Unit 8.2. Multistep Methods

Numerical Analysis

June 2, 2015

Polynomial Approximation

- We assume the solution of the dynamic equation $x(t)$ can be approximated by a polynomial of degree p as

$$x(t) = a_0 + a_1 t + a_2 t^2 + \cdots + a_p t^p. \tag{8.2.1}$$

- Furthermore, we assume the dynamic equation is solved with a fixed time step, h. Thus, $x(t)$ is evaluated at $t = nh$ and we can write

$$x_n = x(nh).$$

- Since the dynamic equation is

$$\frac{dx(t)}{dt} = f(x, t).$$

  We have

$$f(x, t) = a_1 + 2a_2 t + 3a_3 t^2 + \cdots + pa_p t^{p-1}.$$

- $f(x, t)$ is also evaluated at $t = nh$, we can write

$$f_n = f(x(nh), nh).$$

2nd Order Approximation – Trapezoidal Rule

- Approximate $x(t)$ by
$$x(t) = a_0 + a_1 t + a_2 t^2.$$
- Then
$$\begin{aligned} f(x,t) &= a_1 + 2a_2 t \\ f_n &= f(x(nh), nh) = a_1 + 2a_2 nh \\ f_{n+1} &= a_1 + 2a_2(n+1)h \\ f_{n+1} - f_n &= 2a_2 h \end{aligned}$$
- And
$$\begin{aligned} x_n &= a_0 + a_1 nh + a_2 n^2 h^2 \\ x_{n+1} &= a_0 + a_1(n+1)h + a_2(n+1)^2 h^2 \\ &= a_0 + a_1(n+1)h + a_2(n^2+2n+1)h^2 \\ &= x_n + a_1 h + a_2(2n+1)h^2 \\ &= x_n + f_n h + a_2 h^2 \\ &= x_n + f_n h + h(f_{n+1} - f_n)/2 \\ &= x_n + h(f_{n+1} + f_n)/2 \end{aligned}$$
- This is the Trapezoidal rule

2nd Order Forward Integration

- Approximate $x(t)$ by
$$x(t) = a_0 + a_1 t + a_2 t^2.$$
- Then
$$\begin{aligned} f(x,t) &= a_1 + 2a_2 t \\ f_n &= f(x(nh), nh) = a_1 + 2a_2 nh \\ f_{n-1} &= a_1 + 2a_2(n-1)h \\ f_n - f_{n-1} &= 2a_2 h \end{aligned}$$
- And
$$\begin{aligned} x_n &= a_0 + a_1 nh + a_2 n^2 h^2 \\ x_{n+1} &= a_0 + a_1(n+1)h + a_2(n+1)^2 h^2 \\ &= a_0 + a_1(n+1)h + a_2(n^2+2n+1)h^2 \\ &= x_n + a_1 h + a_2(2n+1)h^2 \\ &= x_n + f_n h + a_2 h^2 \\ &= x_n + f_n h + h(f_n - f_{n-1})/2 \\ &= x_n + h(3f_n - f_{n-1})/2 \end{aligned}$$
- 2nd order forward integration formula

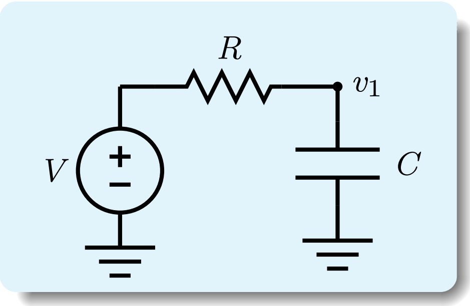
2nd Order Forward Integration, II

- Trapezoidal rule

$$x_{n+1} = x_n + h\frac{f_{n+1} + f_n}{2}$$

- 2nd order forward integration method

$$x_{n+1} = x_n + h\frac{3f_n - f_{n-1}}{2}$$



- Nodal equation:

$$\frac{dv_1}{dt} = \frac{V - v_1}{RC}$$

- Let $x = v_1$ and $f = \dfrac{V - v_1}{RC} = \dfrac{V - x}{RC}$

$$x_{n+1} = x_n + (3V_n - 3x_n - V_{n-1} + x_{n-1})\frac{h}{2RC}$$

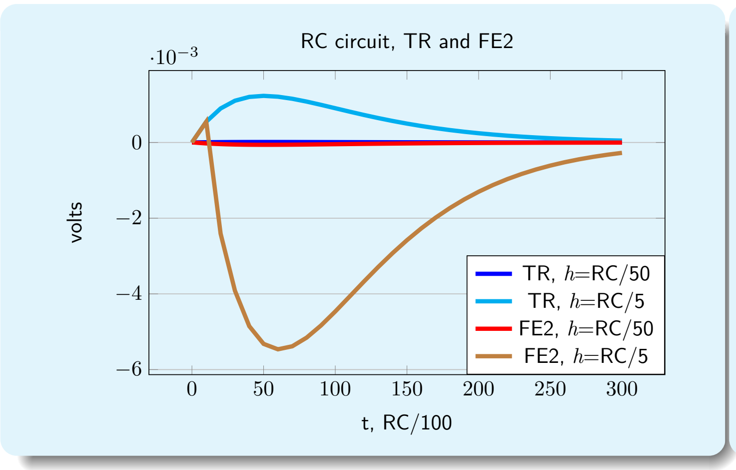
$$= \left(1 - \frac{3h}{2RC}\right)x_n + \frac{h}{2RC}x_{n-1} + (3V_n - V_{n-1})\frac{h}{2RC}$$

