Ch. 2 Multistep Methods

Key Points:

- Basic Idea of Multistep Methods
  - use of previous info...
- Connection of method to interpolation theory
- Brief review of interpolation theory
  (polynomial, Newtonian, Lagrangian forms)
  - Adams Methods — interpolate \( \hat{y}' \) (or \( y' \))
  - Adams Bashforth (4th order explicit)
  - Adams Bashforth (5-step) general
- General theory for multistep methods

  Thm 2.1 — order of multistep

  Thm 2.2 — convergence of multistep
  - root condition

- Backward Differentiation Formulae (interpolate \( \hat{y} \))
  (e.g. Backward Euler, ...)
Multistep Methods (for solving $\dot{y} = f(t, y)$, $y(t_0) = y_0$)

**General idea:** These use information at more than one previous point to advance to the next point (unlike Euler, Heun, Trapezoid, ...)

Recall:

Euler: \[ \dot{y}_{k+1} = y_k + h \frac{\dot{y}_k}{t_k, y_k} \]

Here only information at the previous time value \( \dot{y}_k \) is required to evaluate the formula for \( y_{k+1} \). (i.e. this is a single-step method).

\[ y_k \rightarrow y_{k+1} \]

\[ t_k \rightarrow t_{k+1} \]

An example of a multistep method is a method known as Adams-Bashforth. Here, we use

\[ \dot{y}_{k+1} = \dot{y}_k + \frac{h}{24} \left( 55 \dot{y}_k - 59 \dot{y}_{k-1} + 37 \dot{y}_{k-2} - 9 \dot{y}_{k-3} \right) \]

where

\[ \dot{y}_k = f(t_k, y_k) \]

\[ \dot{y}_{k-1} = f(t_{k-1}, y_{k-1}) \]

\[ \dot{y}_{k-2} = f(t_{k-2}, y_{k-2}) \]

\[ \dot{y}_{k-3} = f(t_{k-3}, y_{k-3}) \]

\[ k = 3, 4, 3, 5, ... \]

(need something else for $k=0,1,2$)

**4th order explicit**

Don't get too used to this notation... we are shifting the $k$'s to something else.
So in order to obtain $\bar{y}_{k+1}$ we need to know $\bar{y}_k, \bar{y}_{k-1}, \bar{y}_{k-2}, \bar{y}_{k-3}$ (i.e. 4 previously calculated values).

![Diagram of time points]

t_0 \rightarrow t_1 \rightarrow t_2 \rightarrow t_3 \rightarrow t_4 \rightarrow \ldots \rightarrow t_k \rightarrow \ldots \rightarrow t_{k+1}

Comments:
- Since we have an initial condition at only one time, one might ask how we "start" this method (not "self-starting"). We need some help to get up to speed (maybe RK?).
- You may also ask if we are even allowed to do this (specify the solution at multiple previous points) [see comment in text, p. 11 after (2.1)].
- How does one come up with such a scheme? (the numbers 55, 59, 37, -9 are not arbitrarily selected)
The general form of multistep methods we consider is

\[ a_0 \tilde{y}_K = a_1 \tilde{y}_{K+1} + a_2 \tilde{y}_{K+2} + \ldots + a_{s+1} \tilde{y}_{K+s+1} = 1 \]

where \( s \geq 1 \) is an integer.

(see also equation 2.8, p. 21 in Iserles)

**Comments:**

- This equation is interpreted as determining \( \tilde{y}_{K+s} \) given that \( \tilde{y}_K, \tilde{y}_{K+1}, \tilde{y}_{K+2}, \ldots, \tilde{y}_{K+s-1} \) are already known (somehow)

- It is conventional to set \( a_s = 1 \)

- The method is explicit if \( b_s = 0 \)

- The method is implicit if \( b_s \neq 0 \)

- In the 4th order explicit Adams-Bashforth scheme note that \( s = 4 \) (and we use a shifted notation on the \( k \)-values)

- The coefficients \( a_j, b_j \) are determined by polynomial interpolation as explained below in more detail.

