§5.5 Adaptive Error Control

$$\frac{dy}{dt} = f(t, y(t)), \quad a \le t \le b, \quad y(a) = \alpha.$$

- Given tolerance ϵ
- Given variable-step method $\phi(t, w, h)$:

$w_0 = \alpha.$
for $j = 0, 1, \cdots$,
  choose step-size $h_j = t_{j+1} - t_j$,
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- only consider **local truncation error** (LTE)

$$\tau_{j+1}(h) = \frac{y(t_{j+1}) - y(t_j)}{h} - \phi\left(t_j, y(t_j), h\right) = O\left(h^n\right)$$

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Approach: Estimate $\tau_{j+1}(h)$ with **order**-$(n+1)$ method

$$\widetilde{w}_{j+1} = \widetilde{w}_j + h\,\widetilde{\phi}\left(t_j, \widetilde{w}_j, h\right), \quad \text{for} \quad j \ge 0.$$

LTE Estimation (I)

- Assume (only for estimating **LTE**)

$$w_j \approx y(t_j), \quad \widetilde{w}_j \approx y(t_j) \quad (1)$$

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$$\begin{aligned}
\tau_{j+1}(h) &\overset{def}{=} \frac{y(t_{j+1}) - y(t_j)}{h} - \phi\left(t_j, y(t_j), h\right) \\
&\overset{w_j \approx y(t_j)}{\approx} \frac{y(t_{j+1}) - \left(w_j + h\,\phi\left(t_j, w_j, h\right)\right)}{h} \\
&= \frac{y(t_{j+1}) - w_{j+1}}{h} = O\left(h^n\right).
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\widetilde{\tau}_{j+1}(h) &\stackrel{def}{=} \frac{y(t_{j+1}) - y(t_j)}{h} - \widetilde{\phi}\left(t_j, y(t_j), h\right) \\
&\stackrel{\widetilde{w}_j \approx y(t_j)}{\approx} \frac{y(t_{j+1}) - \left(\widetilde{w}_j + h\,\widetilde{\phi}\left(t_j, \widetilde{w}_j, h\right)\right)}{h} \\
&= \frac{y(t_{j+1}) - \widetilde{w}_{j+1}}{h} = O\left(h^{n+1}\right).
\end{aligned}$$

- therefore, with assumption (1)

$$\begin{aligned}
w_{j+1} &\approx y(t_j) + h\,\phi\left(t_j, y(t_j), h\right) \\
\tau_{j+1}(h) &\approx \frac{y(t_{j+1}) - w_{j+1}}{h} \\
&= \frac{y(t_{j+1}) - \widetilde{w}_{j+1}}{h} + \frac{\widetilde{w}_{j+1} - w_{j+1}}{h} \\
&= O\left(h^{n+1}\right) + \frac{\widetilde{w}_{j+1} - w_{j+1}}{h} = O\left(h^n\right)
\end{aligned}$$

$$\boxed{\text{LTE estimate: } \tau_{j+1}(h) \approx \frac{\widetilde{w}_{j+1} - w_{j+1}}{h}}$$

step-size selection

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$$K\, h^n \approx \frac{\widetilde{w}_{j+1} - w_{j+1}}{h} \qquad (1)$$

- **Choose** new step-size $q\, h$ so LTE satisfies given tolerance ϵ:
$$\left|\tau_{j+1}(q\, h)\right| \leq \epsilon$$

- Equation (1) implies

$$\left|q^n\, \frac{\widetilde{w}_{j+1} - w_{j+1}}{h}\right| \approx \left|K\, (q\, h)^n\right| \approx \left|\tau_{j+1}(q\, h)\right| \lesssim \epsilon$$

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- compute a <u>conservative</u> value for q:

$$q = \left|\frac{\epsilon\, h}{2\left(\widetilde{w}_{j+1} - w_{j+1}\right)}\right|^{\frac{1}{n}}.$$

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- if $q < 1$, give up current w_{j+1}; otherwise keep it and set $j = j + 1$.
- make restricted step-size change:

  $$h = \begin{cases} 0.1\, h, & \text{if } q \leq 0.1, \\ 4\, h, & \text{if } q \geq 4, \\ q\, h, & \text{if } 0.1 < q < 4. \end{cases}$$

step-size selection

$$\boxed{\text{LTE estimate: } \tau_{j+1}(h) \approx \frac{\widetilde{w}_{j+1} - w_{j+1}}{h}}$$

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- step-size can't be too big: $h = \mathbf{min}\left(h, h_{\mathbf{max}}\right)$

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LTE estimate: $\tau_{j+1}(h) \approx \dfrac{\widetilde{w}_{j+1} - w_{j+1}}{h}$

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- step-size can't be too small:

$$\textbf{if} \quad h < h_{\min} \quad \textbf{then} \quad \textit{declare failure}.$$

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Runge-Kutta-Fehlberg: 4th order method, 5th order estimate

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\begin{aligned}
w_{j+1} &= w_j + \frac{25}{216}k_1 + \frac{1408}{2565}k_3 + \frac{2197}{4104}k_4 - \frac{1}{5}k_5, \\
\widetilde{w}_{j+1} &= w_j + \frac{16}{135}k_1 + \frac{6656}{12825}k_3 + \frac{28561}{56430}k_4 - \frac{9}{50}k_5 + \frac{2}{55}k_6, \quad \text{where}
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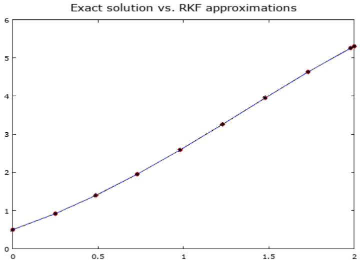
k_1 &= h\,f\left(t_j, w_j\right), \\
k_2 &= h\,f\left(t_j + \frac{h}{4}, w_j + \frac{1}{4}\,k_1\right), \\
k_3 &= h\,f\left(t_j + \frac{3h}{8}, w_j + \frac{3}{32}\,k_1 + \frac{9}{32}\,k_2\right), \\
k_4 &= h\,f\left(t_j + \frac{12h}{13}, w_j + \frac{1932}{2197}\,k_1 - \frac{7200}{2197}\,k_2 + \frac{7296}{2197}\,k_3\right), \\
k_5 &= h\,f\left(t_j + h, w_j + \frac{439}{216}\,k_1 - 8\,k_2 + \frac{3680}{513}\,k_3 - \frac{845}{4104}\,k_4\right), \\
k_6 &= h\,f\left(t_j + \frac{h}{2}, w_j - \frac{8}{27}\,k_1 + 2\,k_2 - \frac{3544}{2565}\,k_3 + \frac{1859}{4104}\,k_4 - \frac{11}{40}\,k_5\right).
\end{aligned}$$

Runge-Kutta-Fehlberg: solution plots

Initial Value ODE $$\frac{dy}{dt} = y - t^2 + 1, \quad 0 \le t \le 2, \quad y(0) = 0.5.$$



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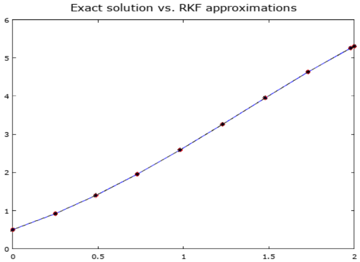

$\boxed{\text{5th order method indeed more accurate at beginning}}$

Runge-Kutta-Fehlberg: truncation errors

Initial Value ODE $\quad \dfrac{dy}{dt} = y - t^2 + 1, \quad 0 \le t \le 2, \quad y(0) = 0.5.$

$$\textbf{actual} \stackrel{def}{=} \left|\frac{y(t_j) - w_j}{h_j}\right|, \quad \textbf{estimate} \stackrel{def}{=} \left|\frac{\widetilde{w}_j - w_j}{h_j}\right|.$$

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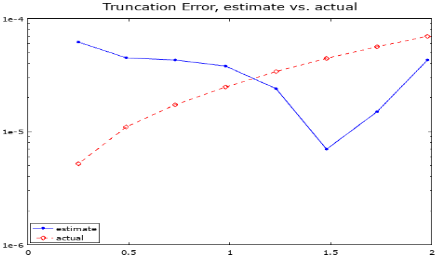

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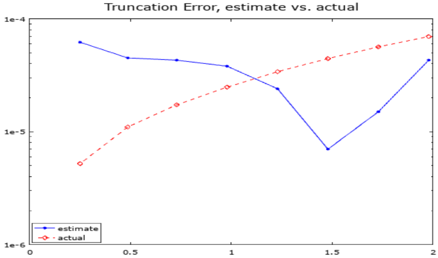
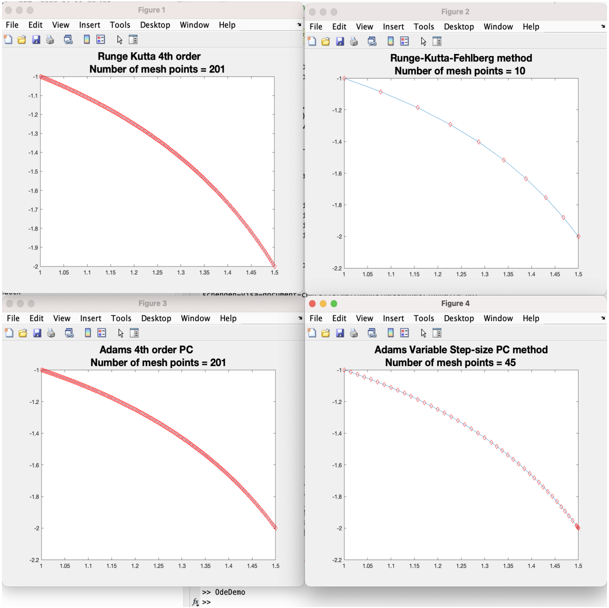