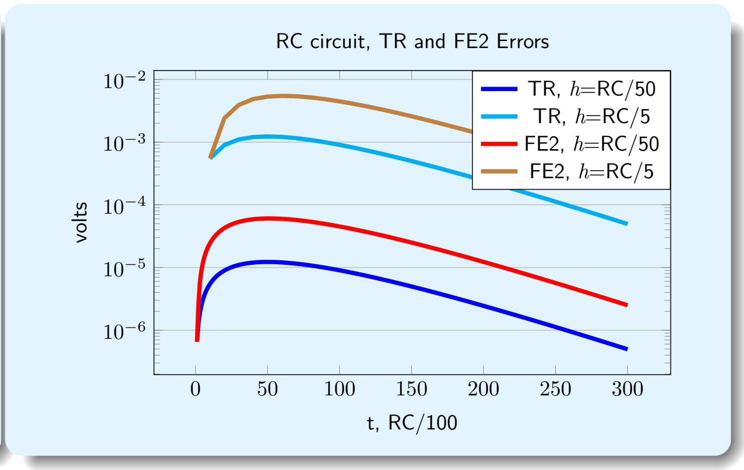
$$V(t) = 1, \quad t \geq 0,$$
$$v_1(0) = 0.$$

Analytical solution:

$$v_1(t) = 1 - \exp(\frac{-t}{RC})$$

2nd Order Forward Integration, III





- Both trapezoidal and 2nd order forward integration methods produce accurate results.
  - Especially for small h.
  - No error accumulation is observed.
- 2nd order forward integration has larger errors than trapezoidal method.

Local Truncation Error – Trapezoidal Rule

- In trapezoidal rule, we have the following approximations
$$x_n = a_0 + a_1 nh + a_2 n^2 h^2$$
$$f_n = a_1 + 2a_2 nh$$
- And the integration formula is
$$x_{n+1} = x_n + h \cdot \frac{f_{n+1} + f_n}{2}$$
- Error in $x(t)$ is dominated by t^3 term
$$x_n = a_0 + a_1 nh + a_2 n^2 h^2 + a_3 n^3 h^3$$
$$x_{n+1} = a_0 + a_1(n+1)h + a_2(n+1)^2 h^2 + a_3(n+1)^3 h^3 \quad (8.2.2)$$
$$= a_0 + a_1(n+1)h + a_2(n^2 + 2n + 1)h^2 + a_3(n^3 + 3n^2 + 3n + 1)h^3 \quad (8.2.3)$$
$$x_n + h \cdot \frac{f_{n+1} + f_n}{2} = a_0 + a_1 nh + a_2 n^2 h^2 + a_3 n^3 h^3$$
$$+ h \cdot \frac{a_1 + 2a_2(n+1)h + 3a_3(n+1)^2 h^2 + a_1 + 2a_2 nh + 3a_3 n^2 h^2}{2} \quad (8.2.4)$$
- Thus
$$x_n + h \cdot \frac{f_{n+1} + f_n}{2} - x_{n+1} = \frac{a_3 h^3}{2} \quad (8.2.5)$$
- Local truncation error for trapezoidal rule is $\dfrac{a_3 h^3}{2}$.

Local Truncation Error – Trapezoidal Rule, II

- For trapezoidal rule, we assume $x(t)$ is a second order polynomial of t.
- If that is the case, we get the exact solution.
- However, if $x(t)$ is a higher order polynomial then the local truncation error is
$$LTE = \frac{a_3 h^3}{2} \quad (8.2.6)$$
- Note that
$$x(t) = x_0 + x' t + \frac{x''}{2} t^2 + \frac{x'''}{3!} t^3 + \cdots + \frac{1}{p!} \cdot \frac{d^p x}{dt^p} t^p \quad (8.2.7)$$
- Thus, $a_3 = \dfrac{x'''}{6}$
- And, the local truncation error for trapezoidal rule is
$$LTE = \frac{h^3}{12} x'''. \quad (8.2.8)$$

Local Truncation Error – 2nd Order Forward Integration

- In 2nd order forward integration method, we approximate

$$x_n = a_0 + a_1 nh + a_2 n^2 h^2$$
$$f_n = a_1 + 2a_2 nh$$

- Integration formula: $x_{n+1} = x_n + h \cdot \frac{3f_n - f_{n-1}}{2}$.
- Error in $x(t)$ is dominated by the t^3 term

$$x_n = a_0 + a_1 nh + a_2 n^2 h^2 + a_3 n^3 h^3$$
$$x_{n+1} = a_0 + a_1(n+1)h + a_2(n^2+2n+1)h^2 + a_3(n^3+3n^2+3n+1)h^3 \quad (8.2.9)$$

$$x_n + h \cdot \frac{3f_n - f_{n-1}}{2} = a_0 + a_1 nh + a_2 n^2 h^2 + a_3 n^3 h^3$$
$$+ h \cdot \frac{3a_1 + 6a_2 nh + 9a_3 n^2 h^2 - a_1 - 2a_2(n-1)h - 3a_3(n-1)^2 h^2}{2}. \quad (8.2.10)$$

- Thus,

$$x_n + h \cdot \frac{f_{n+1} + f_n}{2} - x_{n+1} = -5h^3 \frac{a_3}{2}$$

- And

$$LTE = -5a_3 \frac{h^3}{2} = \frac{-5}{12} x''' h^3. \quad (8.2.11)$$

Local Truncation Error – Forward Euler

- In forward Euler method, we approximate

$$x_n = a_0 + a_1 nh$$
$$f_n = a_1$$

- Integration formula: $x_{n+1} = x_n + h \cdot f_n$.
- Error in $x(t)$ is dominated by the t^2 term

$$x_n = a_0 + a_1 nh + a_2 n^2 h^2$$
$$x_{n+1} = a_0 + a_1(n+1)h + a_2(n^2+2n+1)h^2 \quad (8.2.12)$$

$$x_n + h \cdot f_n = a_0 + a_1 nh + a_2 n^2 h^2 + h(a_1 + 2a_2 nh) \quad (8.2.13)$$

