General 2nd order Runge-Kutta Methods

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

$$w_{j+1} = w_j + h\left(a_1 f(t_j, w_j) + a_2 f\left(t_j + \alpha_2, w_j + \delta_2 f(t_j, w_j)\right)\right).$$

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local truncation error

$$\tau_{j+1}(h) = \frac{y(t_{j+1}) - y(t_j)}{h} - \left(a_1 f(t_j, y(t_j)) + a_2 f\left(t_j + \alpha_2, y(t_j) + \delta_2 f(t_j, y(t_j))\right)\right)$$

$$= y'(t_j) + \frac{h}{2} y''(t_j) + O(h^2)$$

$$- \left((a_1 + a_2) f(t_j, y(t_j)) + a_2 \alpha_2 \frac{\partial f}{\partial t}(t_j, y(t_j)) + a_2 \delta_2 f(t_j, y(t_j)) \frac{\partial f}{\partial y}(t_j, y(t_j)) + O(h^2)\right).$$

local truncation error

$$\begin{aligned}\tau_{j+1}(h) = \;& y'(t_j) + \frac{h}{2} y''(t_j) + O(h^2) \\ & - \Bigg((a_1 + a_2)\, f(t_j, y(t_j)) + a_2\, \alpha_2\, \frac{\partial f}{\partial t}(t_j, y(t_j)) \\ & \quad + \quad a_2\, \delta_2 f(t_j, y(t_j)) \frac{\partial f}{\partial y}(t_j, y(t_j)) + O(h^2) \Bigg) .\end{aligned}$$

where $y'(t_j) = f(t_j, y(t_j))$,

local truncation error

$$
\begin{aligned}
\tau_{j+1}(h) = \;& y'(t_j) + \frac{h}{2} y''(t_j) + O(h^2) \\
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& \quad + \quad a_2\, \delta_2 f(t_j, y(t_j)) \frac{\partial f}{\partial y}(t_j, y(t_j)) + O(h^2) \Bigg) .
\end{aligned}
$$

where $y'(t_j) = f(t_j, y(t_j))$,

$$
y''(t_j) = \frac{d\, f}{d\, t}(t_j, y(t_j)) = \frac{\partial f}{\partial t}(t_j, y(t_j)) + f(t_j, y(t_j)) \frac{\partial f}{\partial y}(t_j, y(t_j)).
$$

For any choice with

$$
a_1 + a_2 = 1, \quad a_2\, \alpha_2 = a_2\, \delta_2 = \frac{h}{2},
$$

we have a second order method

$$
\tau_{j+1}(h) = O(h^2).
$$

local truncation error

$$\tau_{j+1}(h) = y'(t_j) + \frac{h}{2} y''(t_j) + O(h^2)$$
$$- \left((a_1 + a_2)\, f(t_j, y(t_j)) + a_2\, \alpha_2\, \frac{\partial f}{\partial t}(t_j, y(t_j)) \right.$$
$$\left. + \quad a_2\, \delta_2 f(t_j, y(t_j)) \frac{\partial f}{\partial y}(t_j, y(t_j)) + O(h^2) \right).$$

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Four parameters, three equations

General 2nd order Runge-Kutta Methods

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

$$w_{j+1} \quad = \quad w_j + h\left(a_1 f(t_j, w_j) + a_2 f\left(t_j + \alpha_2, w_j + \delta_2 f(t_j, w_j)\right)\right).$$

$$a_1 + a_2 = 1, \quad a_2\,\alpha_2 = a_2\,\delta_2 = \frac{h}{2},$$

- **Midpoint method**: $a_1 = 0, a_2 = 1, \alpha_2 = \delta_2 = \frac{h}{2}$,

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

- **Modified Euler method**: $a_1 = a_2 = \frac{1}{2}, \alpha_2 = \delta_2 = h$,

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

3rd order Runge-Kutta Method (rarely used in practice)

$$w_0 = \alpha;$$
$$\text{for} \quad j = 0, 1, \cdots, N-1,$$

$$w_{j+1} = w_j + \frac{h}{4}\left(f(t_j, w_j) + 3f\left(t_j + \frac{2h}{3}, w_j + \frac{2h}{3} f(t_j + \frac{h}{3}, w_j + \frac{h}{3} f(t_j, w_j)) \right)\right)$$
$$\stackrel{def}{=} w_j + h\,\phi(t_j, w_j).$$