No indication 5th order method $\widetilde{w}_j$ stays more accurate over time

OdeDemo in matlab



§5.6 Multistep Methods

$$\frac{dy}{dt} = f(t, y), \quad a \le t \le b, \quad y(a) = \alpha.$$

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  $$t_j = a + j\,h, \quad \text{for} \quad j = 0, 1, 2, \cdots N, \quad \text{where } h = (b - a)/N.$$

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$$y(t_{j+1}) - y(t_j) = \int_{t_j}^{t_{j+1}} \left(\frac{dy}{dt}\right)\,dt = \int_{t_j}^{t_{j+1}} f(t, y(t))\,dt.$$

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- Approximate the integral with quadratures on function values
  - $f(t_{j+1}, y(t_{j+1}))$,
  - $f(t_j, y(t_j))$,
  - $f(t_{j-1}, y(t_{j-1}))$,
  - $\vdots$

Examples: Constant approximations

$f(t, y(t)) \approx \boxed{f(t_j, y(t_j)),}$ so

$$y(t_{j+1}) - y(t_j) = \int_{t_j}^{t_{j+1}} f(t, y(t))\, dt \approx h\, f(t_j, y(t_j)),$$

leading to Euler's method (*explicit*)

$$w_{j+1} = w_j + h\, f(t_j, w_j), \quad \text{for} \quad j = 0, 1, \cdots$$

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$$y(t_{j+1}) - y(t_j) = \int_{t_j}^{t_{j+1}} f(t, y(t))\, dt \approx h\, f(t_{j+1}, y(t_{j+1})),$$

leading to *backward* Euler's method (*implicit*)

$$w_{j+1} = w_j + h\, f(t_{j+1}, w_{j+1}), \quad \text{for} \quad j = 0, 1, \cdots$$

Both first order methods, but being *implicit* means much more work

Examples: Linear approximations

with points $f(t_j, y(t_j))$ and $\boxed{f(t_{j-1}, y(t_{j-1}))}$

$$f(t, y(t)) \approx \frac{(t - t_{j-1})f(t_j, y(t_j)) + (t_j - t)f(t_{j-1}, y(t_{j-1}))}{h}$$

$$\begin{aligned} \Longrightarrow \quad y(t_{j+1}) - y(t_j) &= \int_{t_j}^{t_{j+1}} f(t, y(t))\, dt \\ &\approx \frac{h}{2}\left(3f(t_j, y(t_j)) - f(t_{j-1}, y(t_{j-1}))\right) \end{aligned}$$

leading to Adams-Bashforth <u>two-step explicit</u> method

$$w_{j+1} = w_j + \frac{h}{2}\left(3f(t_j, w_j) - f(t_{j-1}, w_{j-1})\right)$$

for $\quad j = 1, 2, \cdots$

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$$f(t, y(t)) \approx \frac{(t - t_j) f(t_{j+1}, y(t_{j+1})) + (t_{j+1} - t) f(t_j, y(t_j))}{h}$$

$$\Longrightarrow \quad y(t_{j+1}) - y(t_j) = \int_{t_j}^{t_{j+1}} f(t, y(t))\, dt$$

$$\approx \frac{h}{2}\left(f(t_j, y(t_j)) + f(t_{j+1}, y(t_{j+1}))\right)$$

leading to mid-point method (<u>one-step *implicit*</u>)

$$w_{j+1} = w_j + \frac{h}{2}\left(f(t_j, w_j) + f(t_{j+1}, w_{j+1})\right)$$

for $\quad j = 1, 2, \cdots$

Examples: Linear approximations

with points $f(t_j, y(t_j))$ and $\boxed{f(t_{j-1}, y(t_{j-1}))}$

$$f(t, y(t)) \approx \frac{(t - t_{j-1}) f(t_j, y(t_j)) + (t_j - t) f(t_{j-1}, y(t_{j-1}))}{h}$$

$$\Longrightarrow \quad y(t_{j+1}) - y(t_j) = \int_{t_j}^{t_{j+1}} f(t, y(t))\, dt$$

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leading to mid-point method (<u>one-step *implicit*</u>)

$$w_{j+1} = w_j + \frac{h}{2} \left(f(t_j, w_j) + f(t_{j+1}, w_{j+1})\right)$$

for $\quad j = 1, 2, \cdots$

Both 2nd order methods, but being *implicit* means much more work

m-th order Methods

explicit m-step

$P(t)$ interpolates $f(t, y(t))$ at $f(t_j, y(t_j))$, $f(t_{j-1}, y(t_{j-1}))$, $\cdots$, $\boxed{f(t_{j-m+1}, y(t_{j-m+1}))}$

$$y(t_{j+1}) - y(t_j) = \int_{t_j}^{t_{j+1}} f(t, y(t))\, dt \approx \int_{t_j}^{t_{j+1}} P(t)\, dt$$

$$\stackrel{def}{=} h\left(b_{m-1} f(t_j, y(t_j)) + b_{m-2} f(t_{j-1}, y(t_{j-1})) + \cdots + b_0 f(t_{j-m+1}, y(t_{j-m+1}))\right)$$

leading to *explicit* m-point method, $j =$ m-1,m,m+1, $\cdots$

$$w_{j+1} = w_j + h\left(b_{m-1} f(t_j, w_j) + b_{m-2} f(t_{j-1}, w_{j-1}) + \cdots + b_0 f(t_{j-m+1}, w_{j-m+1})\right)$$

implicit (m-1)-step

$P(t)$ interpolates $f(t, y(t))$ at $\boxed{f(t_{j+1}, y(t_{j+1}))}$, $f(t_j, y(t_j))$, $\cdots$, $f(t_{j-m+2}, y(t_{j-m+2}))$

$$y(t_{j+1}) - y(t_j) = \int_{t_j}^{t_{j+1}} f(t, y(t))\, dt \approx \int_{t_j}^{t_{j+1}} P(t)\, dt$$

$$\stackrel{def}{=} h\left(b_m f(t_{j+1}, y(t_{j+1})) + b_{m-1} f(t_j, y(t_j)) + \cdots + b_0 f(t_{j-m+2}, y(t_{j-m+2}))\right)$$

implicit m-1-point method, $j =$ m-1,m,m+1, $\cdots$

$$w_{j+1} = w_j + h\left(b_{m-1} f(t_{j+1}, w_{j+1}) + b_{m-2} f(t_j, w_j) + b_{m-3} f(t_{j-1}, w_{j-1}) + \cdots + b_0 f(t_{j-m+2}, w_{j-m+2})\right)$$

m-th order Methods

explicit m-step

$P(t)$ interpolates $f(t, y(t))$ at $f(t_j, y(t_j))$, $f(t_{j-1}, y(t_{j-1}))$, $\cdots$, $\boxed{f(t_{j-m+1}, y(t_{j-m+1}))}$

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implicit (m-1)-step

$P(t)$ interpolates $f(t, y(t))$ at $\boxed{f(t_{j+1}, y(t_{j+1}))}$, $f(t_j, y(t_j))$, $\cdots$, $f(t_{j-m+2}, y(t_{j-m+2}))$

$$y(t_{j+1}) - y(t_j) = \int_{t_j}^{t_{j+1}} f(t, y(t))\, dt \approx \int_{t_j}^{t_{j+1}} P(t)\, dt$$

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implicit m-1-point method, $j = \text{m-1,m,m+1}, \cdots$

$$w_{j+1} = w_j + h\left(b_{m-1} f(t_{j+1}, w_{j+1}) + b_{m-2} f(t_j, w_j) + b_{m-3} f(t_{j-1}, w_{j-1}) + \cdots + b_0 f(t_{j-m+2}, w_{j-m+2})\right)$$

