



NTNU

TMA4125 Matematikk 4N

Numerical methods for ordinary differential equations
— Runge–Kutta methods and adaptive stepping

Ronny Bergmann and Douglas R. Q. Pacheco

Department of Mathematical Sciences, NTNU.

March 1, 2022

Introduction

Remember the ODEs we are trying to solve: $\mathbf{y}'(t) = \mathbf{f}(t, \mathbf{y})$

Introduction

Remember the ODEs we are trying to solve: $\mathbf{y}'(t) = \mathbf{f}(t, \mathbf{y})$

Euler's method:

$$\mathbf{k}_1 = \mathbf{f}(t_n, \mathbf{y}_n)$$

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\mathbf{k}_1 \rightarrow \mathcal{O}(h) \text{ convergence}$$

Introduction

Remember the ODEs we are trying to solve: $\mathbf{y}'(t) = \mathbf{f}(t, \mathbf{y})$

Euler's method:

$$\mathbf{k}_1 = \mathbf{f}(t_n, \mathbf{y}_n)$$

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\mathbf{k}_1 \rightarrow \mathcal{O}(h) \text{ convergence}$$

Heun's method:

$$\mathbf{k}_1 = \mathbf{f}(t_n, \mathbf{y}_n)$$

$$\mathbf{k}_2 = \mathbf{f}(t_n + h, \mathbf{y}_n + h\mathbf{k}_1)$$

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h[0.5\mathbf{k}_1 + 0.5\mathbf{k}_2] \rightarrow \mathcal{O}(h^2) \text{ convergence}$$

Introduction

Remember the ODEs we are trying to solve: $\mathbf{y}'(t) = \mathbf{f}(t, \mathbf{y})$

Euler's method:

$$\mathbf{k}_1 = \mathbf{f}(t_n, \mathbf{y}_n)$$

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\mathbf{k}_1 \rightarrow \mathcal{O}(h) \text{ convergence}$$

Heun's method:

$$\mathbf{k}_1 = \mathbf{f}(t_n, \mathbf{y}_n)$$

$$\mathbf{k}_2 = \mathbf{f}(t_n + h, \mathbf{y}_n + h\mathbf{k}_1)$$

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h[0.5\mathbf{k}_1 + 0.5\mathbf{k}_2] \rightarrow \mathcal{O}(h^2) \text{ convergence}$$

Questions:

- ▶ Can we generalise this?
- ▶ Can we do better than $\mathcal{O}(h^2)$?

Runge-Kutta methods

RK methods are **one-step methods** following the general scheme

$$k_i = f\left(t_n + c_i h, y_n + h \sum_{j=1}^s a_{ij} k_j\right), \quad i = 1, \dots, s \quad (s \text{ stages})$$

Runge-Kutta methods

RK methods are **one-step methods** following the general scheme

$$k_i = f\left(t_n + c_i h, y_n + h \sum_{j=1}^s a_{ij} k_j\right), \quad i = 1, \dots, s \quad (s \text{ stages})$$

$$y_{n+1} = y_n + h \sum_{i=1}^s b_i k_i$$

Runge-Kutta methods

RK methods are **one-step methods** following the general scheme

$$k_i = f\left(t_n + c_i h, y_n + h \sum_{j=1}^s a_{ij} k_j\right), \quad i = 1, \dots, s \quad (s \text{ stages})$$

$$y_{n+1} = y_n + h \sum_{i=1}^s b_i k_i$$

The coefficients are all real numbers, presented in the Butcher tableau:

c_1	a_{11}	a_{12}	\dots	a_{1s}
c_2	a_{21}	a_{22}	\dots	a_{2s}
\vdots	\vdots	\vdots	\ddots	\vdots
c_s	a_{s1}	a_{s2}	\dots	a_{ss}
	b_1	b_2	\dots	b_s

Runge-Kutta methods

$$\mathbf{k}_i = \mathbf{f}\left(t_n + c_i h, \mathbf{y}_n + h \sum_{j=1}^s a_{ij} \mathbf{k}_j\right)$$

