RUNGE-KUTTA METHODS

Euler's Method: $y_{n+1} = y_n + h\, f\,(t_n\,,\, y_n)$

Heun's Method $$y_{n+1} = y_n + \frac{h}{2}\left[f\,(t_n\,, y_n) + f\left(t_{n+1}\,, y_n + f\,(t_n\,, y_n\right)\right]$$

The Runge-Kutta Order 4 $$y_{n+1} = y_n + \frac{h}{6}(K_1 + 2K_2 + 2K_3 + K_4)$$

$K_1 = f\,(t_n\,,\, y_n)$

$$K_2 = f\,(t_n + \frac{h}{2}\,,\; y_n + \frac{h}{2}K_1)$$

$$K_3 = f\,(t_n + \frac{h}{2}\,,\; y_n + \frac{h}{2}K_2)$$

$$K_4 = f\,(t_{n+1}\,,\; y_n + h\,K_3)$$

h or Δt

1. How to choose?
2. Why constant and uniform?
3. How to find the total (overall) error?

Richardson's Extrapolation

"Richardson's Extrapolation to the Limit" or "Deferred Approach to the Limit":

Finding a more accurate answer using two inaccurate ones (estimates).

Remember Romberg integration table.

This is applicable to evaluation of functional values, derivatives, integrals, solution of differential equations, etc.

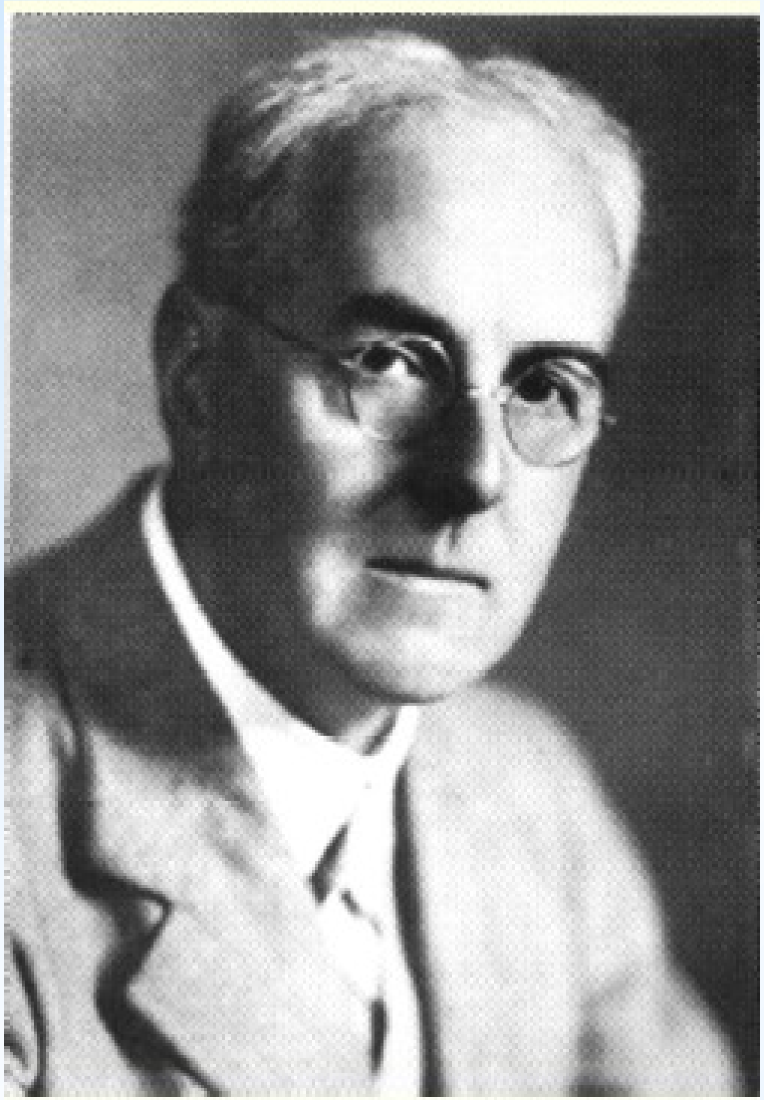
Extrapolating Polynomials

$$f(x) = a_0 + a_p\, x^p + a_{p+1}\, x^{p+1} + \ldots.$$

Remember Taylor series expansion where $(x - x_o)$ is replaced by x

$f(x) \approx a_0$ first-order approximation to f(x)

How do you find a better approximation to f(x)?



Lewis Fry Richardson

English mathematician

1881 – 1953

$$f(x) = a_0 + a_p\ x^p + a_{p+1}\ x^{p+1} + \dots.$$

Compute f(qx) where 0 > q > 1:

$$f(qx) = a_0 + a_p\ (q\,x)^p + a_{p+1}\ (q\,x)^{p+1} + \dots.$$

Solve for $a_p\ x^p$:

$$a_p\ x^p = \frac{f(x) - f(qx)}{1 - q^p} + O\left(x^{p+1}\right)$$

Substitute:

$$a_0 = f(x) - \frac{f(x) - f(qx)}{1 - q^p} + O\left(x^{p+1}\right)$$

Richardson's formula

Higher order approximation to f(0)

Example: $f(x) = \dfrac{e^{x} - 1}{x} \quad , \quad f(0) \; \square \; ?$

Exact solution: $f(0) = 1$

At x = 0.25: $f(0.25) = \dfrac{e^{0.25} - 1}{0.25} = 1.1361017 \quad => \quad 13.6\ \%\ \text{error}$

At x = 0.0125: $f(0.125) = \dfrac{e^{0.125} - 1}{0.125} = 1.0651876 \quad => \quad 6.5\ \%\ \text{error}$

At x = 0:

$$\left.\begin{aligned} f(0) \;&\cong\; a_0 \;\cong\; f(0.25) - \frac{f(0.25) - f(0.125)}{1 - (0.5)} \\ &\cong\; 0.9942736 \quad => \quad 0.6\ \%\ \text{error} \end{aligned}\right\}$$

Richardson's formula

Richardson's Extrapolation for Derivatives:

$$f(x+h) = f(x) + h\, f'(x) + \frac{h^2}{2!} f''(\xi)$$

$$f'(x) = \underbrace{\frac{f(x+h) - f(x)}{h}}_{\text{First-order approximation}} - \underbrace{\frac{h}{2} f''(\xi)}_{O(h)} \qquad , \qquad x < \xi < x+h$$

Find a better approximation to the first derivative, f(x):

$$f'(x) = \underbrace{\frac{f(x+h) - f(x-h)}{2\, h}}_{\text{Second-order approximation}} - \underbrace{\frac{h^2}{3!} f'''(\xi)}_{O(h^2)} \qquad , \qquad x-h < \xi < x+h$$

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + a_2 h^2 + a_4 h^4 + a_6 h^6 + \ldots$$

Define: $$\phi(h) = \frac{f(x+h) - f(x-h)}{2h}$$

Find: $$\lim_{h \to 0} \phi(h)$$

$$\phi(h) = f'(x) - a_2 h^2 - a_4 h^4 - a_6 h^6 - \ldots$$

$$\phi\left(\frac{h}{2}\right) = f'(x) - a_2 \left(\frac{h}{2}\right)^2 - a_4 \left(\frac{h}{2}\right)^4 - a_6 \left(\frac{h}{2}\right)^6 - \ldots$$

Eliminate the terms with a_2: $$f'(x) = \phi\left(\frac{h}{2}\right) + \frac{\phi\left(\frac{h}{2}\right) - \phi(h)}{3} + O\left(h^4\right)$$

Example:

Given $f(x) = e^{-x}$, find f '(0) using second-order evaluation and Richardson's formula

Exact solution: $f'(0) = -e^{-x}$ $\quad f'(0) = -1.000000$

Choose h = 0.1 $\quad f'(0.1) = -e^{0.1} = -1.10517$ => 10.5 % error

$f'(-0.1) = -e^{-0..1} = -0.90484$ => 10.5 % error

$$f'(0) \cong \frac{f(0.1) - f(-0.1)}{2\ (0.1)} = -1.00167 \quad \Rightarrow \quad 0.15\ \%\ \text{error}$$

Use Richardson's extrapolation formula:

h = 0.1 f ’(0.1) = - $e^{0.1}$ = - 1.10517 => 10.5 % error

f ’(- 0.1) = - $e^{-0..1}$ = - 0.90484 => 10.5 % error

$$f'(0) \cong \frac{f(0.1)-f(-0.1)}{2\ (0.1)} = -1.00167 \quad => \quad 0.15\ \%\ \text{error}$$

h = 0.05 f ’(0.1) = - $e^{0.05}$ = - 1.05127 => 5 % error

f ’(- 0.1) = - $e^{-0..05}$ = - 0.95123 => 5 % error

$$f'(0) \cong \frac{f'(0.05)-f'(-0.05)}{2\ (0.05)} = -1.00042 \quad => \quad 0.04\ \%\ \text{error}$$

Use Richardson’s extrapolation formula:

$$f'(0) = f'(0.05) + \frac{f'(0.05)-f'(0.1)}{3} + O\left(h^4\right)$$

Use Richardson's extrapolation formula:

$$f'(0) = f'(0.05) + \frac{f'(0.05) - f'(0.1)}{3} + O\left(h^4\right)$$

$$f'(0) \cong -1.00042 + \frac{-1.00042 + 1.00167}{3} \underbrace{= -1.0000}_{\text{Almost the exact answer}}$$

A GENERAL DICTUM IN NUMERICAL MATH.

