- Will skip Section 5.8, *extrapolation methods for ODEs*.
- Notation and details for Chapter 5 messy and not all trivial.
- Brand new concepts to work through.

Multistep Methods

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

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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 (I): Constant approximations

- $f(t, y(t)) \approx f(t_j, y(t_j))$, 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

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

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leading to *backward* Euler's method

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

Implicit method, **much** harder to handle.

Examples: Linear approximation (II)

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

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

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

leading to Adams-Bashforth two-step explicit method

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

Examples (III): Linear approximation

- with $f(t_{j+1}, y(t_{j+1}))$ and $f(t_j, y(t_j))$

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

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

leading to *implicit* mid-point method

$$w_{j+1} = w_j + \frac{h}{2} \left(f(t_j, w_j) + f(t_{j+1}, w_{j+1}) \right), \quad \text{for} \quad j = 0, 1, \cdots$$

Examples (IV): m-step Explicit Method

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

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

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leading to *explicit* m-point method

$$\begin{aligned} w_{j+1} &= w_j + h\left(b_{m-1} f(t_j, w_j) + b_{m-2} f(t_{j-1}, w_{j-1}) \right. \\ &\quad \left. + \cdots + b_0 f(t_{j-m+1}, w_{j-m+1})\right), \\ &\quad \text{for} \quad j = m-1, m, \cdots \end{aligned}$$

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- $m = 4$: fourth-order Adams-Bashforth method

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

Examples (V): m-step Implicit Method

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

Examples (V): m-step Implicit Method

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

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

Examples (V): m-step Implicit Method

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

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

leading to *implicit* m-point method

$$\begin{aligned} w_{j+1} &= w_j + h\left(b_m f(t_{j+1}, w_{j+1}) + b_{m-1} f(t_j, w_j) \right. \\ &\quad \left. + b_{m-2} f(t_{j-1}, w_{j-1}) + \cdots + b_0 f(t_{j-m+1}, w_{j-m+1})\right), \\ &\quad \text{for} \quad j = m-1, m, \cdots \end{aligned}$$

Examples (V): m-step Implicit Method

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

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leading to *implicit* m-point method

$$\begin{aligned} w_{j+1} &= w_j + h\left(b_m f(t_{j+1}, w_{j+1}) + b_{m-1} f(t_j, w_j)\right. \\ &\quad \left. + b_{m-2} f(t_{j-1}, w_{j-1}) + \cdots + b_0 f(t_{j-m+1}, w_{j-m+1})\right), \\ &\quad \text{for} \quad j = m-1, m, \cdots \end{aligned}$$

- $m = 3$: fourth-order Adams-Moulton method

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

- **General m-step method**

$$
\begin{aligned}
w_{j+1} \quad = \quad & a_{m-1}w_j + a_{m-1}w_{j-1} + \cdots + a_0 w_{j-m+1} \\
& + h\left(b_m f\left(t_{j+1}, w_{j+1}\right) + b_{m-1} f\left(t_j, w_j\right)\right. \\
& \left. + b_{m-2} f\left(t_{j-1}, w_{j-1}\right) + \cdots + b_0 f\left(t_{j-m+1}, w_{j-m+1}\right)\right).
\end{aligned}
$$

- **explicit** if $b_m = 0$; **implicit** if $b_m \neq 0$.

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w_{j+1} \quad = \quad & a_{m-1}w_j + a_{m-1}w_{j-1} + \cdots + a_0 w_{j-m+1} \\
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& \left. + b_{m-2} f(t_{j-1}, w_{j-1}) + \cdots + b_0 f(t_{j-m+1}, w_{j-m+1})\right).
\end{aligned}
$$

- **explicit** if $b_m = 0$; **implicit** if $b_m \neq 0$.

$$\boxed{\textbf{LTE: } \text{assume } w_i \approx y(t_i), i \leq j}$$

$$
\begin{aligned}
\tau_{j+1}(h) \stackrel{def}{=} \quad & \frac{y(t_{j+1}) - (a_{m-1}y(t_j) + a_{m-1}y(t_{j-1}) + \cdots + a_0 y(t_{j-m+1}))}{h} \\
& - \left(b_m f(t_{j+1}, y(t_{j+1})) + b_{m-1} f(t_j, y(t_j))\right. \\
& \left. + b_{m-2} f(t_{j-1}, y(t_{j-1})) + \cdots + b_0 f(t_{j-m+1}, y(t_{j-m+1}))\right).
\end{aligned}
$$

example fourth-order Adams-Moulton method (I)

$$f(t, y(t)) = P(t) + R(t), \quad \text{with}$$

$$\begin{aligned} P(t) &= L_3(t) f(t_{j+1}, y(t_{j+1})) + L_2(t) f(t_j, y(t_j)) \\ &\quad + L_1(t) f(t_{j-1}, y(t_{j-1})) + L_0(t) f(t_{j-2}, y(t_{j-2})), \\ R(t) &= \frac{f^{(4)}(\xi_t, y(\xi_t))}{4!}(t - t_{j+1})(t - t_j)(t - t_{j-1})(t - t_{j-2}). \end{aligned}$$

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$$\begin{aligned} y(t_{j+1}) - y(t_j) &= \int_{t_j}^{t_{j+1}} f(t, y(t))\, dt = \int_{t_j}^{t_{j+1}} (P(t) + R(t))\, dt \\ &= f(t_{j+1}, y(t_{j+1})) \int_{t_j}^{t_{j+1}} L_3(t)\, dt + f(t_j, y(t_j)) \int_{t_j}^{t_{j+1}} L_2(t)\, dt \\ &\quad f(t_{j-1}, y(t_{j-1})) \int_{t_j}^{t_{j+1}} L_1(t)\, dt + f(t_{j-2}, y(t_{j-2})) \int_{t_j}^{t_{j+1}} L_0(t)\, dt \\ &\quad + \int_{t_j}^{t_{j+1}} \frac{f^{(4)}(\xi_t, y(\xi_t))}{4!}(t - t_{j+1})(t - t_j)(t - t_{j-1})(t - t_{j-2})\, dt \end{aligned}$$

example fourth-order Adams-Moulton method (II)

- 4-point interpolation on $f(t, y(t))$

$$
\begin{aligned}
y(t_{j+1}) = & \; y(t_j) + \int_{t_j}^{t_{j+1}} (P(t) + R(t))\, dt \\
= & \; y(t_j) + \\
& \frac{h}{24}(9f(t_{j+1}, y(t_{j+1})) + 19f(t_j, y(t_j)) - 5f(t_{j-1}, y(t_{j-1})) + f(t_{j-2}, y(t_{j-2})) \\
& + \frac{f^{(4)}(\xi, y(\xi))}{4!} \int_{t_j}^{t_{j+1}} (t - t_{j+1})(t - t_j)(t - t_{j-1})(t - t_{j-2})\, dt
\end{aligned}
$$

example fourth-order Adams-Moulton method (II)