- 4th-order Adams-Bashforth method (explicit, 4-step)

$$w_{j+1} = w_j + \frac{h}{24}\left(55 f(t_j, w_j) - 59 f(t_{j-1}, w_{j-1}) + 37 f(t_{j-2}, w_{j-2}) - 9 f(t_{j-3}, w_{j-3})\right).$$

m-th order Methods

explicit m-step

$P(t)$ interpolates $f(t, y(t))$ at $f(t_j, y(t_j))$, $f(t_{j-1}, y(t_{j-1}))$, $\cdots$, $\boxed{f(t_{j-m+1}, y(t_{j-m+1}))}$

m-th order Methods

explicit m-step

$P(t)$ interpolates $f(t, y(t))$ at $f(t_j, y(t_j))$, $f(t_{j-1}, y(t_{j-1}))$, $\cdots$, $\boxed{f(t_{j-m+1}, y(t_{j-m+1}))}$

$$
\begin{aligned}
y(t_{j+1}) - y(t_j) = \int_{t_j}^{t_{j+1}} f(t, y(t))\, dt &\approx \int_{t_j}^{t_{j+1}} P(t)\, dt \\
&\overset{def}{=} h\left(b_{m-1} f(t_j, y(t_j)) + b_{m-2} f(t_{j-1}, y(t_{j-1}))\right. \\
&\qquad \left. + \cdots + b_0 f(t_{j-m+1}, y(t_{j-m+1}))\right)
\end{aligned}
$$

m-th order Methods

explicit m-step

$P(t)$ interpolates $f(t, y(t))$ at $f(t_j, y(t_j))$, $f(t_{j-1}, y(t_{j-1}))$, $\cdots$, $\boxed{f(t_{j-m+1}, y(t_{j-m+1}))}$

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m-th order Methods

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$$\stackrel{def}{=} h\left(b_{m-1} f(t_j, y(t_j)) + b_{m-2} f(t_{j-1}, y(t_{j-1})) + \cdots + b_0 f(t_{j-m+1}, y(t_{j-m+1}))\right)$$

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implicit (m-1)-step

$P(t)$ interpolates $f(t, y(t))$ at $\boxed{f(t_{j+1}, y(t_{j+1}))}$, $f(t_j, y(t_j))$, $\cdots$, $f(t_{j-m+2}, y(t_{j-m+2}))$

m-th order Methods

explicit m-step

$P(t)$ interpolates $f(t, y(t))$ at $f(t_j, y(t_j))$, $f(t_{j-1}, y(t_{j-1}))$, $\cdots$, $\boxed{f(t_{j-m+1}, y(t_{j-m+1}))}$

$$y(t_{j+1}) - y(t_j) = \int_{t_j}^{t_{j+1}} f(t, y(t))\, dt \approx \int_{t_j}^{t_{j+1}} P(t)\, dt$$

$$\stackrel{def}{=} h\left(b_{m-1} f(t_j, y(t_j)) + b_{m-2} f(t_{j-1}, y(t_{j-1})) + \cdots + b_0 f(t_{j-m+1}, y(t_{j-m+1}))\right)$$

leading to *explicit* m-point method, $j =$ m-1,m,m+1, $\cdots$

$$w_{j+1} = w_j + h\left(b_{m-1} f(t_j, w_j) + b_{m-2} f(t_{j-1}, w_{j-1}) + \cdots + b_0 f(t_{j-m+1}, w_{j-m+1})\right)$$

implicit (m-1)-step

$P(t)$ interpolates $f(t, y(t))$ at $\boxed{f(t_{j+1}, y(t_{j+1}))}$, $f(t_j, y(t_j))$, $\cdots$, $f(t_{j-m+2}, y(t_{j-m+2}))$

$$y(t_{j+1}) - y(t_j) = \int_{t_j}^{t_{j+1}} f(t, y(t))\, dt \approx \int_{t_j}^{t_{j+1}} P(t)\, dt$$

$$\stackrel{def}{=} h\left(b_m f(t_{j+1}, y(t_{j+1})) + b_{m-1} f(t_j, y(t_j)) + \cdots + b_0 f(t_{j-m+2}, y(t_{j-m+2}))\right)$$

m-th order Methods

explicit m-step

$P(t)$ interpolates $f(t, y(t))$ at $f(t_j, y(t_j))$, $f(t_{j-1}, y(t_{j-1}))$, $\cdots$, $\boxed{f(t_{j-m+1}, y(t_{j-m+1}))}$

$$y(t_{j+1}) - y(t_j) = \int_{t_j}^{t_{j+1}} f(t, y(t))\, dt \approx \int_{t_j}^{t_{j+1}} P(t)\, dt$$

$$\stackrel{def}{=} h\left(b_{m-1} f(t_j, y(t_j)) + b_{m-2} f(t_{j-1}, y(t_{j-1})) + \cdots + b_0 f(t_{j-m+1}, y(t_{j-m+1}))\right)$$

leading to *explicit* m-point method, $j =$ m-1,m,m+1, $\cdots$

$$w_{j+1} = w_j + h\left(b_{m-1} f(t_j, w_j) + b_{m-2} f(t_{j-1}, w_{j-1}) + \cdots + b_0 f(t_{j-m+1}, w_{j-m+1})\right)$$

implicit (m-1)-step

$P(t)$ interpolates $f(t, y(t))$ at $\boxed{f(t_{j+1}, y(t_{j+1}))}$, $f(t_j, y(t_j))$, $\cdots$, $f(t_{j-m+2}, y(t_{j-m+2}))$

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$$\stackrel{def}{=} h\left(b_m f(t_{j+1}, y(t_{j+1})) + b_{m-1} f(t_j, y(t_j)) + \cdots + b_0 f(t_{j-m+2}, y(t_{j-m+2}))\right)$$

implicit m-1-point method, $j =$ m-1,m,m+1, $\cdots$

$$w_{j+1} = w_j + h\left(b_{m-1} f(t_{j+1}, w_{j+1}) + b_{m-2} f(t_j, w_j) + b_{m-3} f(t_{j-1}, w_{j-1}) + \cdots + b_0 f(t_{j-m+2}, w_{j-m+2})\right)$$

- 4th-order Adams-Bashforth method (explicit, 4-step)

$$w_{j+1} = w_j + \frac{h}{24}\left(55 f(t_j, w_j) - 59 f(t_{j-1}, w_{j-1}) + 37 f(t_{j-2}, w_{j-2}) - 9 f(t_{j-3}, w_{j-3})\right).$$

- 4th-order Adams-Moulton method (implicit, 3-step)

$$w_{j+1} = w_j + \frac{h}{24}\left(9 f(t_{j+1}, w_{j+1}) + 19 f(t_j, w_j) - 5 f(t_{j-1}, w_{j-1}) + f(t_{j-2}, w_{j-2})\right).$$

m-th order Methods, LTE

explicit m-step

$P(t)$ interpolates $f(t, y(t))$ at $f(t_j, y(t_j))$, $f(t_{j-1}, y(t_{j-1}))$, $\cdots$, $\boxed{f(t_{j-m+1}, y(t_{j-m+1}))}$

m-th order Methods, LTE

explicit m-step

$P(t)$ interpolates $f(t, y(t))$ at $f(t_j, y(t_j))$, $f(t_{j-1}, y(t_{j-1}))$, $\cdots$, $\boxed{f(t_{j-m+1}, y(t_{j-m+1}))}$

$$f(t, y(t)) = P(t) + R(t)$$

$$R(t) = \frac{f^{(m)}(\xi_t, y(\xi_t))}{m!} \prod_{k=j-m+1}^{j} (t - t_k)$$

m-th order Methods, LTE

explicit m-step

$P(t)$ interpolates $f(t, y(t))$ at $f(t_j, y(t_j))$, $f(t_{j-1}, y(t_{j-1}))$, $\cdots$, $\boxed{f(t_{j-m+1}, y(t_{j-m+1}))}$

$$f(t, y(t)) = P(t) + R(t)$$

$$R(t) = \frac{f^{(m)}(\xi_t, y(\xi_t))}{m!} \prod_{k=j-m+1}^{j} (t - t_k)$$

$$y(t_{j+1}) - y(t_j) = \int_{t_j}^{t_{j+1}} (P(t) + R(t))\ dt$$

$$\stackrel{def}{=} h\left(b_{m-1} f(t_j, y(t_j)) + b_{m-2} f(t_{j-1}, y(t_{j-1}))\right.$$

$$\left. + \cdots + b_0 f(t_{j-m+1}, y(t_{j-m+1}))\right) + \int_{t_j}^{t_{j+1}} R(t)\, dt$$

m-th order Methods, LTE

explicit m-step

$P(t)$ interpolates $f(t, y(t))$ at $f(t_j, y(t_j))$, $f(t_{j-1}, y(t_{j-1}))$, $\cdots$, $\boxed{f(t_{j-m+1}, y(t_{j-m+1}))}$

$$f(t, y(t)) = P(t) + R(t)$$

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$$y(t_{j+1}) - y(t_j) = \int_{t_j}^{t_{j+1}} (P(t) + R(t))\; dt$$

$$\stackrel{def}{=} h\left(b_{m-1} f(t_j, y(t_j)) + b_{m-2} f(t_{j-1}, y(t_{j-1}))\right.$$

$$\left. + \cdots + b_0 f(t_{j-m+1}, y(t_{j-m+1}))\right) + \int_{t_j}^{t_{j+1}} R(t)\, dt$$

$$\textbf{LTE} \stackrel{def}{=} \tau_{j+1}(h) = \frac{1}{h} \int_{t_j}^{t_{j+1}} R(t)\, dt$$