  * Adams Methods: interpolate \( \tilde{y} \) (i.e. \( \tilde{y}' \))

  * Backward Differentiation: interpolate \( \tilde{y} \)
Adams Methods

\[ \bar{y}(t) = \hat{y}(t) \quad \text{at} \quad 5 \text{ previous points} \]

\[ \hat{y}(t) = \tilde{f}(t, \bar{y}) \quad \text{at} \quad \tilde{y}_k, \tilde{y}_{k-1}, \tilde{y}_{k-2}, ..., \tilde{y}_{k-5} \]

\[ f(t) = \text{a polynomial of degree 5-1} \]

Then, the scheme is found by integrating the polynomial (essentially interpolation)

\[ \bar{y}_{k+1} = \bar{y}_k + \int_{t_k}^{t_{k+1}} f(t, \bar{y}) \, dt \]

\[ \bar{y}(t) = \bar{y}(t) \quad \text{at} \quad 5 \text{ previous points} \]

\[ \tilde{y}(t) = \tilde{y}(t) \quad \text{at} \quad \tilde{y}_k, \tilde{y}_{k+1}, \tilde{y}_{k+2}, ..., \tilde{y}_{k+5} \]

\[ \hat{y}_k = \hat{y}(t) \quad \text{at} \quad \hat{y}_k, \hat{y}_{k-1}, \hat{y}_{k-2}, ..., \hat{y}_{k-5} \]

Backward Difference Formula (BDF) Methods

Interpolate \( \bar{y} \) at \( 6 \) previous points \((\bar{y}_k, \bar{y}_{k+1}, ..., \bar{y}_{k+6})\)

\[ \frac{\bar{y}_{k+1} - \bar{y}_k}{t_{k+1} - t_k} = \hat{g}(t_k) \]

where \( \hat{g}(t) \) is a polynomial of degree 5.

Then the scheme is found by differentiating \( \hat{g}(t) \)

and setting it equal to \( f(t_{k+1}, \bar{y}_{k+1}) \) at \( t_{k+1} \) to get \( \bar{y}_{k+1} \).
Some examples

**EX 1** (explicit 2-step method) - Adams-type

$$Y_{k+2} = Y_{k+1} + \int_{t_{k+1}}^{t_{k+2}} b(t) \, dt$$

where $b(t)$ interpolates $n$ points $(t_k, f(t_k, Y_k))$.

$$b(t) = A + B(t - t_k)$$

and

$$t_{k+2} - t_{k+1} = \frac{A}{B}$$

Integrating gives

$$\int_{t_{k+1}}^{t_{k+2}} b(t) \, dt = A (t_{k+2} - t_{k+1}) + \frac{1}{2} B (t_{k+2} - t_{k+1})^2$$

which simplifies to

$$t_{k+2} - t_{k+1} = A \cdot h + h^2 B$$

So

$$Y_{k+2} = Y_{k+1} + A \cdot h + \frac{3}{2} h^2 B$$

$$= Y_{k+1} + \frac{1}{h} (Y_{k+1} - Y_k) \cdot h - \frac{1}{2} h (Y_{k+1} - Y_k)$$

$$= Y_{k+1} - \frac{3}{2} h Y_{k+1} - \frac{1}{2} Y_k$$

$$(Y_{k+2} = Y_{k+1} + h \left[ \frac{3}{2} f(t_{k+1}, Y_{k+1}) - \frac{1}{2} f(t_k, Y_k) \right]$$

(see also eq. 2.6, p. 20 in Iserles)
EX 2  (4th order explicit Adams-Bashforth) (s = 4)

\[ y_{k+4} = \hat{y}_{k+4} + \left( \frac{\hat{p}(t)}{t_{k+3}} \right) \Delta t \]

where

\[ \hat{p}(t) \text{ polynomial that interpolates} \]

\[ (t_{k+1}, \hat{y}_{k+1}) \quad (t_{k+2}, \hat{y}_{k+2}) \]

\[ (t_{k+3}, \hat{y}_{k+3}) \]

\[ \text{cubic} \]

\[ y_{k+1}, y_{k+2}, y_{k+3} \]

\[ \text{then insert } \hat{p}(t) \text{ into above integral to obtain scheme.} \]

... tedious but doable...

