Multi-step methods:

An m-step multi-step method for solving the IVP

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

has a difference equation for finding the approximation w_{i+1} at the mesh point t_{i+1}, represented by the following equation, where m is an integer greater than 1:

$$w_{i+1} = a_{m-1} w_i + a_{m-2} w_{i-1} + \cdots + a_0 w_{i+1-m}$$

$$+ h \left[b_m f(t_{i+1}, w_{i+1}) + b_{m-1} f(t_i, w_i) + \cdots \right.$$

$$\left. \cdots + b_0 f(t_{i+1-m}, w_{i+1-m}) \right], \qquad \text{— (1)}$$

for ~~where~~ $i = m-1, m, \ldots N-1$; where $h = \frac{b-a}{N}$,

$a_0, a_1, \ldots a_{m-1}$ and $b_0, b_1, \ldots b_m$ are constants,

and the starting values

$$w_0 = \alpha, \; w_1 = \alpha_1, \ldots \; w_{m-1} = \alpha_{m-1}$$

are specified.

When $b_m = 0$ the method is called explicit or open, because (1) can be used to compute w_{i+1} explicitly in terms of previously determined values. When $b_m \neq 0$, the method is called implicit or closed, because w_{i+1} occurs on both sides of (1).

Note that computation of w_{i+1} involves previous values $w_0, w_1 \ldots w_{m-1}$ in m-step method, [since $i+1-m \ge 0 \Rightarrow i \ge m-1$], to start an m-step method first m values, $w_0, w_1 \ldots w_{m-1}$ are required to compute using another method.

Derivation of multistep method:

Recall IVP.

$$y' = f(t, y), \quad a \le t \le b, \quad y(a) = \alpha.$$

Integrate over $[t_i, t_{i+1}]$,

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

which implies

$$y(t_{i+1}) = y(t_i) + \int_{t_i}^{t_{i+1}} f(t, y(t))\,dt. \quad \text{— (2)}$$

We cannot integrate $f(t, y(t))$ without knowing $y(t)$. We use numerical integration instead by using interpolating polynomial $P(t)$ to $f(t, y(t))$, one that is determined by some of the previously obtained data points $(t_0, w_0), (t_1, w_1), \ldots (t_i, w_i)$. If we assume $y(t_i) \approx w_i$, then (2) becomes

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

We can use any interpolation, but it is most convenient to use the Newton backward-difference formula.

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

$(t_i, f(t_i, y(t_i))), (t_{i-1}, f(t_{i-1}, y(t_{i-1}))), \ldots$

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

Since $P_{m-1}(t)$ is an interpolatory polynomial of degree (3)
$m-1$, there exists some ξ_i in (t_{i+1-m}, t_{i+1}) ~~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 $t = t_i + sh$, with $dt = h\,ds$, into $P_{m-1}(t)$ and the error term implies that

$$f(t, y(t)) = \sum_{k=0}^{m-1}(-1)^k\binom{-s}{k}\nabla^k f(t_i, y(t_i)) + \frac{f^{(m)}(\xi_i, y(\xi_i))}{m!}\prod_{j=i+1-m}^{i}(t-t_j)$$

and

$$\int_{t_i}^{t_{i+1}} f(t, y(t))\,dt = \sum_{k=0}^{m-1}(-1)^k\nabla^k f(t_i, y(t_i))\int_{t_i}^{t_{i+1}}\binom{-s}{k}dt$$

$$+\int_{t_i}^{t_{i+1}}\frac{f^{(m)}(\xi_i, y(\xi_i))}{m!}\prod_{j=i+1-m}^{i}(t-t_j)\,dt$$

$$= \sum_{k=0}^{m-1}\nabla^k f(t_i, y(t_i))\,h\,(-1)^k\int_0^1\binom{-s}{k}ds \; ; \qquad \boxed{t = t_i + sh}$$

$$+\frac{h^{m+1}}{m!}\int_0^1 s(s+1)\cdots(s+m-1)\,f^{(m)}(\xi_i, y(\xi_i))\,ds.$$

Recall that $\nabla P_n = P_n - P_{n-1}$, where $\{P_n\}_{n=0}^{\infty}$ is a sequence
$n \geq 1$.

$$\nabla^k P_n = \nabla(\nabla^{k-1}P_n) \qquad k \geq 2$$

$$\binom{-s}{k} = \frac{-s(-s-1)\cdots(-s-k+1)}{k!}$$

$$= \frac{s(s+1)\cdots(s+k-1)}{k!}\cdot(-1)^k.$$

The integral $(-1)^k \int_0^1 \binom{-s}{k} ds$ for various values of k can be computed.