$$= \frac{1}{m!\, h} \int_{t_j}^{t_{j+1}} f^{(m)}(\xi_t, y(\xi_t)) \prod_{k=j-m+1}^{j} (t - t_k)\; dt$$

$$\stackrel{book}{=\!=} \frac{f^{(m)}(\xi, y(\xi))}{m!\, h} \int_{t_j}^{t_{j+1}} \prod_{k=j-m+1}^{j} (t - t_k)\; dt$$

m-th order Methods, LTE

explicit m-step

$P(t)$ interpolates $f(t, y(t))$ at $f(t_j, y(t_j))$, $f(t_{j-1}, y(t_{j-1}))$, $\cdots$, $\boxed{f(t_{j-m+1}, y(t_{j-m+1}))}$

$$f(t, y(t)) = P(t) + R(t)$$

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implicit (m-1)-step

$P(t)$ interpolates $f(t, y(t))$ at $\boxed{f(t_{j+1}, y(t_{j+1}))}$, $f(t_j, y(t_j))$, $\cdots$, $f(t_{j-m+2}, y(t_{j-m+2}))$

m-th order Methods, LTE

explicit m-step

$P(t)$ interpolates $f(t, y(t))$ at $f(t_j, y(t_j))$, $f(t_{j-1}, y(t_{j-1}))$, $\cdots$, $\boxed{f(t_{j-m+1}, y(t_{j-m+1}))}$

$$f(t, y(t)) = P(t) + R(t)$$

$$R(t) = \frac{f^{(m)}\left(\xi_t, y(\xi_t)\right)}{m!} \prod_{k=j-m+1}^{j} (t - t_k)$$

$$y(t_{j+1}) - y(t_j) = \int_{t_j}^{t_{j+1}} \left(P(t) + R(t)\right)\, dt$$

$$\stackrel{def}{=} h\left(b_{m-1} f(t_j, y(t_j)) + b_{m-2} f(t_{j-1}, y(t_{j-1}))\right.$$

$$\left. + \cdots + b_0 f(t_{j-m+1}, y(t_{j-m+1}))\right) + \int_{t_j}^{t_{j+1}} R(t)\, dt$$

$$\textbf{LTE} \stackrel{def}{=} \tau_{j+1}(h) = \frac{1}{h} \int_{t_j}^{t_{j+1}} R(t)\, dt$$

$$= \frac{1}{m!\, h} \int_{t_j}^{t_{j+1}} f^{(m)}\left(\xi_t, y(\xi_t)\right) \prod_{k=j-m+1}^{j} (t - t_k)\, dt$$

$$\stackrel{book}{=} \frac{f^{(m)}\left(\xi, y(\xi)\right)}{m!\, h} \int_{t_j}^{t_{j+1}} \prod_{k=j-m+1}^{j} (t - t_k)\, dt$$

implicit (m-1)-step

$P(t)$ interpolates $f(t, y(t))$ at $\boxed{f(t_{j+1}, y(t_{j+1}))}$, $f(t_j, y(t_j))$, $\cdots$, $f(t_{j-m+2}, y(t_{j-m+2}))$

$$f(t, y(t)) = P(t) + R(t)$$

$$R(t) = \frac{f^{(m)}\left(\xi_t, y(\xi_t)\right)}{m!} \prod_{k=j-m+2}^{j+1} (t - t_k)$$

m-th order Methods, LTE

explicit m-step

$P(t)$ interpolates $f(t, y(t))$ at $f(t_j, y(t_j))$, $f(t_{j-1}, y(t_{j-1}))$, $\cdots$, $\boxed{f(t_{j-m+1}, y(t_{j-m+1}))}$

$$f(t, y(t)) = P(t) + R(t)$$

$$R(t) = \frac{f^{(m)}(\xi_t, y(\xi_t))}{m!} \prod_{k=j-m+1}^{j} (t - t_k)$$

$$y(t_{j+1}) - y(t_j) = \int_{t_j}^{t_{j+1}} (P(t) + R(t))\, dt$$

$$\stackrel{def}{=} h\left(b_{m-1} f(t_j, y(t_j)) + b_{m-2} f(t_{j-1}, y(t_{j-1}))\right.$$

$$\left. + \cdots + b_0 f(t_{j-m+1}, y(t_{j-m+1}))\right) + \int_{t_j}^{t_{j+1}} R(t)\, dt$$

$$\textbf{LTE} \stackrel{def}{=} \tau_{j+1}(h) = \frac{1}{h} \int_{t_j}^{t_{j+1}} R(t)\, dt$$

$$= \frac{1}{m!\, h} \int_{t_j}^{t_{j+1}} f^{(m)}(\xi_t, y(\xi_t)) \prod_{k=j-m+1}^{j} (t - t_k)\, dt$$

$$\stackrel{book}{=\!=} \frac{f^{(m)}(\xi, y(\xi))}{m!\, h} \int_{t_j}^{t_{j+1}} \prod_{k=j-m+1}^{j} (t - t_k)\, dt$$

implicit (m-1)-step

$P(t)$ interpolates $f(t, y(t))$ at $\boxed{f(t_{j+1}, y(t_{j+1}))}$, $f(t_j, y(t_j))$, $\cdots$, $f(t_{j-m+2}, y(t_{j-m+2}))$

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m-th order Methods, LTE

explicit m-step

$P(t)$ interpolates $f(t, y(t))$ at $f(t_j, y(t_j))$, $f(t_{j-1}, y(t_{j-1}))$, $\cdots$, $\boxed{f(t_{j-m+1}, y(t_{j-m+1}))}$

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implicit (m-1)-step

$P(t)$ interpolates $f(t, y(t))$ at $\boxed{f(t_{j+1}, y(t_{j+1}))}$, $f(t_j, y(t_j))$, $\cdots$, $f(t_{j-m+2}, y(t_{j-m+2}))$

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4th-order Methods

- 4th-order Adams-Bashforth method (explicit, 4-step)

$$w_{j+1} = w_j + \frac{h}{24}\left(55f(t_j, w_j) - 59f(t_{j-1}, w_{j-1}) + 37f(t_{j-2}, w_{j-2}) - 9f(t_{j-3}, w_{j-3})\right).$$

- 4th-order Adams-Moulton method (implicit, 3-step)

$$w_{j+1} = w_j + \frac{h}{24}\left(9f(t_{j+1}, w_{j+1}) + 19f(t_j, w_j) - 5f(t_{j-1}, w_{j-1}) + f(t_{j-2}, w_{j-2})\right).$$

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Adams-Bashforth

$$\mathbf{LTE} \stackrel{def}{=} \frac{f^{(4)}(\xi, y(\xi))}{4!\, h} \int_{t_j}^{t_{j+1}} \prod_{k=j-3}^{j} (t - t_k)\, dt$$

$$= \frac{f^{(4)}(\xi, y(\xi))}{4!\, h} \int_0^h t\,(t+h)\,(t+2\,h)\,(t+3\,h)\,dt$$

$$= \boxed{\tfrac{251}{720}} f^{(4)}(\xi, y(\xi))\; h^4$$

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Adams-Moulton

$$\textbf{LTE} \stackrel{def}{=} \frac{f^{(4)}(\xi, y(\xi))}{4!\,h} \int_{t_j}^{t_{j+1}} \prod_{k=j-2}^{j+1} (t - t_k)\, dt$$

$$= \frac{f^{(4)}(\xi, y(\xi))}{4!\,h} \int_0^h (t-h)\,t\,(t+h)\,(t+2\,h)\, dt$$

$$= -\boxed{\tfrac{19}{720}} f^{(4)}(\xi, y(\xi))\; h^4$$

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To be explicit or implicit?

- Explicit methods cheaper than implicit.
- Implicit methods smaller LTE and more reliable (more later)

experiment

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$$w_{j+1} = w_j + \frac{h}{24}\left(55f(t_j, w_j) - 59f(t_{j-1}, w_{j-1}) + 37f(t_{j-2}, w_{j-2}) - 9f(t_{j-3}, w_{j-3})\right).$$

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$$\frac{dy}{dt} = y - t^2 + 1, \quad 0 \leq t \leq 2, \quad y(a) = 0.5, \quad \text{for } N = 10, h = 0.2, t_j = 0.2j, 0 \leq j \leq N.$$

experiment

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Adams-Bashforth method:
4 initial values to start

experiment

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Adams-Moulton method:
3 initial values to start