- Thus,

$$x_n + h \cdot f_n - x_{n+1} = -a_2 h^2.$$

- And

$$LTE = -a_2 h^2 = \frac{-1}{2} x'' h^2. \quad (8.2.14)$$

Local Truncation Error – Backward Euler

- In backward Euler method, we approximate

$$x_n = a_0 + a_1 nh$$
$$f_n = a_1$$

- Integration formula: $x_{n+1} = x_n + h \cdot f_{n+1}$.
- Error in $x(t)$ is dominated by the t^2 term

$$x_n = a_0 + a_1 nh + a_2 n^2 h^2$$
$$x_{n+1} = a_0 + a_1(n+1)h + a_2(n^2 + 2n + 1)h^2 \quad (8.2.15)$$

$$x_n + h \cdot f_{n+1} = a_0 + a_1 nh + a_2 n^2 h^2 + h\big(a_1 + 2a_2(n+1)h\big) \quad (8.2.16)$$

- Thus,

$$x_n + h \cdot f_{n+1} - x_{n+1} = a_2 h^2.$$

- And

$$LTE = a_2 h^2 = \frac{1}{2} x'' h^2. \quad (8.2.17)$$

Local Truncation Errors

- Local truncation errors for the integration methods discussed so far

Forward Euler:	$\frac{-1}{2} x'' h^2$
Backward Euler:	$\frac{1}{2} x'' h^2$
Trapezoidal rule:	$\frac{1}{12} x''' h^3$
2nd order forward integration:	$\frac{-5}{12} x''' h^3$

- Euler methods have the same LTE but with opposite signs.
- Trapezoidal method, indeed, has the smallest LTE, so far.
- As $h \to 0$, $LTE \to 0$, thus all these methods can be very accurate.
    - Trapezoidal rule may be more efficient.

3rd Order Integration – Forward Method

- 3rd order approximation: $x(t) = a_0 + a_1 t + a_2 t^2 + a_3 t^3$.

$$f_n = a_1 + 2a_2 nh + 3a_3 n^2 h^2$$
$$f_{n-1} = a_1 + 2a_2(n-1)h + 3a_3(n-1)^2 h^2$$
$$f_{n-2} = a_1 + 2a_2(n-2)h + 3a_3(n-2)^2 h^2$$

$$f_n - f_{n-1} = 2a_2 h + 3a_3(2n-1)h^2$$
$$f_{n-1} - f_{n-2} = 2a_2 h + 3a_3(2n-3)h^2$$
$$f_n - 2f_{n-1} + f_{n-2} = 6a_3 h^2$$

$$\begin{aligned} x_{n+1} &= a_0 + a_1(n+1)h + a_2(n+1)^2 h^2 + a_3(n+1)^3 h^3 \\ &= a_0 + a_1(n+1)h + a_2(n^2+2n+1)h^2 + a_3(n^3+3n^2+3n+1)h^3 \\ &= x_n + a_1 h + a_2(2n+1)h^2 + a_3(3n^2+3n+1)h^3 \\ &= x_n + hf_n + a_2 h^2 + a_3(3n+1)h^3 \\ &= x_n + hf_n + h(f_n - f_{n-1} + 3a_3 h^2)/2 + a_3 h^3 \\ &= x_n + hf_n + h(f_n - f_{n-1})/2 + 5a_3 h^3/2 \\ &= x_n + hf_n + h(f_n - f_{n-1})/2 + h(f_n - 2f_{n-1} + f_{n-2}) \cdot 5/12 \\ &= x_n + h(23f_n - 16f_{n-1} + 5f_{n-2})/12 \end{aligned}$$

3rd Order Integration – Backward Method

- 3rd order approximation: $x(t) = a_0 + a_1 t + a_2 t^2 + a_3 t^3$.

$$f_n = a_1 + 2a_2 nh + 3a_3 n^2 h^2$$
$$f_{n-1} = a_1 + 2a_2(n-1)h + 3a_3(n-1)^2 h^2$$
$$f_{n+1} = a_1 + 2a_2(n+1)h + 3a_3(n+1)^2 h^2$$

$$f_{n+1} - f_n = 2a_2 h + 3a_3(2n+1)h^2$$
$$f_n - f_{n-1} = 2a_2 h + 3a_3(2n-1)h^2$$
$$f_n - 2f_{n-1} + f_{n-2} = 6a_3 h^2$$

$$\begin{aligned} x_{n+1} &= a_0 + a_1(n+1)h + a_2(n+1)^2 h^2 + a_3(n+1)^3 h^3 \\ &= x_n + a_1 h + a_2(2n+1)h^2 + a_3(3n^2+3n+1)h^3 \\ &= x_n + hf_n + a_2 h^2 + a_3(3n+1)h^3 \\ &= x_n + hf_n + h(f_{n+1} - f_n - 3a_3 h^2)/2 + a_3 h^3 \\ &= x_n + hf_n + h(f_{n+1} - f_n)/2 - a_3 h^3/2 \\ &= x_n + hf_n + h(f_{n+1} - f_n)/2 - h(f_{n+1} - 2f_n + f_{n-1})/12 \\ &= x_n + h(5f_{n+1} + 8f_n - f_{n-1})/12 \end{aligned}$$

3rd Order Integration Methods

- Thus, the 3rd order integration methods with constant steps are
- 3rd order forward integration

$$x_{n+1} = x_n + h \cdot \frac{23f_n - 16f_{n-1} + 5f_{n-2}}{12} \tag{8.2.18}$$

  - To carry out the integration, the value of the derivatives of the previous three time points are needed.
  - Integration is straightforward since f_{n+1} is not required.
- 3rd order backward integration

$$x_{n+1} = x_n + h \cdot \frac{5f_{n+1} + 8f_n - f_{n-1}}{12} \tag{8.2.19}$$

  - To carry out the integration, the value of the derivatives of the previous two time points are needed.
  - f_{n+1}, which is a function of x_{n+1}, is needed and solved for.
  - If the system is nonlinear, Newton's method is usually required.
  - Stamps can be derived to form the linear system.