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$$\stackrel{def}{=} w_j + h\,\phi(t_j, w_j).$$

local truncation error

$$\tau_{j+1}(h) = \frac{y(t_{j+1})y(t_j)}{h} - \phi(t_j, y(t_j)) = O(h^3).$$

4th order Runge-Kutta Method

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

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

4 function evaluations per step

Example

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

exact solution $\quad y(t) = (1+t)^2 - 0.5\, e^t.$

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t_i	Exact	Euler $h = 0.025$	Modified Euler $h = 0.05$	Runge-Kutta Order Four $h = 0.1$
0.0	0.5000000	0.5000000	0.5000000	0.5000000
0.1	0.6574145	0.6554982	0.6573085	0.6574144
0.2	0.8292986	0.8253385	0.8290778	0.8292983
0.3	1.0150706	1.0089334	1.0147254	1.0150701
0.4	1.2140877	1.2056345	1.2136079	1.2140869
0.5	1.4256394	1.4147264	1.4250141	1.4256384

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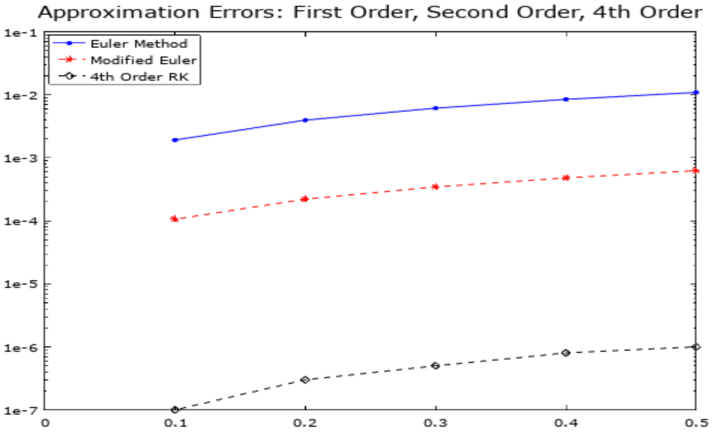

Adaptive Error Control (I)

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

Consider a variable-step method with a well-chosen function $\phi(t, w, h)$:

- $w_0 = \alpha$.
- for $j = 0, 1, \cdots$,
  - **choose** step-size $h_j = t_{j+1} - t_j$,
  - **set** $w_{j+1} = w_j + h_j \, \phi(t_j, w_j, h_j)$.

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Adaptively choose step-size to satisfy given tolerance

Adaptive Error Control (II)

- Given an **order-n** method
  - $w_0 = \alpha$.
  - for $j = 0, 1, \cdots,$

$$w_{j+1} = w_j + h\,\phi\left(t_j, w_j, h\right), \quad h = t_{j+1} - t_j,$$

  - **local truncation error** (LTE)

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

- Given tolerance $\tau > 0$, we would like to estimate **largest** step-size h for which

$$|\tau_{j+1}(h)| \lesssim \tau.$$

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

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

LTE Estimation (I)

- Assume $\quad w_j \approx y(t_j), \quad \widetilde{w}_j \approx y(t_j)$ (only estimating **LTE**).

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

- $\widetilde{\phi}(t, w, h)$ is order-$(n+1)$ method,

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

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- therefore

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

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

step-size selection (I)

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

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- Since $\tau_{j+1}(h) = O\left(h^n\right)$, **assume**

  $\tau_{j+1}(h) \approx K\, h^n$ where K is independent of h.

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- K should satisfy

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

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

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

step-size selection (II)

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

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$$\text{new step-size estimate: } q\,h \lesssim \left| \frac{\epsilon\,h}{\widetilde{w}_{j+1} - w_{j+1}} \right|^{\frac{1}{n}} h$$

Summary

- Given **order-n** method

$$w_{j+1} = w_j + h\,\phi\,(t_j, w_j, h)\,, \quad h = t_{j+1} - t_j, \quad j \geq 0,$$

- and given **order-$(n+1)$** method

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

- for each j, compute

$$\begin{aligned} w_{j+1} &= w_j + h\,\phi\,(t_j, w_j, h)\,, \\ \widetilde{w}_{j+1} &= w_j + h\,\widetilde{\phi}\,(t_j, w_j, h)\,, \end{aligned}$$