Adams-Bashforth method:
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Adams-Moulton method:
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$$\begin{aligned} w_{j+1} &= w_j+\frac{h}{24}\left(9f(t_{j+1},w_{j+1})+19f(t_j,w_j)-5f(t_{j-1},w_{j-1})+f(t_{j-2},w_{j-2})\right) \\ &= \frac{1}{24}\left(\boxed{1.8w_{j+1}}+27.8w_j-w_{j-1}+0.2w_{j-2}-0.192j^2-0.192j+4.736\right) \end{aligned}$$

experiment

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experiment

t_j	Exact	Bashforth	Error	Moulton	Error
0.0	0.5				
0.2	0.8293				
0.4	1.2141				
0.6	1.6489			1.6489	$6.5e-06$
0.8	2.1272	2.1273	$8.28e-05$	2.1272	$1.6e-05$
1.0	2.6409	2.6411	0.0002219	2.6408	$2.93e-05$
1.2	3.1799	3.1803	0.0004065	3.1799	$4.78e-05$
1.4	3.7324	3.7331	0.0006601	3.7323	$7.31e-05$
1.6	4.2835	4.2845	0.0010093	4.2834	0.0001071
1.8	4.8152	4.8167	0.0014812	4.815	0.0001527
2.0	5.3055	5.3076	0.0021119	5.3053	0.0002132

experiment

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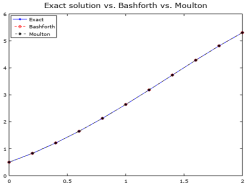

experiment

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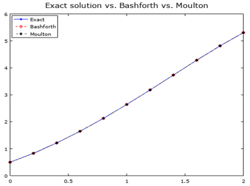

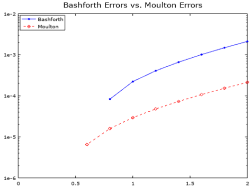

§5.7 Predictor-Corrector Methods

- 4th-order Adams-Bashforth method (explicit, less accurate)

$$w_{j+1} = w_j + \frac{h}{24}\left(55f(t_j, w_j) - 59f(t_{j-1}, w_{j-1}) + 37f(t_{j-2}, w_{j-2}) - 9f(t_{j-3}, w_{j-3})\right).$$

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- 4th-order Adams-Moulton method (implicit, more accurate)

$$w_{j+1} = w_j + \frac{h}{24}\left(9f(t_{j+1}, w_{j+1}) + 19f(t_j, w_j) - 5f(t_{j-1}, w_{j-1}) + f(t_{j-2}, w_{j-2})\right).$$

- Predictor-Corrector (PC)

`Adams4PC` $\stackrel{def}{=}$ <u>One</u> fixed-point iteration on Moulton, with Bashforth initial guess

§5.7 Predictor-Corrector Methods

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- Predictor-Corrector (PC)

`Adams4PC` $\stackrel{def}{=}$ <u>One</u> fixed-point iteration on Moulton, with Bashforth initial guess

- **Initialization**: 3 steps of 4-th order Runge-Kutta.
- Adams-Bashforth **Predictor**:

$$w_{j+1}^{\mathbf{p}} \quad \stackrel{def}{=} \quad w_j + \frac{h}{24}\left(55f(t_j, w_j) - 59f(t_{j-1}, w_{j-1}) + 37f(t_{j-2}, w_{j-2}) - 9f(t_{j-3}, w_{j-3})\right)$$