If anything at all is known about the errors in a process, that knowledge can be exploited to improve the process.

$$\phi(h) = L - \sum_{k=1}^{\infty} a_{2k}\, h^{2k}$$

L: Objective to be evaluated (can be derivative, definite integral, etc.

ϕ (h): Known function of chosen h

Procedure: Select a convenient h, compute numbers

$$\underbrace{D(n,1)}_{\text{First estimates of L}} = \varphi\left(\frac{h}{2^n}\right) \quad , \quad n = 1, 2, 3, \ldots$$

$$D(n,1) = \underbrace{L}_{\text{Objective}} + \sum_{k=1}^{\infty} \underbrace{A(k,1)}_{-\,a_{2k}} \left(\frac{h}{2^n}\right)^{2k}$$

Richardson's Extrapolation for derivatives

$$D(n, m+1) = \frac{4^m}{4^m - 1} D(n, m) - \frac{1}{4^m - 1} D(n-1, m)$$

D (1 , 1)			
D (2 , 1)	D (2 , 2)		
D (3 , 1)	D (3 , 2)	D (3 , 3)	
D (4 , 1)	D (4 , 2)	D (4 , 3)	D (4 , 4)

- Accuracy increases as we move down the table in any column because h is decreased by half at each step.
- Accuracy increases as we move to the right in any row because of order-of-magnitude decrease in h.
- Note that smaller h does not always leads to higher accuracy. The accumulation of round-off error eventually catches up with the process.

Richardson's Extrapolation for Integrals:

$$T(n, m+1) = \frac{4^m}{4^m - 1} T(n, m) - \frac{1}{4^m - 1} T(n-1, m)$$

Example:

Exact solution:

$$\int_0^4 f(x)\, dx = \int_0^4 2^x\, dx = 21.640426$$

Richardson's extrapolation table:

Start with Trap Rule

One Panel (n = 1)	34.0		
Two Panels (n = 2)	25.0	22.0	
Four Panels (n = 4)	22.5	21.666	21.6444

Percent Errors:

One Panel (n = 1)	- 57.1 %		
Two Panels (n = 2)	- 15.5 %	- 1.7 %	
Four Panels (n = 4)	- 4.0 %	- 0.12 %	- 0.02 %

Richardson's Extrapolation for Solving ODE's:

Richardson's recursive formula: $$A\,(k\,,\,m+1)\;=\;\frac{2^{p+m-1}A(k,m)-A(k-1,m)}{2^{p+m-1}-1}$$

Example:

Given ODE: $$\frac{dy}{dt}=f(t,y)=-y\quad,\quad y(0)=1$$

Use Euler's method with : $$h=\frac{0.25}{2^{k-1}}\quad,\quad k=1,2,3,\ldots$$

Exact solution: y (0.25) = 0.7788008

N	Richardson's extrapolation table			
1	0.75			
2	0.765625	0.78125		
4	0.772476	0.7793274	0.7786865	
8	0.7756999	0.7789236	0.778789	0.7788036

N	Percent Errors			
1	3.7			
2	1.7	- 0.3		
4	0.8	- 0.07	0.015	
8	0.4	- 0.02	0.0015	- 0.00036

Selecting step size, h:

Given ODE: $$\frac{dy}{dt} = f(t, y) \quad , \quad y(t_0) = y_0$$

Exact (unknown) solution at t_n: $$y(t_n) = y^*$$

Local error from step t_{n-1} to t_n with step size h_1: $$E_{local} = C\, h_1^{p+1}$$

Numerical solution of order p at t_n: $$y_{n,h_1} = y^* + C\, h_1^{p+1}$$

Repeat the numerical solution with step size : $$h_2 = \frac{h_1}{2}$$

Numerical solution of order p at t_n: $$y_{n,h_2} \cong y^* + 2\,C\, h_2^{p+1}$$

$$y_{n,h_1} = y^* + C\,h_1^{p+1}$$

$$y_{n,h_2} \cong y^* + 2\,C\,h_2^{p+1}$$

Combine these two equations and solve for y^*:

$$y^* \cong \frac{y_{n,h_1} - 2^p\,y_{n,h_2}}{1 - 2^p}$$

Error in $y_{n,h1}$:

$$E_{local} \cong y_n^* - y_{n,h_1} = \frac{2^p\left(y_{n,h_2} - y_{n,h_1}\right)}{2^p - 1} = C\,h_1^{p+1}$$

$$C \cong \frac{2^p}{2^p - 1}\,\frac{y_{n,h_2} - y_{n,h_1}}{h_1^{p+1}}$$

$$E_{local,max} \cong C\,h_{max}^{p+1} = \frac{2^p}{2^p - 1}\,\frac{y_{n,h_2} - y_{n,h_1}}{h_1^{p+1}}\,h_{max}^{p+1} \le \varepsilon$$

$$h_{max} \le h_1\left[\frac{\varepsilon\left(2^p - 1\right)}{2^p\left|y_{n,h_2} - y_{n,h_1}\right|}\right]^{\frac{1}{p+1}}$$

Maximum step size for the local error not to exceed ε.

The above procedure is rather expensive when we want to check h at every step of the calculation. We need to have an inexpensive method with less number of calculations.

Consider two methods of order p and q such that $p+1 \leq q$

Define: $y_{n,p} = y_n^* + A_{p+1}\, h^{p+1} + O(h^{p+2})$

$$y_{n,q} = y_n^* + B_{q+1}\, h^{q+1} + O(h^{q+2})$$

Subtract side by side: $y_{n,q} - y_{n,p} = A_{p+1}\, h^{p+1} + O(h^{p+2})$

Therefore: $E_n \cong y_{n,q} - y_{n,p}$ This is the local error in $y_{n,p}$

Runge-Kutta-Fehlberg Order 4

$$y_{n+1} = y_n + h\left(\frac{25}{216}F_1 + \frac{1408}{2565}F_3 + \frac{2197}{4104}F_4 - \frac{1}{5}F_5\right)$$

$$F_1 = f\,(t_n\,,y_n)$$

$$F_2 = f\left(t_n + \frac{1}{4}h\,,\,y_n + \frac{1}{4}h\,F_1\right)$$

$$F_3 = f\left(t_n + \frac{3}{8}h\;,\;y_n + \frac{3}{32}h\,F_1 + \frac{9}{32}h\,F_2\right)$$

$$F_4 = f\left(t_n + \frac{12}{13}h\;,\;y_n + \frac{1932}{2197}h\,F_1 - \frac{7200}{2197}h\,F_2 + \frac{7296}{2197}h\,F_3\right)$$

$$F_5 = f\left(t_n + h\;,\;y_n + \frac{439}{216}h\,F_1 - 8\,h\,F_2 + \frac{3680}{513}h\,F_3 - \frac{845}{4104}h\,F_4\right)$$

Runge-Kutta-Fehlberg Order 5

$$y_{n+1} = y_n + h\left(\frac{16}{135}F_1 + \frac{6656}{12825}F_3 + \frac{28561}{56430}F_4 - \frac{9}{50}F_5 + \frac{2}{55}F_6\right)$$

$$F_1 = f\,(t_n\,, y_n)$$

$$F_2 = f\left(t_n + \frac{1}{4}h\,, y_n + \frac{1}{4}h\,F_1\right)$$

$$F_3 = f\left(t_n + \frac{3}{8}h\ ,\ y_n + \frac{3}{32}h\,F_1 + \frac{9}{32}h\,F_2\right)$$

$$F_4 = f\left(t_n + \frac{12}{13}h\ ,\ y_n + \frac{1932}{2197}h\,F_1 - \frac{7200}{2197}h\,F_2 + \frac{7296}{2197}h\,F_3\right)$$

$$F_5 = f\left(t_n + h\ ,\ y_n + \frac{439}{216}h\,F_1 - 8\,h\,F_2 + \frac{3680}{513}h\,F_3 - \frac{845}{4104}h\,F_4\right)$$

$$F_6 = f\left(t_n + \frac{1}{2}h\ ,\ y_n - \frac{8}{27}h\,F_1 + 2\,h\,F_2 - \frac{3544}{2565}h\,F_3 + \frac{1859}{4104}h\,F_4 - \frac{11}{40}h\,F_5\right)$$

Multi-step Methods

Multi-step (multi-procedure) methods require information on the solution of more than one point, and hence they are **not self-starting**.