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

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

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

$$
\begin{aligned}
w_{j+1} &= w_j + \frac{25}{216}k_1 + \frac{1408}{2565}k_3 + \frac{2197}{4104}k_4 - \frac{1}{5}k_5, \\
\widetilde{w}_{j+1} &= w_j + \frac{16}{135}k_1 + \frac{6656}{12825}k_3 + \frac{28561}{56430}k_4 - \frac{9}{50}k_5 + \frac{2}{55}k_6, \quad \text{where}
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k_1 = h\,f\left(t_j, w_j\right),
$$

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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}
$$

Dormand-Prince (ode45): 4^{th} order method, 5^{th} order estimate

$$
\begin{aligned}
k_1 &= h\, f\left(t_j, w_j\right), \\
k_2 &= h\, f\left(t_j + \frac{h}{5}, w_j + \frac{1}{5}\, k_1\right), \\
k_3 &= h\, f\left(t_j + \frac{3h}{10}, w_j + \frac{3}{40}\, k_1 + \frac{9}{40}\, k_2\right), \\
k_4 &= h\, f\left(t_j + \frac{4h}{5}, w_j + \frac{44}{45}\, k_1 - \frac{56}{15}\, k_2 + \frac{32}{9}\, k_3\right), \\
k_5 &= h\, f\left(t_j + \frac{8h}{9}, w_j + \frac{19372}{6561}\, k_1 - \frac{25360}{2187}\, k_2 + \frac{64448}{6561}\, k_3 - \frac{212}{729}\, k_4\right), \\
k_6 &= h\, f\left(t_j + h, w_j - \frac{9017}{3168}\, k_1 - \frac{355}{33}\, k_2 + \frac{46732}{5247}\, k_3 + \frac{49}{176}\, k_4 - \frac{5103}{18656}\, k_5\right), \\
w_{j+1} &= w_j + \frac{35}{384} k_1 + \frac{500}{1113} k_3 + \frac{125}{192} k_4 - \frac{2187}{6784} k_5 + \frac{11}{84} k_6, \\
k_7 &= h\, f\left(t_{j+1}, w_{j+1}\right).
\end{aligned}
$$

$$
\widetilde{w}_{j+1} = w_j + \frac{5179}{57600} k_1 + \frac{7571}{16695} k_3 + \frac{393}{640} k_4 - \frac{92097}{339200} k_5 + \frac{187}{2100} k_6 + \frac{1}{40} k_7.
$$

Runge-Kutta-Fehlberg vs. Dormand-Prince

- Both methods require 6 function evaluations per step.
- Runge-Kutta-Fehlberg ensures a small **LTE** of fourth order method.
- Dormand-Prince chooses coefficients to minimize **LTE** of fifth order method.
- Dormand-Prince better allows an extrapolation step for better integration accuracy.
- Dormand-Prince is basis for `ode45` in matlab.

Runge-Kutta-Fehlberg: step-size selection procedure

- compute a conservative value for q:

$$q = \left| \frac{\epsilon\, h}{\mathbf{2}\left(\widetilde{w}_{j+1} - w_{j+1}\right)} \right|^{\frac{1}{4}}.$$

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

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

- step-size can't be too small:

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

Runge-Kutta-Fehlberg: example

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

exact solution $$y(t) = (1 + t)^2 - 0.5\, e^t.$$

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t_i	Exact	Euler $h = 0.025$	Modified Euler $h = 0.05$	Runge-Kutta Order Four $h = 0.1$
0.0	0.5000000	0.5000000	0.5000000	0.5000000
0.1	0.6574145	0.6554982	0.6573085	0.6574144
0.2	0.8292986	0.8253385	0.8290778	0.8292983
0.3	1.0150706	1.0089334	1.0147254	1.0150701
0.4	1.2140877	1.2056345	1.2136079	1.2140869
0.5	1.4256394	1.4147264	1.4250141	1.4256384

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t_j	h_j	$y(t_j)$	w_j	$\widetilde{w}_j$
0.00000	0.00000	0.50000	0.50000	0.50000
0.25000	0.25000	0.92049	0.92049	0.92049
0.48655	0.23655	1.39649	1.39649	1.39649
0.72933	0.24278	1.95374	1.95375	1.95375
0.97933	0.25000	2.58642	2.58643	2.58643
1.22933	0.25000	3.26045	3.26046	3.26046
1.47933	0.25000	3.95208	3.95210	3.95210
1.72933	0.25000	4.63081	4.63083	4.63083
1.97933	0.25000	5.25747	5.25749	5.25749
2.00000	0.02067	5.30547	5.30549	5.30549