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```
function [w,t] = Adams4PC(FunFcn, Intv, alpha, N)
a     = Intv(1);
b     = Intv(2);
h     = (b-a)/N;
w     = zeros(N+1,1);
t     = a + h*(0:N)';
w(1) = alpha;
%
% RK4 for the first 3 steps
h2    = h/2;
for i = 1:3
    k1 = h* FunFcn(t(i),w(i));
    k2 = h* FunFcn(t(i)+h2,w(i)+k1/2);
    k3 = h* FunFcn(t(i)+h2,w(i)+k2/2);
    k4 = h* FunFcn(t(i)+h,w(i)+k3);
    w(i+1) = w(i) + (k1+2*k2+2*k3+k4)/6;
end
%
% main loop
p = h*[-9/24  37/24 -59/24 55/24];
c = h*[ 1/24 -5/24   19/24 9/24 ];
f = FunFcn(t(1:4), w(1:4));
for i = 4:N
    wp      = w(i) + p*f;
    fp      = FunFcn(t(i+1),wp);
    w(i+1) = w(i) + c *[f(2:end);fp];
    f       =[f(2:end); FunFcn(t(i+1),w(i+1))];
end
```

Adaptive Error Control (I)

$$\frac{dy}{dt} = f(t, y(t)), \quad a \leq t \leq b, \quad y(a) = \alpha.$$

$\boxed{\text{Variable-step method based on } \texttt{Adams4PC}}$

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$\boxed{\text{Assumptions}}$

- Given tolerance $\tau > 0$,
- $w_i \approx y(t_i)$ for all $i \leq j$.

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- Try to make sure **LTE** $|\tau_{j+1}(h_{j+1})| \lesssim \tau$

$\boxed{\text{Approach}}$

for $j = 0, 1, \cdots$,

- **run** Runge-Kutta $\boxed{\text{initially or if}}$ step-size changes,
- **reset** step-size $h_j = t_{j+1} - t_j$ if tolerance requires,
- **compute** w_{j+1} with `Adams4PC`.

Adaptive Error Control (II)

- 4th-order Adams-Bashforth **Predictor**

$$w^{\mathbf{p}}_{j+1} = w_j + \frac{h}{24}\left(55f(t_j, w_j) - 59f(t_{j-1}, w_{j-1}) + 37f(t_{j-2}, w_{j-2}) - 9f(t_{j-3}, w_{j-3})\right) \approx y_{j+1} - \frac{251}{720} f^{(4)}(\xi, y(\xi))\, h^5$$

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$$w_{j+1} = w_j + \frac{h}{24}\Big(9f(t_{j+1}, w^{\mathbf{p}}_{j+1}) + 19f(t_j, w_j) - 5f(t_{j-1}, w_{j-1}) + f(t_{j-2}, w_{j-2})\Big) \approx y_{j+1} + \frac{19}{720} f^{(4)}(\widetilde{\xi}, y(\widetilde{\xi}))\, h^5$$

$$\boxed{\textbf{Assume } h^5\, f^{(4)}(\xi, y(\xi)) \approx h^5\, f^{(4)}(\widetilde{\xi}, y(\widetilde{\xi}))}$$

$$\frac{w_{j+1} - w^{\mathbf{p}}_{j+1}}{h} \approx \frac{270}{720} f^{(4)}(\widetilde{\xi}, y(\widetilde{\xi}))\, h^4$$

Adaptive Error Control (II)

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$$\frac{w_{j+1} - w_{j+1}^{\mathbf{p}}}{h} \approx \frac{270}{720} f^{(4)}(\widetilde{\xi}, y(\widetilde{\xi}))\, h^4 \implies \frac{19}{720} f^{(4)}(\widetilde{\xi}, y(\widetilde{\xi}))\, h^4 \approx \frac{19}{270}\, \frac{w_{j+1} - w_{j+1}^{\mathbf{p}}}{h},$$

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step-size selection

$$\boxed{\text{LTE estimate: } \tau_{j+1}(h) = \frac{y_{j+1} - w_{j+1}}{h} \approx -\frac{19}{270}\,\frac{w_{j+1} - w^{\mathbf{p}}_{j+1}}{h}}$$

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- K $\boxed{\text{should}}$ satisfy

$$K\, h^4 \approx -\frac{19}{270}\,\frac{w_{j+1} - w^{\mathbf{p}}_{j+1}}{h} \qquad (1)$$

- **Choose** new step-size $q\,h$ so LTE satisfies given tolerance ϵ:

$$\left|\tau_{j+1}(q\,h)\right| \leq \epsilon$$

- Equation (1) implies

$$\left|q^4\,\frac{19}{270}\,\frac{w_{j+1} - w^{\mathbf{p}}_{j+1}}{h}\right| \approx \left|K\,(q\,h)^4\right| \approx \left|\tau_{j+1}(q\,h)\right| \lesssim \epsilon$$

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$$q = 1.5 \left(\frac{\epsilon\, h}{\left| w_{j+1} - w_{j+1}^{\mathbf{p}} \right|} \right)^{\frac{1}{4}}.$$

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$$h = \begin{cases} \mathbf{max}(q, 0.1)\,h, & \text{if } q < 1, \\ \mathbf{min}(q, 4)\,h, & \text{if } q > 2, \\ h & \text{if } 1 \le q \le 2, \end{cases}$$

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- step-size can't be too big: $h = \mathbf{min}\,(h, h_{\mathbf{max}})$
- step-size can't be too small:

if $h < h_{\mathbf{min}}$ **then** *declare failure.*

cf. step-size selection

Adaptive Runger-Kutta

Summary: Adams 4th-order Predictor-Corrector Method

For each j,

- compute 4th-order Adams-Bashforth **Predictor**

$$w_{j+1}^{\mathbf{p}} = w_j + \frac{h}{24}\left(55f(t_j, w_j) - 59f(t_{j-1}, w_{j-1}) + 37f(t_{j-2}, w_{j-2}) - 9f(t_{j-3}, w_{j-3})\right)$$

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- new step-size $q\,h$ should satisfy

$$q\,h \lesssim 1.5\,h\left(\frac{\epsilon\,h}{\left|w_{j+1} - w_{j+1}^{\mathbf{p}}\right|}\right)^{\frac{1}{4}}.$$

- if $q < 1$, give up current w_{j+1}; otherwise keep it and set $j = j + 1$.
- additional safeguards on step-size.

Adaptive `Adams4PC`

Initial Value ODE $$\frac{dy}{dt} = y - t^2 + 1, \quad 0 \leq t \leq 2, \quad y(0) = 0.5$$

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t_j	h_j	$y(t_j)$	w_j	$\lvert\mathbf{LTE}\rvert$	$\lvert y(t_j) - w_j\rvert$
0	0	0.5	0.5	0	0
0.1257	0.1257	0.70023	0.70023	$4.051e-05$	$5e-07$
0.2514	0.1257	0.9231	0.92309	$4.051e-05$	$1.1e-06$
0.37711	0.1257	1.1674	1.1674	$4.051e-05$	$1.7e-06$
0.50281	0.1257	1.4318	1.4317	$4.051e-05$	$2.2e-06$
0.62851	0.1257	1.7146	1.7146	$4.61e-05$	$2.8e-06$
0.75421	0.1257	2.0143	2.0143	$5.21e-05$	$3.5e-06$
0.87991	0.1257	2.3287	2.3287	$5.913e-05$	$4.3e-06$
1.0056	0.1257	2.6557	2.6557	$6.706e-05$	$5.4e-06$
1.1313	0.1257	2.9926	2.9926	$7.604e-05$	$6.6e-06$
1.257	0.1257	3.3367	3.3367	$8.622e-05$	$8e-06$
1.3827	0.1257	3.6845	3.6845	$9.777e-05$	$9.7e-06$
1.4857	0.10301	3.9698	3.9697	$7.029e-05$	$1.08e-05$
1.5887	0.10301	4.2528	4.2528	$7.029e-05$	$1.2e-05$
1.6917	0.10301	4.531	4.531	$7.029e-05$	$1.33e-05$
1.7948	0.10301	4.8017	4.8016	$7.029e-05$	$1.51e-05$
1.8978	0.10301	5.0616	5.0615	$7.76e-05$	$1.72e-05$
1.9233	0.025558	5.124	5.124	$3.918e-07$	$1.77e-05$
1.9489	0.025558	5.1855	5.1855	$3.918e-07$	$1.81e-05$
1.9744	0.025558	5.246	5.246	$3.918e-07$	$1.86e-05$
2.0	0.025558	5.3055	5.3055	$3.918e-07$	$1.91e-05$

Adaptive Adams4PC

Initial Value ODE $$\frac{dy}{dt} = y - t^2 + 1, \quad 0 \le t \le 2, \quad y(0) = 0.5$$

t_j	h_j	$y(t_j)$	w_j	$\|\mathbf{LTE}\|$	$\|y(t_j) - w_j\|$
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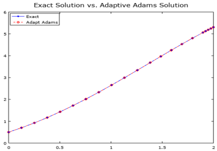
1.257	0.1257	3.3367	3.3367	$8.622e-05$	$8e-06$
1.3827	0.1257	3.6845	3.6845	$9.777e-05$	$9.7e-06$
1.4857	0.10301	3.9698	3.9697	$7.029e-05$	$1.08e-05$
1.5887	0.10301	4.2528	4.2528	$7.029e-05$	$1.2e-05$
1.6917	0.10301	4.531	4.531	$7.029e-05$	$1.33e-05$
1.7948	0.10301	4.8017	4.8016	$7.029e-05$	$1.51e-05$
1.8978	0.10301	5.0616	5.0615	$7.76e-05$	$1.72e-05$
1.9233	0.025558	5.124	5.124	$3.918e-07$	$1.77e-05$
1.9489	0.025558	5.1855	5.1855	$3.918e-07$	$1.81e-05$
1.9744	0.025558	5.246	5.246	$3.918e-07$	$1.86e-05$
2.0	0.025558	5.3055	5.3055	$3.918e-07$	$1.91e-05$



Adaptive `Adams4PC`

Initial Value ODE $\quad \frac{dy}{dt} = y - t^2 + 1, \quad 0 \le t \le 2, \quad y(0) = 0.5$

t_j	h_j	$y(t_j)$	w_j	$\lvert\textbf{LTE}\rvert$	$\lvert y(t_j) - w_j\rvert$
0	0	0.5	0.5	0	0
0.1257	0.1257	0.70023	0.70023	$4.051e-05$	$5e-07$
0.2514	0.1257	0.9231	0.92309	$4.051e-05$	$1.1e-06$
0.37711	0.1257	1.1674	1.1674	$4.051e-05$	$1.7e-06$
0.50281	0.1257	1.4318	1.4317	$4.051e-05$	$2.2e-06$
0.62851	0.1257	1.7146	1.7146	$4.61e-05$	$2.8e-06$
0.75421	0.1257	2.0143	2.0143	$5.21e-05$	$3.5e-06$
0.87991	0.1257	2.3287	2.3287	$5.913e-05$	$4.3e-06$
1.0056	0.1257	2.6557	2.6557	$6.706e-05$	$5.4e-06$
1.1313	0.1257	2.9926	2.9926	$7.604e-05$	$6.6e-06$
1.257	0.1257	3.3367	3.3367	$8.622e-05$	$8e-06$
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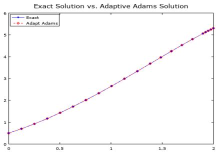

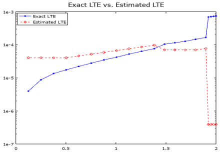

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Initial Value ODE $\quad \dfrac{dy}{dt} = y - t^2 + 1, \quad 0 \le t \le 2, \quad y(0) = 0.5$

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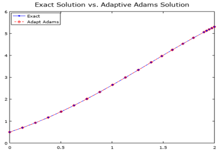

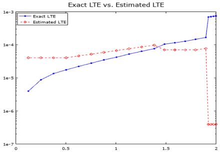

$\boxed{\text{Estimated LTE is neither upper bound nor accurate}}$

Multistep vs. Runge-Kutta

- Multistep methods cheaper than Runge-Kutta.
- Multistep methods require Runge-Kutta for every step-size change.