- They are however more efficient (faster) than R-K methods.

- You may even hope that they may solve the instability problem of R-K methods.

Example using Euler's method:

$$\frac{dy(t)}{dt} = f\big(t,y(t)\big) \quad , \quad y(t_0) = y_0 \qquad \Rightarrow \qquad y_{n+1} = y_n + h\, f(t_n,y_n) + \underbrace{O(h^2)}_{\text{Local error}}$$

$$y_1 \cong y_0 + h\, f(t_0,y_0)$$

$$y_2 \cong y_1 + h\, f(t_1,y_1)$$

etc.

If y_1 is also known (besides y_0), what can you do for a better estimation of y_2?

Example using Euler's method:

$$\frac{dy(t)}{dt} = f\big(t, y(t)\big) \quad , \quad y(t_0) = y_0 \quad \underbrace{\text{and } \; y(t_1) \cong y_1}_{\substack{\text{Somehow known very accurately, maybe} \\ \text{from a very accurate numerical calculation}}}$$

$$y_2 = ?$$

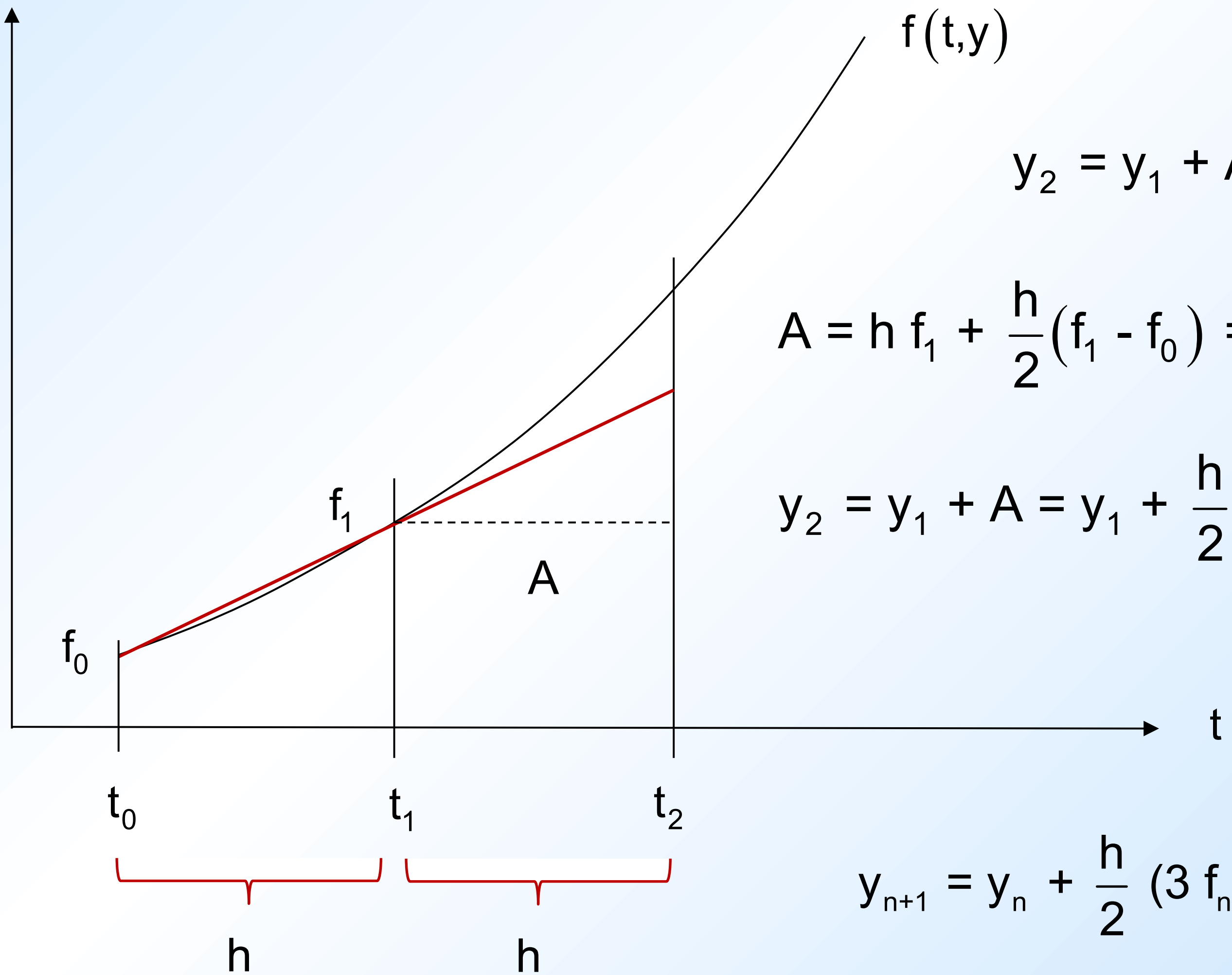
Find y_2 (and the rest of the points, y_3, y_4, etc.) fitting a first degree polynomial to $f(t_0,y_0)$ and $f(t_1,y_1)$, extend to the next panel, and find the area.

$$y_2 = y_1 + \frac{h}{2}\big(3\, f(t_1,y_1) - f(t_0,y_0)\big) = y_1 + \frac{h}{2}(3\, f_1 - f_0)$$

$$y_{n+1} = y_n + \frac{h}{2}(3\, f_n - f_{n-1}) \quad , \quad n = 1, 2, 3, \ldots$$

Local truncation error: $E_{local} = \dfrac{5}{12} h^3 \, f''(\xi)$ How do you find this?

$$\frac{dy}{dt} = f(t,y)$$



$$y_2 = y_1 + A$$

$$A = h\,f_1 + \frac{h}{2}\left(f_1 - f_0\right) = \frac{h}{2}\left(3\,f_1 - f_0\right)$$

$$y_2 = y_1 + A = y_1 + \frac{h}{2}\left(3\,f_1 - f_0\right)$$

$$y_{n+1} = y_n + \frac{h}{2}\,(3\,f_n - f_{n-1})$$

Adams-Bashfort Open Formulae:

Order two: $y_{n+1} = y_n + \dfrac{h}{2}(3\,f_n - f_{n-1})$, $n = 1, 2, 3, \ldots$

Local truncation error: $\dfrac{5}{12} h^3 f''(\xi)$ => O(2)

Order three: $y_{n+1} = y_n + \dfrac{h}{12}(23\,f_n - 16\,f_{n-1} + 5\,f_{n-2})$, $n = 2, 3, 4, \ldots$

Local truncation error: $\dfrac{9}{24} h^4 f'''(\xi)$ => O(3)

Order four: $y_{n+1} = y_n + \dfrac{h}{24}(55\,f_n - 59\,f_{n-1} + 37\,f_{n-2} - 9\,f_{n-3})$, $n = 3, 4, 5, \ldots$

Local truncation error: $\dfrac{251}{720} h^5 f^{(4)}(\xi)$ => O(4)