Example: (1) $k=0$: $\quad (-1)^k \int_0^1 \binom{-s}{k} ds = \int_0^1 \binom{-s}{0} ds = 1$

(2) $k=1$: $\quad (-1)^k \int_0^1 \binom{-s}{k} ds = (-1) \int_0^1 \binom{-s}{1} ds = \int_0^1 s\, ds = \frac{1}{2}$.

(3) $k=2$: $\quad (-1)^k \int_0^1 \binom{-s}{k} ds = \int_0^1 \binom{-s}{2} ds = \int_0^1 \frac{s(s+1)}{2} ds = \frac{5}{12}$

(4) $k=3$: $\quad (-1)^3 \int_0^1 \binom{-s}{3} ds = \int_0^1 \frac{s(s+1)(s+2)}{6} ds = \frac{1}{6}\int_0^1 (s^3+3s^2+2s) ds$

$$= \frac{1}{6}\left[\frac{1}{4}+1+1\right] = \frac{1}{6}\cdot\frac{9}{4} = \frac{3}{8}.$$

(5) $k=4$: $\quad (-1)^4 \int_0^1 \binom{-s}{4} ds = \frac{251}{720}$;

(6) $k=5$: $\quad (-1)^5 \int_0^1 \binom{-s}{4} = \frac{95}{288}$

~~As a consequence~~

Note that since we are looking for $t = t_i + sh$, ~~so~~ $t > t_i$ [for integral over $[t_i, t_{i+1}]$], $s > 0$.

So $s(s+1)\cdots(s+m-1)$ does not change sign on $[0,1]$.

the weighted mean value theorem gives us

$$\frac{h^{m+1}}{m!}\int_0^1 s(s+1)\cdots(s+m-1) f^{(m)}(z_i, y(z_i))\, ds$$

$$= \frac{h^{m+1}}{m!} f^{(m)}(\mu_i, y(\mu_i)) \int_0^1 s(s+1)\cdots(s+m-1)\, ds$$

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

As a consequence

$$\int_{t_i}^{t_{i+1}} f(t, y(t))\,dt = h\left[f(t_i, y(t_i)) + \frac{1}{2}\nabla f(t_i, y(t_i)) + \frac{5}{12}\nabla^2 f(t_i, y(t_i))\right.$$

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

By dropping the remainder term, (error term), we form the Adams-Bashforth Explicit methods:

<u>Two step explicit method:</u>

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

$$w_{i+1} = w_i + \frac{h}{2}\left[3 f(t_i, w_i) - f(t_{i-1}, w_{i-1})\right]$$

where $i = 1, 2, \ldots N-1$.

<u>Three step explicit method:</u>

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

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

where $i = 2, 3 \ldots N-1$,

<u>Four step explicit method:</u>

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

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

where $i = 3, 4, \ldots N-1$.

Local truncation error for Adams-Bashforth method:

Let $y(t)$ be the solution of IVP

$$y' = f(t, y), \quad a \le t \le b, \quad y(a) = \alpha.$$

and

$$w_{i+1} = a_{m-1} w_i + a_{m-2} w_{i-1} + \cdots + a_0 w_{i+1-m}$$
$$+ h\left[b_m f(t_{i+1}, w_{i+1}) + b_{m-1} f(t_i, w_i) + \cdots + b_0 f(t_{i+1-m}, w_{i+1-m})\right]$$

is the $(i+1)^{th}$ step in a multistep method, the local truncation error at this step is

$$\tau_{i+1}(h) = \frac{y(t_{i+1}) - a_{m-1} y(t_i) - \cdots - a_0 y(t_{i+1-m})}{h}$$
$$- \left[b_m f(t_{i+1}, y(t_{i+1})) + \cdots + b_0 f(t_{i+1-m}, y(t_{i+1-m}))\right]$$

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

Example: (1) Two step method of Adams-Bashforth by local truncation

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

since in this case $m=2$.

(2) three step method, local truncation error is $\tau_{i+1}(h) = \frac{3}{8} y^{(4)}(\mu_i) h^3$, $\mu_i \in (t_{i-2}, t_{i+1})$

(3) Four step method local truncation error is

$$\tau_{i+1}(h) = \frac{251}{720} y^{(5)}(\mu_i) h^4.$$

$$\mu_i \in (t_{i-3}, t_{i+1})$$

Adams-Moulton Implicit methods:

Implicit methods are derived by using $(t_{i+1}, f(t_{i+1}, y(t_{i+1})))$ as an additional interpolation data point in the approximation of the integral

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

Some of the more common implicit methods are as follows:

Adam-Moulton Two-step Implicit method:

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

$$w_{i+1} = w_i + \frac{h}{12}\left[5 f(t_{i+1}, w_{i+1}) + 8 f(t_i, w_i) - f(t_{i-1}, w_{i-1})\right],$$

where $i = 1, 2, \dots N-1$. The local truncation error is

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

Adam-Moulton Three step implicit method:

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

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

where $i = 2, 3 \dots N-1$. The local truncation error is

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

Adam-Moulton four step implicit method:

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

$$w_{i+1} = w_i + \frac{h}{720}\left[251 f(t_{i+1}, w_{i+1}) + 646 f(t_i, w_i) - 264 f(t_{i-1}, w_{i-1}) + 106 f(t_{i-2}, w_{i-2}) - 19 f(t_{i-3}, w_{i-3})\right]$$

where $i = 3, 4, \dots N-1$. The local truncation error is

$$\tau_{i+1}(h) = -\frac{3}{160} y^{(6)}(\mu_i) h^5, \quad \mu_i \in (t_{i-3}, t_{i+1}).$$

<u>Remarks</u> In the derivation of Adams-Moulton implicit methods, we use interpolating polynomial $P_m(t)$ of degree m interpolating the data points

$(t_{i+1}, f(t_{i+1}, y(t_{i+1})))$, $(t_i, f(t_i, y(t_i)))$, $(t_{i-1}, f(t_{i-1}, y(t_{i-1})))$,

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

These are $m+1$ data points to find $P_m(t)$.

Using Newton backward difference formula, we can derive the implicit methods as we did before in finding explicit methods.

<u>Predictor - Corrector methods:</u>

Implicit Adams-Moulton methods are higher order compared with explicit Adams-Bashforth explicit methods. We expect better results with implicit methods. However implicit methods are difficult to implement compared with explicit methods. Predictor-corrector methods are designed to reduce the complexity of implicit methods as follows: suppose we want to use Adams-Moulton ~~three~~ step implicit method at $(i+1)$ step $(i \geq 3)$. First we apply Adams-Bashforth four step method to find $w_{i+1}^{(0)}$ and then use it in the Adams-Moulton ~~three~~ step method [in RHS for w_{i+1}], to find $w_{i+1}^{(1)}$. We treat $w_{i+1}^{(1)}$ as an approximation to $y(t_{i+1})$ which is an improvement of approximation obtained from Adams-Bashforth explicit method. Then we proceed to find w_{i+2}, i.e. the next time step.

To write down explicitely the method:

suppose $w_0 = \alpha$, $w_1 = \alpha_1$, $w_2 = \alpha_2$, $w_3 = \alpha_3$ are known.

$$w_{4p} = w_3 + \frac{h}{24}\left[55 f(t_3, w_3) - 59 f(t_2, w_2) + 37 f(t_1, w_1) - 9 f(t_0, w_0)\right]$$

to find w_{4p} from Adams-Bashforth four step ~~explicit method~~ explicit method. This step is called predictor.

The approximation w_{4p} is improved by using it in the right hand side of Adams-Moulton three step implicit method as a corrector: This gives

$$w_4 = w_3 + \frac{h}{24}\left[9 f(t_4, w_{4p}) + 19 f(t_3, w_3) - 5 f(t_2, w_2) + f(t_1, w_1)\right].$$

The only new function value to be evaluated is $f(t_4, w_{4p})$. The value w_4 is then used as the approximation to $y(t_4)$.

The technique of using the Adams-Bashforth four step explicit method as a predictor and the Adams-Moulton ~~method as~~ three step implicit method as a corrector is repeated to find w_{5p} and w_5, the initial & final approximation to $y(t_5)$. This procedure is continued until we find an approximation to $y(t_N) = y(b)$.

Higher order equations and systems of ODE:

An m^{th} order systems of first order initial-value problems has the form

$$\left.\begin{aligned}
\frac{du_1}{dt} &= f_1(t, u_1, u_2, \ldots u_m), \\
\frac{du_2}{dt} &= f_2(t, u_1, u_2, \ldots u_m), \\
&\vdots \\
\frac{du_m}{dt} &= f_m(t, u_1, u_2, \ldots u_m),
\end{aligned}\right] \text{(1)}$$

for $a \le t \le b$, with initial conditions:

$$u_1(a) = \alpha_1, \; u_2(a) = \alpha_2, \; \ldots, \; u_m(a) = \alpha_m. \Big\} \text{(2)}$$

The objective is to find m functions $u_1(t), u_2(t), \ldots u_m(t)$ that satisfy each of the differential equations together with all the initial conditions.

<u>Definition:</u> The function $f(t, y_1, y_2, \ldots y_m)$ defined on the set $D = \{(t, u_1, u_2, \ldots u_m) : a \le t \le b, \; -\infty < u_i < \infty, \; i = 1, 2, \ldots m\}$

is said to satisfy a Lipschitz condition on D in the variables $u_1, u_2, \ldots u_m$, if a constant $L > 0$ exists with

$$|f(t, u_1, u_2, \ldots u_m) - f(t, z_1, z_2, \ldots z_m)| \le L \sum_{j=1}^{m} |u_j - z_j|$$

for all $(t, u_1, u_2, \ldots u_m)$ and $(t, z_1, z_2, \ldots z_m)$ in D.

