Computational Techniques
Module 7: Ordinary Differential Equations (Initial Value Problems)

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Background

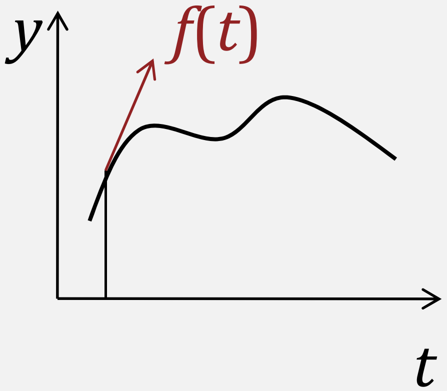
- Given:

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

$$y(t_0) = y_0$$

⇩

$$y(t)$$



Compare with Integration

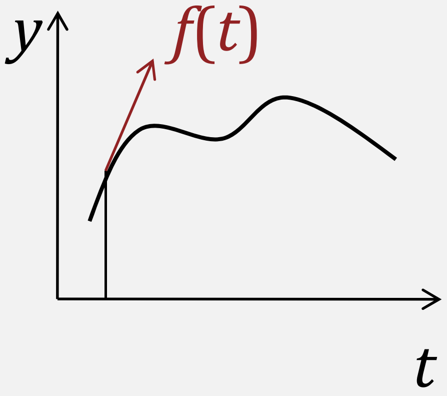
- Given:

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

$$y(t_0) = y_0$$

$$\Downarrow$$

$$y(t)$$

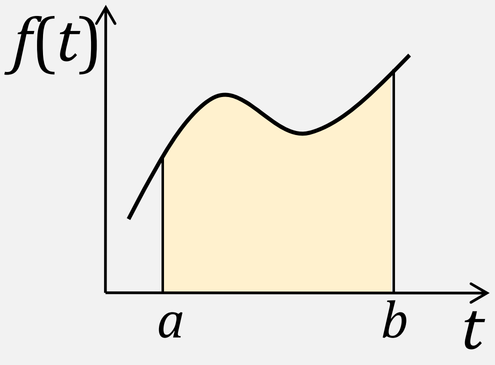


- Given:

$$f(t)$$

$$\Downarrow$$

$$\int_a^b f(t)\,dt$$



Example: Plug Flow Reactor

- Design Equation for volume of PFR

$$V = F_{A0} \int_0^X \frac{dX}{-r(X)}$$

  - Volume of PFR is given by area under the curve $\frac{1}{-r(X)}$

- Conversion from a PFR

$$F \frac{dC_A}{dV} = -r(C_A) \quad \Rightarrow \quad F_{A0} \frac{dX}{dV} = r(X)$$

Numerical Method

- To solve: $$\frac{dy}{dt} = f(y,t)$$

$$\Downarrow$$

$$\lim_{\Delta t \to 0} \frac{y_{i+1} - y_i}{\Delta t} = f(y_i, t_i)$$

$$\Downarrow$$

$$y_{i+1} = y_i + \Delta t . \underbrace{S(y_i, t_i)}$$

Numerical methods focus on using appropriate value of "slope" $S(y,t)$ to improve accuracy

Geometric Interpretation

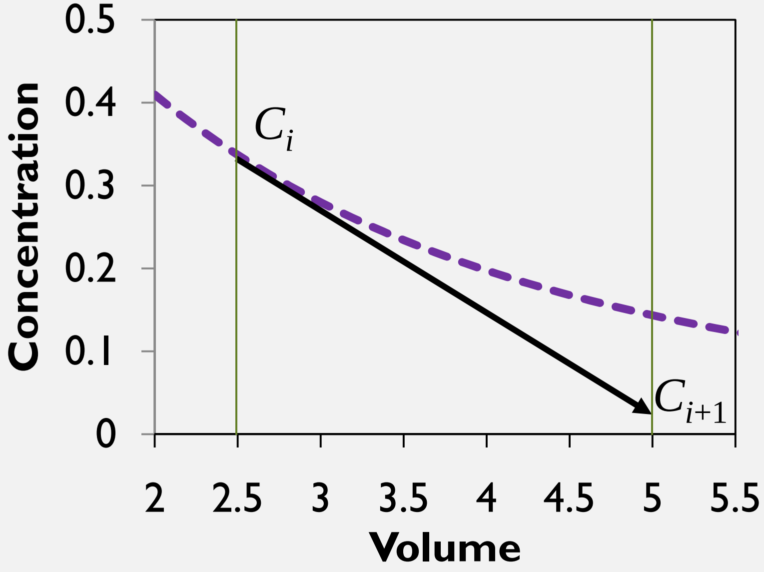
$$y(i+1) = y(i) + h \times \text{Slope}(i)$$

