

Runge-Kutta

Sunday, November 1, 2020

5:29 PM

Recall local truncation error $\tau_{i+1}(h) := \frac{1}{h} (y_{i+1} - (y_i + h \phi(t_i, y_i)))$

for the method $w_{i+1} = w_i + h \phi(t_i, w_i)$.

Euler's method has $\tau(h) = O(h)$. Higher-order methods do better, e.g., $O(h^2)$

We saw higher-order Taylor methods based on Taylor expansions of f

(recall: our IVP is $y' = f(t, y)$, $y(a) = y_0$, $t \in [a, b]$)

This lecture: a better way to get higher-order methods

Background: Taylor's Thm in 2D

Thm 5.13 Suppose $f(t, y)$ and all its partial derivatives of order $\leq n+1$

are continuous on $D = \{ (t, y) : a \leq t \leq b, c \leq y \leq d \}$, and let

$(t_0, y_0) \in D$. Then $\forall (t, y) \in D$, $\exists \xi$ between t and t_0

and $\exists \mu$ between y and y_0 with

$$f(t, y) = \underbrace{P_n(t, y)}_{\text{Taylor polynomial}} + \underbrace{R_n(t, y)}_{\text{error/remainder}}$$

where

$$\begin{aligned} P_n(t, y) = & \underbrace{f(t_0, y_0)}_{0^{\text{th}} \text{ order}} + \underbrace{(t - t_0) \frac{\partial f}{\partial t}(t_0, y_0) + (y - y_0) \frac{\partial f}{\partial y}(t_0, y_0)}_{1^{\text{st}} \text{ order terms}} \\ & + \underbrace{\frac{(t - t_0)^2}{2!} \frac{\partial^2 f}{\partial t^2}(t_0, y_0) + (t - t_0)(y - y_0) \frac{\partial^2 f}{\partial t \partial y}(t_0, y_0) + \frac{(y - y_0)^2}{2!} \frac{\partial^2 f}{\partial y^2}(t_0, y_0)}_{2^{\text{nd}} \text{ order terms}} \\ & + \dots + \underbrace{\frac{1}{n!} \sum_{j=0}^n \binom{n}{j} (t - t_0)^{n-j} (y - y_0)^j \frac{\partial^n f}{\partial t^{n-j} \partial y^j}(t_0, y_0)}_{n^{\text{th}} \text{ order terms}} \end{aligned}$$

Recall
 $\binom{n}{j} = \frac{n!}{(n-j)!j!}$

and the remainder term is

$$R_n(t, y) = \frac{1}{(n+1)!} \sum_{j=0}^{n+1} \binom{n+1}{j} (t - t_0)^{n+1-j} (y - y_0)^j \frac{\partial^{n+1} f}{\partial t^{n+1-j} \partial y^j}(\xi, \mu)$$

Idea of Runge-Kutta

Carl Runge 1856-1927, Martin Kutta 1867-1944

A family of methods, not a single method

$$y(t+h) = y(t) + \underbrace{h \cdot y'(t)}_{\substack{f(t,y) \\ \text{via ODE}}} + \underbrace{\frac{h^2}{2} y''(t)}_{f'(t,y)} + O(h^3)$$

So our 1st order Taylor method (Euler's method) is $\phi(t,y) = f(t,y)$

$$w_{i+1} = w_i + h \phi(t_i, w_i) \quad \left. \vphantom{w_{i+1}} \right\} \text{Generic form of one-step methods} \\ \text{(of which RK belongs)}$$

and 2nd order Taylor method is $\phi(t,y) = f(t,y) + \frac{h}{2} f'(t,y)$
etc. $\xrightarrow{\text{ } T^{(2)} \text{ } }$

Focus on \nearrow for now. We'd like to avoid calculating $f'(t,y)$.

Let's approximate it with Taylor Series! (if you haven't noticed yet, that's the theme of this class)

How many terms to keep in the Taylor Series?

We already have a $O(h^2)$ error in ϕ , so let's keep at some amount

It gets a bit messy.