Runge-Kutta-Fehlberg: solution plots

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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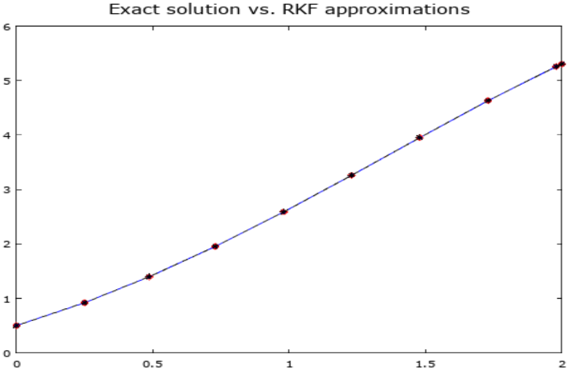

Runge-Kutta-Fehlberg: solution errors

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

Runge-Kutta-Fehlberg: solution errors

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Runge-Kutta-Fehlberg: truncation errors

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

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

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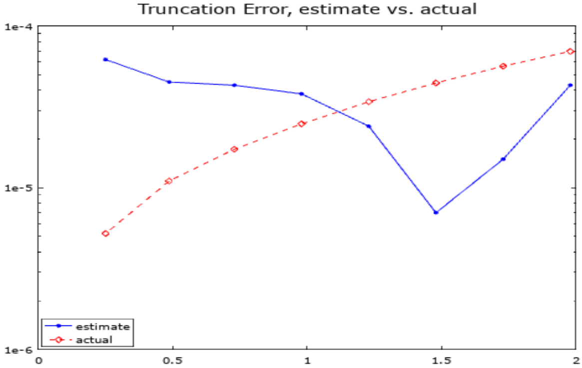

- Will skip Section 5.8, *extrapolation methods for ODEs*.
- Notation and details for Chapter 5 messy and not all trivial.
- Brand new concepts to work through.

Multistep Methods

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

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- Choose positive integer N, and select mesh points

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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 (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

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

Examples (I): Constant approximations

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

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

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

leading to Adams-Bashforth two-step explicit method

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

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

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

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

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
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- $m = 3$: 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} \;=\;& a_{m-1} w_j + a_{m-1} w_{j-1} + \cdots + a_0 w_{j-m+1} \\
& + h\left(b_m f(t_{j+1}, w_{j+1}) + b_{m-1} f(t_j, w_j)\right. \\
& \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}
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- **explicit** if $b_m = 0$; **implicit** if $b_m \neq 0$.

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

LTE: assume $w_i \approx y(t_i), i \leq j$

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

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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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}$$

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

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)

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

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

$$= y(t_j) +$$

$$\frac{h}{24}(9f(t_{j+1}, y(t_{j+1})) + 19f(t_j, y(t_j)) - 5f(t_{j-1}, y(t_{j-1})) + f(t_{j-2}, y(t_{j-2}))$$

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

- 3-step fourth-order Adams-Moulton method

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

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

$$= -\frac{19}{720} f^{(4)}(\xi, y(\xi))\, h^4.$$

example fourth-order Adams-Bashforth method

- 4-step and fourth-order

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

example fourth-order Adams-Bashforth method

- 4-step and fourth-order

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

To be explicit or not to be?

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

example fourth-order Adams-Bashforth method

- 4-step and fourth-order

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

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

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

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

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

- 4 initial values to start.

experiment

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

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

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

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

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

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

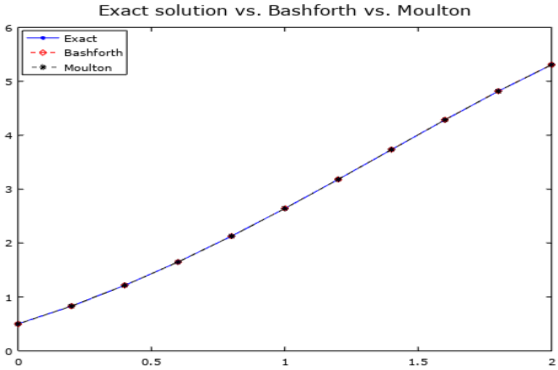
- 3 initial values to start.