General Approach – Backward Integration

- To find the k'th order backward integration formula, assume

$$x_{n+1} = x_n + h(b_0 f_{n+1} + b_1 f_n + b_2 f_{n-1} + b_3 f_{n-2} \cdots + b_{k-1} f_{n-k+2})$$

- For convenience, let $n = 0$ and $h = 1$.

$$x_1 = x_0 + b_0 f_1 + b_1 f_0 + b_2 f_{-1} + b_3 f_{-2} \cdots + b_{k-1} f_{-k+2} \tag{8.2.20}$$

- If x is a polynomial of degree less than k, then the above equation is exact.
- If x is order 1, then

$$x = a_0 + a_1 t$$
$$f = x' = a_1$$

This equation holds for any value of t, then $\forall k, f_k = a_1$. And we have

$$\begin{aligned} x_0 &= a_0, \\ x_1 &= a_0 + a_1 \\ &= x_0 + b_0 f_1 + b_1 f_0 + b_2 f_{-1} + b_3 f_{-2} \cdots + b_{k-1} f_{-k+2} \\ &= a_0 + a_1(b_0 + b_1 + b_2 + b_3 \cdots + b_{k-1}) \end{aligned}$$

Or,

$$b_0 + b_1 + b_2 + \cdots + b_{k-1} = 1. \tag{8.2.21}$$

General Approach – Backward Integration, II

- If x is of order 2

$$
\begin{aligned}
x &= a_0 + a_1 t + a_2 t^2 \\
x_1 &= a_0 + a_1 + a_2 \\
x_0 &= a_0 \\
f &= a_1 + 2a_2 t
\end{aligned}
$$

- And we have

$$
\begin{aligned}
x_1 &= a_0 + a_1 + a_2 \\
&= x_0 + b_0 f_1 + b_1 f_0 + b_2 f_{-1} + b_3 f_{-2} \cdots + b_{k-1} f_{-k+2} \\
&= a_0 + b_0(a_1 + 2a_2) + b_1 a_1 + b_2(a_1 - 2a_2) + \cdots + b_{k-1}(a_1 - 2(k-2)a_2) \\
&= a_0 + a_1(b_0 + b_1 + b_2 + \cdots + b_{k-1}) + 2a_2(b_0 - b_2 - \cdots - (k-2)b_{k-1}) \\
&= a_0 + a_1 + 2a_2(b_0 - b_2 - \cdots - (k-2)b_{k-1})
\end{aligned}
$$

- Thus,

$$
b_0 - b_2 - 2b_3 - \cdots - (k-2)b_{k-1} = \frac{1}{2}. \tag{8.2.22}
$$

General Approach – Backward Integration, III

- If x is of order 3

$$
\begin{aligned}
x &= a_0 + a_1 t + a_2 t^2 + a_3 t^3 \\
x_1 &= a_0 + a_1 + a_2 + a_3 \\
x_0 &= a_0 \\
f &= a_1 + 2a_2 t + 3a_3 t^2
\end{aligned}
$$

- And we have

$$
\begin{aligned}
x_1 &= a_0 + a_1 + a_2 + a_3 \\
&= x_0 + b_0 f_1 + b_1 f_0 + b_2 f_{-1} + b_3 f_{-2} \cdots + b_{k-1} f_{-k+2} \\
&= a_0 + b_0(a_1 + 2a_2 + 3a_3) + b_1 a_1 + b_2(a_1 - 2a_2 + 3a_3) + \cdots \\
&\quad + b_{k-1}(a_1 - 2(k-2)a_2 + 3(k-2)^2 a_3) \\
&= a_0 + a_1(b_0 + b_1 + b_2 + \cdots + b_{k-1}) + 2a_2(b_0 - b_2 - \cdots - (k-2)2b_{k-1}) \\
&\quad + 3a_3(b_0 + b_2 + 4b_3 + \cdots + (k-2)^2 b_{k-1}) \\
&= a_0 + a_1 + a_2 + 3a_3(b_0 + b_2 + 4b_3 + \cdots + (k-2)^2 b_{k-1})
\end{aligned}
$$

- Thus,

$$
b_0 + b_2 + b_3 + \cdots + (k-2)^2 b_{k-1} = \frac{1}{3}. \tag{8.2.23}
$$

General Approach – Backward Integration, IV

- Combining all k constraints, we have

$$\begin{bmatrix} 1 & 1 & 1 & 1 & \cdots & 1 \\ 1 & 0 & -1 & -2 & \cdots & -(k-2) \\ 1 & 0 & 1 & 4 & \cdots & (k-2)^2 \\ 1 & 0 & -1 & -8 & \cdots & -(k-2)^3 \\ \vdots & \vdots & \vdots & \vdots & \cdots & \vdots \\ 1 & 0 & (-1)^{k-1} & (-2)^{k-1} & \cdots & (-k+2)^{k-1} \end{bmatrix} \begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_{k-1} \end{bmatrix} = \begin{bmatrix} 1 \\ 1/2 \\ 1/3 \\ 1/4 \\ \vdots \\ 1/k \end{bmatrix} \qquad (8.2.24)$$

- Coefficients $b_0, b_1, b_2, \cdots, b_{k-1}$, can be solved from the above equation and we have a general k'th order backward integration formula

$$x_1 = x_0 + h(b_0 f_1 + b_1 f_0 + b_2 f_{-1} + b_3 f_{-2} + \cdots + b_{k-1} f_{-k+2})$$

- Or

$$\begin{aligned} x(t+h) =& x(t) + h\big(b_0 f(t+h) + b_1 f(t) + b_2 f(t-h) + b_3 f(t-2h) \\ &+ \cdots + b_{k-1} f(t-(k-2)h)\big). \end{aligned}$$

General Approach – Backward Integration, V

- 2nd order backward integration formula

$$\begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} b_0 \\ b_1 \end{bmatrix} = \begin{bmatrix} 1 \\ 1/2 \end{bmatrix}$$

$$b_0 = 1/2, \qquad b_1 = 1/2.$$

- Thus, the 2nd order backward integration formula is

$$x(t+h) = x(t) + h\big(f(t+h) + f(t)\big)/2.$$

- 3rd order backward integration formula

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & 0 & -1 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} b_0 \\ b_1 \\ b_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1/2 \\ 1/3 \end{bmatrix}$$

$$b_0 = 5/12, \qquad b_1 = 8/12, \qquad b_2 = -1/12.$$

- Thus, the 3rd order backward integration formula is

$$x(t+h) = x(t) + h\big(5f(t+h) + 8f(t) - f(t-h)\big)/12.$$

- Higher order formulas can be found in the same way.