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& + \frac{f^{(4)}(\xi, y(\xi))}{4!} \int_{t_j}^{t_{j+1}} (t - t_{j+1})(t - t_j)(t - t_{j-1})(t - t_{j-2})\, dt
\end{aligned}
$$

- 3-step fourth-order Adams-Moulton method

$$
\begin{aligned}
w_{j+1} &= w_j + \frac{h}{24}\,(9f(t_{j+1}, w_{j+1}) + 19f(t_j, w_j) - 5f(t_{j-1}, w_{j-1}) + f(t_{j-2}, w_{j-2})) \\
\textbf{LTE} &= \frac{f^{(4)}(\xi, y(\xi))}{4!\, h} \int_{t_j}^{t_{j+1}} (t - t_{j+1})(t - t_j)(t - t_{j-1})(t - t_{j-2})\, dt \\
&= -\frac{19}{720} f^{(4)}(\xi, y(\xi))\, h^4.
\end{aligned}
$$

example fourth-order Adams-Bashforth method

- 4-step and fourth-order

$$
\begin{aligned}
w_{j+1} &= w_j + \\
&\quad \frac{h}{24}\left(55f(t_j, w_j) - 59f(t_{j-1}, w_{j-1}) + 37f(t_{j-2}, w_{j-2}) - 9f(t_{j-3}, w_{j-3})\right) \\
\textbf{LTE} &= \frac{251}{720} f^{(4)}(\xi, y(\xi))\, h^4.
\end{aligned}
$$

example fourth-order Adams-Bashforth method

- 4-step and fourth-order

$$
\begin{aligned}
w_{j+1} &= w_j + \\
&\quad \frac{h}{24}\left(55f(t_j, w_j) - 59f(t_{j-1}, w_{j-1}) + 37f(t_{j-2}, w_{j-2}) - 9f(t_{j-3}, w_{j-3})\right) \\
\textbf{LTE} &= \frac{251}{720} f^{(4)}(\xi, y(\xi))\, h^4.
\end{aligned}
$$

$\boxed{\text{To be explicit or not to be?}}$

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

example fourth-order Adams-Bashforth method

- 4-step and fourth-order

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\begin{aligned}
w_{j+1} &= w_j + \\
&\quad \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) \\
\textbf{LTE} &= \frac{251}{720} f^{(4)}(\xi, y(\xi))\, h^4.
\end{aligned}
$$

To be explicit or not to be?

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

To be multistep or not to be?

- Multistep methods cheaper than Runge-Kutta.
- Multistep methods do not self-start.

experiment

$$\begin{aligned} \frac{dy}{dt} &= y - t^2 + 1, \quad 0 \le t \le 2, \quad y(a) = 0.5, \\ \text{exact solution } y(t) &= (t+1)^2 - 0.5\, e^t. \end{aligned}$$

experiment

$$\begin{aligned} \frac{dy}{dt} &= y - t^2 + 1, \quad 0 \le t \le 2, \quad y(a) = 0.5, \\ \text{exact solution } y(t) &= (t+1)^2 - 0.5\, e^t. \end{aligned}$$

- $N = 10, h = 0.2, t_j = 0.2j, 0 \le j \le N.$

experiment

$$\begin{aligned} \frac{dy}{dt} &= y - t^2 + 1, \quad 0 \le t \le 2, \quad y(a) = 0.5, \\ \text{exact solution } y(t) &= (t+1)^2 - 0.5\, e^t. \end{aligned}$$

- $N = 10, h = 0.2, t_j = 0.2j, 0 \le j \le N.$
- Adams-Bashforth method

$$\begin{aligned} w_{j+1} &= w_j + \\ &\quad \frac{h}{24}\left(55f(t_j, w_j) - 59f(t_{j-1}, w_{j-1}) + 37f(t_{j-2}, w_{j-2}) - 9f(t_{j-3}, w_{j-3})\right) \\ &= \frac{1}{24}\left(35w_j - 11.8w_{j-1} + 7.4w_{j-2} - 1.8w_{j-3} - 0.192j^2 - 0.192j + 4.736\right). \end{aligned}$$

- 4 initial values to start.

experiment

$$\begin{aligned} \frac{dy}{dt} &= y - t^2 + 1, \quad 0 \le t \le 2, \quad y(a) = 0.5, \\ \text{exact solution } y(t) &= (t+1)^2 - 0.5\, e^t. \end{aligned}$$

- $N = 10, h = 0.2, t_j = 0.2j, 0 \le j \le N.$

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$$\begin{aligned} \frac{dy}{dt} &= y - t^2 + 1, \quad 0 \le t \le 2, \quad y(a) = 0.5, \\ \text{exact solution } y(t) &= (t+1)^2 - 0.5\, e^t. \end{aligned}$$

- $N = 10, h = 0.2, t_j = 0.2j, 0 \le j \le N.$
- Adams-Moulton method

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

experiment

$$\begin{aligned} \frac{dy}{dt} &= y - t^2 + 1, \quad 0 \le t \le 2, \quad y(a) = 0.5, \\ \text{exact solution } y(t) &= (t+1)^2 - 0.5\, e^t. \end{aligned}$$

- $N = 10, h = 0.2, t_j = 0.2j, 0 \le j \le N.$
- Adams-Moulton method

$$\begin{aligned} w_{j+1} &= w_j + \frac{h}{24}\left(9f(t_{j+1}, w_{j+1}) + 19f(t_j, w_j) - 5f(t_{j-1}, w_{j-1}) + f(t_{j-2}, w_{j-2})\right) \\ &= \frac{1}{24}\left(1.8w_{j+1} + 27.8w_j - w_{j-1} + 0.2w_{j-2} - 0.192j^2 - 0.192j + 4.736\right) \\ &= \frac{1}{22.2}\left(27.8w_j - w_{j-1} + 0.2w_{j-2} - 0.192j^2 - 0.192j + 4.736\right) \end{aligned}$$

