These are the lecture notes for CSC349A Numerical Analysis taught by Rich Little in the Spring of 2018. They roughly correspond to the material covered in each lecture in the classroom but the actual classroom presentation might deviate significantly from them depending on the flow of the course delivery. They are provided as a reference to the instructor as well as supporting material for students who miss the lectures. They are simply notes to support the lecture so the text is not detailed and they are not thoroughly checked. Use at your own risk. They are complimentary to the handouts. Many thanks to all the guidance and materials I received from Dale Olesky who has taught this course for many years and George Tzanetakis.

1 Runge-Kutta Methods

Advantage of Taylor methods of order n

- global truncation error of $O(h^n)$ insures high accuracy (even for $n = 3, 4$ or 5)

Disadvantage

- high order derivatives of $f(x, y(x))$ may be difficult and expensive to evaluate.

Runge-Kutta methods are higher order formulas (they can have any order ≥ 1) that require function evaluations only of $f(x, y(x))$, and not of any of its derivatives.

1.1 Taylor Polynomial with 2 Variables

This is accomplished using the Taylor polynomial for a function of 2 variables:

$$
\begin{aligned}
f(x+h, y+k) = f(x,y) &+ hf_x(x,y) + kf_y(x,y) \\
&+ \frac{h^2}{2} f_{xx}(x,y) + hkf_{xy}(x,y) + \frac{k^2}{2} f_{yy}(x,y) \\
&+ \frac{h^3}{6} f_{xxx}(x,y) + \frac{h^2k}{2} f_{xxy}(x,y) + \frac{hk^2}{2} f_{xyy}(x,y) + \frac{k^3}{6} f_{yyy}(x,y) \\
&+ \cdots
\end{aligned}
$$

where $f_x \equiv \frac{\partial f}{\partial x}$, $f_{xy} \equiv \frac{\partial^2 f}{\partial x \partial y}$, etc.

The derivation of Runge-Kutta methods and an understanding of why they work requires the Taylor polynomial for a function of 2 variables, but this Taylor polynomial is not required to use these methods to numerically approximate the solution of a differential equation.

It is only needed in the derivation and we will derive the second-order Runge-Kutta methods a little later.

Runge-Kutta methods are so-called one-step methods (as also are Eulers method and all Taylor methods): that is, they are of the form

$$y_{i+1} = y_i + h\Phi(x_i, y_i, h)$$

for some (possibly very complicated) function Φ.

That is, each computed approximation $y_i + 1$ is computed using only the value y_i at the previous grid point, along with the values of x_i, the step size h, and of course the function $f(x, y(x))$ that specifies the differential equation.

1.2 General Form of RK Methods of Order m

A Runge-Kutta method of order m is of the form:

$$y_{i+1} = y_i + \sum_{j=1}^{m} a_j k_j$$

where the a_j are constants and the k_j are functions of the form,

$$\begin{aligned} k_1 &= hf(x_i, y_i) \\ k_j &= hf(x_i + \alpha_j h, y_i + \sum_{l=1}^{j-1} \beta_{jl} k_l), \text{ for } 2 \leq j \leq m \end{aligned}$$

Examples: Derive the general forms for $m = 1, 2, 3$, and 4.

Each of these formuals defines a whole class of Runge-Kutta methods of order m.

Our goal is to take the formula for any fixed value of $m \geq 1$, and determine values for the parameters:

- $\{a_1\}$ when $m = 1$
- $\{a_1, a_2, \alpha_2, \beta_{21}\}$ when $m = 2$

- $\{a_1, a_2, a_3, \alpha_2, \alpha_3, \beta_{21}, \beta_{31}, \beta_{32}\}$ when $m = 3$
- $\{a_1, a_2, a_3, a_4, \alpha_2, \alpha_3, \alpha_4, \beta_{21}, \beta_{31}, \beta_{32}, \beta_{41}, \beta_{42}, \beta_{43}\}$ when $m = 4$

so that the resulting Runge-Kutta method has as high an order as possible (i.e., its local truncation error is as small as possible).

2 Derivation of Runge-Kutta Methods

This is accomplished by choosing the unknown parameters $\{a_i\}, \{\alpha_i\}$, and $\{\beta_{ij}\}$ so that the Runge-Kutta formula

$$y_{i+1} = y_i + \sum_{j=1}^{m} a_j k_j$$

is identical to the Taylor series expansion

$$y(x_{i+1}) = y(x_i) + hy'(x_i) + \frac{h^2}{2}y''(x_i) + \frac{h^3}{6}y'''(x_i) + \cdots$$

to as many terms as possible.