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

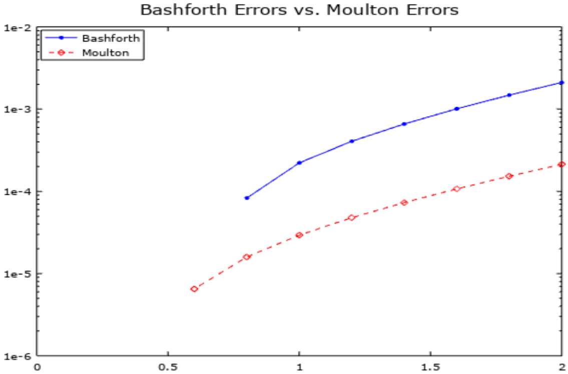
Solution plot

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



Error plot

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



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:

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

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

Assumptions

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

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

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

Assumptions

- Given tolerance $\tau > 0$,
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Goals

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

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

Assumptions

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

Goals

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

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**:

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

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

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

Adaptive Error Control (III)

- Adams-Moulton **Corrector**:

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

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

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

Adaptive Error Control (IV)

- **Predictor LTE**:

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

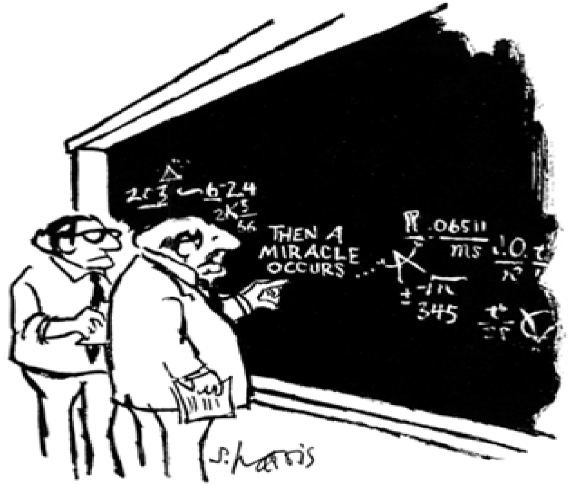
- **Corrector LTE**:

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

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

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

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



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

step-size selection (I)

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

step-size selection (I)

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

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

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

step-size selection (I)

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

  assume $\left|\tau_{j+1}(h)\right| \approx K\,h^4$ where K is independent of h.

- K should satisfy

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

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

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

step-size selection (II)

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

step-size selection (II)

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

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

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

step-size selection (II)

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

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

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

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

Review: Predictor-Corrector Methods

- Adams-Bashforth **Predictor**:

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

- Adams-Moulton **Corrector**:

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

Summary

- 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**:

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

- 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:

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

step-size selection procedure

- compute a conservative value for q:

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

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

step-size selection procedure

- compute a conservative value for q:

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

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

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

step-size selection procedure

- compute a conservative value for q:

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

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

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

- step-size can't be too big:

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

step-size selection procedure

- compute a conservative value for q:

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- make restricted step-size change:

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

- step-size can't be too big:

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

- step-size can't be too small:

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

Adaptive Adams 4th order Predictor Corrector: solution plots

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

exact solution $\qquad y(t) = (1+t)^2 - 0.5\, e^t.$

Adaptive Adams 4th order Predictor Corrector: solution plots

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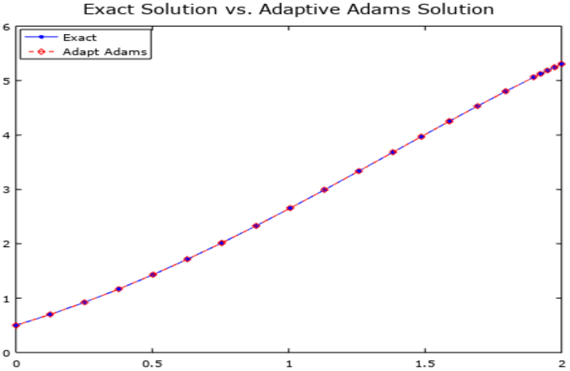

Solution Data

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	$8.622e-05$	$8e-06$
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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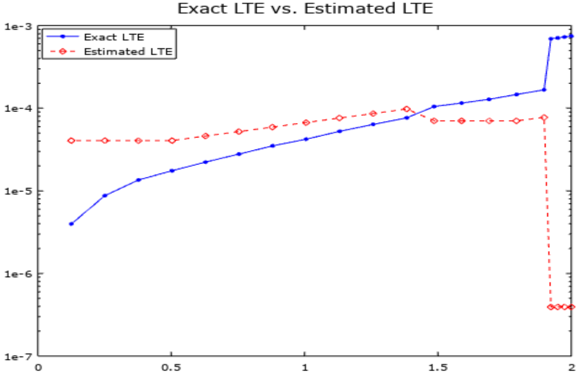