`OdeDemo: matlab` code on *bcourses* running different ODE solvers.

§5.9 Predator and Prey Model

$$\begin{array}{lrcll} \text{Notation:} & x & \stackrel{def}{=} & \text{prey population,} & y \stackrel{def}{=} \text{predator population.} \\ \text{Dynamics:} & x' & = & \alpha x - \beta\, x\, y, & y' = -\gamma y + \delta\, x\, y. \end{array}$$

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- prey population x increases when alone, decreases with predator
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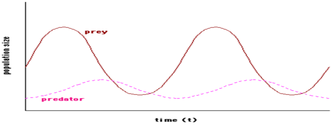
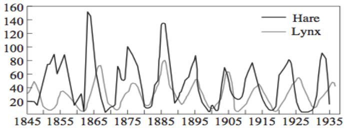
Circle of life: Boom and Bust dynamics



Circle of life from Canada



Hungry fox y catches squirrel x (best wildlife photo, 2019)

Lynx and Hare in the Canadian snow

System of ODEs

single initial value ODE $$\frac{dy}{dt} = f(t, y), \quad a \leq t \leq b, \quad y(a) = \alpha.$$

System of ODEs

single initial value ODE $\dfrac{dy}{dt} = f(t, y), \quad a \le t \le b, \quad y(a) = \alpha.$

System of m first-order ODEs:

$$
\begin{aligned}
\frac{du_1}{dt} &= f_1(t, u_1, u_2, \cdots, u_m), \\
\frac{du_2}{dt} &= f_2(t, u_1, u_2, \cdots, u_m), \\
&\vdots \\
\frac{du_m}{dt} &= f_m(t, u_1, u_2, \cdots, u_m), \quad a \le t \le b,
\end{aligned}
$$

with m initial conditions

$$u_1(a) = \alpha_1, \quad u_2(a) = \alpha_2, \cdots, u_m(a) = \alpha_m.$$

Systems of ODEs in vector form

$$\mathbf{u} \stackrel{def}{=} \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_m \end{pmatrix}, \quad \alpha \stackrel{def}{=} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_m \end{pmatrix}.$$

$$\mathbf{f}(t, \mathbf{u}) \stackrel{def}{=} \begin{pmatrix} f_1(t, u_1, u_2, \cdots, u_m) \\ f_2(t, u_1, u_2, \cdots, u_m) \\ \vdots \\ f_m(t, u_1, u_2, \cdots, u_m) \end{pmatrix}$$

System of m first-order ODEs:

$$\frac{d\mathbf{u}}{dt} = \mathbf{f}(t, \mathbf{u}), \quad a \leq t \leq b \quad (1)$$

with initial condition

$$\mathbf{u}(a) = \alpha \quad (2)$$

Systems of ODEs in vector form

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Higher order ODEs

$$y^{(m)} = f\left(t, y, y', \cdots, y^{(m-1)}\right), \quad a \le t \le b \quad (3)$$

for some $m > 1$, with initial conditions

$$y(a) = \alpha, \quad y'(a) = \alpha', \cdots, y^{(m-1)}(a) = \alpha^{(m-1)} \quad (4)$$

Systems of ODEs in vector form

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Magic: re-write problem (3)+(4) $\Longrightarrow$ (1)+(2):

$$\mathbf{u} = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_m \end{pmatrix} \stackrel{def}{=} \begin{pmatrix} y \\ y' \\ \vdots \\ y^{(m-1)} \end{pmatrix}, \quad \alpha \stackrel{def}{=} \begin{pmatrix} \alpha \\ \alpha' \\ \vdots \\ \alpha^{(m-1)} \end{pmatrix}$$

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$$\Longrightarrow \frac{d\mathbf{u}}{dt} = \begin{pmatrix} y' \\ y'' \\ \vdots \\ y^{(m)} \end{pmatrix} = \begin{pmatrix} u_2 \\ u_3 \\ \vdots \\ u_m \\ f(t, u_1, u_2, \cdots, u_m) \end{pmatrix} \stackrel{def}{=} \mathbf{f}(t, \mathbf{u})$$

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Higher order ODEs

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$$\Longrightarrow \mathbf{u}(a) = \alpha$$

$\boxed{\text{Every ODE} = \text{first order ODE}}$

example

$$
\begin{aligned}
x'' &= \alpha y - \beta\, x\, y, \\
y'' &= -\gamma x + \delta\, x\, y.
\end{aligned}
$$

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$$
\mathbf{u} = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} \stackrel{def}{=} \begin{pmatrix} x \\ x' \\ y \\ y' \end{pmatrix}
$$

example

$$
\begin{aligned}
x'' &= \alpha y - \beta\, x\, y, \\
y'' &= -\gamma x + \delta\, x\, y.
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$$

$$
\Longrightarrow \frac{d\mathbf{u}}{dt} = \begin{pmatrix} x' \\ x'' \\ y' \\ y'' \end{pmatrix} = \begin{pmatrix} u_2 \\ \alpha\, u_3 - \beta\, u_1\, u_3 \\ u_4 \\ -\gamma\, u_1 + \delta\, u_1\, u_3 \end{pmatrix} \stackrel{def}{=} \mathbf{f}\,(t, \mathbf{u})
$$

Vector Lipschitz condition (I)

Definition: The function $f\left(t, \mathbf{u}\right)$ for $\mathbf{u} = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_m \end{pmatrix} \in \mathbf{R}^m$ defined

on the set

$$\mathcal{D} \overset{def}{=} \{(t, \mathbf{u}) \quad | \quad a \leq t \leq b, \quad -\infty < u_j < \infty, \quad 1 \leq j \leq m.\}$$

satisfies a Lipschitz condition on $\mathcal{D}$ if

$$|f\left(t, \mathbf{u}\right) - f\left(t, \mathbf{z}\right)| \leq L \sum_{j=1}^{m} \left|u_j - z_j\right|, \quad \text{where} \quad z = \begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_m \end{pmatrix},$$

for a constant L and all $\left(t, \mathbf{u}\right), \left(t, \mathbf{z}\right) \in \mathcal{D}$.

Vector Lipschitz condition (II)

$$\mathcal{D} \stackrel{def}{=} \{(t, \mathbf{u}) \quad | \quad a \leq t \leq b, \quad -\infty < u_j < \infty, \quad 1 \leq j \leq m.\}$$

Theorem: $f(t, \mathbf{u})$ satisfies a Lipschitz condition with Lipschitz constant L on $\mathcal{D}$ if

$$\left| \frac{\partial f}{\partial u_j}(t, \mathbf{u}) \right| \leq L, \quad j = 1, 2, \cdots, m.$$

$$\mathcal{D} \stackrel{def}{=} \{(t, \mathbf{u}) \quad | \quad a \leq t \leq b, \quad -\infty < u_j < \infty, \quad 1 \leq j \leq m.\}$$

System of m first-order ODEs:

$$\frac{d\mathbf{u}}{dt} = \mathbf{f}\left(t, \mathbf{u}\right), \quad a \leq t \leq b, \quad \text{with} \quad \mathbf{u}\left(a\right) = \alpha.$$

Theorem: Suppose that $f_j\left(t, \mathbf{u}\right)$ satisfies a Lipschitz condition with Lipschitz constant L on $\mathcal{D}$ for all $1 \leq j \leq m$. Then the system of initial value ODEs has a unique solution $\mathbf{u} = \mathbf{u}(t)$ for all $t \in [a, b]$.

scalar ODE method $\Longrightarrow$ **vector** ODE method

scalar initial value ODE	$\dfrac{dy}{dt} = f(t, y), \quad a \le t \le b, \quad y(a) = \alpha$
vector initial value ODEs	$\dfrac{d\mathbf{u}}{dt} = \mathbf{f}\left(t, \mathbf{u}\right), \quad a \le t \le b, \quad \mathbf{u}\left(a\right) = \alpha$

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<u>scalar</u> Runge-Kutta 4^{th} order method:

- $\mathbf{w}_0 = \alpha$
- for $j = 0, 1, \cdots$

$$
\begin{aligned}
\mathbf{k}_1 &= h\,\mathbf{f}(t_j, \mathbf{w}_j), \\
\mathbf{k}_2 &= h\,\mathbf{f}(t_j + \frac{h}{2}, \mathbf{w}_j + \frac{1}{2}\mathbf{k}_1), \\
\mathbf{k}_3 &= h\,\mathbf{f}(t_j + \frac{h}{2}, \mathbf{w}_j + \frac{1}{2}\mathbf{k}_2), \\
\mathbf{k}_4 &= h\,\mathbf{f}(t_{j+1}, \mathbf{w}_j + \mathbf{k}_3), \\
\mathbf{w}_{j+1} &= \mathbf{w}_j + \frac{1}{6}\left(\mathbf{k}_1 + 2\mathbf{k}_2 + 2\mathbf{k}_3 + \mathbf{k}_4\right)
\end{aligned}
$$

scalar ODE method $\Longrightarrow$ **vector** ODE method

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\end{aligned}$$

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\mathbf{k}_4 &= h\,\mathbf{f}(t_{j+1}, \mathbf{w}_j + \mathbf{k}_3),\\
\mathbf{w}_{j+1} &= \mathbf{w}_j + \frac{1}{6}\left(\mathbf{k}_1 + 2\mathbf{k}_2 + 2\mathbf{k}_3 + \mathbf{k}_4\right)
\end{aligned}$$

scalar ODE method $\Longrightarrow$ **vector** ODE method

scalar initial value ODE $\quad \dfrac{dy}{dt} = f(t, y), \quad a \le t \le b, \quad y(a) = \alpha$

vector initial value ODEs $\quad \dfrac{d\mathbf{u}}{dt} = \mathbf{f}(t, \mathbf{u}), \quad a \le t \le b, \quad \mathbf{u}(a) = \alpha$

<u>scalar</u> Runge-Kutta 4$^{\text{th}}$ order method:

- $\mathbf{w}_0 = \alpha$
- for $j = 0, 1, \cdots$

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Identical appearance!!!

example: Lotka-Volterra predator-prey model

- `matlab` function *lotka*

$$
\begin{aligned}
x' &= x - 0.01\,x\,y, \\
y' &= -y + 0.02\,x\,y.
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$$[t, y] = \textbf{ode45}(@\text{lotka}, [0, 40], [2, 1]);$$

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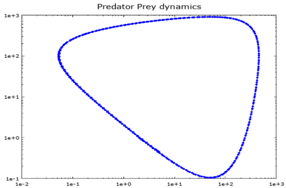
Predator Prey dynamics: circle of life



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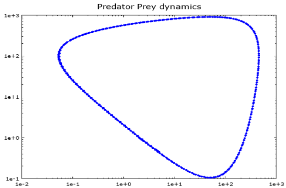