Euler's Explicit Method:

Slope computed at the location i

Euler's Implicit Method:

Slope computed at the final location $(i+1)$



Explicit vs. Implicit Methods

- Explicit method
  - $y_{i+1} = y_i + \Delta t . S(y_i, t_i)$
  - Slope $S(y,t)$ depends on *already known* quantities
  - y_{i+1} is computed directly from the above expression
- Implicit method
  - $y_{i+1} = y_i + \Delta t . S(y_{i+1}, t_{i+1})$
  - Slope $S(y,t)$ depends implicitly on *unknown* quantities
  - Y_{i+1} computed by solving the above nonlinear equation

Runge Kutta Class of Methods

- Multi-point methods to improve accuracy
- Explicit Methods

Overview

- Runge-Kutta Family of Methods
  - Euler's methods
  - Explicit vs. Implicit Methods
  - Higher order Runge-Kutta methods
  - Error analysis and Stability
- Predictor-Corrector Methods
- Adam-Moulton's Family of Methods
- Adaptive Step Sizing
- Stiff ODE Solvers

Runge-Kutta Methods (RK-2)

$$y_{i+1} = y_i + h[w_1 k_1 + w_2 k_2]$$

$$k_1 = f(y_i, t_i)$$

$$k_2 = f\left((y_i + q_{21}[hk_1]), (t_i + p_2 h)\right)$$

$$w_1 + w_2 = 1$$

$$w_2 p_2 = 1/2$$

$$w_2 q_{21} = 1/2$$

p_2	q_{21}	q_{22}
	w_1	w_2

Runge-Kutta Methods (RK-2)

$$y_{i+1} = y_i + h[w_1 k_1 + w_2 k_2]$$

$$k_1 = f(y_i, t_i)$$

$$k_2 = f\left((y_i + q_{21}[hk_1]), (t_i + p_2 h)\right)$$

$$w_1 + w_2 = 1$$

$$w_2 p_2 = 1/2$$

$$w_2 q_{21} = 1/2$$

0.5	0.5	–
	0	1

Mid-Point Method

Runge-Kutta Methods (RK-2)

$$y_{i+1} = y_i + h[w_1 k_1 + w_2 k_2]$$

$$k_1 = f(y_i, t_i)$$

$$k_2 = f\left((y_i + q_{21}[hk_1]), (t_i + p_2 h)\right)$$

$$w_1 + w_2 = 1$$

$$w_2 p_2 = 1/2$$

$$w_2 q_{21} = 1/2$$

1	1	–
	0.5	0.5

Heun's Method

Runge-Kutta Methods (RK-2)

$$y_{i+1} = y_i + h[w_1 k_1 + w_2 k_2]$$

$$k_1 = f(y_i, t_i)$$

$$k_2 = f\left((y_i + q_{21}[hk_1]), (t_i + p_2 h)\right)$$

$$w_1 + w_2 = 1$$

$$w_2 p_2 = 1/2$$

$$w_2 q_{21} = 1/2$$

0.75	0.75	–
	$1/3$	$2/3$

Ralston's Method

Runge-Kutta Methods (RK-n)

$$y_{i+1} = y_i + h\sum_{m=1}^{n} w_m k_m$$

$$k_1 = f\left(y_i, t_i\right)$$

$$k_m = f\left(\left(y_i + h\left[q_{m1}k_1 + \ldots + q_{m,m-1}k_{m-1}\right]\right), \left(t_i + p_m h\right) \right)$$

Runge-Kutta Methods (RK-4)

$p2$	$q21$	–	–	–
$p3$	$q31$	$q32$	–	–
$p4$	$q41$	$q42$	$q43$	–
	$w1$	$w2$	$w3$	$w4$

0.5	0.5	–	–	–
0.5	0	0.5	–	–
1	0	0	1	–
	$\frac{1}{6}$	$\frac{2}{6}$	$\frac{2}{6}$	$\frac{1}{6}$

"Classical"