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h \sum_{i=1}^s b_i \mathbf{k}_i$$

Euler's method:

$$\mathbf{k}_1 = \mathbf{f}(t_n, \mathbf{y}_n)$$

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h \mathbf{k}_1$$

c_1	a_{11}	a_{12}	\dots	a_{1s}
c_2	a_{21}	a_{22}	\dots	a_{2s}
\vdots	\vdots	\vdots	\ddots	\vdots
c_s	a_{s1}	a_{s2}	\dots	a_{ss}
	b_1	b_2	\dots	b_s

Runge-Kutta methods

$$\mathbf{k}_i = \mathbf{f}\left(t_n + c_i h, \mathbf{y}_n + h \sum_{j=1}^s a_{ij} \mathbf{k}_j\right)$$

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h \sum_{i=1}^s b_i \mathbf{k}_i$$

(????) method:

0		0	0
1		1	0
<hr/>			
		$\frac{1}{2}$	$\frac{1}{2}$

c_1		a_{11}	a_{12}	\dots	a_{1s}
c_2		a_{21}	a_{22}	\dots	a_{2s}
\vdots		\vdots	\vdots	\ddots	\vdots
c_s		a_{s1}	a_{s2}	\dots	a_{ss}
		b_1	b_2	\dots	b_s

Runge-Kutta methods

$$k_i = f\left(t_n + c_i h, y_n + h \sum_{j=1}^s a_{ij} k_j\right)$$

$$y_{n+1} = y_n + h \sum_{i=1}^s b_i k_i$$

Heun (3rd-order):

0	0	0	0
1/3	1/3	0	0
2/3	0	2/3	0
	1/4	0	3/4

c_1	a_{11}	a_{12}	\dots	a_{1s}
c_2	a_{21}	a_{22}	\dots	a_{2s}
\vdots	\vdots	\vdots	\ddots	\vdots
c_s	a_{s1}	a_{s2}	\dots	a_{ss}
	b_1	b_2	\dots	b_s

Consistency

$$\begin{array}{c|cccc}
 c_1 & a_{11} & a_{12} & \dots & a_{1s} \\
 c_2 & a_{21} & a_{22} & \dots & a_{2s} \\
 \vdots & \vdots & \vdots & \ddots & \vdots \\
 c_s & a_{s1} & a_{s2} & \dots & a_{ss} \\
 \hline
 & b_1 & b_2 & \dots & b_s
 \end{array}$$

Consistency

c_1	a_{11}	a_{12}	\dots	a_{1s}
c_2	a_{21}	a_{22}	\dots	a_{2s}
\vdots	\vdots	\vdots	\ddots	\vdots
c_s	a_{s1}	a_{s2}	\dots	a_{ss}
	b_1	b_2	\dots	b_s

Theorem

An RK method is **order- p consistent** if, and only if **all the conditions up to p** in the table are satisfied

Consistency

p	Conditions
1	$\sum_{i=1}^s b_i = 1$
2	$\sum_{i=1}^s b_i c_i = \frac{1}{2}$
3	$\sum_{i=1}^s b_i c_i^2 = \frac{1}{3}$ $\sum_{i=1}^s \sum_{j=1}^s b_i a_{ij} c_j = \frac{1}{6}$
4	$\sum_{i=1}^s b_i c_i^3 = \frac{1}{4}$ $\sum_{i=1}^s \sum_{j=1}^s b_i c_i a_{ij} c_j = \frac{1}{8}$ $\sum_{i=1}^s \sum_{j=1}^s b_i a_{ij} c_j^2 = \frac{1}{12}$ $\sum_{i=1}^s \sum_{j=1}^s \sum_{k=1}^s b_i a_{ij} a_{jk} c_k = \frac{1}{24}$

c_1	a_{11}	a_{12}	\dots	a_{1s}
c_2	a_{21}	a_{22}	\dots	a_{2s}
\vdots	\vdots	\vdots	\ddots	\vdots
c_s	a_{s1}	a_{s2}	\dots	a_{ss}
	b_1	b_2	\dots	b_s