ADAMS-BASHFORT OPEN FORMULAE

$$y_{i+1} = y_i + h\sum_{k=1}^{n}\alpha_{nk}\, f_{i-k+1} + O(h^{n+1})$$

Order of the Formula (n)	k = 1 α_{n1}	k = 2 α_{n2}	k = 3 α_{n3}	k = 4 α_{n4}	k = 5 α_{n5}	k = 6 α_{n6}	Local Truncation Error, $O(h^{n+1})$
1	1						$\frac{1}{2}h^2 f'(\xi)$
2	$\frac{3}{2}$	$-\frac{1}{2}$					$\frac{5}{12}h^3 f''(\xi)$
3	$\frac{23}{12}$	$-\frac{16}{12}$	$\frac{5}{12}$				$\frac{9}{24}h^4 f'''(\xi)$
4	$\frac{55}{24}$	$-\frac{59}{24}$	$\frac{37}{24}$	$-\frac{9}{24}$			$\frac{251}{720}h^5 f^{(4)}(\xi)$
5	$\frac{1901}{720}$	$-\frac{2774}{720}$	$\frac{2616}{720}$	$-\frac{1274}{720}$	$\frac{251}{720}$		$\frac{475}{1440}h^6 f^{(5)}(\xi)$
6	$\frac{4277}{1440}$	$-\frac{7923}{1440}$	$\frac{9982}{1440}$	$-\frac{7298}{1440}$	$\frac{2877}{1440}$	$-\frac{475}{1440}$	$\frac{19087}{60480}h^7 f^{(6)}(\xi)$

EXAMPLE ON MULTI-STEP METHODS

$\dfrac{dy}{dt} = y\cos(t)$	IC: $y(0) = 1$
Exact Solution:	$y(t) = e \sin(t)$

Use Heun's method to start and 3-point Adams-Bashfort open formula to proceed:

Heun's Method

$$y_{n+1} = y_n + \frac{h}{2}\left[f\left(t_n, y_n\right) + f\left(t_{n+1}, y_n + h\, f\left(t_n, y_n\right)\right)\right]$$

Adams-Bashfort open order 3:

$$y^p_{n+1} = y_n + \frac{h}{12}\left(23\, f_n - 16\, f_{n-1} + 5\, f_{n-2}\right)$$

t	y (t)	Heun's			
	Exact	y_n	% Error		
0	0	1.0			
0.25	1.28070	1.27639	0.34		
0.5	1.61515	1.60492	0.63		
0.75	1.97712	1.95996	0.87		
1.0	2.31978	2.29591	1.03		
1.25	2.58309	2.55358	1.14		
1.5	2.71148	2.67858	1.21		
1.75	2.67510	2.64153	1.25		
2.0	2.48258	2.45139	1.26		

t	y (t)	Heun's		Adams-Bashfort	
	Exact	y_n	% Error	y_n	% Error
0	0	1.0		1.0	
0.25	1.28070	1.27639	0.34		
0.5	1.61515	1.60492	0.63		
0.75	1.97712	1.95996	0.87	1.97172	0.27
1.0	2.31978	2.29591	1.03	2.32236	- 0.11
1.25	2.58309	2.55358	1.14	2.58942	- 0.25
1.5	2.71148	2.67858	1.21	2.71148	- 0.04
1.75	2.67510	2.64153	1.25	2.66317	0.45
2.0	2.48258	2.45139	1.26	2.45679	1.04

Note that, the order of the starter method is better be greater than the order of the rest of the solution in order to reduce the beginning errors which may accumulate later on.

This is not so in the above example.

Example: Error calculation of Adams-Bashfort open formulae:

Prove the following

$$y_{n+1} = y_n + \frac{h}{2}\left[3\,f_n - f_{n-1}\right] + \frac{5}{12}\,h^3\,f\,''(\xi)$$

$$y_{n+1} = y_n + \frac{h}{12}\left[23\,f_n - 16\,f_{n-1} + 5\,f_{n-2}\right] + \frac{9}{24}\,h^4\,f\,'''(\xi)$$

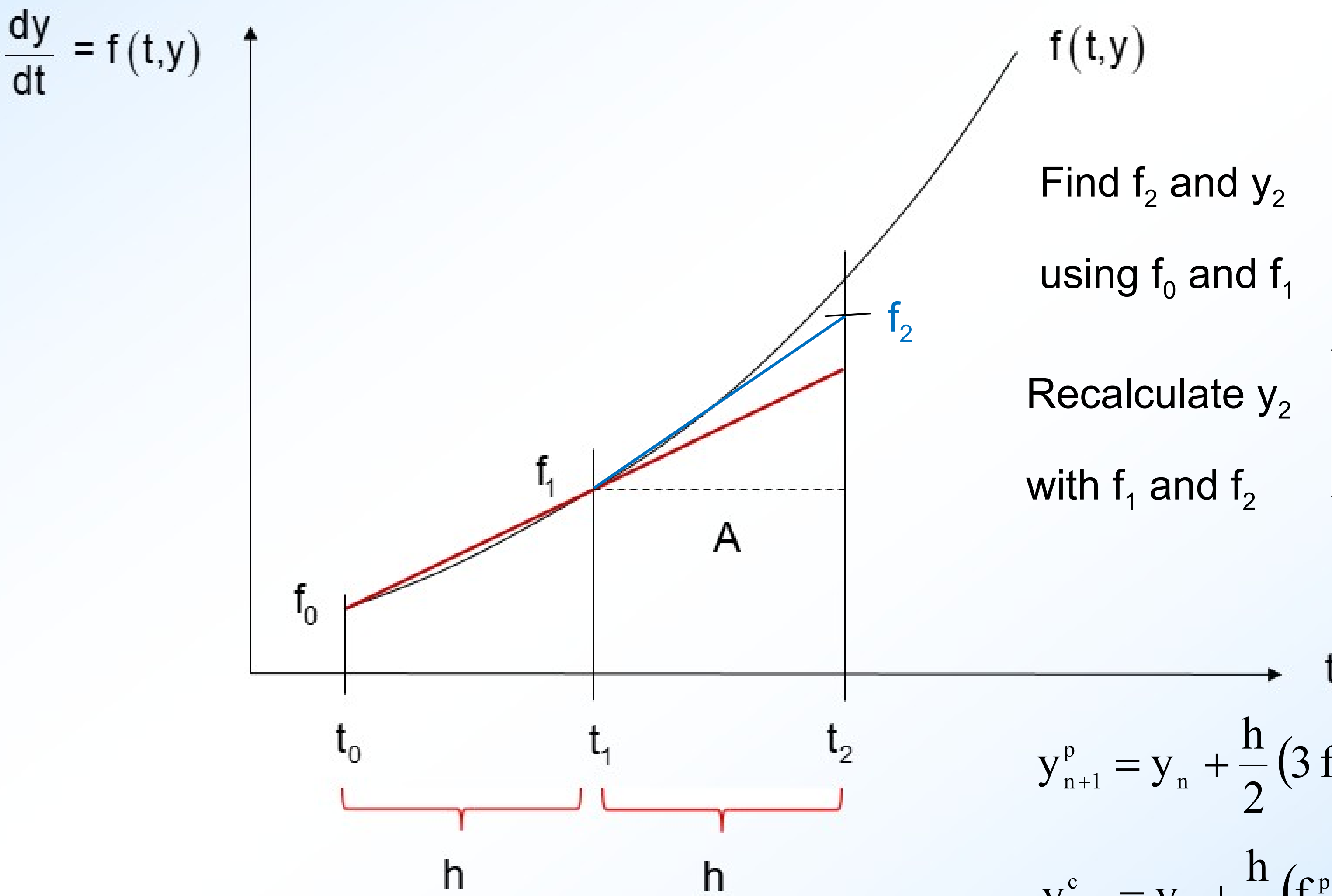
Predictor-Corrector Procedures

The idea behind the predictor-corrector methods is to use a suitable combination of an explicit and an implicit technique to obtain a method with better convergence characteristics.

