CSC349A Numerical Analysis

Lecture 20

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Higher-Order Taylor Series Methods

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Higher order methods can be obtained by keeping more terms from the Taylor expansion.

$$
\begin{aligned}
y(x_{i+1}) &= y(x_i) + hy'(x_i) + \frac{h^2}{2}y''(x_i) + \cdots \\
&\qquad + \frac{h^n}{n!}y^{(n)}(x_i) + \frac{h^{n+1}}{(n+1)!}y^{(n+1)}(\xi_i) \\
&= y(x_i) + hf(x_i, y(x_i)) + \frac{h^2}{2}f'(x_i, y(x_i)) + \cdots \\
&\qquad + \frac{h^n}{n!}f^{(n-1)}(x_i, y(x_i)) + O(h^{n+1})
\end{aligned}
$$

The Taylor Method of Order n

Dropping the $O(h^{n+1})$ remainder term in the above Taylor expansion, gives a numerical method

$$y_{i+1} = y_i + hf(x_i, y_i) + \frac{h^2}{2} f'(x_i, y_i) + \cdots + \frac{h^n}{n!} f^{(n-1)}(x_i, y_i)$$

for any integer $n \geq 1$.
This is called **the Taylor method of order** n (as its local truncation error is $O(h^{n+1})$, and thus its global truncation error is $O(h^n)$).
Euler's method is just the case when $n = 1$.

Example 1 - Taylor Method of Order 2

Solve the differential equation $y' = y - x^2 + 1$ with $y(0) = 0.5$ and step size $h = 0.2$ using the Taylor Method of order $n = 2$.

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

Example 1 continued

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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.

General Form of RK Methods

Runge-Kutta methods are so-called one-step methods (as also are Euler's 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.

General Form of RK Methods of Order m

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

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

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

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

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

Example 2 - Derive the general forms for $m = 1, 2, 3,$ and 4.

Example 2 - Derive the general forms for $m = 1, 2, 3$, and 4.

The Goal given General Form of Order m

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).

Deriving RK Methods of Order m

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

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

is identical to the Taylor series expansion

$$y_{i+1} = y_i + hy_i' + \frac{h^2}{2} y_i'' + \frac{h^3}{6} y_i''' + \cdots$$

to as many terms as possible.

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Derivation of First Order RK Method

Case m = 1
The only Runge-Kutta method of first order

$$y_{i+1} = y_i + ha_1 f(x_i, y_i)$$

is when $a_1 = 1$. That is, Euler's 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 $O(h^m)$.

Taylor Polynomial with 2 Variables

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.

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

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

Derivation of second order R-K

Case m = 2

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

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

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

Derivation of Second Order RK Method

But, also by Taylors Theorem

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

Derivation of Second Order RK Method

In summary, the second order Runge-Kutta general form is

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

and the second order Taylor expansion is

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

These two are equal only when

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

Examples - Heun's Method

Let $a_1 = a_2 = 1/2, \alpha_2 = \beta_{21} = 1$, which gives

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

Examples - Midpoint Method

Let $a_1 = 0, a_2 = 1, \alpha_2 = \beta_{21} = 1/2$, which gives

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

Example 2

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

Example 2 - Iterative refinement

We can make this an iterative process by plugging our current approximation of y_{i+1} into Heun's for the Euler approximation.

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

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

where

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

$$k_2 = f\left(x_i + \frac{h}{2}, y_i + \frac{h}{2}k_1\right)$$

$$k_3 = f(x_i + h, y_i - hk_1 + 2hk_2)$$

Derivation of Fourth Order RK Methods

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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 $O(h^4)$:

$$y_{i+1} = y_i + \frac{h}{6}(k_1 + 2_2 + 2k_3 + k_4)$$

where

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

$$k_2 = f\left(x_i + \frac{h}{2}, y_i + \frac{h}{2}k_1\right)$$

$$k_3 = f\left(x_i + \frac{h}{2}, y_i + \frac{h}{2}k_2\right)$$

$$k_4 = f(x_i + h, y_i + hk_3)$$

Classical Fourth Order RK Method Graphically

Example 3

Use the classical 4th-order RK method with $h = 0.2$ and $y(0) = 0.5$ to solve $y' = y - x^2 + 1$.

Example 3 continued