Theorem

An RK method is **order- p consistent** if, and only if **all the conditions up to p** in the table are satisfied

Consistency

Heun's method:

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

p	Conditions
1	$\sum_{i=1}^s b_i = 1$
2	$\sum_{i=1}^s b_i c_i = \frac{1}{2}$
3	$\sum_{i=1}^s b_i c_i^2 = \frac{1}{3}$ $\sum_{i=1}^s \sum_{j=1}^s b_i a_{ij} c_j = \frac{1}{6}$
4	$\sum_{i=1}^s b_i c_i^3 = \frac{1}{4}$ $\sum_{i=1}^s \sum_{j=1}^s b_i c_i a_{ij} c_j = \frac{1}{8}$ $\sum_{i=1}^s \sum_{j=1}^s b_i a_{ij} c_j^2 = \frac{1}{12}$ $\sum_{i=1}^s \sum_{j=1}^s \sum_{k=1}^s b_i a_{ij} a_{jk} c_k = \frac{1}{24}$

Error estimation

One-step methods: $\mathbf{y}_{n+1} = \mathbf{y}_n + h\Phi(t_n, \mathbf{y}_n, h)$

Question: for a method Φ , how can we estimate the error $\epsilon_n = |\mathbf{y}_n - \mathbf{y}(t_n)|$, if we don't know the exact solution $\mathbf{y}(t)$?

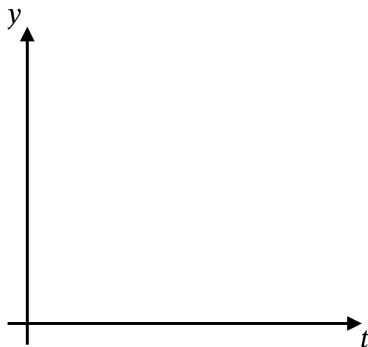
Error estimation

One-step methods: $\mathbf{y}_{n+1} = \mathbf{y}_n + h\Phi(t_n, \mathbf{y}_n, h)$

Question: for a method Φ , how can we estimate the error $\epsilon_n = |\mathbf{y}_n - \mathbf{y}(t_n)|$, if we don't know the exact solution $\mathbf{y}(t)$?

Idea

Why not use a more accurate method $\hat{\Phi}$ to compute $\hat{\epsilon}_n = |\mathbf{y}_n - \hat{\mathbf{y}}_n|$?



Error estimation

If $\hat{\epsilon}_{n+1} > \text{tol}$, we might want to reduce the time-step size h and recompute the step... but how can we estimate a good h_{new} ?

Error estimation

If $\hat{\epsilon}_{n+1} > \text{tol}$, we might want to reduce the time-step size h and recompute the step... but how can we estimate a good h_{new} ?

- ▶ Since $\hat{\Phi}$ is convergent of order $p + 1$, we can write

$$\hat{y}_{n+1} - y(t_n + h) = Ah^{p+1}$$

Error estimation

If $\hat{\epsilon}_{n+1} > \text{tol}$, we might want to reduce the time-step size h and recompute the step... but how can we estimate a good h_{new} ?

- ▶ Since $\hat{\Phi}$ is **convergent of order $p + 1$** , we can write

$$\hat{y}_{n+1} - y(t_n + h) = Ah^{p+1}$$

- ▶ Since Φ is **consistent of order p** , we can write

$$\frac{y(t_n+h) - y(t_n)}{h} - \Phi(t_n, y(t_n), h) = Bh^p, \text{ that is,}$$

Error estimation

If $\hat{\epsilon}_{n+1} > \text{tol}$, we might want to reduce the time-step size h and recompute the step... but how can we estimate a good h_{new} ?