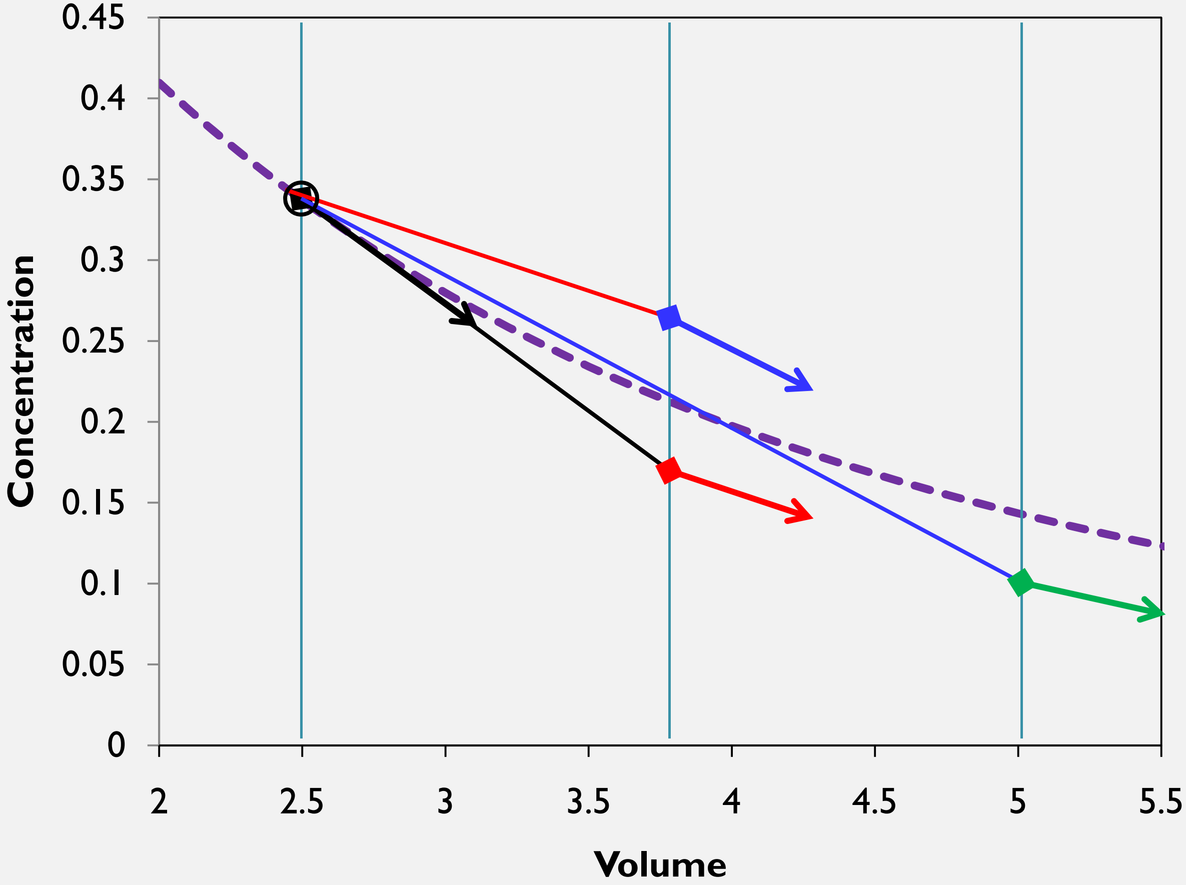
0.5	0.5	–	–	–
0.5	$\frac{\sqrt{2}-1}{2}$	$\frac{2-\sqrt{2}}{2}$	–	–
1	0	$\frac{-1}{\sqrt{2}}$	$\frac{2+\sqrt{2}}{2}$	–
	$\frac{1}{6}$	$\frac{2-\sqrt{2}}{6}$	$\frac{2+\sqrt{2}}{6}$	$\frac{1}{6}$

RK-Gill

$\frac{1}{4}$	$\frac{1}{4}$	–	–	–
$\frac{3}{8}$	$\frac{3}{32}$	$\frac{9}{32}$	–	–
$\frac{12}{13}$	$\frac{1932}{2197}$	$\frac{-7200}{2197}$	$\frac{7296}{2197}$	–
	$\frac{25}{216}$	$\frac{1408}{2565}$	$\frac{2197}{4104}$	$\frac{-1}{5}$