Multi-Step Backward Integration Formulas

- Adams-Moulton's formulas
- 4th order backward integration formula

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 0 & -1 & -2 \\ 1 & 0 & 1 & 4 \\ 1 & 0 & -1 & -8 \end{bmatrix} \begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 1/2 \\ 1/3 \\ 1/4 \end{bmatrix}$$

$$b_0 = 9/24, \qquad b_1 = 19/24, \qquad b_2 = -5/24, \qquad b_3 = 1/24.$$

- Thus, the 4th order backward integration formula is

$$x(t+h) = x(t) + h\big(9f(t+h) + 19f(t) - 5f(t-h) + f(t-2h)\big)/24.$$

Multi-Step Backward Integration Formulas, II

- 5th order backward integration formula

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & -1 & -2 & -3 \\ 1 & 0 & 1 & 4 & 9 \\ 1 & 0 & -1 & -8 & -27 \\ 1 & 0 & 1 & 16 & 81 \end{bmatrix} \begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix} = \begin{bmatrix} 1 \\ 1/2 \\ 1/3 \\ 1/4 \\ 1/5 \end{bmatrix}$$

$$b_0 = 251/720, b_1 = 646/720, b_2 = -264/720, b_3 = 106/720, b_4 = -19/720.$$

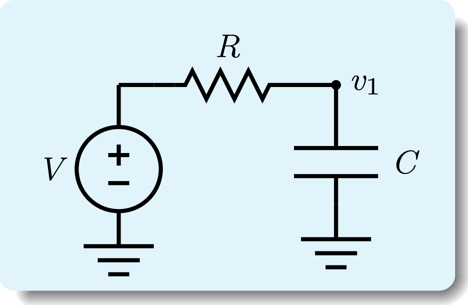
- Thus, the 5th order backward integration formula is

$$\begin{aligned} x(t+h) =& x(t) + h\big(251f(t+h) + 646f(t) - 264f(t-h) + 106f(t-2h) \\ & - 19f(t-3h)\big)/720. \end{aligned}$$

Multi-Step Backward Integration Formulas, III

- For the simple RC circuit, we have

$$\frac{dx}{dt} = \frac{V - x}{RC}.$$



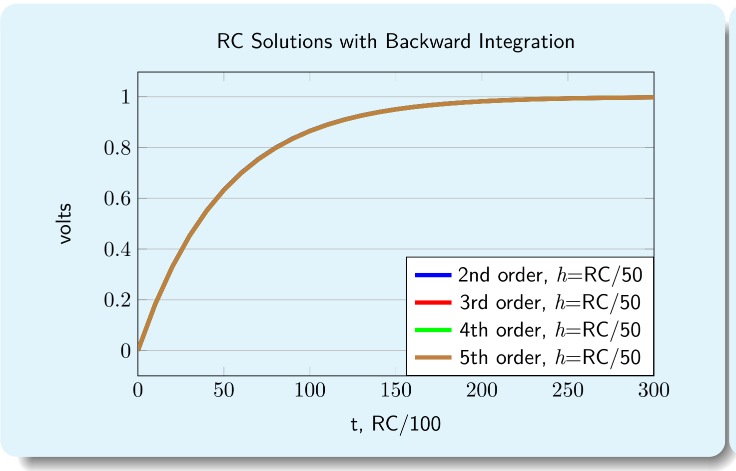
- Using fixed step backward integration method

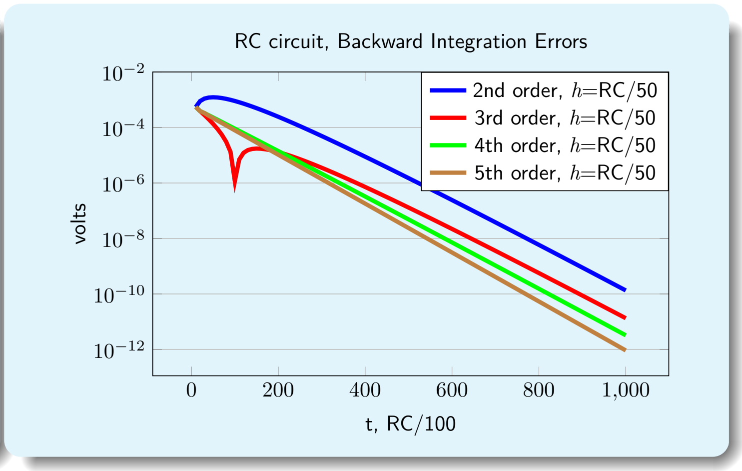
$$\begin{aligned} x(t+h) =& x(t) + \frac{h}{RC}\Big(b_0(V - x(t+h)) + b_1(V - x(t)) \\ &+ \cdots + b_{k-1}(V - x(t-(k-2)h)\Big) \\ =& x(t) + \frac{hV}{RC} - \frac{h}{RC}\Big(b_0 x(t+h) + b_1 x(t) \\ &+ \cdots + b_{k-1} x(t-(k-2)h)\Big) \end{aligned}$$

- Or

$$\begin{aligned} x(t+h) =& (1 + \frac{hb_0}{RC})^{-1}\Big(\frac{hV}{RC} + x(t)(1 - \frac{hb_1}{RC}) \\ &- \frac{h}{RC}\Big(b_2 x(t-h) + \cdots + b_{k-1} x(t-(k-2)h)\Big)\Big). \end{aligned}$$

Multi-Step Backward Integration Formulas, IV





- Higher order integration methods can deliver higher accuracy.
- A k'th order integration method needs $k-1$ previous time points.
  - For example, 3rd order integration method needs two past time points
    - The first two time steps cannot be used
  - It is common to use lower order methods for the first few time points, and then switch to higher order ones.