- ▶ Since $\hat{\Phi}$ is **convergent of order $p + 1$** , we can write

$$\hat{y}_{n+1} - y(t_n + h) = Ah^{p+1}$$

- ▶ Since Φ is **consistent of order p** , we can write

$$\frac{y(t_n+h) - y(t_n)}{h} - \Phi(t_n, y(t_n), h) = Bh^p, \text{ that is,}$$

$$y(t_n + h) - [y(t_n) + h\Phi(t_n, y(t_n), h)] = Bh^{p+1}$$

Error estimation

If $\hat{\epsilon}_{n+1} > \text{tol}$, we might want to reduce the time-step size h and recompute the step... but how can we estimate a good h_{new} ?

- ▶ Since $\hat{\Phi}$ is **convergent of order $p + 1$** , we can write

$$\hat{y}_{n+1} - y(t_n + h) = Ah^{p+1}$$

- ▶ Since Φ is **consistent of order p** , we can write

$$\frac{y(t_n+h) - y(t_n)}{h} - \Phi(t_n, y(t_n), h) = Bh^p, \text{ that is,}$$

$$y(t_n + h) - [y(t_n) + h\Phi(t_n, y(t_n), h)] = Bh^{p+1}$$

Hence, we get

$$|\hat{y}_{n+1} - y_{n+1}| \approx |A + B|h^{p+1}$$

Error estimation

If $\hat{\epsilon}_{n+1} > \text{tol}$, we might want to reduce the time-step size h and recompute the step... but how can we estimate a good h_{new} ?

- ▶ Since $\hat{\Phi}$ is **convergent of order $p + 1$** , we can write

$$\hat{y}_{n+1} - y(t_n + h) = Ah^{p+1}$$

- ▶ Since Φ is **consistent of order p** , we can write

$$\frac{y(t_n+h)-y(t_n)}{h} - \Phi(t_n, y(t_n), h) = Bh^p, \text{ that is,}$$

$$y(t_n + h) - [y(t_n) + h\Phi(t_n, y(t_n), h)] = Bh^{p+1}$$

Hence, we get

$$\hat{\epsilon}_{n+1} = |\hat{y}_{n+1} - y_{n+1}| \approx |A + B|h^{p+1}$$

Time-step control

$$\hat{\epsilon}_{n+1} \approx Ch^{p+1}$$

$$\hat{\epsilon}_{new} \approx Ch_{new}^{p+1} \Rightarrow$$

Time-step control

$$\hat{\epsilon}_{n+1} \approx Ch^{p+1}$$

$$\hat{\epsilon}_{new} \approx Ch_{new}^{p+1} \Rightarrow$$

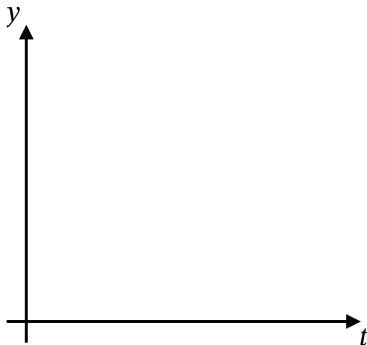
$$\hat{\epsilon}_{new} < tol \quad \Leftrightarrow \quad h_{new} < \left[\left(\frac{tol}{\hat{\epsilon}_{n+1}} \right)^{\frac{1}{p+1}} \right] h$$

Time-step control

$$\hat{\epsilon}_{n+1} \approx Ch^{p+1}$$

$$\hat{\epsilon}_{new} \approx Ch_{new}^{p+1} \Rightarrow$$

$$\hat{\epsilon}_{new} < tol \Leftrightarrow h_{new} < \left[\left(\frac{tol}{\hat{\epsilon}_{n+1}} \right)^{\frac{1}{p+1}} \right] h$$



Time-step control: Heun + Euler

$$y' = 2 + 2^{-t} - \sin(0.25\pi y), \quad y(0) = 2, \quad h = 0.5, \quad \text{tol} = 0.01$$