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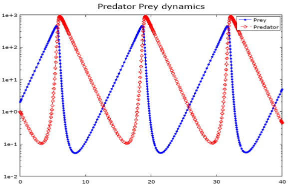

§5.10 Stability Analysis for one-step methods

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Review: convergence analysis for Euler method

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Definition: A *method* is **stable** if

- Small changes (perturbation) to ODE (due to the method) imply small changes to *numerical* solution.

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Then

- The method is <u>stable</u>
- The method is <u>convergent</u> $\iff$ <u>consistent</u> $\iff$

$$\phi(t,y,0) = f(t,y) \quad a \le t \le b.$$

-

$$|y(t_j) - w_j| \le \frac{\tau(h)}{L}\, e^{L(t_j - a)}, \quad \tau(h) \stackrel{def}{=} \mathbf{max}_{0 \le j \le N} |\tau_j(h)|\,.$$

Example: Modified Euler's Method, assuming $\left|\frac{\partial f}{\partial y}\right| \leq \widehat{L}$

$w_0 = \alpha$, and for $j = 0, 1, \cdots$

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$$\begin{aligned}
|\phi(t, w, h) - \phi(t, \widehat{w}, h)| \quad &\leq \quad \frac{\widehat{L}}{2}|w - \widehat{w}| \\
&\quad + \frac{\widehat{L}}{2}\left|w + h\,f(t, w) - \widehat{w} - h\,f(t, \widehat{w})\right| \\
&\leq \quad \left(\widehat{L} + \frac{1}{2}h\widehat{L}^2\right)|w - \widehat{w}| \stackrel{def}{=} L\,|w - \widehat{w}|
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Stability Analysis: multistep methods (I)

single ODE $$\frac{dy}{dt} = f(t, y), \quad a \le t \le b, \quad y(a) = \alpha.$$

Consider multistep method, $w_0 = \alpha$, $w_1 = \alpha_1$, $\cdots$, $w_{m-1} = \alpha_{m-1}$,

- for $j = m-1, m, m+1, \cdots$

$$\begin{aligned} w_{j+1} &= a_{m-1}\, w_j + a_{m-2}\, w_{j-1} + \cdots + a_0\, w_{j+1-m} \\ &\quad + h\, F\left(t_j, w_{j+1}, w_j, \cdots, w_{j+1-m}\right), \quad x_j = a + j\, h. \end{aligned}$$

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- local truncation error

$$\textbf{LTE } \tau_{j+1}(h) \stackrel{def}{=} \frac{y(t_{j+1}) - (a_{m-1}\, y(t_j) + a_{m-2}\, y(t_{j-1}) + \cdots + a_0\, y(t_{j+1-m}))}{h} - F\left(t_j, y(t_{j+1}), y(t_j), \cdots, y(t_{j+1-m})\right).$$

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Assumptions on F

- If $f \equiv 0$, then $F \equiv 0$
- $$\begin{aligned} &\left|F\left(t_j, u_{j+1}, u_j, \cdots, u_{j+1-m}\right) - F\left(t_j, \widehat{u}_{j+1}, \widehat{u}_j, \cdots, \widehat{u}_{j+1-m}\right)\right| \\ &\quad \le L\left(|u_{j+1} - \widehat{u}_{j+1}| + \cdots + |u_{j+1-m} - \widehat{u}_{j+1-m}|\right) \end{aligned}$$

Stability Analysis: multistep methods (II)

- *Definition*: **consistency**

$$\mathbf{lim}_{h\to 0}\mathbf{max}_{m\le j\le N}|\tau_j(h)| = 0, \quad \mathbf{lim}_{h\to 0}\mathbf{max}_{0\le j\le m-1}|y(t_j)-\alpha_j| = 0.$$

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- *Definition*: **convergence**

$$\mathbf{lim}_{h\to 0}\mathbf{max}_{0\le j\le N}\,|y(t_j)-w_j| = 0$$

Both similar to single-step case.

Stability Analysis: multistep methods (II)

- *Definition*: **consistency**

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- *Definition*: **convergence**

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Both similar to single-step case.

But stability will be different and much bigger issue

Stability Analysis: multistep methods (III)

single ODE $$\frac{dy}{dt} = f(t, y) = 0, \quad a \leq t \leq b, \quad y(a) = \alpha.$$

Solution is $y \equiv \alpha$.

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$$\begin{aligned} w_{j+1} &= a_{m-1}\, w_j + a_{m-2}\, w_{j-1} + \cdots + a_0\, w_{j+1-m} \\ &\quad + h\, F\left(t_j, w_{j+1}, w_j, \cdots, w_{j+1-m}\right), \\ &= a_{m-1}\, w_j + a_{m-2}\, w_{j-1} + \cdots + a_0\, w_{j+1-m}. \quad (F \equiv 0) \end{aligned}$$

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Minimum requirements on method

- $w_{j+1} \equiv \alpha$ for all j.
- w_{j+1} remains close to α in finite precision.

Finite recurrence relations (I)

Given $w_0 = \alpha_0,\ w_1 = \alpha_1, \cdots, w_{m-1} = \alpha_{m-1}$,

- for $j = m-1, m, m+1, \cdots$

$$w_{j+1} = a_{m-1}\, w_j + a_{m-2}\, w_{j-1} + \cdots + a_0\, w_{j+1-m} \quad (1)$$

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$$w_{j+1} \quad = \quad a_{m-1}\, w_j + a_{m-2}\, w_{j-1} + \cdots + a_0\, w_{j+1-m} \quad (1)$$

- To solve for w_j for all j, **assume**

$$\frac{w_{k+1}}{w_k} = \lambda \quad \text{for all} \quad k \quad (2)$$

- Recurrence becomes

$$\mathbf{P}(\lambda) \quad = \quad 0, \quad \mathbf{P}(\mu) \stackrel{def}{=} \mu^m - \left(a_{m-1}\,\mu^{m-1} + a_{m-2}\,\mu^{m-2} + \cdots + a_0\right).$$

- thus $\mu = \lambda$ must be a root of $\mathbf{P}(\mu) = 0$.
- $w_j \equiv 1$ satisfies (1) $\Longrightarrow \mu = 1$ should be a root of $\mathbf{P}(\mu) = 0$.

Finite recurrence relations (II)

- Recurrence relation

$$w_{j+1} \quad = \quad a_{m-1}\, w_j + a_{m-2}\, w_{j-1} + \cdots + a_0\, w_{j+1-m}.$$

- **characteristic polynomial**

$$\mathbf{P}(\mu) \quad \stackrel{def}{=} \quad \mu^m - \left(a_{m-1}\, \mu^{m-1} + a_{m-2}\, \mu^{m-2} + \cdots + a_0\right).$$

- If $\mathbf{P}(\mu)$ has m **distinct** roots $\mu_1, \cdots, \mu_m$, then

$$w_j = c_1\, \mu_1^j + c_2\, \mu_2^j + \cdots + c_m\, \mu_m^j, \quad j = 0, 1, \cdots m-1, m, \cdots$$

  for constants $c_1, c_2, \cdots c_m$ determined by the equations for $0 \le j \le m-1$.

Finite recurrence relations (III)

- Example recurrence relation

$$w_{j+1} \quad = \quad 3\,w_j - 2\,w_{j-1}. \quad (m = 2.)$$

- **characteristic polynomial**

$$\mathbf{P}(\mu) \quad = \quad \mu^2 - 3\,\mu^1 + 2 = (\mu - 1)(\mu - 2).$$

- Roots of $\mathbf{P}(\mu)$ are 1 and 2.
- recurrence solution

$$w_j = c_1 + c_2\,2^j, \quad j = 0, 1, 2, 3, \cdots$$

where

$$w_0 = c_1 + c_2, \quad w_1 = c_1 + 2\,c_2, \quad \text{or, equivalently}$$

$$c_1 = 2w_0 - w_1, \quad c_2 = w_1 - w_0.$$

Finite recurrence relations (IV)

- Example recurrence relation

$$w_{j+1} \quad = \quad 2\,w_j - 1\,w_{j-1}. \quad (m = 2.)$$

- **characteristic polynomial**

$$\mathbf{P}(\mu) \quad = \quad \mu^2 - 2\,\mu^1 + 1 = (\mu - 1)^2.$$

- Roots of $\mathbf{P}(\mu)$ are 1 and 1.
- recurrence solution

$$w_j = c_1 + j\,c_2, \quad j = 0, 1, 2, 3, \cdots$$

where

$$w_0 = c_1, \quad w_1 = w_1 - w_0.$$

Root conditions

Multistep method with $w_0 = \alpha$, $w_1 = \alpha_1, \cdots, w_{m-1} = \alpha_{m-1}$,

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w_{j+1} &= a_{m-1}\, w_j + a_{m-2}\, w_{j-1} + \cdots + a_0\, w_{j+1-m} \\
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root condition: every root μ_i of $\mathbf{P}(\mu)$ must satisfy $|\mu_i| \leq 1$

Assume multistep method satisfies root condition.

- **strongly stable**: $\mu = 1$ is only root of $\mathbf{P}(\mu)$ with magnitude 1.
- **weakly stable**: $\mathbf{P}(\mu)$ has more than one distinct root with magnitude 1.

Otherwise method is **unstable.**

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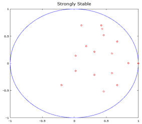
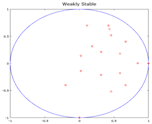


- **weakly stable**:



single ODE $$\frac{dy}{dt} = f(t,y), \quad a \le t \le b, \quad y(a) = \alpha.$$

Theorem: Assume multistep method with $w_0 = \alpha$, $w_1 = \alpha_1, \cdots, w_{m-1} = \alpha_{m-1}$,

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Assume the method is **consistent**, then

- The method is stable $\iff$ it satisfies root condition $\iff$ it is convergent.

example fourth-order methods

- 4-step Adams-Bashforth

$$
\begin{aligned}
w_{j+1} &= w_j + h\, F\left(t_j, w_j, w_{j-1}, w_{j-2}, w_{j-3}\right) \quad \text{where} \\
F\left(t_j, w_j, w_{j-1}, w_{j-2}, w_{j-3}\right) &= \frac{h}{24}\left(55 f(t_j, w_j) - 59 f(t_{j-1}, w_{j-1}) + 37 f(t_{j-2}, w_{j-2}) - 9 f(t_{j-3}, w_{j-3})\right)
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Roots of $\mathbf{P}(\mu)$ are $\pm 1, \pm\sqrt{-1}$

- satisfies root condition
- **weakly stable**, all roots have magnitude 1