Here is an example using Euler's method:

Predictor: $$y_{n+1}^{p} = y_n + h\, f(t_n, y_n)$$

Corrector: $$y_{n+1}^{c} = y_n + \frac{h}{2}\left[f(t_n, y_n) + f(t_{n+1}, y_{n+1}^{p})\right]$$



Find f_2 and y_2 using f_0 and f_1 — Predictor

Recalculate y_2 with f_1 and f_2 — Corrector

$$y^{p}_{n+1} = y_n + \frac{h}{2}\left(3\,f_n - f_{n-1}\right)$$

$$y^{c}_{n+1} = y_n + \frac{h}{2}\left(f^{p}_{n+1} + f_n\right)$$

ADAMS CLOSED FORMULAE

$$y_{i+1} = y_i + h \sum_{k=1}^{n} \alpha_{nk} f_{i-k+1} + O(h^{n+1})$$

Order of the Formula (n)	k = 1 α_{n1}	k = 2 α_{n2}	k = 3 α_{n3}	k = 4 α_{n4}	k = 5 α_{n5}	k = 6 α_{n6}	Local Truncation Error, $O(h^{n+1})$
1	1						$-\frac{1}{2} h^2 f'(\xi)$
2	$\frac{1}{2}$	$\frac{1}{2}$					$-\frac{1}{12} h^3 f''(\xi)$
3	$\frac{5}{12}$	$\frac{8}{12}$	$-\frac{1}{12}$				$-\frac{1}{24} h^4 f'''(\xi)$
4	$\frac{9}{24}$	$\frac{19}{24}$	$-\frac{5}{24}$	$\frac{1}{24}$			$-\frac{19}{720} h^5 f^{(4)}(\xi)$
5	$\frac{251}{720}$	$\frac{646}{720}$	$-\frac{264}{720}$	$\frac{106}{720}$	$-\frac{19}{720}$		$-\frac{27}{1440} h^6 f^{(5)}(\xi)$
6	$\frac{475}{1440}$	$\frac{1427}{1440}$	$-\frac{798}{1440}$	$\frac{482}{1440}$	$-\frac{173}{1440}$	$\frac{27}{1440}$	$-\frac{863}{60480} h^7 f^{(6)}(\xi)$

ADAMS-MOULTON PREDICTOR-CORRECTOR METHODS

Order	Predictor-Corrector Formulae	Local Error
2	$y^p_{n+1} = y_n + \frac{h}{2}\left(3 f_n - f_{n-1}\right)$ $y^c_{n+1} = y_n + \frac{h}{2}\left(f^p_{n+1} + f_n\right)$	$\lvert E_{n+1}\rvert \cong \frac{1}{6}\lvert y^p_{n+1} - y^c_{n+1}\rvert$
3	$y^p_{n+1} = y_n + \frac{h}{12}\left(23 f_n - 16 f_{n-1} + 5 f_{n-2}\right)$ $y^c_{n+1} = y_n + \frac{h}{12}\left(5 f^p_{n+1} + 8 f_n - f_{n-1}\right)$	$\lvert E_{n+1}\rvert \cong \frac{1}{10}\lvert y^p_{n+1} - y^c_{n+1}\rvert$
4	$y^p_{n+1} = y_n + \frac{h}{24}\left(55 f_n - 59 f_{n-1} + 37 f_{n-2} - 9 f_{n-3}\right)$ $y^c_{n+1} = y_n + \frac{h}{24}\left(9 f^p_{n+1} + 19 f_n - 5 f_{n-1} + f_{n-2}\right)$	$\lvert E_{n+1}\rvert \cong \frac{19}{270}\lvert y^p_{n+1} - y^c_{n+1}\rvert$

ILL-conditioned ODE: $\dfrac{dy}{dt} = 3y - t^2 \quad , \quad y(0) = \dfrac{2}{27}$

General solution: $y(t) = C e^{3t} + \dfrac{t^2}{3} + \dfrac{2t}{9} + \dfrac{2}{27}$

Particular solution: $y(t) = \dfrac{t^2}{3} + \dfrac{2t}{9} + \dfrac{2}{27}$

Parasitic solution

Example: $\dfrac{du_1}{dx} = 2u_2(x) \quad , \quad u_1(0) = 3 \qquad \dfrac{du_2}{dx} = 2u_1(x) \quad , \quad u_2(0) = -3$

General Solution: $u_1(x) = A e^{2x} + B e^{-2x} \qquad u_2(x) = A e^{2x} - B e^{-2x}$

Apply initial conditions: A = 0 and B = 3

The component with the positive exponential will dominate with any numerical method

Stiff ODE: Any ODE with a rapidly decreasing transient solution requires an extremely small step size for an accurate solution.

$$\frac{dy(t)}{d\,t} = \lambda\,\big(y(t) - g(t)\big) + \frac{dg(t)}{d\,t} \quad , \quad \lambda << 0$$ and g(t) smooth and slowly varying

Solution: $$y(t) = \underbrace{\big[y(0) - g(0)\big]\, e^{\lambda t}} + g(t)$$ h must be very very small

Will soon be insignificant besides g(t)

But, (λ h) will govern the stability. So h must be small as well.

For any resonable h for g(t) will give small (λ h).

For a system of equations $$\frac{dy(t)}{dt} = A\left(y(t) - g(t)\right) + \frac{dg(t)}{dt}$$

the eigenvalues of A correspond to λ. If all the eigenvalues have negative real parts, the solution will converge to g(t) as t goes to infinity.

Example: $$\frac{du}{dt} = 98\,u + 198\,v \qquad \frac{dv}{dt} = -\,99\,u + 199\,v$$

Exact solution:
$$u(t) = 2\,e^{-t} - e^{-100\,t}$$
$$v(t) = -\,e^{-t} + e^{-100\,t}$$

Rapidly decaying terms
requiring a very small step size

One answer to stiff ODE's is to use implicit methods: $y_{n+1} = y_n + h\,f\left(t_{n+1}, y_{n+1}\right)$

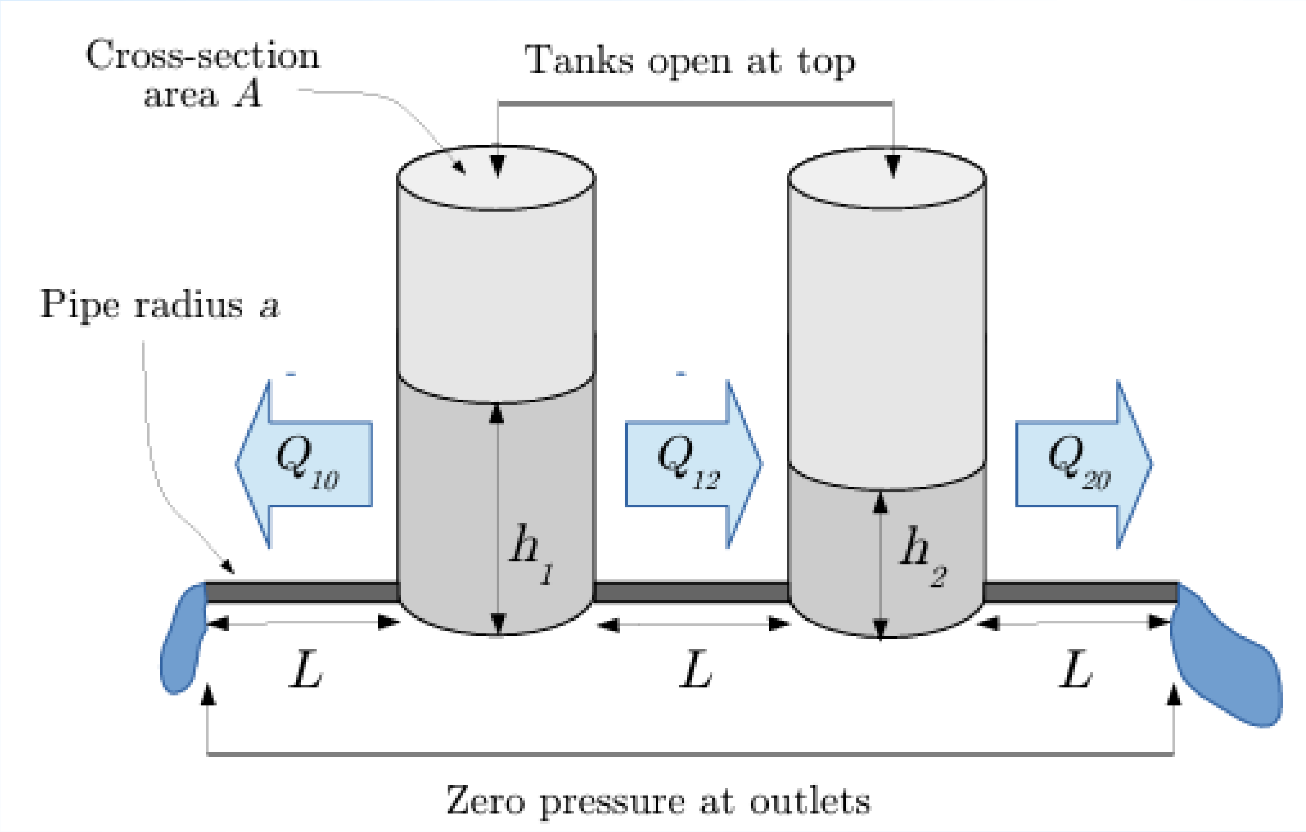
There exist other methods of solving ODE’s which we will not discuss in detail.