Circle of life: Predator and Prey/Boom And Bust

- Canadian Lynx and Snowshoe Hares in Canadian Boreal Forest

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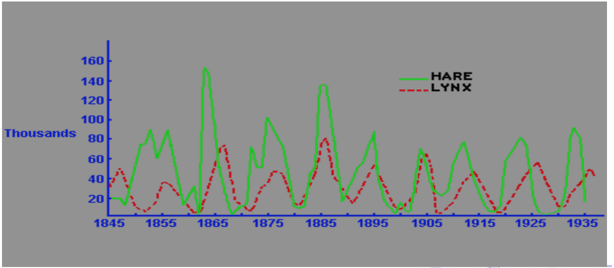

Predator and Prey Model

- 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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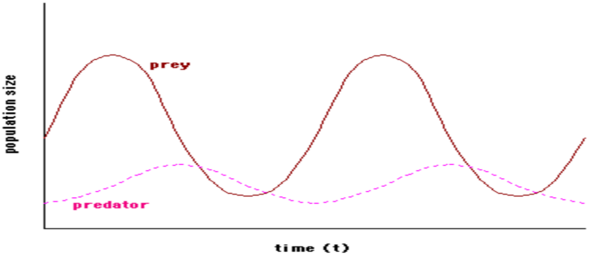

System of ODEs

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

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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

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

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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

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

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System of m first-order ODEs:

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

Theorem: Suppose that $f_j(t, \mathbf{u})$ satisfies a Lipschitz condition with Lipschitz constant L on $\mathcal{D}$ for all $1 \le j \le m$. 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 $$\frac{dy}{dt} = f(t, y), \quad a \le t \le b, \quad y(a) = \alpha.$$

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Runge-Kutta 4^{th} 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{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}$$

example: Lotka-Volterra predator-prey model

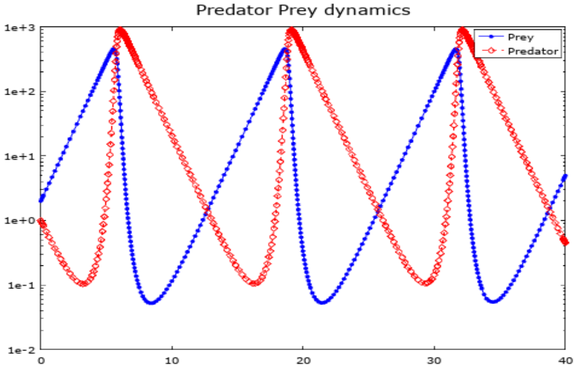
- `matlab` function *lotka*

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

- `matlab` command

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

Predator Prey dynamics



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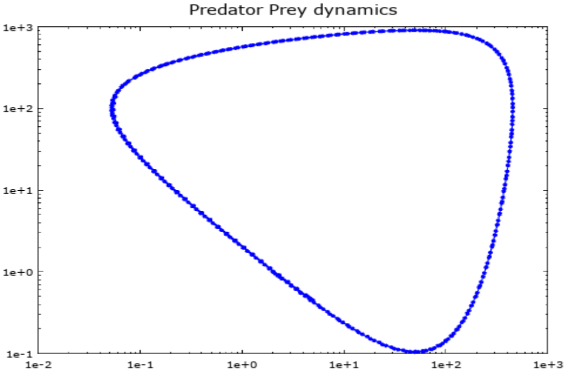

Stability Analysis for one-step methods

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- for $j = 0, 1, \cdots$
$$w_{j+1} = w_j + h\,\phi(t_j, w_j, h).$$
- **LTE**
$$\tau_j(h) = \frac{y(t_{j+1}) - y(t_j)}{h} - \phi(t_j, y(t_j), h).$$

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least of requirements of an ODE method:

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  least of requirements of an ODE method:

- *Definition*: **convergent**

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

Prior analysis on Euler's Method

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

Stability of Euler method

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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:

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

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

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

Review: Well-posed problem

Definition in English: ODE is well-posed if

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

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

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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> $\iff$

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

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

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

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