RK-Fehlberg

Classical RK-4 Method
(PFR Problem with h = 2.5)



$$k_1 = f_i$$

$$k_2 = f_{i+\frac{k_1}{2}}$$

$$k_3 = f_{i+\frac{k_2}{2}}$$

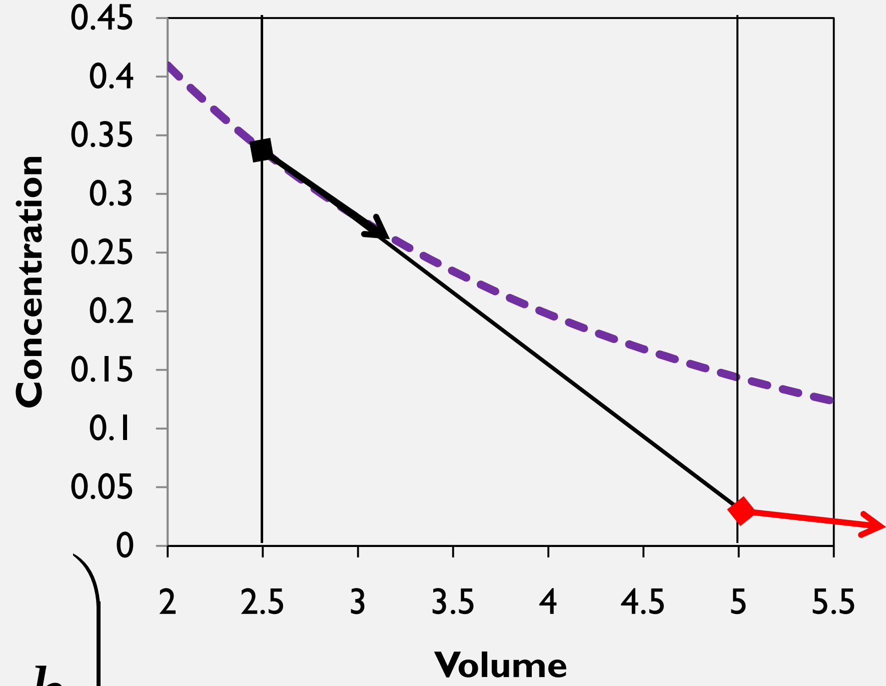
$$k_4 = f_{i+k_3}$$

Heun's Method

- RK-2 variant gives:

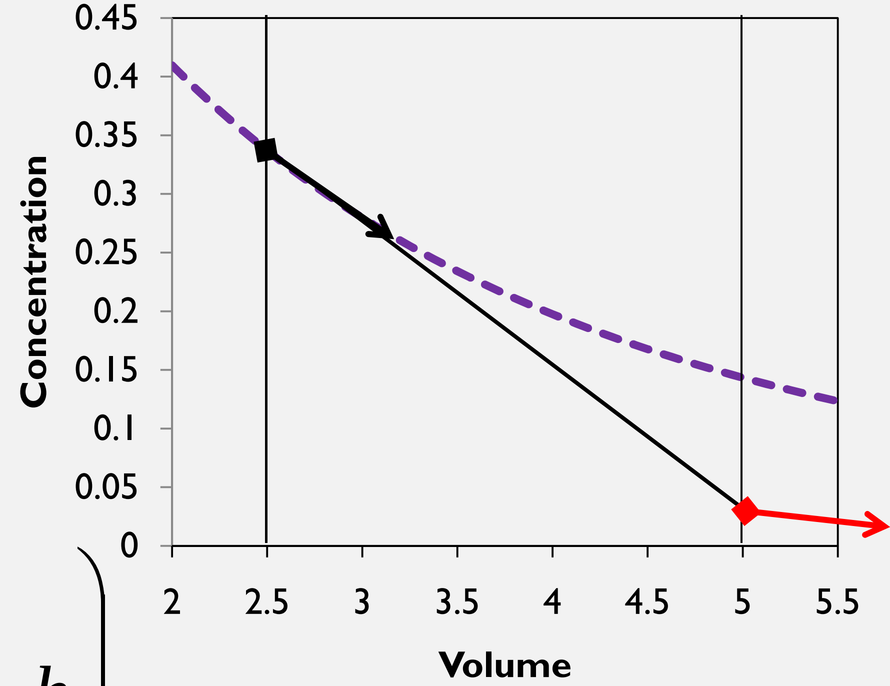
$$k_1 = f\left(y_i, t_i\right)$$

$$k_2 = f\left(\left(y_i + hk_1\right), \underbrace{t_i + h}_{t_{i+1}}\right)$$



Heun's Method

- RK-2 variant gives:



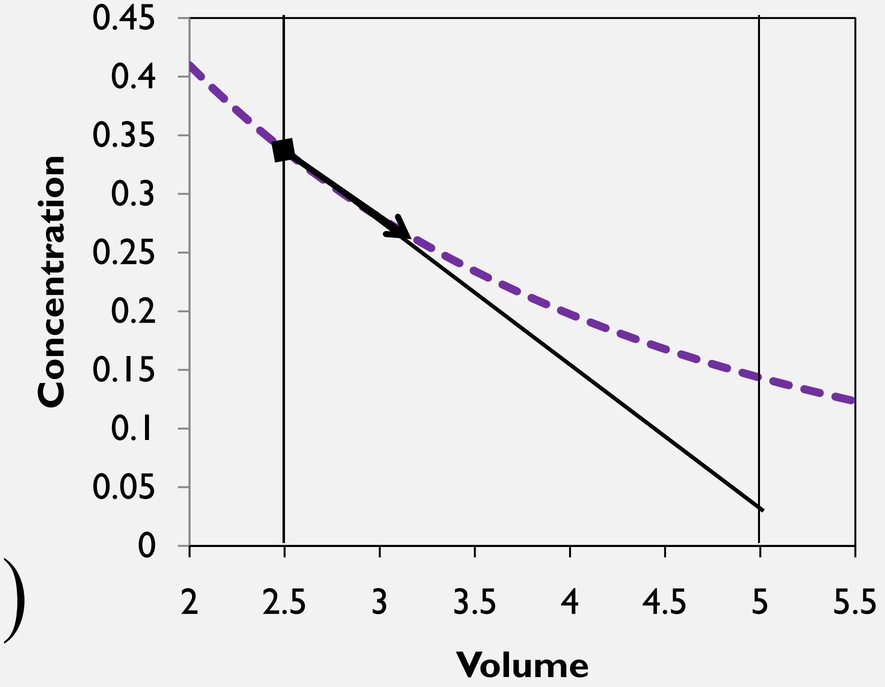
$$k_1 = f(y_i, t_i)$$

$$k_2 = f\left(\underbrace{(y_i + hk_1)}_{\bar{y}_{i+1}}, \underbrace{t_i + h}_{t_{i+1}}\right)$$

$$y_{i+1} = y_i + \frac{h}{2}[k_1 + k_2]$$

$$y_{i+1} = y_i + \frac{h}{2}[f(y_i, t_i) + f(\bar{y}_{i+1}, t_{i+1})]$$

Heun's Method



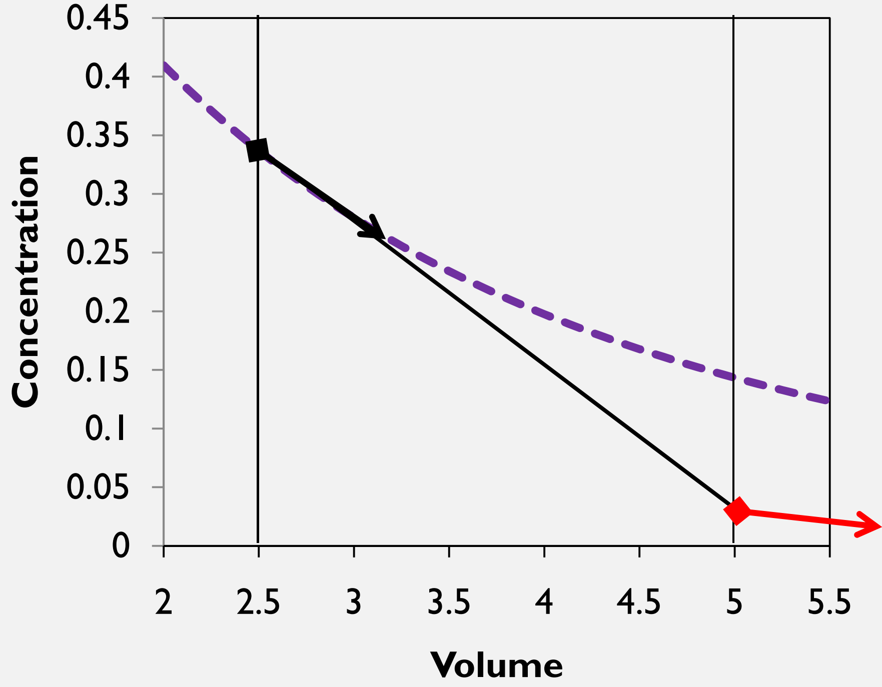
- Predictor:

$$k_1 = f(y_i, t_i)$$

$$\bar{y}_{i+1}^{0} = y_i + hf(y_i, t_i)$$

- Corrector:

Heun's Method



- Predictor:

$$k_1 = f(y_i, t_i)$$

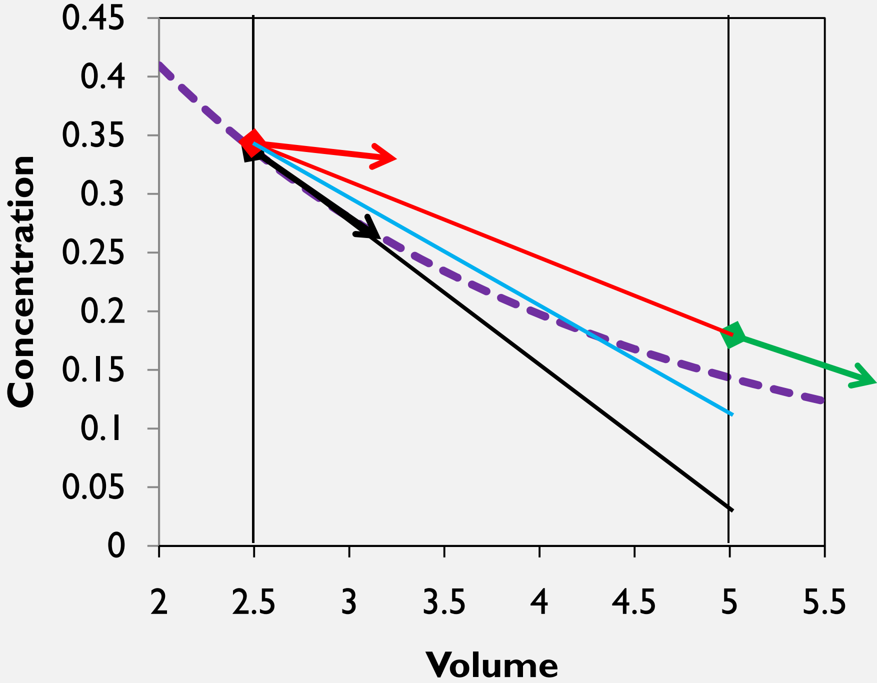
$$\bar{y}_{i+1}^{0} = y_i + hf(y_i, t_i)$$

- Corrector:

$$k_2^0 = f\left(\bar{y}_{i+1}^{0}, t_{i+1}\right)$$

$$\bar{y}_{i+1}^{1} = y_i + \frac{h}{2}\left[k_1 + k_2^0\right]$$

Heun's Method



- Predictor:

$$k_1 = f\left(y_i, t_i\right)$$

$$\bar{y}_{i+1}^{0} = y_i + hf\left(y_i, t_i\right)$$

- Corrector:

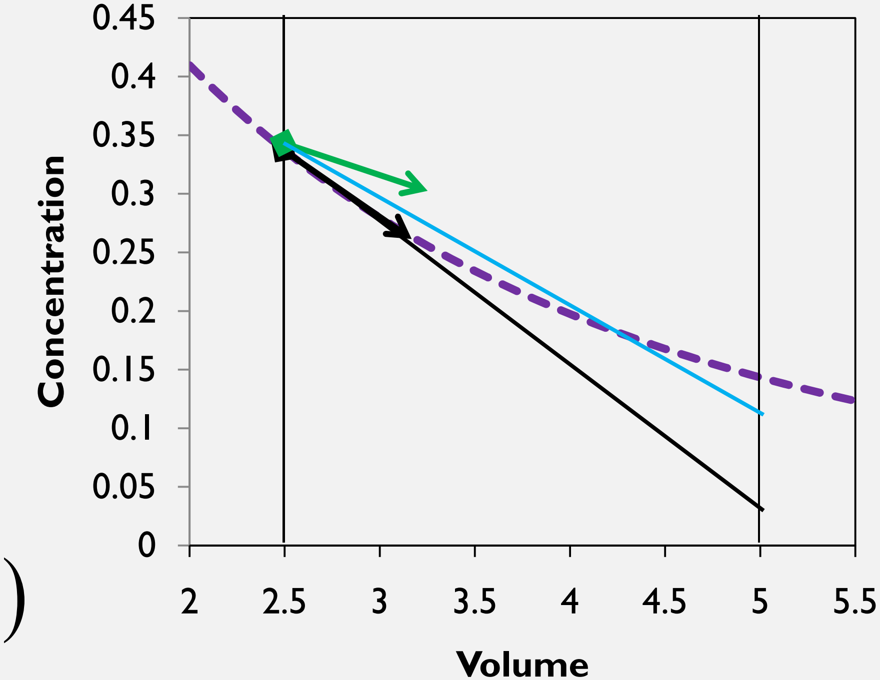
$$k_2^0 = f\left(\bar{y}_{i+1}^{0}, t_{i+1}\right)$$