One such method is called Bulirsch-Stoer method. It combines two ideas:

1. Richardson’s extrapolation to the limit; and
2. Rational function (Padé) approximation rather than power (Taylor) series.

See the book «Numerical Recipies».

SYSTEM OF ODE's



$$\frac{d\,h_1(t)}{d\,t} = -2\,h_1 + h_2 \quad , \quad h_1(0) = h_{1,0}$$

$$\frac{d\,h_2(t)}{d\,t} = h_1 - 2\,h_2 \quad , \quad h_2(0) = h_{2,0}$$

Consider:

$$\frac{d\,y(x)}{d\,x} = f\big(x,\, y(x),\, z(x)\big) \quad , \quad y(0) = y_0$$

$$\frac{d\,z(x)}{d\,x} = g\big(x,\, y(x),\, z(x)\big) \quad , \quad z(0) = z_0$$

All the methods that we have discussed so far are applicable.

Euler's Method:

$$y_{n+1} = y_n + h\, f\big(x_n,\, y_n,\, z_n\big)$$

$$z_{n+1} = z_n + h\, g\big(x_n,\, y_n,\, z_n\big)$$

The Runge-Kutta Order Four: $$y_{n+1} = y_n + \frac{h}{6}\left(K_1 + 2\,K_2 + 2\,K_3 + K_4\right)$$

$$z_{n+1} = z_n + \frac{h}{6}\left(L_1 + 2\,L_2 + 2\,L_3 + L_4\right)$$

$$K_1 = f\left(x_n,\, y_n,\, z_n\right) \qquad L_1 = g\left(x_n,\, y_n,\, z_n\right)$$

$$K_2 = f\left(x_n+\frac{h}{2},\, y_n+\frac{h}{2}K_1,\, z_n+\frac{h}{2}L_1\right) \qquad L_2 = g\left(x_n+\frac{h}{2},\, y_n+\frac{h}{2}K_1,\, z_n+\frac{h}{2}L_1\right)$$

$$K_3 = f\left(x_n+\frac{h}{2},\, y_n+\frac{h}{2}K_2,\, z_n+\frac{h}{2}L_2\right) \qquad L_3 = g\left(x_n+\frac{h}{2},\, y_n+\frac{h}{2}K_2,\, z_n+\frac{h}{2}L_2\right)$$

$$K_4 = f\left(x_{n+1},\, y_n+h\,K_3,\, z_n+h\,L_3\right) \qquad L_4 = g\left(x_{n+1},\, y_n+h\,K_3,\, z_n+h\,L_3\right)$$

Example:

The Kermack - McKendrick model for the course of an epidemic in a population is given by the system of ODE's:

$$\frac{dy_1}{dt} = -c\, y_1\, y_2 \qquad \frac{dy_2}{dt} = c\, y_1\, y_2 - d\, y_2 \qquad \frac{dy_3}{dt} = d\, y_2$$

where y_1 represents the number of people susceptible to the disease, y_2 represents infected people that are still in circulation, and y_3 represents infected people that are removed from the population through isolation, death, or recovery and immunity. The parameters c and d represent the infection rate and removal rate, respectively.

Use the parameter values c = 1 and d = 5, along with initial values $y_1(0) = 95$, $y_2(0) = 5$, and $y_3(0) = 0$.

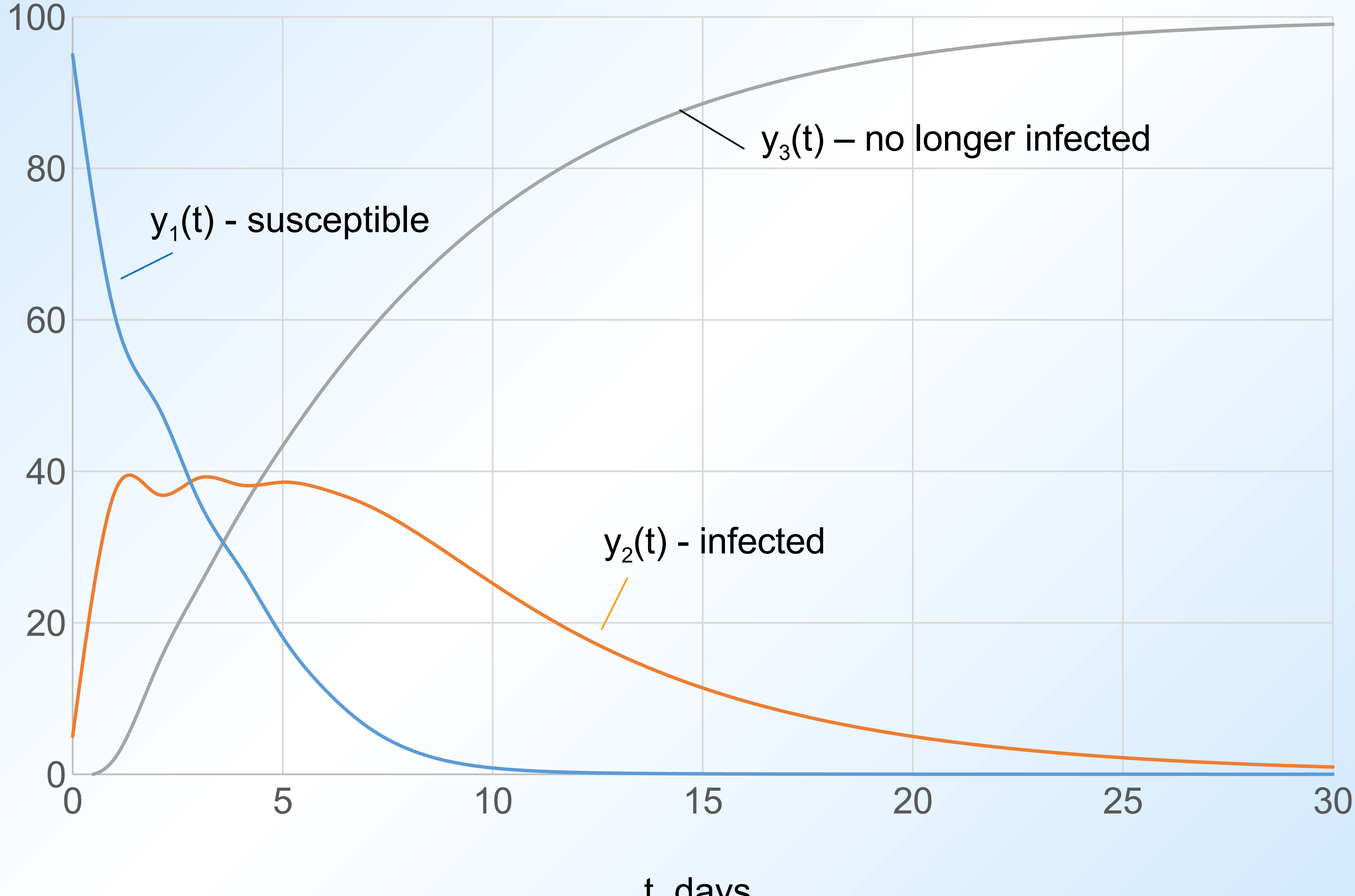
$$\frac{dy_1}{dt} = -\,y_1\,y_2 = f_1\left(t\,,\,y_1\,,\,y_2\,,\,y_3\right) \quad , \quad y_{1,0} = 95$$

$$\frac{dy_2}{dt} = y_1\,y_2 - 5\,y_2 = f_2\left(t\,,\,y_1\,,\,y_2\,,\,y_3\right) \quad , \quad y_{2,0} = 5$$

$$\frac{dy_3}{dt} = 5\,y_2 = f_3\left(t\,,\,y_1\,,\,y_2\,,\,y_3\right) \quad , \quad y_{3,0} = 0$$

Use a numerical method of your choice (not Euler's method) to find $y_1(t)$, $y_2(t)$, and $y_3(t)$ (t is in months) and plot all on the same graph. You may use any suitable step size, h, such as h = 0.1.

Choose h = 1/30 (one day) and Heun's method (Runge-Kutta order two).