<u>Theorem</u>: Suppose that

$$D = \{(t, u_1, u_2, \dots u_m) : a \le t \le b, \ -\infty < u_i < \infty, \ 1 \le i \le m\}$$ (5)

and let $f_i(t, u_1, u_2 \dots u_m)$ for each $i = 1, 2, \dots m$, be continuous and satisfy a Lipschitz condition on D. Then the system of first-order differential equations (1) ~~and~~ subject to initial conditions (2) has a unique solution $u_1(t), u_2(t), \dots u_m(t)$, for $a \le t \le b$.

Methods to solve systems of first-order differential equations are generalizations of the methods for a single first order equation discussed earlier.

We can also write the system of differential equations in (1) as

$$\frac{dU}{dt} = F(t, U),$$

and initial conditions in (2) as $U(a) = \alpha$, where

$$U(t) = (u_1(t), u_2(t), \dots u_m(t))^T,$$

$$F(t, U) = (f_1(t, U), f_2(t, U), \dots f_m(t, U))^T,$$

& $f_i(t, U) = f_i(t, u_1, u_2, \dots u_m)$, $\alpha = (\alpha_1, \alpha_2 \dots \alpha_m)^T$.

Here $(\cdot, \cdot, \dots \cdot)^T$ denotes the transpose of $(\cdot, \cdot, \dots \cdot)$.

Therefore we have IVP for the system

$$\frac{dU}{dt} = F(t, U)$$

$$U(a) = \alpha.$$

We can write Euler's method for the system as (1)

$$w_0 = \alpha,$$
$$w_{i+1} = w_i + h F(t_i, w_i). \quad \Big] \; (3)$$

where w_i is an approximation to $u(t_i)$, $i = 0, 1, \ldots N$.

$$w_i = (\omega_{1,i}, \omega_{2,i}, \omega_{3,i}, \ldots \omega_{m,i})^T$$

$$F(t_i, \omega_i) = (f_1(t_i, \omega_i), f_2(t_i, \omega_i), \ldots f_m(t_i, \omega_i))^T$$

$$f_j(t_i, \omega_i) = f_j(t_i, w_{1,i}, w_{2,i}, \ldots \omega_{m,i}).$$

$w_{j,i}$ is approximation to $u_j(t_i)$.

Therefore (3) can be written as

$$w_0 = (\omega_{1,0}, \omega_{2,0}, \ldots \omega_{m,0}) = (\alpha_1, \alpha_2, \ldots \alpha_m).$$

$$w_{j,i+1} = w_{j,i} + h f_j(t_i, w_{1,i}, \omega_{2,i}, \ldots \omega_{m,i})$$

for $1 \leq j \leq m$ and $i = 0, 1, \ldots N-1$.

Similarly we can write the methods that we developed earlier.

Higher order equations

A general mth order IVP:

$$y^{(m)}(t) = f(t, y, y', \ldots y^{(m-1)}), \quad a \leq t \leq b,$$

with initial conditions $y(a) = \alpha_1$, $y'(a) = \alpha_2$, $\ldots$ $y^{(m-1)}(a) = \alpha_m$

can be converted into a system of first order differential equations as follows:

Let
$$u_1(t) = y(t)$$
$$u_2(t) = y'(t)$$
$$\vdots$$
$$u_m(t) = y^{(m-1)}(t).$$

Then
$$\frac{du_1}{dt} = \frac{dy}{dt} = u_2;$$
$$\frac{du_2}{dt} = \frac{dy'}{dt} = u_3;$$
$$\vdots$$
$$\frac{du_m}{dt} = \frac{dy^{(m-1)}}{dt} = y^{(m)} = f(t, y, y', \dots y^{(m-1)})$$
$$= f(t, u_1, u_2 \dots u_m)$$

we have
$$\frac{du_1}{dt} = u_2$$
$$\frac{du_2}{dt} = u_3$$
$$\vdots$$
$$\frac{du_m}{dt} = f(t, u_1, u_2 \dots u_m)$$

and initial conditions
$u_1(a) = y(a) = \alpha_1$, $u_2(a) = y'(a) = \alpha_2$, ... $u_m(a) = y^{(m-1)}(a) = \alpha_m$

i.e. $u_1(a) = \alpha_1$, $u_2(a) = \alpha_2$, ... $u_m(a) = \alpha_m$.

we get a system of m equations of first order differential equations in m unknowns
$u_1, u_2 \dots u_m$