LTE for Backward Integration Methods

- k'th order backward integration formula

$$x_{n+1} = x_n + h\big(b_0 f_{n+1} + b_1 f_n + b_2 f_{n-1} + b_3 f_{n-2} + \cdots + b_{k-1} f_{n-k+2}\big).$$

  where x is assumed to be a k'th order polynomial.
- In that case, the integration formula is exact, i.e., no errors. Otherwise, local truncation error is dominated by t^{k+1} term.

$$\begin{aligned} x(t) &= a_0 + a_1 t + a_2 t^2 + \cdots + a_k t^k + a_{k+1} t^{k+1} \\ x(t+h) &= a_0 + a_1(t+h) + a_2(t+h)^2 + \cdots + a_k(t+h)^k + a_{k+1}(t+h)^{k+1} \\ f(t) &= a_1 + 2a_2 t + 3a_3 t^2 + \cdots + k a_k t^{k-1} + (k+1)a_{k+1} t^k. \end{aligned}$$

- Let $t = 0$ and $h = 1$

$$\begin{aligned} x_1 &= a_0 + a_1 + a_2 + \cdots + a_k + a_{k+1} \\ f_j &= a_1 + 2a_2 j + 3a_3 j^2 + \cdots + k a_k j^{k-1} + (k+1)a_{k+1} j^k \\ x_1 &= x_0 + h(b_0 f_1 + b_1 f_0 + b_2 f_{-1} + \cdots + b_{k-1} f_{-k+2}) \end{aligned}$$

LTE for Backward Integration Methods, II

- In deriving the backward integration formulas, we have matched the coefficients up to the k'th term.
- Thus, we need to consider a_{k+1} term only.
- Coefficients for a_{k+1} term in $x_0 + h(b_0 f_1 + \cdots + b_{k-1} f_{-k+2}) - x_1$ is

$$\begin{aligned} RHS: &\quad 1 \\ LHS: &\quad b_0(k+1) + b_1 \cdot 0 + b_2(k+1)(-1)^k + b_3(k+1)(-2)^k + \cdots \\ &\quad + b_{k-1}(k+1)(-k+2)^k \end{aligned}$$

- Thus,

$$LTE = \Big((k+1)\Big(b_0 + b_2(-1)^k + b_3(-2)^k + \cdots + b_{k-1}(-k+2)^k\Big) - 1\Big) a_{k+1} h^{k+1}.$$

LTE for Backward Integration Methods, III

$$LTE = \Big((k+1)\Big(b_0 + b_2(-1)^k + b_3(-2)^k + \cdots + b_{k-1}(-k+2)^k\Big) - 1\Big) a_{k+1} h^{k+1}.$$

- 2nd order integration

$$b_0 = 1/2, \quad b_1 = 1/2,$$
$$LTE = (3\frac{1}{2} - 1) a_3 h^3 = \frac{1}{2} a_3 h^3.$$

- 3rd order integration

$$b_0 = 5/12, \quad b_1 = 8/12, \quad b_2 = -1/12$$
$$LTE = \Big(4\Big(\frac{5}{12} - \frac{(-1)^3}{12}\Big) - 1\Big) a_4 h^4 = a_4 h^4.$$

- 4th order integration

$$b_0 = 9/24, \quad b_1 = 19/24, \quad b_2 = -5/24, \quad b_3 = 1/24,$$
$$LET = \Big(5\Big(\frac{9}{24} - (-1)^4 \frac{5}{24} + (-2)^4 \frac{1}{24}\Big) - 1\Big) a_5 h^5 = \frac{19}{6} \times a_5 h^5.$$

- Note: $a_{k+1} = \dfrac{1}{(k+1)\,!} \dfrac{d^{k+1}x}{dt^{k+1}}$.

General Approach – Forward Integration

- To find the k'th order forward integration formula, assume

$$x_{n+1} = x_n + h(b_1 f_n + b_2 f_{n-1} + b_3 f_{n-2} \cdots + b_k f_{n-k+1})$$

- For convenience, let $n = 0$ and $h = 1$.

$$x_1 = x_0 + b_1 f_0 + b_2 f_{-1} + b_3 f_{-2} \cdots + b_k f_{-k+1} \tag{8.2.25}$$

- If x is a polynomial of degree less than k, then the above equation is exact.
- If x is order 1, then

$$x = a_0 + a_1 t$$
$$f = x' = a_1$$

This equation holds for any value of t, then $\forall k, f_k = a_1$. And we have

$$\begin{aligned} x_0 &= a_0, \\ x_1 &= a_0 + a_1 \\ &= x_0 + b_1 f_0 + b_2 f_{-1} + b_3 f_{-2} \cdots + b_k f_{-k+1} \\ &= a_0 + a_1(b_1 + b_2 + b_3 \cdots + b_k) \end{aligned}$$

Or,

$$b_1 + b_2 + \cdots + b_k = 1. \tag{8.2.26}$$

General Approach – Forward Integration, II

- If x is of order 2

$$
\begin{aligned}
x &= a_0 + a_1 t + a_2 t^2 \\
x_1 &= a_0 + a_1 + a_2 \\
x_0 &= a_0 \\
f &= a_1 + 2a_2 t
\end{aligned}
$$