Time-step control: Heun + Euler

$$y' = 2 + 2^{-t} - \sin(0.25\pi y), \quad y(0) = 2, \quad h = 0.5, \quad \text{tol} = 0.01$$

First step:

- ▶ Evaluate $k_1 = f(t_n, y_n) = 2$
- ▶ Compute Euler step: $y_{n+1}^{\text{Euler}} = y_n + hk_1 = 3$
- ▶ Evaluate $k_2 = f(t_n + h, y_n + hk_1) = 2$
- ▶ Compute $y_{n+1} = y_n + h \left[\frac{k_1}{2} + \frac{k_2}{2} \right] = 3$

Time-step control: Heun + Euler

$$y' = 2 + 2^{-t} - \sin(0.25\pi y), \quad y(0) = 2, \quad h = 0.5, \quad \text{tol} = 0.01$$

First step:

- ▶ Evaluate $k_1 = f(t_n, y_n) = 2$
- ▶ Compute Euler step: $y_{n+1}^{\text{Euler}} = y_n + hk_1 = 3$
- ▶ Evaluate $k_2 = f(t_n + h, y_n + hk_1) = 2$
- ▶ Compute $y_{n+1} = y_n + h \left[\frac{k_1}{2} + \frac{k_2}{2} \right] = 3$

Error estimate: $\hat{\epsilon}_{n+1} = |3 - 3| = 0 < \text{tol}$

Time-step control: Heun + Euler

$$y' = 2 + 2^{-t} - \sin(0.25\pi y), \quad y(0) = 2, \quad h = 0.5, \quad \text{tol} = 0.01$$

First step:

- ▶ Evaluate $k_1 = f(t_n, y_n) = 2$
- ▶ Compute Euler step: $y_{n+1}^{\text{Euler}} = y_n + hk_1 = 3$
- ▶ Evaluate $k_2 = f(t_n + h, y_n + hk_1) = 2$
- ▶ Compute $y_{n+1} = y_n + h \left[\frac{k_1}{2} + \frac{k_2}{2} \right] = 3$

Error estimate: $\hat{e}_{n+1} = |3 - 3| = 0 < \text{tol}$

⇒ No need to recompute step!

⇒ We can keep h as it is,
or even increase it a bit...

Time-step control: Heun + Euler

$$y' = 2 + 2^{-t} - \sin(0.25\pi y), \quad y_1 = 3, \quad h = 0.5, \quad \text{tol} = 0.01$$

Second step:

- ▶ Evaluate $k_1 = f(t_n, y_n) = 2$
- ▶ Compute Euler step: $y_{n+1}^{\text{Euler}} = y_n + hk_1 = 4$
- ▶ Evaluate $k_2 = f(t_n + h, y_n + hk_1) = 2.5$
- ▶ Compute $y_{n+1} = y_n + h \left[\frac{k_1}{2} + \frac{k_2}{2} \right] = 4.125$

Time-step control: Heun + Euler

$$y' = 2 + 2^{-t} - \sin(0.25\pi y), \quad y_1 = 3, \quad h = 0.5, \quad \text{tol} = 0.01$$

Second step:

- ▶ Evaluate $k_1 = f(t_n, y_n) = 2$
- ▶ Compute Euler step: $y_{n+1}^{\text{Euler}} = y_n + hk_1 = 4$
- ▶ Evaluate $k_2 = f(t_n + h, y_n + hk_1) = 2.5$
- ▶ Compute $y_{n+1} = y_n + h \left[\frac{k_1}{2} + \frac{k_2}{2} \right] = 4.125$

Error estimate: $\hat{\epsilon}_{n+1} = |4.125 - 4| = 0.125 > \text{tol}$

Time-step control: Heun + Euler

$$y' = 2 + 2^{-t} - \sin(0.25\pi y), \quad y_1 = 3, \quad h = 0.5, \quad \text{tol} = 0.01$$

Second step:

- ▶ Evaluate $k_1 = f(t_n, y_n) = 2$
- ▶ Compute Euler step: $y_{n+1}^{\text{Euler}} = y_n + hk_1 = 4$
- ▶ Evaluate $k_2 = f(t_n + h, y_n + hk_1) = 2.5$
- ▶ Compute $y_{n+1} = y_n + h \left[\frac{k_1}{2} + \frac{k_2}{2} \right] = 4.125$

Error estimate: $\hat{\epsilon}_{n+1} = |4.125 - 4| = 0.125 > \text{tol}$

⇒ Reduce h and recompute the step:

$$h_{\text{new}} < \left[\left(\frac{\text{tol}}{\hat{\epsilon}_{n+1}} \right)^{\frac{1}{p+1}} \right] h = \left(\frac{0.01}{0.125} \right)^{\frac{1}{2}} \times 0.5 \approx 0.14$$

Time-step control: embedded RK

We can combine a higher-order method and a lower-order method as:

c_1	a_{11}	a_{12}	\dots	a_{1s}
c_2	a_{21}	a_{22}	\dots	a_{2s}
\vdots	\vdots	\vdots	\ddots	\vdots
c_s	a_{s1}	a_{s2}	\dots	a_{ss}
	b_1	b_2	\dots	b_s
	b_1^*	b_2^*	\dots	b_s^*

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h \sum_{i=1}^s b_i \mathbf{k}_i, \quad \mathcal{O}(h^{p+1})$$

$$\mathbf{y}_{n+1}^* = \mathbf{y}_n + h \sum_{i=1}^s b_i^* \mathbf{k}_i, \quad \mathcal{O}(h^p)$$

Time-step control: embedded RK

We can combine a **higher-order method** and a **lower-order method** as:

c_1	a_{11}	a_{12}	\dots	a_{1s}
c_2	a_{21}	a_{22}	\dots	a_{2s}
\vdots	\vdots	\vdots	\ddots	\vdots
c_s	a_{s1}	a_{s2}	\dots	a_{ss}
	b_1	b_2	\dots	b_s
	b_1^*	b_2^*	\dots	b_s^*

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h \sum_{i=1}^s b_i \mathbf{k}_i, \quad \mathcal{O}(h^{p+1})$$

$$\mathbf{y}_{n+1}^* = \mathbf{y}_n + h \sum_{i=1}^s b_i^* \mathbf{k}_i, \quad \mathcal{O}(h^p)$$

Therefore, we get simply $\hat{\epsilon}_{n+1} = |\mathbf{y}_{n+1} - \mathbf{y}_{n+1}^*| = h \left| \sum_{i=1}^s (b_i - b_i^*) \mathbf{k}_i \right|,$

Time-step control: embedded RK

We can combine a **higher-order method** and a **lower-order method** as:

c_1	a_{11}	a_{12}	\dots	a_{1s}
c_2	a_{21}	a_{22}	\dots	a_{2s}
\vdots	\vdots	\vdots	\ddots	\vdots
c_s	a_{s1}	a_{s2}	\dots	a_{ss}
	b_1	b_2	\dots	b_s
	b_1^*	b_2^*	\dots	b_s^*

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h \sum_{i=1}^s b_i \mathbf{k}_i, \quad \mathcal{O}(h^{p+1})$$

$$\mathbf{y}_{n+1}^* = \mathbf{y}_n + h \sum_{i=1}^s b_i^* \mathbf{k}_i, \quad \mathcal{O}(h^p)$$

Therefore, we get simply $\hat{\epsilon}_{n+1} = |\mathbf{y}_{n+1} - \mathbf{y}_{n+1}^*| = h \left| \sum_{i=1}^s (b_i - b_i^*) \mathbf{k}_i \right|$,

so we can easily compute

$$h_{new} < \left[\left(\frac{\text{tol}}{\hat{\epsilon}_{n+1}} \right)^{\frac{1}{p+1}} \right] h$$