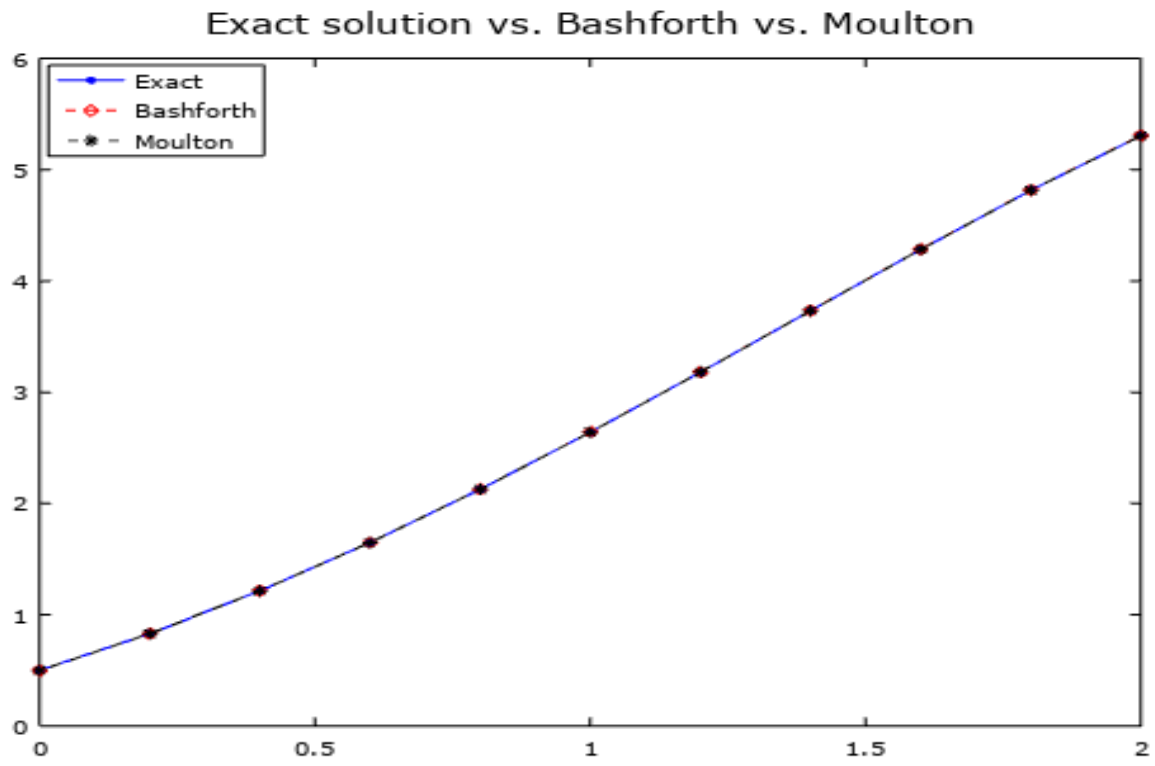
- 3 initial values to start.

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

Solution plot

$$\begin{aligned} \frac{dy}{dt} &= y - t^2 + 1, \quad 0 \le t \le 2, \quad y(a) = 0.5, \\ \text{exact solution } y(t) &= (t+1)^2 - 0.5\, e^t. \end{aligned}$$



Error plot

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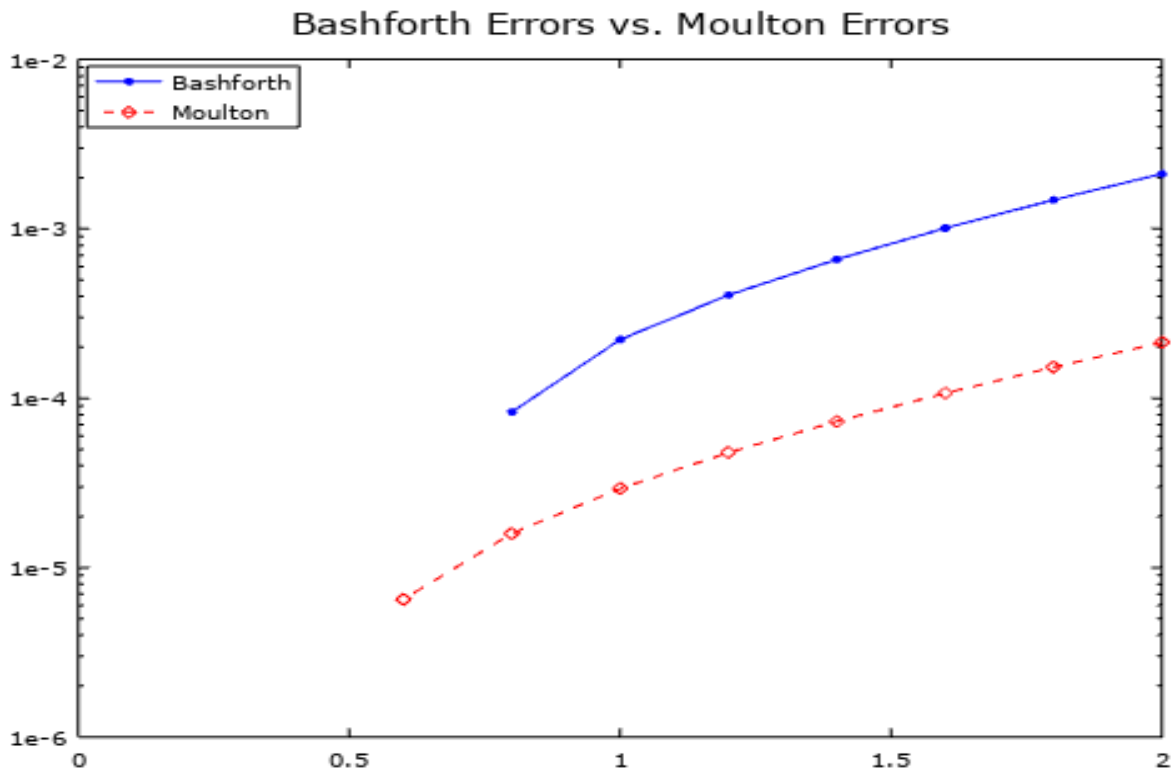

Predictor-Corrector Methods (I)

- Adams-Moulton method is non-linear equation for w_{j+1}

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

- Adams-Bashforth method explicit but less accurate:

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

$\boxed{\text{Fixed-point iteration on Moulton, with Bashforth initial guess}}$

Predictor-Corrector Methods (II)

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

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

- Adams-Moulton **Corrector**:

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

```
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)

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

Variable-step method based on Adams-Bashforth and Adams-Moulton

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Assumptions

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

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Goals

- Make sure **LTE** $|\tau_{j+1}(h_{j+1})| \le \tau$

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- Given tolerance $\tau > 0$,
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Goals

- Make sure **LTE** $|\tau_{j+1}(h_{j+1})| \le \tau$

Approach

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

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

Adaptive Error Control (II)

- Adams-Bashforth **Predictor**:

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

- Adams-Bashforth interpolation relation, $y_i \stackrel{def}{=} y(t_i)$:

$$\begin{aligned} y_{j+1} &= y_j + \frac{h}{24}\left(55f(t_j, y_j) - 59f(t_{j-1}, y_{j-1}) + 37f(t_{j-2}, y_{j-2}) - 9f(t_{j-3}, y_{j-3})\right) \\ &\quad + \frac{251}{720} f^{(4)}(\xi, y(\xi))\, h^5 \\ &= w_{j+1}^{\mathbf{p}} + \frac{251}{720} f^{(4)}(\xi, y(\xi))\, h^5. \end{aligned}$$

Adaptive Error Control (III)

- Adams-Moulton **Corrector**:

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

- Adams-Moulton interpolation relation, $y_i \stackrel{def}{=} y(t_i)$:

$$\begin{aligned} y_{j+1} &= y_j + \frac{h}{24}\left(9f(t_{j+1}, y_{j+1}) + 19f(t_j, y_j) - 5f(t_{j-1}, y_{j-1}) + f(t_{j-2}, y_{j-2})\right) \\ &\quad - \frac{19}{720} f^{(4)}(\widetilde{\xi}, y(\widetilde{\xi}))\, h^5 \\ &\approx w_j + \frac{h}{24}\left(9f(t_{j+1}, w_{j+1}^{\mathbf{p}}) + 19f(t_j, w_j) - 5f(t_{j-1}, w_{j-1}) + f(t_{j-2}, w_{j-2})\right) \\ &\quad - \frac{19}{720} f^{(4)}(\widetilde{\xi}, y(\widetilde{\xi}))\, h^5 \\ &\approx w_{j+1} - \frac{19}{720} f^{(4)}(\widetilde{\xi}, y(\widetilde{\xi}))\, h^5. \end{aligned}$$

Adaptive Error Control (IV)

- **Predictor LTE**:

$$y_{j+1} \approx w_{j+1}^{\mathbf{p}} + \frac{251}{720} f^{(4)}(\xi, y(\xi))\, h^5.$$

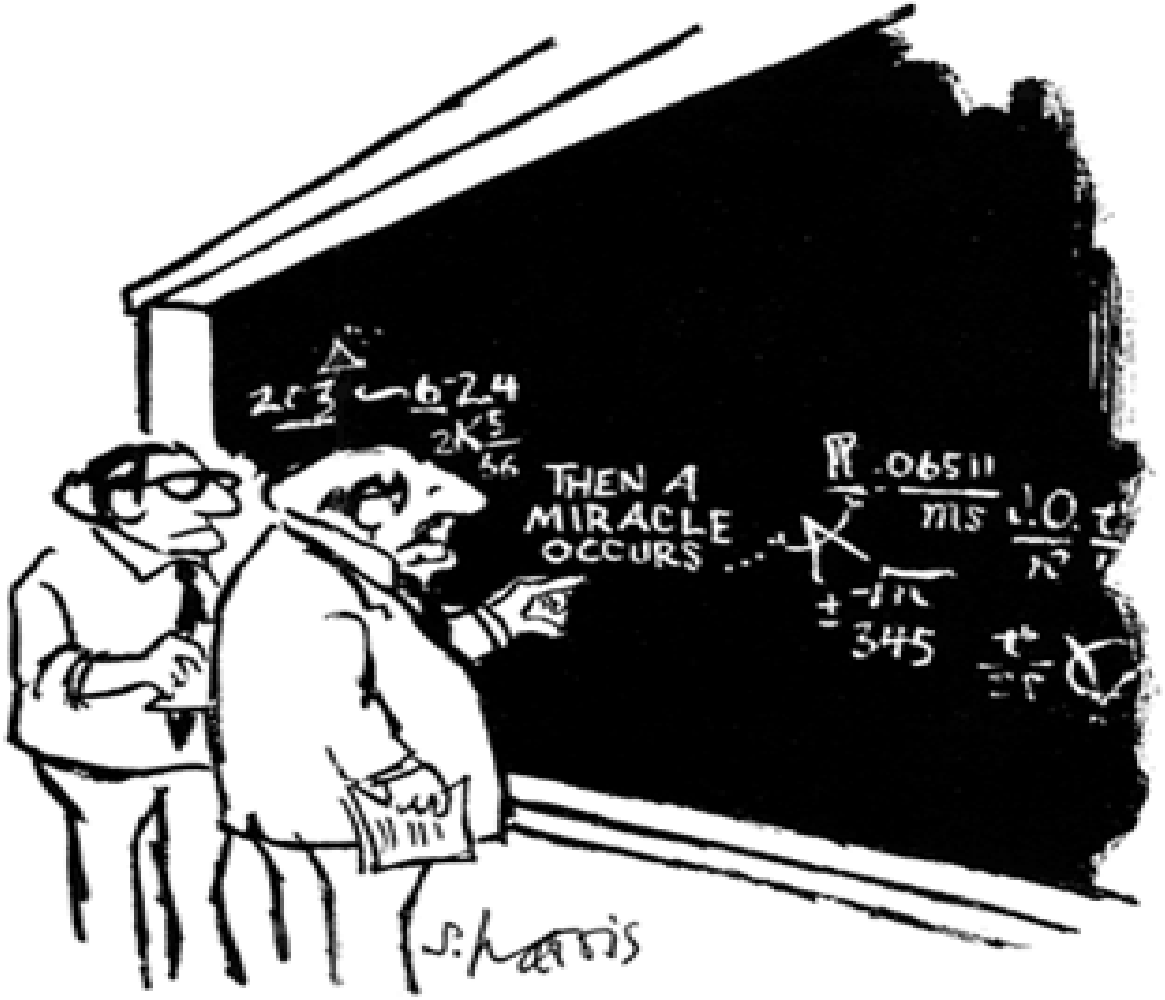
- **Corrector LTE**:

$$y_{j+1} \approx w_{j+1} - \frac{19}{720} f^{(4)}(\widetilde{\xi}, y(\widetilde{\xi}))\, h^5.$$

- <u>**Assume**</u> $f^{(4)}(\xi, y(\xi)) \approx f^{(4)}(\widetilde{\xi}, y(\widetilde{\xi}))$:

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

$$\boxed{\tau_{j+1}(h) = \frac{y_{j+1} - w_{j+1}}{h} \approx -\frac{19}{270}\, \frac{w_{j+1} - w_{j+1}^{\mathbf{p}}}{h}}.$$



"I think you should be more explicit here in step two."

step-size selection (I)

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

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