- And we have

$$
\begin{aligned}
x_1 &= a_0 + a_1 + a_2 \\
&= x_0 + b_1 f_0 + b_2 f_{-1} + b_3 f_{-2} \cdots + b_k f_{-k+1} \\
&= a_0 + b_1 a_1 + b_2(a_1 - 2a_2) + b_3(a_1 - 4a_2) + \cdots + b_k(a_1 - 2(k-1)a_2) \\
&= a_0 + a_1(b_1 + b_2 + \cdots + b_k) + 2a_2(-b_2 - 2b_3 - \cdots - (k-1)b_k) \\
&= a_0 + a_1 + 2a_2(-b_2 - 2b_3 - \cdots - (k-1)b_k)
\end{aligned}
$$

- Thus,

$$
-b_2 - 2b_3 - \cdots - (k-1)b_k = \frac{1}{2}. \tag{8.2.27}
$$

General Approach – Forward Integration, III

- If x is of order 3

$$
\begin{aligned}
x &= a_0 + a_1 t + a_2 t^2 + a_3 t^3 \\
x_1 &= a_0 + a_1 + a_2 + a_3 \\
x_0 &= a_0 \\
f &= a_1 + 2a_2 t + 3a_3 t^2
\end{aligned}
$$

- And we have

$$
\begin{aligned}
x_1 =& a_0 + a_1 + a_2 + a_3 \\
=& x_0 + b_1 f_0 + b_2 f_{-1} + b_3 f_{-2} \cdots + b_k f_{-k+1} \\
=& a_0 + b_1 a_1 + b_2(a_1 - 2a_2 + 3a_3) + b_3(a_1 - 2 \cdot 2a_2 + 3 \cdot 4a_3) + \cdots \\
& + b_k(a_1 - 2(k-1)a_2 + 3(k-1)^2 a_3) \\
=& a_0 + a_1(b_1 + b_2 + b_3 + \cdots + b_k) + 2a_2(-b_2 - 2b_3 - \cdots - (k-1)b_k) \\
& + 3a_3(b_2 + 4b_3 + \cdots + (k-1)^2 b_k) \\
=& a_0 + a_1 + a_2 + 3a_3(b_2 + 4b_3 + \cdots + (k-1)^2 b_k)
\end{aligned}
$$

- Thus,

$$
b_2 + 4b_3 + \cdots + (k-1)^2 b_k = \frac{1}{3}. \tag{8.2.28}
$$

General Approach – Forward Integration, IV

- Combining all k constraints, we have

$$\begin{bmatrix} 1 & 1 & 1 & 1 & \cdots & 1 \\ 0 & -1 & -2 & -3 & \cdots & -(k-1) \\ 0 & 1 & 4 & 9 & \cdots & (k-1)^2 \\ 0 & -1 & -8 & -27 & \cdots & -(k-1)^3 \\ \vdots & \vdots & \vdots & \vdots & \cdots & \vdots \\ 0 & (-1)^{k-1} & (-2)^{k-1} & (-3)^{k-1} & \cdots & (-k+1)^{k-1} \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ \vdots \\ b_k \end{bmatrix} = \begin{bmatrix} 1 \\ 1/2 \\ 1/3 \\ 1/4 \\ \vdots \\ 1/k \end{bmatrix} \tag{8.2.29}$$

- Coefficients $b_1, b_2, b_3, \cdots, b_k$, can be solved from the above equation and we have a general k'th order forward integration formula

$$x_1 = x_0 + h(b_1 f_0 + b_2 f_{-1} + b_3 f_{-2} + \cdots + b_k f_{-k+1})$$

- Or

$$\begin{aligned} x(t+h) =& x(t) + h\big(b_1 f(t) + b_2 f(t-h) + b_3 f(t-2h) \\ &+ \cdots + b_k f(t-(k-1)h)\big). \end{aligned}$$

General Approach – Forward Integration, V

- 2nd order forward integration formula

$$\begin{bmatrix} 1 & 1 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1/2 \end{bmatrix}$$

$$b_1 = 3/2, \qquad b_2 = -1/2.$$

- Thus, the 2nd order forward integration formula is

$$x(t+h) = x(t) + h\big(3f(t) - f(t-h)\big)/2.$$

- 3rd order forward integration formula

$$\begin{bmatrix} 1 & 1 & 1 \\ 0 & -1 & -2 \\ 0 & 1 & 4 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 1/2 \\ 1/3 \end{bmatrix}$$

$$b_1 = 23/12, \qquad b_2 = -16/12, \qquad b_3 = 5/12.$$

- Thus, the 3rd order forward integration formula is

$$x(t+h) = x(t) + h\big(23f(t) - 16f(t-h) + 5f(t-2h)\big)/12.$$

Multi-Step Forward Integration Formulas

- Adams-Bashforth's formulas
- 4th order forward integration formula

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & -1 & -2 & -3 \\ 0 & 1 & 4 & 9 \\ 0 & -1 & -8 & -27 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix} = \begin{bmatrix} 1 \\ 1/2 \\ 1/3 \\ 1/4 \end{bmatrix}$$

$$b_1 = 55/24, \qquad b_2 = -59/24, \qquad b_3 = 37/24, \qquad b_4 = -9/24.$$

- Thus, the 4th order forward integration formula is

$$x(t+h) = x(t) + h\big(55f(t) - 59f(t-h) + 37f(t-2h) - 9f(t-3h)\big)/24.$$

Multi-Step Forward Integration Formulas, II

- 5th order forward integration formula

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 0 & -1 & -2 & -3 & -4 \\ 0 & 1 & 4 & 9 & 16 \\ 0 & -1 & -8 & -27 & -64 \\ 0 & 1 & 16 & 81 & 256 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \end{bmatrix} = \begin{bmatrix} 1 \\ 1/2 \\ 1/3 \\ 1/4 \\ 1/5 \end{bmatrix}$$

$$b_1 = 1901/720, b_2 = -2774/720, b_3 = 2616/720, b_4 = -1274/720, b_5 = 251/720.$$

