aligned}w_0 &= \alpha, \quad w_1 = \alpha_1, \quad w_2 = \alpha_2 \quad \text{and for } i = 1, 2, \dots, N-1 \\w_{i+1} &= w_i + \frac{h}{24} [9f(t_{i+1}, w_{i+1}) + 19f(t_i, w_i) - 5f(t_{i-1}, w_{i-1}) + f(t_{i-2}, w_{i-2})]\end{aligned}$$

Truncation error:  $\tau_{i+1}(h) = -\frac{19}{720}y^{(5)}(\mu_i)h^4$  for some  $\mu_i \in (t_{i-2}, t_{i+1})$

# Adams-Moulton Implicit Methods

## Adams-Moulton Four-step implicit method

$$\begin{aligned}w_0 &= \alpha, \quad w_1 = \alpha_1, \quad w_2 = \alpha_2, \quad w_3 = \alpha_3, \quad \text{and for } i = 3, 4, \dots, N-1 \\w_{i+1} &= w_i + \frac{h}{720} [251f(t_{i+1}, w_{i+1}) + 646f(t_i, w_i) \\&\quad - 264f(t_{i-1}, w_{i-1}) + 106f(t_{i-2}, w_{i-2}) - 19f(t_{i-3}, w_{i-3})]\end{aligned}$$

Truncation error:  $\tau_{i+1}(h) = -\frac{3}{160}y^{(6)}(\mu_i)h^5$  for some  $\mu_i \in (t_{i-3}, t_{i+1})$



# Example

## Example

Consider the initial value problem

$$y' = y - t^2 + 1, \quad 0 \leq t \leq 2, \quad y(0) = 0.5$$

Use the exact values given from  $y(t) = (t + 1)^2 - 0.5e^t$  as starting values and  $h = 0.2$  to compare the approximations from by

- (a) the explicit Adams-Bashforth four-step method and
- (b) the implicit Adams-Moulton three-step method.

Given  $f(t, y) = y - t^2 + 1$ ,  $h = 0.2$  and  $t_i = 0.2i$

(a) The Adams-Bashforth four-step method: for  $i = 3, 4, \dots, 9$

$$w_{i+1} = w_i + \frac{h}{24} [55f(t_i, w_i) - 59f(t_{i-1}, w_{i-1}) + 37f(t_{i-2}, w_{i-2}) - 9f(t_{i-3}, w_{i-3})]$$

on simplification using given information this becomes:

$$w_{i+1} = \frac{1}{24} [35w_i - 11.8w_{i-1} + 7.4w_{i-2} - 1.8w_{i-3} - 0.192i^2 - 0.192i + 4.736]$$



## Example

(b) The Adams-Moulton three-step method:

$$w_{i+1} = w_i + \frac{h}{24} [9f(t_{i+1}, w_{i+1}) + 19f(t_i, w_i) - 5f(t_{i-1}, w_{i-1}) + f(t_{i-2}, w_{i-2})]$$

on simplification this becomes:

$$w_{i+1} = \frac{1}{24} [1.8w_{i+1} + 27.8w_i - w_{i-1} + 0.2w_{i-2} - 0.192i^2 - 0.192i + 4.736]$$

collecting all  $w_{i+1}$  terms on LHS we get, for  $i = 2, 3, \dots, 9$ .

$$w_{i+1} = \frac{1}{22.2} [27.8w_i - w_{i-1} + 0.2w_{i-2} - 0.192i^2 - 0.192i + 4.736]$$

# Example

$t_i$	Exact	Adams-Bashforth $w_i$	Error	Adams-Moulton $w_i$	Error
0.0	0.5000000				
0.2	0.8292986				
0.4	1.2140877				
0.6	1.6489406			1.6489341	0.0000065
0.8	2.1272295	2.1273124	0.0000828	2.1272136	0.0000160
1.0	2.6408591	2.6410810	0.0002219	2.6408298	0.0000293
1.2	3.1799415	3.1803480	0.0004065	3.1798937	0.0000478
1.4	3.7324000	3.7330601	0.0006601	3.7323270	0.0000731
1.6	4.2834838	4.2844931	0.0010093	4.2833767	0.0001071
1.8	4.8151763	4.8166575	0.0014812	4.8150236	0.0001527
2.0	5.3054720	5.3075838	0.0021119	5.3052587	0.0002132



**ANY  
QUESTIONS?**