- Since $\quad \tau_{j+1}(h) = O\left(h^4\right)$,

  <u>assume</u> $\quad |\tau_{j+1}(h)| \approx K\,h^4 \quad$ where K is independent of h.

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- K should satisfy

$$K\,h^4 \approx \left|\frac{19}{270}\,\frac{w_{j+1} - w_{j+1}^{\mathbf{p}}}{h}\right|.$$

- **Assume** LTE for new step-size $q\,h$ satisfies given tolerance τ:

$$|\tau_{j+1}(q\,h)| \leq \tau, \quad \text{need to estimate } q.$$

step-size selection (II)

$$\boxed{\text{LTE estimate: } K\,h^4 \approx |\tau_{j+1}(h)| \approx \left| \frac{19}{270}\,\frac{w_{j+1} - w_{j+1}^{\mathbf{p}}}{h} \right|}$$

step-size selection (II)

$$\boxed{\text{LTE estimate: } K\,h^4 \approx |\tau_{j+1}(h)| \approx \left|\frac{19}{270}\,\frac{w_{j+1} - w_{j+1}^{\mathbf{p}}}{h}\right|}$$

- **Assume** LTE for $q\,h$ satisfies given tolerance τ:

$$\begin{aligned} |\tau_{j+1}(q\,h)| &\approx \left|K\,(q\,h)^4\right| = q^4\,\left|K\,h^4\right| \\ &\approx q^4\,\left|\frac{19}{270}\,\frac{w_{j+1} - w_{j+1}^{\mathbf{p}}}{h}\right| \leq \tau. \end{aligned}$$

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$$\boxed{\text{new step-size estimate: } q\,h \lesssim \left|\frac{270\tau\,h}{19(w_{j+1} - w_{j+1}^{\mathbf{p}})}\right|^{\frac{1}{4}}\,h}$$

Review: Predictor-Corrector Methods

- Adams-Bashforth **Predictor**:

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

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Summary

- Adams-Bashforth **Predictor**:

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

$$q\,h \lesssim \left|\frac{270\tau\,h}{19(w_{j+1} - w_{j+1}^{\mathbf{p}})}\right|^{\frac{1}{4}} h.$$

step-size selection procedure

- compute a conservative value for q:

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

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

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- step-size can't be too big:

$$h = \mathbf{min}\left(h, h_{\mathbf{max}}\right).$$

- step-size can't be too small:

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

Adaptive Adams 4th order Predictor Corrector: solution plots

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

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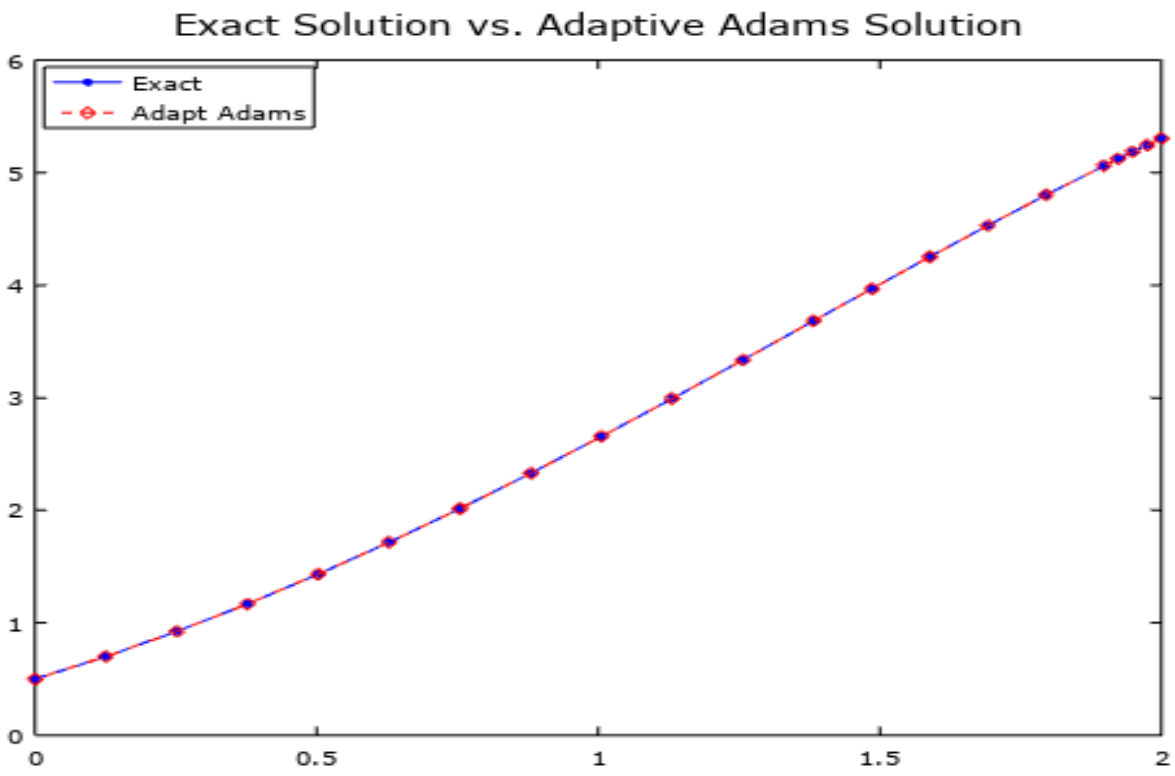

Solution Data

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	$3.918e-07$	$1.81e-05$

Adaptive Adams 4th order Predictor Corrector: LTE errors

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

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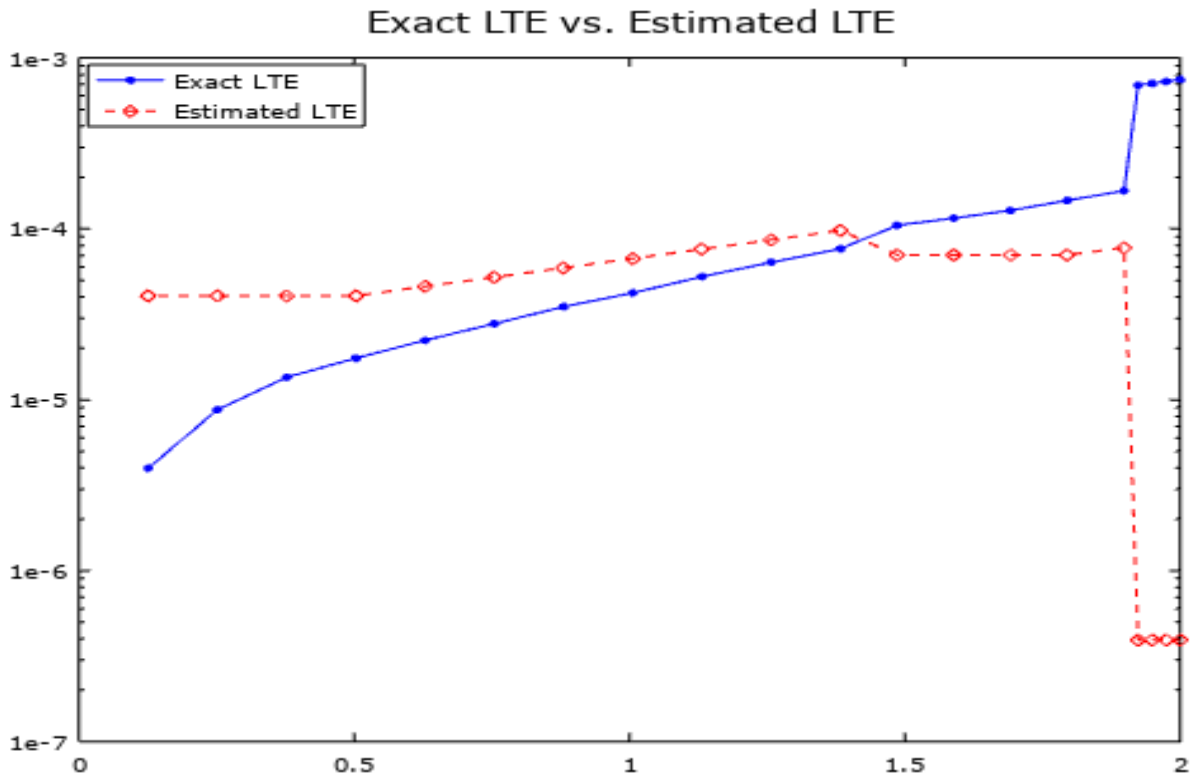


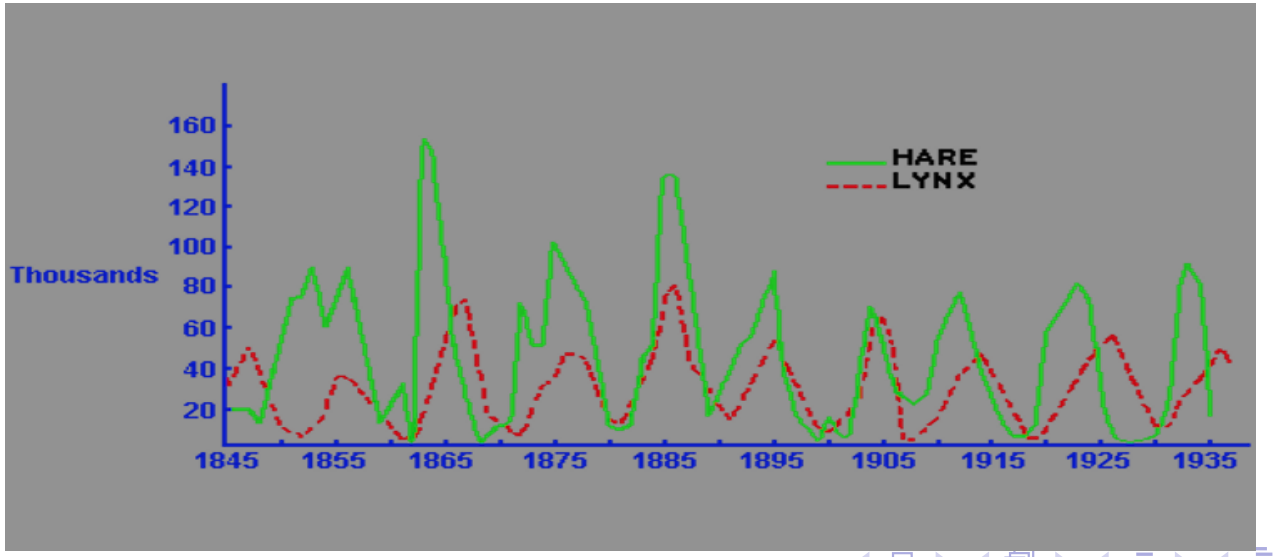
Circle of life: Predator and Prey/Boom And Bust

- Canadian Lynx and Snowshoe Hares in Canadian Boreal Forest

Circle of life: Predator and Prey/Boom And Bust

- Canadian Lynx and Snowshoe Hares in Canadian Boreal Forest