100
80
60
40
20
0
0
5
10
15
20
25
30
y3(t) – no longer infected
y1(t) - susceptible
y2(t) - infected
t, days

Examples of System of First-order ODE's

- Predator-prey systems (Rabbits and Foxes)
- Chemistry and biochemistry (Chemical rate equations)
- Dilution problems
- Coupled spring-mass systems
- Electrical circuits
- SIR model of an epidemic (Susceptible, Infected, Recovered)
- Growth and decay problems
- Temperature problems
- Trajectories of planets, comets, etc.

HIGHER-ORDER ODE's

Second-order ODE: $$\frac{d^2y(x)}{d\,x^2} = f\left(x,\, y(x),\, y'(x)\right)$$

Two conditions must be specified for the solution:

$$\left.\begin{array}{l} \text{At } x = 0 \quad y(0) = y_0 \quad \text{and} \\ \left.\dfrac{d\,y}{d\,x}\right|_{x=0} = y'(0) \end{array}\right\} \quad \text{Initial-value problem}$$

$$\left.\begin{array}{l} \text{At } x = 0 \quad y(0) = y_0 \quad \text{and} \\ \text{At } x = L \quad y(L) = y_L \end{array}\right\} \quad \text{Boundary-value problem}$$

Note that derivative conditions may also be specified at the boundaries

SECOND-ORDER ODE - INITIAL VALUE PROBLEM

$$\frac{d^2y(x)}{d\,x^2} = f\left(x, y(x), y'(x)\right)$$

At $x = 0$ $\quad y(0) = y_0$ and

$$\left.\frac{d\,y}{d\,x}\right|_{x=0} = y'(0)$$

Define
$$\frac{dy(x)}{d\,x} = z(x) = g(x, y, z) \quad , \quad z(0) = z_0$$

$$\frac{dz(x)}{d\,x} = f\left(x, y(x), z(x)\right) \quad , \quad y(0) = y_0$$

All the methods that we have discussed so far are applicable.

SECOND-ORDER ODE - INITIAL VALUE PROBLEM

Given:	$y'' = -y$	$y(0) = 0$	$y'(0) = 1$
Exact solution:	$y(t) = \sin(t)$	$y'(t) = \cos(t)$	

t	0	0.1	0.2	0.3	0.4	0.5	1.0
y_{exact}	0	0.0998	0.1987	0.2955	0.3894	0.4794	0.8415
y_{Euler}	0	0.100	0.200	0.299	0.396	0.440	0.940
y'_{exact}	1.0	0.995	0.980	0.995	0.921	0.878	0.540
y'_{Euler}	1.0	1.0	0.990	0.970	0.940	0.900	0.660

BOUNDARY-VALUE PROBLEMS

Second-order ODE: $$\frac{d^2y(x)}{d\,x^2} = f\left(x,\, y(x),\, y'(x)\right)$$

$$\left.\begin{array}{l} \text{At } x = 0 \quad y(0) = y_0 \quad \text{and} \\ \\ \text{At } x = L \quad y(L) = y_L \end{array}\right\} \text{Boundary-value problem}$$

Note that derivative conditions may also be specified at the boundaries

There are two methods of solution: **Matrix Method** - f is a linear function of y and all the derivatives of y

Shooting Method - A trial-and-error solution

Matrix Method

Given: $\dfrac{d^2y(x)}{d\,x^2} = f\big(x, y(x), y'(x)\big)$, $y(a) = \alpha$, $y(b) = \beta$

Select a set of equally-spaced points, x_0, x_1, ..., x_n, x_{n+1}, on the interval [a,b]

$$x_i = a + i\,h \quad , \quad h = \frac{b - a}{n + 1} \quad , \quad 0 \le i \le n + 1$$

Approximate the derivatives using standart central-difference formula

$$y'(x) \cong \frac{y(x + h) - y(x - h)}{2\,h} = \frac{y_{i+1} - y_{i-1}}{2\,h}$$

$$y''(x) \cong \frac{y(x + h) - 2\,y(x) + y(x - h)}{h^2} = \frac{y_{i+1} - 2\,y_i + y_{i-1}}{h^2}$$

The problem becomes:

$$y_0 = \alpha \quad \text{(given)}$$

$$\frac{y_{i-1} - 2\,y_i + y_{i+1}}{h^2} = f\left(x_i,\, y_i,\, \frac{y_{i+1} - y_{i-1}}{2\,h}\right) \quad , \quad 1 \le i \le n$$

$$y = \beta \quad \text{(given)}$$

This is usually a non-linear system of equations in n unkowns, y_1, y_2, ..., y_n.

The solution of such a sytem of non-linear equations is seldom easy.

IF the "**f**" **function is linear in y and y'**, only then the solution is easier

because we can form a matrix:

First derivatives with finite differences:

Two-point forward difference $$y'(x) \cong \frac{y_{i+1} - y_i}{h} + O(h)$$

Two-point backward difference $$y'(x) \cong \frac{y_i - y_{i-1}}{h} + O(h)$$

Three-point forward difference $$y'(x) \cong \frac{-3\,y_i + 4\,y_{i+1} - y_{i+2}}{2\,h} + O(h^2)$$

Three-point backward difference $$y'(x) \cong \frac{y_{i-2} - 4\,y_{i-1} + 3\,y_i}{2\,h} + O(h^2)$$

Three-point central difference $$y'(x) \cong \frac{y_{i+1} - y_{i-1}}{2\,h} + O(h^2)$$

Five-point central difference $$y'(x) \cong \frac{-y_{i+2} + 8\,y_{i+1} - 8\,y_{i-1} + y_{i-2}}{12\,h} + O(h^4)$$

Example

Solve the following second-order ODE with the given boundary conditions:

$$-2\,\frac{d^2y}{dx^2} + y = e^{-0.2x} \quad , \quad y(0) = 1 \quad , \quad \left.\frac{dy}{dx}\right|_{x=1} = -y$$

Divide the solution domain into eight subintervals, and use the central difference approximation for all the derivatives in the given ODE and the boundary conditions. Compare the numerical solution with the exact solution:

Exact solution: $$y = -0.2108\,e^{x/\sqrt{2}} + 0.1238\,e^{-x/\sqrt{2}} + \frac{e^{-0.2x}}{0.92}$$

Note: When there is an exact solution, numerical solution becomes unnecessary.

Given ODE: $$-2\,\frac{d^2y}{dx^2} + y = e^{-0.2\,x}$$

Corresponding finite difference equation:

$$-2\left(\frac{y_{i-1} - 2\,y_i + y_{i+1}}{h^2}\right) + y_i = e^{-0.2\,x_i} \quad , \quad i = 1, 2, ..., 7$$

Re-arrange: $$-2\,y_{i-1} + \left(4 + h^2\right) y_i - 2\,y_{i+1} = h^2\,e^{-0.2\,x_i} \quad , \quad i = 1, 2, ..., 7$$

Boundary conditions: $y_0 = 1$ at $x = 0$

$$\left.\frac{dy}{dx}\right|_{x=1} \cong \frac{y_9 - y_7}{2\,h} = -\,y_8 \quad \Rightarrow \quad y_9 = y_7 - 2\,h\,y_8$$

$$
\begin{pmatrix}
4+h^2 & -2 & 0 & 0 & 0 & 0 & 0 & 0 \\
-2 & 4+h^2 & -2 & 0 & 0 & 0 & 0 & 0 \\
0 & -2 & 4+h^2 & -2 & 0 & 0 & 0 & 0 \\
0 & 0 & -2 & 4+h^2 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -2 & 4+h^2 & -2 & 0 & 0 \\
0 & 0 & 0 & 0 & -2 & 4+h^2 & -2 & 0 \\
0 & 0 & 0 & 0 & 0 & -2 & 4+h^2 & -2 \\
0 & 0 & 0 & 0 & 0 & 0 & -4 & 4+4h+h^2
\end{pmatrix}
\begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \\ y_7 \\ y_8 \end{pmatrix}
=
\begin{pmatrix}
2+h^2\ e^{-0.2x_1} \\
h^2\ e^{-0.2x_2} \\
h^2\ e^{-0.2x_3} \\
h^2\ e^{-0.2x_4} \\
h^2\ e^{-0.2x_5} \\
h^2\ e^{-0.2x_6} \\
h^2\ e^{-0.2x_7} \\
h^2\ e^{-0.2x_8}
\end{pmatrix}
$$