An alternate way to look at this and derive the coefficients is to recognize this scheme as having the form

\[ \hat{y}_{k+4} = \hat{y}_{k+3} + \Delta t \left[ \beta_0 \hat{y}_{k+1} + \beta_1 \hat{y}_{k+2} + \beta_2 \hat{y}_{k+3} + \beta_3 \hat{y}_{k+4} \right] \]

and requiring that this formula be exact if

\[ y' = 1, t, t^2, \text{ or } t^3 \]

(then \( \beta \) would coincide exactly)

\[ y = t, \frac{t^2}{2}, \frac{t^3}{3}, \frac{t^4}{4}, \frac{t^5}{5} \text{ with } \hat{y}' \]
\[
\begin{align*}
Y' &= 1 \\
Y &= t + C_0 \\
\frac{1}{2} (t_{k+4})^2 &= \frac{1}{2} (t_{k+3})^2 + h \left[ \beta_0 t_{k+1} + \beta_1 t_{k+2} + \beta_2 t_{k+3} \right] \\
Y' &= t \\
Y &= \frac{1}{2} t^2 + C_0 \\
\frac{1}{3} (t_{k+4})^3 &= \frac{1}{3} (t_{k+3})^3 + h \left[ \beta_0 t_{k+1}^2 + \beta_1 t_{k+2}^2 + \beta_2 t_{k+3}^2 \right] \\
Y' &= t^3 \\
Y &= \frac{1}{4} t^4 + C_0 \\
\frac{1}{4} (t_{k+4})^4 &= \frac{1}{4} (t_{k+3})^4 + h \left[ \beta_0 t_{k+1}^3 + \beta_1 t_{k+2}^3 + \beta_2 t_{k+3}^3 \right]
\end{align*}
\]

Note that the four equations (\(\ast\)) must hold for any values of \(t\) so let's choose them conveniently,

\[
\begin{align*}
t_k &= 0 \\
t_{k+1} &= 1 \\
t_{k+2} &= 2 \\
t_{k+3} &= 3 \\
t_{k+4} &= 4 \\
h &= 1.
\end{align*}
\]
So...

\[ 4 = 3 + \beta_0 + \beta_1 + \beta_2 + \beta_3 \]

\[ 16 \beta = 9 + 2[0 + \beta_1 + 2 \beta_2 + 3 \beta_3] \]

\[ 64 = 27 + 3[0 + \beta_1 + 4 \beta_2 + 9 \beta_3] \]

\[ 256 = 81 + 4[0 + \beta_1 + 8 \beta_2 + 27 \beta_3] \]

\[
\begin{bmatrix}
1 & 1 & 1 & 1 \\
0 & 1 & 2 & 3 \\
0 & 1 & 4 & 9 \\
-1 & -8 & 27 & \\
\end{bmatrix}
\begin{bmatrix}
\beta_0 \\
\beta_1 \\
\beta_2 \\
\beta_3 \\
\end{bmatrix}
= 
\begin{bmatrix}
1 \\
7/2 \\
37/3 \\
175/4 \\
\end{bmatrix}
\]

solving \[ \beta_0 = -\frac{9}{24}, \beta_1 = \frac{37}{24}, \beta_2 = -\frac{59}{24}, \beta_3 = \frac{55}{24} \]

So the scheme is

\[
y_{k+4} = y_{k+3} + \frac{h}{24} \begin{bmatrix}
-9 & 37 & y_{k+1} & -59 & y_{k+2} & 55 & y_{k+3} \\
\end{bmatrix}
\]

Adams-Bashforth (4th order explicit)

compare form, p. 23 in notes...
**EX 3** (BDF with \( s=1 \): Backward Euler)

\[
\ddot{y}(t_{k+1}) = \ddot{f}(t_{k+1}, y_{k+1})
\]

where \( \ddot{y} \) interpolates \((t_{k+1}, y_{k+1})\) and \((t_k, \dot{y}_k)\).