- Boom And Bust



Predator and Prey Model

- Notation

$$x \stackrel{def}{=} \text{predator population}, \quad y \stackrel{def}{=} \text{prey population}.$$

- population dynamics,

$$\begin{aligned} \frac{dx}{dt} &= -\alpha y + \beta\, x\, y, \\ \frac{dy}{dt} &= \gamma x - \delta\, x\, y. \end{aligned}$$

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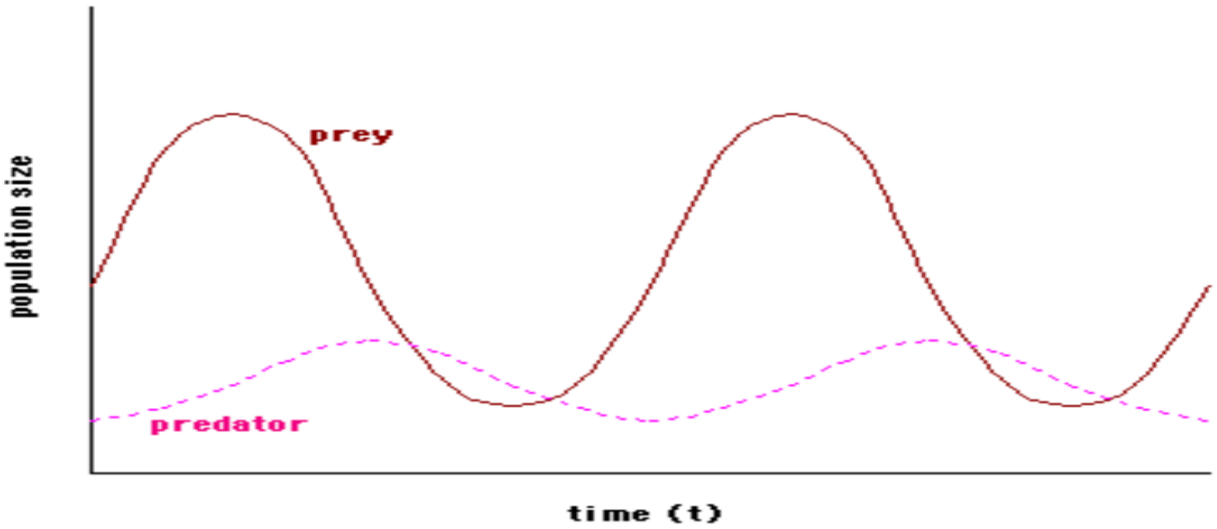
- Solution: Boom and Bust



System of ODEs

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

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

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

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

System of ODEs: vector form

$$\mathbf{u} \stackrel{def}{=} \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_m \end{pmatrix}, \quad \mathbf{f}(t, \mathbf{u}) \stackrel{def}{=} \begin{pmatrix} f_1(t, u_1, u_2, \cdots, u_m) \\ f_2(t, u_1, u_2, \cdots, u_m) \\ \vdots \\ f_m(t, u_1, u_2, \cdots, u_m) \end{pmatrix}, \quad \alpha \stackrel{def}{=} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_m \end{pmatrix}.$$

System of m first-order ODEs:

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

with initial condition

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

Higher order ODEs

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

for some $m > 1$, with initial conditions

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

Higher order ODEs

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for some $m > 1$, with initial conditions

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

$$\mathbf{u} = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_m \end{pmatrix} \stackrel{def}{=} \begin{pmatrix} y \\ y' \\ \vdots \\ y^{(m-1)} \end{pmatrix}, \quad \mathbf{f}(t, \mathbf{u}) \stackrel{def}{=} \begin{pmatrix} u_2 \\ u_3 \\ \vdots \\ u_m \\ f(t, u_1, u_2, \cdots, u_m) \end{pmatrix}.$$

Higher order ODEs

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

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System of m first-order ODEs:

$$\frac{d\mathbf{u}}{dt} = \mathbf{f}(t, \mathbf{u}), \quad a \le t \le b, \quad \text{with} \quad \mathbf{u}(a) = \alpha \stackrel{def}{=} \begin{pmatrix} \alpha \\ \alpha' \\ \vdots \\ \alpha^{(m-1)} \end{pmatrix}.$$

Vector Lipschitz condition (I)

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

on the set

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

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

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

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

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 $t \in [a, b]$.

Recall a scalar method

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