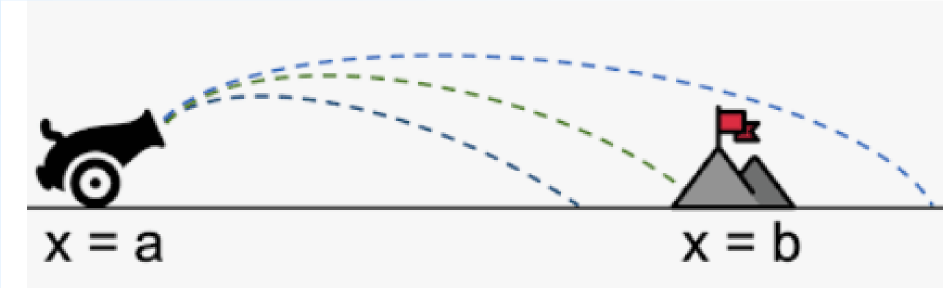
where $h = 1/8$ and $x_i = i\,h$ for $i = 1, 2, \ldots, 8$

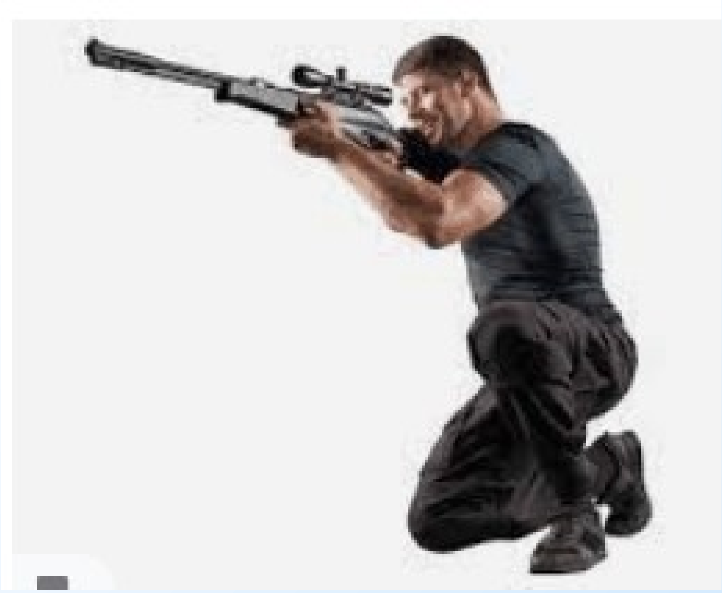
	Matrix	Exact
y_0 =	1.00000	1.00000
y_1 =	0.94323	0.94317
y_2 =	0.88620	0.88612
y_3 =	0.82867	0.82857
y_4 =	0.77036	0.77025
y_5 =	0.71101	0.71087
y_6 =	0.65031	0.65014
y_7 =	0.58797	0.58778
y_8 =	0.52366	0.52344

Shooting Method

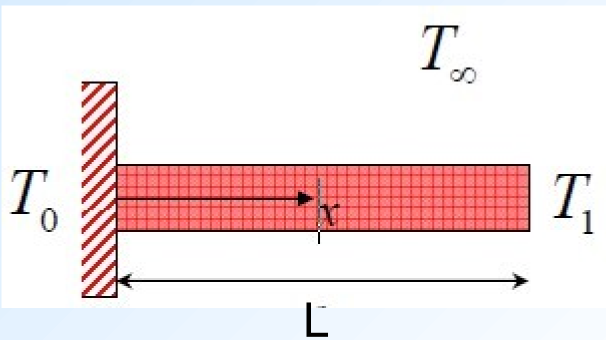
- Applicable to both linear & non-linear Boundary Value (BV) problems.
- Easy to implement
- No guarantee of convergence
- Approach:
  - Convert a BV problem into an initial value problem
  - Solve the resulting problem iteratively (trial & error)
  - Linear ODEs allow a quick linear interpolation
  - Non-linear ODEs will require an iterative approach similar to our root finding techniques.

Shoothing to hit the target by adjusting the aim (slope) of the gun or a rifle.





Cooling Fin Example



h = heat transfer coefficient

k = thermal conductivity

P = perimeter of the fin

A = cross sectional area of the fin

T_∞ = ambient temperature

$$\frac{d^2T}{dx^2} - \frac{h\,P}{k\,A}\left(T - T_\infty\right) = 0$$

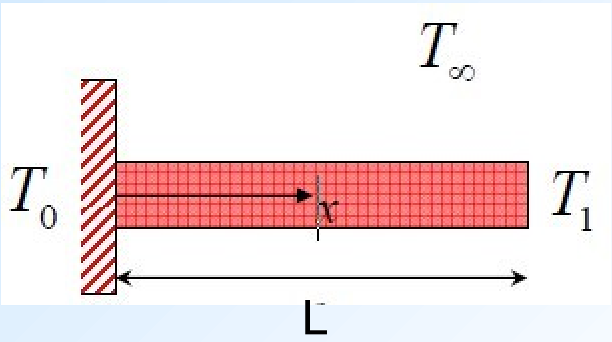
$$T(x = 0) = T_0$$

$$T(x = L) = T_L$$

Analytical solution:

$$m^2 = \frac{h\,P}{k\,A} \qquad \theta(x) = T(x) - T_\infty$$

$$\frac{d^2\theta}{dx^2} - m^2\,\theta = 0$$



$$\frac{d^2\theta}{dx^2} - m^2\,\theta = 0$$

$$\theta(x) = C_1\, e^{m\,x} + C_2\, e^{-m\,x}$$

$$\theta(x) = T(x) - T_\infty$$

$$m^2 = \frac{h\,P}{k\,A}$$

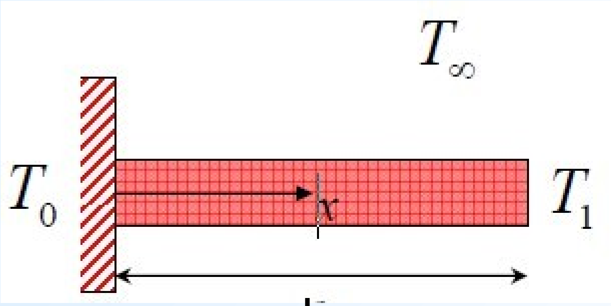
Boundary Conditions:

$$T(0) = T_0 \quad => \quad \theta(0) = T_0 - T_\infty = \theta_0$$

$$T(L) = T_L \quad => \quad \theta(L) = T_L - T_\infty = \theta_L$$

Apply BC's and solve for C_1 and C_2

$$\frac{\theta(x)}{\theta_0} = \frac{\left(\theta_L/\theta_0\right)\,\sinh(m\,x) + \sinh\left(m\,(L - x)\right)}{\sinh(m\,L)}$$



$$\frac{d^2T}{dx^2} - \frac{h\,P}{k\,A}\left(T - T_\infty\right) = 0$$

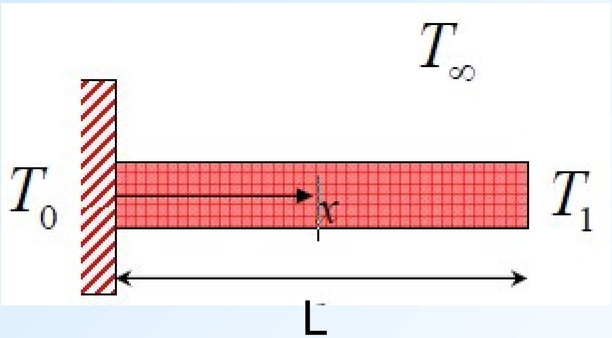
BC's: $T(0) = T_0$

$T(L) = T_L$

1. Re-write as two first-order ODE's: $\dfrac{dT}{dx} = z \quad , \quad T(0) = T_0$

$$\frac{dz}{dx} = \frac{h\,P}{k\,A}(T - T_\infty) \quad , \quad z(0) = ?$$

2. We need an initial value for z. **Guess z_1**



3. Integrate the two equations using RK4 and z_1; this will yield a solution at x = L

4. Integrate the two equations again using a 2nd guess for $z(0) = z_2$.

5. Linearly interpolate the *z* results to obtain the correct initial condition

(Note: this only works for Linear ODEs.)

Example: $$z_3 = z_2 + \frac{z_1 - z_2}{T_1 - T_2}\left(T_L - T_2\right)$$