$$k_2^m = f\left(\bar{y}_{i+1}^{m}, t_{i+1}\right)$$

$$\bar{y}_{i+1}^{1} = y_i + \frac{h}{2}\left[k_1 + k_2^0\right]$$

$$\bar{y}_{i+1}^{m+1} = y_i + \frac{h}{2}\left[k_1 + k_2^m\right]$$

Heun's Method



- Predictor:

$$k_1 = f\left(y_i, t_i\right)$$

$$\overline{y}_{i+1}^{0} = y_i + hf\left(y_i, t_i\right)$$

- Corrector:

$$k_2^m = f\left(\overline{y}_{i+1}^m, t_{i+1}\right)$$

$$\overline{y}_{i+1}^{m+1} = y_i + \frac{h}{2}\left[k_1 + k_2^m\right]$$

Embedded R-K Method

Cash-Karp Parameters for Embedded Runga-Kutta Method								
i	a_i	b_{ij}					c_i	c_i^*
1							$\frac{37}{378}$	$\frac{2825}{27648}$
2	$\frac{1}{5}$	$\frac{1}{5}$					0	0
3	$\frac{3}{10}$	$\frac{3}{40}$	$\frac{9}{40}$				$\frac{250}{621}$	$\frac{18575}{48384}$
4	$\frac{3}{5}$	$\frac{3}{10}$	$-\frac{9}{10}$	$\frac{6}{5}$			$\frac{125}{594}$	$\frac{13525}{55296}$
5	1	$-\frac{11}{54}$	$\frac{5}{2}$	$-\frac{70}{27}$	$\frac{35}{27}$		0	$\frac{277}{14336}$
6	$\frac{7}{8}$	$\frac{1631}{55296}$	$\frac{175}{512}$	$\frac{575}{13824}$	$\frac{44275}{110592}$	$\frac{253}{4096}$	$\frac{512}{1771}$	$\frac{1}{4}$
$j =$		1	2	3	4	5		

From: Numerical Recipes for C

Summary of ODE-IVP Methods

Method	**# Pts.**	**Starting**	**GTE**	**Comment**
Runge-Kutta Family of Methods				
Euler's	1	$y(0)$	$\mathcal{O}(h^1)$	Easy
Euler-Implicit	1	$y(0)$	$\mathcal{O}(h^1)$	Globally Stable
Heun's	2	$y(0)$	$\mathcal{O}(h^2)$	Like Trapezoidal
Midpoint	2	$y(0)$	$\mathcal{O}(h^2)$	
RK-Gill (RK4)	4	$y(0)$	$\mathcal{O}(h^4)$	First choice!
Second Order Heun's Methods				
RK-2	See above			
Predic. – Corr.	2	$y(0)$	$\mathcal{O}(h^{\textbf{2 or 3}})$	Higher accuracy
Crank–Nicholson	2	$y(0)$	$\mathcal{O}(h^2)$	Implicit: Stable!

Summary of ODE-IVP Methods

Method	**# Pts.**	**Starting**	**GTE**	**Comment**
Multi-Point Methods (non-self starting)				
Heun's (P-C)	2	$y(0)$, $y(-1)$	$\mathcal{O}(h^3)$	Higher accuracy
Adam-Moulton	4	$y(0) \ldots y(-3)$	$\mathcal{O}(h^5)$	Implicit: Stable!
Adam-Bashfort	4	$y(0) \ldots y(-3)$	$\mathcal{O}(h^5)$	
Advanced Techniques				
Stiff Systems	Use implicit methods			
Richardson's	$y(\text{new}) = y(h/2) + \Delta/15$			
Adaptive Step Size	h scales as $\Delta^{0.2}$			