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Runge-Kutta 4th order method:

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

$$
\begin{aligned}
k_1 &= h\, f(t_j, w_j), \\
k_2 &= h\, f(t_j + \frac{h}{2}, w_j + \frac{1}{2} k_1), \\
k_3 &= h\, f(t_j + \frac{h}{2}, w_j + \frac{1}{2} k_2), \\
k_4 &= h\, f(t_{j+1}, w_j + k_3), \\
w_{j+1} &= w_j + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)
\end{aligned}
$$

scalar method is vector method

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\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}
$$

example: Lotka-Volterra predator-prey model

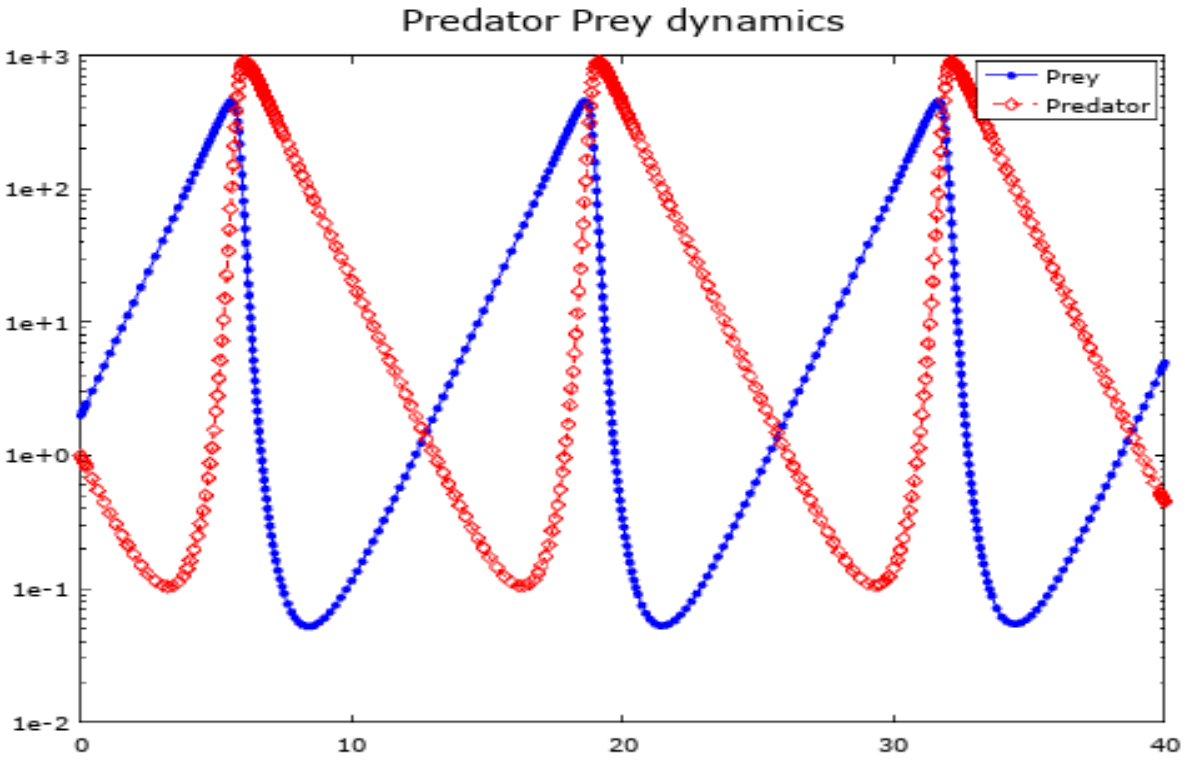
- `matlab` function *lotka*

$$\begin{aligned} x' &= x - 0.01\,x\,y, \\ y' &= -y + 0.02\,x\,y. \end{aligned}$$

- `matlab` command

$$[t, y] = \textbf{ode45}(\text{@lotka}, [0, 40], [2, 1]);$$

Predator Prey dynamics



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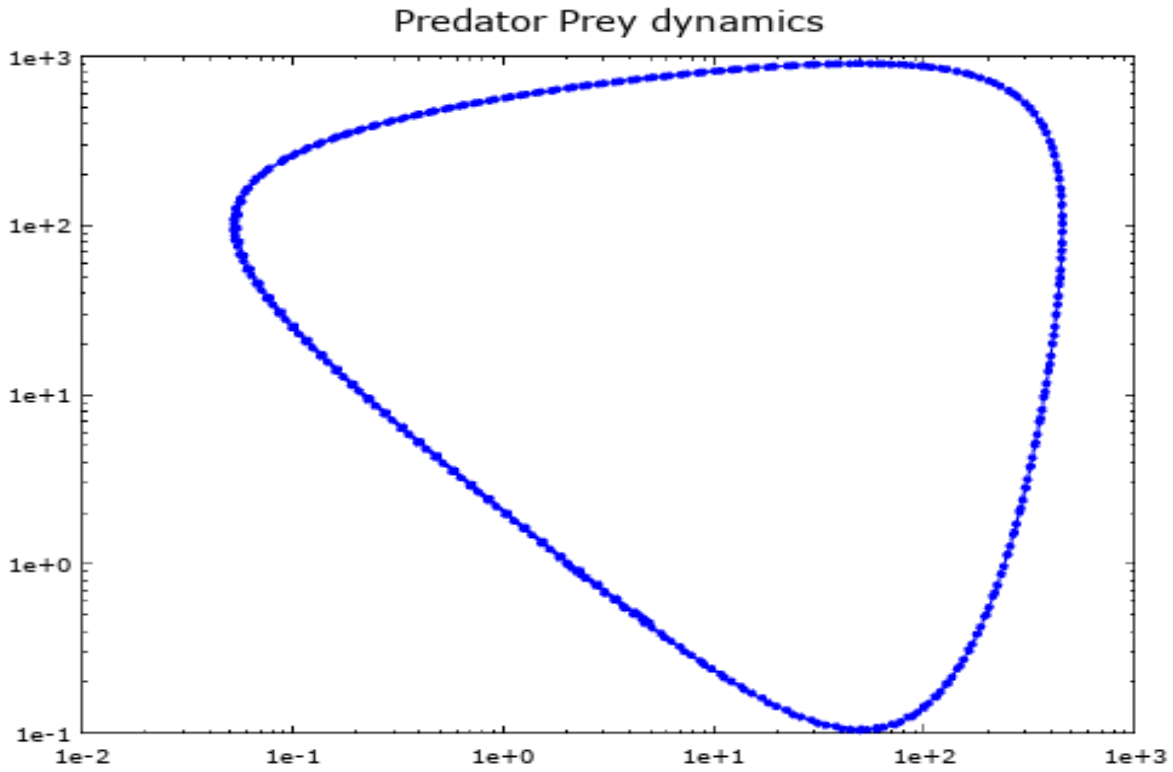

Stability Analysis for one-step methods

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

$$w_{j+1} = w_j + h\,\phi(t_j, w_j, h).$$

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$$\tau_j(h) = \frac{y(t_{j+1}) - y(t_j)}{h} - \phi(t_j, y(t_j), h).$$

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$$\mathbf{lim}_{h\to 0}\mathbf{max}_{0\le j\le N}\,|\tau_j(h)| = 0, \quad x_j = a + j\,h.$$

least of requirements of an ODE method:

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least of requirements of an ODE method:

- *Definition*: **convergent**

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

Prior analysis on Euler's Method

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$$\begin{aligned} |f(t, y_1) - f(t, y_2)| &\leq L\,|y_1 - y_2| \quad \text{on domain} \\ D &= \{(t, y) \quad | \quad a \leq t \leq b, \quad -\infty < y < \infty\}. \end{aligned}$$

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Let $w_0, w_1, \cdots, w_N$ be the approximations generated by Euler's method for some positive integer N. Then for each $j = 0, 1, \cdots, N$,

$$|y(t_j) - w_j| \le \frac{hM}{2L}\left(e^{L(t_j - a)} - 1\right),$$

where $h = (b - a)/N, \quad t_j = a + j\,h$, $M = \mathbf{max}_{t \in [a,b]}\,|y''(t)|$.

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Euler method:

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

$$w_{j+1} = w_j + h\, f(t_j, w_j).$$

- **LTE**

$$|\tau_j(h)| = \left| \frac{y(t_{j+1}) - y(t_j)}{h} - f(t_j, y(t_j)) \right| = \frac{h}{2} \left| \frac{df}{dt} \left(\widetilde{t}_j, y(\widetilde{t}_j) \right) \right| \longrightarrow 0.$$

- prior convergence analysis:

$$|y(t_j) - w_j| \le \frac{M\, h}{2L} \left| e^{L(b-a)} - 1 \right| \longrightarrow 0.$$

Review: Well-posed problem

Definition in English: ODE is well-posed if

- A unique ODE solution exists, and