This is just a linear function

\[
\ddot{y}(t) = \dot{y}_k + \frac{(\ddot{y}_{k+1} - \dot{y}_k)(t - t_k)}{h}
\]

So \( \ddot{y}(t) = \frac{\ddot{y}_{k+1} - \dot{y}_k}{h} \)

and the scheme is...

\[
\ddot{y}_{k+1} = \frac{1}{h} \int_{t_k}^{t_{k+1}} f(t_{k+1}, \ddot{y}_{k+1}) dt
\]

**EX 4** (BDF with \( s=2 \))

Here, \( \ddot{y}(t) \) interpolates \((t_k, y_k)\)
\((t_{k+1}, y_{k+1})\)
\((t_{k+2}, y_{k+2})\)

... a little work shows

\[
\ddot{y}(t) = A + B (t-t_k) + C (t-t_k)(t-t_{k+1})
\]

where \( A = y_k \), \( B = \frac{y_{k+1} - y_k}{h} \), \( C = \frac{y_{k+2} - 2y_{k+1} + y_k}{h^2} \)

So that...

\[
\ddot{y}_{k+2} = \frac{4}{3} \ddot{y}_{k+1} + \frac{1}{3} \ddot{y}_k = \frac{2}{3} h \ddot{f}(t_{k+2}, \ddot{y}_{k+2})
\]
We'd like to now address the issue of "order of the method".
As we did for the previous chapter (see Def. p. 8 in ISERLES),
we can characterize the order of the method by inserting the
exact solution into the formula for the scheme. In the
present context, then, we have an "order p" method if

\[ a_0 \bar{y}(t_k) + a_1 \bar{y}(t_{k+1}) + \ldots + a_p \bar{y}(t_{k+p}) - h \left[ b_0 \bar{y}(t_k, \bar{y}(t_k)) + b_1 \bar{y}(t_{k+1}, \bar{y}(t_{k+1})) + \ldots + b_p \bar{y}(t_{k+p}, \bar{y}(t_{k+p})) \right] = O(h^{p+1}) \]

\[ t_{k+1} = t_k + h, \ldots, t_{k+p} = t_k + ph \]

Multistep Method of order \( p \), as \( h \rightarrow 0 \).

Comment:
- previously, we had taken the approach of writing
  \( \bar{y}(t_{k+1}, \bar{y}(t_k)) = \bar{y}(t_k) + \bar{y}'(t_k) + \frac{1}{2} \bar{y}''(t_k) + \ldots \)
  etc.

  (i.e. Taylor Expand \( \bar{y} \) and \( \bar{y}' \) everywhere and see
  what remains...)

- we'll do the same here but we'll introduce some
  notation, as in ISERLES, to help streamline things...

  etc.

... the result will be Thm 2.1 (ISERLES, p.22)
Let \( \psi(t, \bar{y}) \equiv \sum_{m=0}^{s} a_m \bar{y}(t+mh) - h \sum_{m=0}^{s} b_m \bar{y}'(t+mh) \)

Assume \( \bar{y} \) is analytic and that its radius of convergence is greater than the maximum size of \( mh \) — i.e. \( \exists h \)

So
\[
\bar{y}(t+mh) = \sum_{k=0}^{\infty} \frac{1}{k!} \bar{y}(t)(mh)^k = \bar{y}(t) + mh \bar{y}'(t) + \frac{1}{2!}(mh)^2 \bar{y}''(t) + \ldots
\]

and
\[
\bar{y}'(t+mh) = \sum_{k=0}^{\infty} \frac{1}{k!} \bar{y}'(t)(mh)^k = \bar{y}'(t) + mh \bar{y}''(t) + h^2 \bar{y}'''(t) + \ldots
\]