Recall chain rule $f'(t,y) := \frac{d}{dt} f(t,y) = \frac{\partial}{\partial t} f(t,y) + \frac{\partial}{\partial y} f(t,y) \cdot \frac{dy}{dt} \stackrel{y'=f}{=}$

so

$$T^{(2)}(t,y) = \underbrace{f(t,y)}_{(1)} + \underbrace{\frac{h}{2} \frac{\partial f}{\partial t}(t,y)}_{(2)} + \underbrace{\frac{h}{2} \frac{\partial f}{\partial y}(t,y) \cdot f(t,y)}_{(3)}$$

Idea: can we find α , α and β such that

$$T^{(2)}(t,y) = \alpha \cdot f(t + \alpha, y + \beta) + O(h^2) \quad ?$$

Taylor expand (20) about $f(t,y)$

\swarrow match

$$\alpha \cdot f(t + \alpha, y + \beta) = \alpha \left(\underbrace{f(t,y)}_{(1)} + \underbrace{\alpha \frac{\partial f}{\partial t}(t,y)}_{(2)} + \underbrace{\beta \frac{\partial f}{\partial y}(t,y)}_{(3)} \right) + \alpha R_1(t + \alpha, y + \beta)$$

So matching terms

$$(1) \Rightarrow \boxed{\alpha = 1}$$

$$(2) \Rightarrow \alpha \alpha = h/2 \quad \text{so} \quad \boxed{\alpha = h/2}$$

$$(3) \Rightarrow \alpha \beta = h/2 \cdot f(t,y) \quad \text{so} \quad \boxed{\beta = h/2 f(t,y)}$$

and if $f(t, y)$ and all of its partial derivatives up to degree ≤ 2 are bounded, then $R_1(\dots) = O(h^2)$ ✓

We just derived the

Midpoint Method, a.k.a. Improved Euler (an example of a Runge-Kutta method)

$$w_0 = y_0$$

$$w_{i+1} = w_i + h \cdot f\left(t_i + \frac{h}{2}, w_i + \frac{h}{2} f(t_i, w_i)\right)$$

still "single step" but we call it "multistage"

Another way to write it:

Given w_i , $K_1 = h f(t_i, w_i)$

$$K_2 = h f\left(t_i + \frac{h}{2}, w_i + \frac{1}{2} K_1\right)$$

$$w_{i+1} = w_i + K_2$$

⚠ Twice the cost per iteration, compared to Euler, but usually definitely worth it.

General form of Runge-Kutta methods

We can generalize above, adding more parameters to get higher-orders

RK methods. All s -stage explicit Runge-Kutta methods can be described by their "Butcher array"

0					
c_1	a_{11}				
c_2	a_{21}	a_{22}			
\vdots	\vdots	\vdots	\ddots		
c_{s-1}	$a_{s-1,1}$	$a_{s-1,2}$	\dots	$a_{s-1,s-1}$	
	b_1	b_2	\dots	b_{s-1}	b_s

meaning

$$K_1 = h f(t_i, w_i)$$

$$K_2 = h f(t_i + c_1 h, w_i + a_{11} K_1)$$

$$K_3 = h f(t_i + c_2 h, w_i + a_{21} K_1 + a_{22} K_2)$$

$$\vdots$$

$$K_s = h f(t_i + c_{s-1} h, w_i + a_{s-1,1} K_1 + \dots)$$

$$w_{i+1} = w_i + b_1 K_1 + b_2 K_2 + \dots + b_s K_s$$

Ex Improved Euler

$$K_1 = h f(t_i, w_i)$$

$$K_2 = h f\left(t_i + \frac{h}{2}, w_i + \frac{1}{2} K_1\right)$$

$$w_{i+1} = w_i + K_2$$

$b_2 = 1, b_1 = 0$

Butcher array

0		
$\frac{1}{2}$	$\frac{1}{2}$	
	0	1

Ex Modified Euler (also a 2-stage, 2nd order method)

Our book defines it as $w_{i+1} = w_i + \frac{h}{2} \left[f(t_i, w_i) + f(t_{i+1}, w_i + h f(t_i, w_i)) \right]$

So the Butcher array is

0	
1	1
	$\frac{1}{2} \quad \frac{1}{2}$

$$= w_i + \underbrace{\frac{1}{2} h f(t_i, w_i)}_{K_1} + \underbrace{\frac{1}{2} h f(t_i + h, w_i + h f(t_i, w_i))}_{K_2}$$

$b_1 = \frac{1}{2}$ $b_2 = \frac{1}{2}$ $c_1 = 1$ $a_{11} = 1$

Another ex. of a 2-stage, 2nd order method is Heun's 2-stage method

not the same as our book's
3-stage, 3rd order Heun's method.

0	
$\frac{2}{3}$	$\frac{2}{3}$
	$\frac{1}{4} \quad \frac{3}{4}$

← note: b_i 's always sum to 1

(for consistency)

There are systematic ways to derive these, but complicated and... it only has to be done once. We can just use them

The zoo of RK methods: higher-order RK, and which ones to use?