- Small changes (perturbation) to ODE imply small changes to solution.

Review: Well-posed problem

The initial-value problem

$$\frac{dy}{dt} = f(t, y), \quad a \le t \le b, \quad y(a) = \alpha, \tag{5.2}$$

is said to be a **well-posed problem** if:

- A unique solution, $y(t)$, to the problem exists, and
- There exist constants $\varepsilon_0 > 0$ and $k > 0$ such that for any ε, with $\varepsilon_0 > \varepsilon > 0$, whenever $\delta(t)$ is continuous with $|\delta(t)| < \varepsilon$ for all t in $[a, b]$, and when $|\delta_0| < \varepsilon$, the initial-value problem

$$\frac{dz}{dt} = f(t, z) + \delta(t), \quad a \le t \le b, \quad z(a) = \alpha + \delta_0, \tag{5.3}$$

has a unique solution $z(t)$ that satisfies

$$|z(t) - y(t)| < k\varepsilon \quad \text{for all } t \text{ in } [a, b].$$

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Theorem

Suppose $D = \{(t, y) \mid a \le t \le b \text{ and } -\infty < y < \infty\}$. If f is continuous and satisfies a Lipschitz condition in the variable y on the set D, then the initial-value problem

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

is well-posed. ∎

Well-posed problem vs. Stable method

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Well-posed problem vs. Stable method

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A *method* is **stable**

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

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

Theorem: Suppose a one-step method with $w_0 = \alpha$,

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

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Suppose that $\phi(t, w, h)$ is continuous and satisfies Lipschitz condition with Lipschitz constant L, for $0 < h < h_0$.

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Then

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

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

-

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

example: Modified Euler's Method

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

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

Solution: For Modified Euler's Method,

$$\phi(t, w, h) = \frac{h}{2}\left(f(t, w) + f(t + h, w + h\, f(t, w))\right).$$

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&= \frac{1}{2}\left(f(t, w) - f(t, \widehat{w})\right) \\
&+ \frac{1}{2}\left(f(t + h, w + h\, f(t, w)) - f(t + h, \widehat{w} + h\, f(t, \widehat{w}))\right).
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\end{aligned}$$

$$\begin{aligned}
|\phi(t, w, h) - \phi(t, \widehat{w}, h)| &\leq \frac{L}{2}|w - \widehat{w}| \\
&\quad + \frac{L}{2}\left|w + h\, f(t, w) - \widehat{w} - h\, f(t, \widehat{w})\right| \\
&\leq \left(L + \frac{1}{2}hL^2\right)|w - \widehat{w}|.
\end{aligned}$$