Then
\[
\psi(t, \bar{y}) = \sum_{m=0}^{s} a_m \left[ \bar{y}(t) + \sum_{k=1}^{\infty} \frac{1}{k!} \bar{y}^{(k)}(t)(mh)^k \right] - h \sum_{m=0}^{s} b_m \left[ \sum_{k=0}^{\infty} \frac{1}{k!} \bar{y}^{(k+1)}(t)(mh)^k \right]
\]

\[
= \bar{y}(t) \left( \sum_{m=0}^{s} a_m \right) + \sum_{k=1}^{\infty} \frac{1}{k!} \bar{y}^{(k)}(t) \left( \sum_{m=0}^{s} a_m m^k \right)
\]

\[-h \sum_{m=0}^{s} b_m \left( \sum_{j=1}^{\infty} \frac{1}{(j-1)!} \bar{y}^{(j)}(t) m^j \right) = \bar{y}(t) \left( \sum_{m=0}^{s} a_m \right) + \sum_{k=1}^{\infty} \frac{1}{k!} \bar{y}^{(k)}(t) \left( \sum_{m=0}^{s} a_m m^k \right)
\]

\[-h \left( \sum_{k=1}^{\infty} \frac{1}{k!} \bar{y}^{(k)}(t) \left( \sum_{m=0}^{s} b_m m^{k-1} \right) \right)
\]
\[ \Psi(t, \chi) = \chi(t) \left( \sum_{m=0}^{s} \frac{a_m}{m!} \right) + \sum_{k=1}^{\alpha_0} \left[ \left( \sum_{m=0}^{s} m^k a_m \right) - k \left( \sum_{m=0}^{s} m^{k-1} b_m \right) \right] \frac{1}{k!} \chi^{(k)}(\xi(t)) \]

In order for this method to be order \( \mathcal{O} \) (i.e. \( \Psi \sim \mathcal{O}(h^{p+1}) \))
we need

\[ \sum_{m=0}^{s} a_m = 0 \]
\[ \sum_{m=0}^{s} m^k a_m = k \sum_{m=0}^{s} m^{k-1} b_m \quad \text{for} \quad k=1,2,3,\ldots,p \]

with
\[ \sum_{m=0}^{s} m^{p+1} a_m = (p+1) \sum_{m=0}^{s} m^p b_m \]

These conditions can be expressed in terms of the polynomials

\[ \rho(w) = \sum_{m=0}^{s} a_m w^m \]
\[ \sigma(w) = \sum_{m=0}^{s} b_m w^m \]

(see book page 22 for further details...)
The resulting theorem can be expressed in terms of \( \rho(w) \) and \( \sigma(w) \)...

**Thm 2.1**

Our generic multistep method is of order \( p \geq 1 \) if and only if there exists \( c \neq 0 \) such that

\[
\rho(w) - \sigma(w) = c (w-1)^{p+1} \sim O \left( \left| w-1 \right|^{p+2} \right)
\]

as \( w \to 1 \).

**Comments:**

- The local error properties of the method can be characterized in terms of polynomials defined in the above way by the coefficients \( q_0, q_1, \ldots, q_p, b_0, b_1, \ldots, b_p \).

A second Theorem tells us about convergence of these methods...

**Thm 2.2. (The Dahlquist Equivalence Thm)**

Suppose the error in the starting values \( y_1, y_2, \ldots, y_{s-1} \) tends to zero as \( h \to 0^+ \). Our generic multistep method is convergent if and only if it is of order \( p \geq 1 \) and the polynomial \( \rho(w) \) has all its zeros inside the closed complex unit disc and all its zeros of unit modulus are simple. (Root condition, see p. 24)
What do these results tell us for our specific examples?...

**EX 1**

\[
Y_{k+2} = \frac{3}{2} Y_{k+1} + \frac{1}{2} Y_k
\]

\[
s = 2 \quad a_0 = 0 \quad b_0 = -\frac{1}{2}
\]

\[
a_1 = -1 \quad b_1 = \frac{1}{2}
\]

\[
a_2 = 1 \quad b_2 = 0
\]

\[
\rho(w) = \sum_{m=0}^{\infty} c_m w^m = a_0 + a_1 w + a_2 w^2 = -w + w^2 = w(w-1)
\]

\[
\sigma(w) = \sum_{m=0}^{\infty} b_m w^m = b_0 + b_1 w + b_2 w^2 = -\frac{1}{2} + \frac{3}{2} w
\]