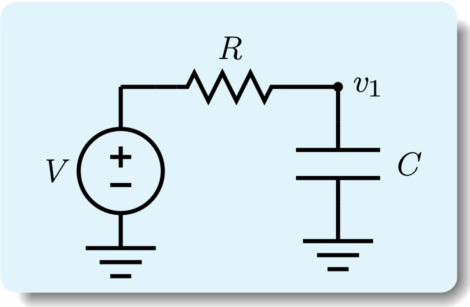
- Thus, the 5th order forward integration formula is

$$\begin{aligned} x(t+h) =& x(t) + h\big(1901f(t) - 2774f(t-h) + 2616(t-2h) - 1274(t-3h) \\ &+ 251(t-4h)\big)/720. \end{aligned}$$

Multi-Step Forward Integration Formulas, III

- For the simple RC circuit, we have

$$\frac{dx}{dt} = \frac{V - x}{RC}.$$



- Using fixed step forward integration method

$$\begin{aligned} x(t+h) =& x(t) + \frac{h}{RC}\Big(b_1(V - x(t)) + b_2(V - x(t-h)) \\ & + \cdots + b_k(V - x(t-(k-1)h)\Big) \\ =& x(t) + \frac{hV}{RC} - \frac{h}{RC}\Big(b_1 x(t) + b_2 x(t-h) \\ & + \cdots + b_k x(t-(k-1)h))\Big) \end{aligned}$$

- Or

$$x(t+h) = \frac{hV}{RC} + x(t)(1 - \frac{hb_1}{RC}) - \frac{h}{RC}\Big(b_2 x(t-h) + \cdots + b_k x(t-(k-1)h)\Big).$$

LTE for Forward Integration Methods

- k'th order forward integration formula

$$x_{n+1} = x_n + h\big(b_1 f_n + b_2 f_{n-1} + b_3 f_{n-2} + \cdots + b_k f_{n-k+1}\big).$$

where x is assumed to be a k'th order polynomial.

- In that case, the integration formula is exact, i.e., no errors. Otherwise, local truncation error is dominated by t^{k+1} term.

$$\begin{aligned} x(t) &= a_0 + a_1 t + a_2 t^2 + \cdots + a_k t^k + a_{k+1} t^{k+1} \\ x(t+h) &= a_0 + a_1(t+h) + a_2(t+h)^2 + \cdots + a_k(t+h)^k + a_{k+1}(t+h)^{k+1} \\ f(t) &= a_1 + 2a_2 t + 3a_3 t^2 + \cdots + k a_k t^{k-1} + (k+1)a_{k+1} t^k. \end{aligned}$$

- Let $t = 0$ and $h = 1$

$$\begin{aligned} x_1 &= a_0 + a_1 + a_2 + \cdots + a_k + a_{k+1} \\ f_j &= a_1 + 2a_2 j + 3a_3 j^2 + \cdots + k a_k j^{k-1} + (k+1)a_{k+1} j^k \\ x_1 &= x_0 + h(b_1 f_0 + b_2 f_{-1} + b_3 f_{-2} + \cdots + b_k f_{-k+1}) \end{aligned}$$

LTE for Forward Integration Methods, II

- In deriving the forward integration formulas, we have matched the coefficients up to the k'th term.
- Thus, we need to consider a_{k+1} term only.
- Coefficients for a_{k+1} term

$$
\begin{aligned}
LHS :& \quad 1 \\
RHS :& b_1 \cdot 0 + b_2(k+1)(-1)^k + b_3(k+1)(-2)^k + \cdots \\
& \quad + b_k(k+1)(-k+1)^k
\end{aligned}
$$

- Thus,

$$LTE = \left((k+1)\left(b_2(-1)^k + b_3(-2)^k + \cdots + b_k(-k+1)^k\right) - 1\right) a_{k+1} h^{k+1}.$$

LTE for Forward Integration Methods, III

$$LTE = \left((k+1)\left(b_2(-1)^k + b_3(-2)^k + \cdots + b_k(-k+1)^k\right) - 1\right) a_{k+1} h^{k+1}.$$

- 2nd order integration

$$
\begin{aligned}
& b_1 = 3/2, \quad b_2 = -1/2, \\
& LTE = (3\frac{-1}{2} - 1) a_3 h^3 = \frac{-5}{2} a_3 h^3.
\end{aligned}
$$

- 3rd order integration

$$
\begin{aligned}
& b_1 = 23/12, \quad b_2 = -16/12, \quad b_3 = 5/12 \\
& LTE = \left(4\left(\frac{-16}{12} - \frac{5 \times (-2)^3}{12}\right) - 1\right) a_4 h^4 = -9 a_4 h^4.
\end{aligned}
$$

- 4th order integration

$$
\begin{aligned}
& b_1 = 55/24, \quad b_2 = -59/24, \quad b_3 = 37/24, \quad b_4 = -9/24, \\
& LET = \left(5\left(\frac{-59}{24} \times (-1)^4 + \frac{37}{24} \times (-2)^4 - \frac{9}{24} \times (-3)^4\right) - 1\right) a_5 h^5 = \frac{-251}{6} \times a_5 h^5.
\end{aligned}
$$

- Note: $a_{k+1} = \dfrac{1}{(k+1)\,!} \dfrac{d^{k+1} x}{dt^{k+1}}$.

LTE comparisons

- LTE for backward and forward integration formulas

Order	Backward integration	Forward integration
2nd order	$\frac{1}{2}a_3h^3$	$\frac{-5}{2}a_3h^3$
3rd order	a_4h^4	$-9a_4h^4$
4th order	$\frac{19}{6}a_5h^5$	$\frac{-251}{6}a_5h^5$

- Note: $a_k = \frac{1}{k!}\frac{d^kx}{dt^k}$.
- Backward integration methods are usually more accurate.
  - The order of error is the same but the coefficients are very different.
- But forward integration maybe easier to solve for.

Summary

- Polynomial approximation and dynamic equation solutions
- 3rd order backward integration formula
- 3rd order forward integration formula
- General approach in deriving integration formulas and their local truncation errors
  - Backward and forward integration methods
  - Higher order integration methods tends to have smaller local truncation errors.