Case m = 1

The only Runge-Kutta method of first order is when $a_1 = 1$. That is, Eulers method

$$y_{i+1} = y_i + hf(x_i, y_i)$$

For each value of $m \geq 2$, there are an infinite number of Runge-Kutta formulas, each one having local truncation error $O(h^{m+1})$ and thus global truncation error $O(h^m)$.

2.1 Derivation of second order R-K

$$\begin{aligned} y(x_{i+1}) = {} & y(x_i) + a_1 hf(x_i, y_i) \\ & + a_2 hf(x_i + \alpha_2 h, y_i + \beta_{21} hf(x_i, y_i)) \end{aligned}$$

Using the Taylor exapnsion for $f(x_i + \alpha_2 h, y_i + \beta_{21} h f(x_i, y_i))$, we get

$$\begin{aligned} y(x_{i+1}) = y(x_i) + a_1 h f(x_i, y_i) + a_2 h[& f(x_i, y_i) + \alpha_2 h f_x(x_i, y_i) \\ & + \beta_{21} h f(x_i, y_i) f_y(x_i, y_i) + O(h^2)] \\ = y(x_i) + [a_1 + a_2] h f(x_i, y_i) + h^2 [& a_2 \alpha_2 f_x(x_i, y_i) \\ & + a_2 \beta_{21} f(x_i, y_i) f_y(x_i, y_i)] + O(h^3) \end{aligned}$$

But, also by Taylors Theorem

$$\begin{aligned} y(x_{i+1}) =& y(x_i) + h y'(x_i) + \frac{h^2}{2} y''(x_i) + O(h^3) \\ =& y(x_i) + h f(x_i, y_i) + \frac{h^2}{2} f'(x_i, y_i) + O(h^3) \\ =& y(x_i) + h f(x_i, y_i) + \frac{h^2}{2} [f_x(x_i, y_i) + f(x_i, y_i) f_y(x_i, y_i)] \\ & + O(h^3) \end{aligned}$$

These two are equal only when

$$a_1 + a_2 = 1, a_2 \alpha_2 = 1/2, a_2 \beta_{21} = 1/2$$

2.2 Examples

1. **Heun's Method:** Let $a_1 = a_2 = 1/2, \alpha_2 = \beta_{21} = 1$, which gives

$$y_{i+1} = y_i + \frac{h}{2} [f(x_i, y_i) + f(x_i + h, y_i + h f(x_i, y_i))]$$

2. **Midpoint Method:** Let $a_1 = 0, a_2 = 1, \alpha_2 = \beta_{21} = 1/2$, which gives

$$y_{i+1} = y_i + h f(x_i + \frac{h}{2}, y_i + \frac{h}{2} f(x_i, y_i))$$

3. Use Heun's Method to solve $y' = 4e^{0.8x} - 0.5y$ from $x = 0$ to $x = 4$ with $h = 1$ and $y_0 = 2$.

2.3 Derivation of Third Order RK Methods

Case m = 3 It can be shown that any solution of a certain system of 6 nonlinear equations in 8 unknowns gives a third-order Runge-Kutta Method.

One common solution is

$$a_1 = \frac{1}{6}, a_2 = \frac{2}{3}, a_3 = \frac{1}{6}, \alpha_2 = \frac{1}{2}, \alpha_3 = 1, \beta_{21} = \frac{1}{2}, \beta_{31} = -1, \beta_{32} = 2$$

which gives the third-order Runge-Kutta method

$$y_{i+1} = y_i + \frac{1}{6}(k_1 + 4k_2 + k_3)$$

where

$$\begin{aligned} k_1 &= hf(x_i, y_i) \\ k_2 &= hf\left(x_i + \frac{h}{2}, y_i + \frac{k_1}{2}\right) \\ k_3 &= hf(x_i + h, y_i - k_1 + 2k_2) \end{aligned}$$

2.4 Derivation of Fourth Order RK Methods

Case m = 4 The 13 Runge-Kutta parameters are obtained by solving 11 nonlinear equations in 13 unknowns. One solution is called the **"classical" Runge-Kutta method**, which has global truncation error of $O(h^4)$:

$$y_{i+1} = y_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

where

$$\begin{aligned} k_1 &= hf(x_i, y_i) \\ k_2 &= hf\left(x_i + \frac{h}{2}, y_i + \frac{k_1}{2}\right) \\ k_3 &= hf\left(x_i + \frac{h}{2}, y_i + \frac{k_2}{2}\right) \\ k_4 &= hf(x_i + h, y_i + k_3) \end{aligned}$$