**Note:** \(\ln w \approx \ln(1 + (w-1)) \sim (w-1) - \frac{1}{2} (w-1)^2 + \frac{1}{3} (w-1)^3 + \ldots\)

So

\[
\rho(w) - \sigma(w) \ln w = w(w-1) - \frac{1}{2} (3w-1)[(w-1) - \frac{1}{2} (w-1)^2 + \frac{1}{3} (w-1)^3 + \ldots]
\]

\[
= (w-1) \left\{ w - \frac{1}{2} (3w-1) \left[ 1 - \frac{1}{2} (w-1) + \frac{1}{3} (w-1)^2 + \ldots \right] \right\}
\]

\[
= (w-1) \left\{ w - \frac{1}{2} (3w-1) \left[ \frac{3}{2} - \frac{1}{2} w + \frac{1}{3} (w-1)^2 + \ldots \right] \right\}
\]

\[
= (w-1) \left\{ w - \frac{1}{2} (9w^2 - 3 - w) - \frac{1}{6} (3w-1)(w-1)^2 + \ldots \right\}
\]

\[
\ln(1+x) = x - \frac{1}{2} x^2 + \frac{1}{3} x^3 - \frac{1}{4} x^4 + \ldots \quad -1 < x \leq 1
\]
\( p(w) - 0(w) \sim (w-1) \left\{ -\frac{1}{4} \left( -3w^2 + 6w - 3 \right) - \frac{1}{6} \frac{3(w-1)(w-1)^2}{(w-1)^2} \right\} \)

\( \sim (w-1) \left\{ -\frac{1}{4} \left( -3w^2 + 6w - 3 \right) - \frac{1}{6} \frac{3w-1}{(w-1)^2} \right\} \)

\( \sim (w-1)^3 \left\{ \frac{3}{4} \frac{(w-1)^2}{(w-1)^2} + O(w-1) \right\} \)

\( \sim (w-1)^3 \left\{ -\frac{1}{2}w + \frac{11}{12} + O(w-1) \right\} \)

So this method is order 2 looks like \((w-1)^2\)!

Also note

\( p(w) = w(w-1) \) obeys the root condition

\( \Rightarrow \text{method is convergent.} \)
Back to Adams-Bashforth (4th order explicit)

This method is often used together with the Adams-Moulton method in a predictor-corrector scheme.

Adams-Moulton (implicit 4th order scheme)

$$\bar{Y}_{k+3} = \bar{Y}_{k+2} + \frac{h}{24} \left[ 9 \bar{Y}'_{k+3} + 19 \bar{Y}'_{k+2} - 5 \bar{Y}'_{k+1} + \bar{Y}'_{k} \right]$$

Adams-Bashforth (explicit 4th order scheme) (slightly rewritten)

$$\bar{Y}_{k+3} = \bar{Y}_{k+2} + \frac{h}{24} \left[ -9 Y'_{k+1} + 37 Y'_{k} - 59 Y'_{k-1} + 55 Y'_{k-2} \right]$$

Idea:
- Predict: $\bar{Y}_{k+3}$ using AB
- Evaluate: $F(t_{k+3}, \bar{Y}_{k+3})$ to estimate $Y'_{k+3}$ in AM
- Correct: use AM to get a new $\bar{Y}_{k+3}$
- Evaluate: $F(t_{k+3}, \bar{Y}_{k+3})$ and repeat the correction AM

Note: This is similar to Heun's method

$$\begin{align*}
\hat{Y}_{k+1} &= Y_k + f(t_k, Y_k) \\
Y_{k+1} &= Y_k + \frac{1}{2} \left[ f(t_k, Y_k) + f(t_{k+1}, \hat{Y}_{k+1}) \right]
\end{align*}$$

i.e. Euler/Trapezoid Predictor/Corrector.
Recall that the interpolation error associated with a polynomial of degree at most \( n-1 \) that interpolates \( f \) at \( n \) distinct points \( t_1, t_2, \ldots, t_n \) (\( f \) is sufficiently smooth) is

\[
f(t) - P_{n-1}(t) = \frac{f^{(n)}(\theta)}{n!} \prod_{i=1}^{n} (t-t_i) \quad \theta \in (t_1, t_n)
\]

(e.g. Heath, p. 324; Isersas A.2.2.2)

Note that if the points are equally spaced,

\[
t_1, t_2, t_3, \ldots, t_n
\]