Runge-Kutta Methods

CS/SE 4X03

Ned Nedialkov

McMaster University

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Outline

Implicit trapezoidal method

- Consider $y'(t) = f(t, y)$, $y(t_i) = y_i$
- From $y(t_{i+1}) = y(t_i) + \int_{t_i}^{t} f(s, y(s))ds$,

$$y(t_{i+1}) = y(t_i) + \int_{t_i}^{t_{i+1}} f(s, y(s))ds$$

- Use the trapezoidal rule for the integral

$$\begin{aligned} y(t_{i+1}) &= y(t_i) + \int_{t_i}^{t_{i+1}} f(s, y(s))ds \\ &\approx y(t_i) + \frac{h}{2}[f(t_i, y(t_i)) + f(t_{i+1}, y(t_{i+1}))] \end{aligned}$$

- From

$$y(t_{i+1}) \approx y(t_i) + \frac{h}{2}[f(t_i, y(t_i)) + f(t_{i+1}, y(t_{i+1}))]$$

write

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

This is the implicit trapezoidal method

- We have to solve a nonlinear system in general for y_{i+1}

- Local truncation error is

$$d_i = \frac{y(t_{i+1}) - y(t_i)}{h} - \frac{1}{2}[f(t_i, y(t_i)) + f(t_{i+1}, y(t_{i+1}))]$$

- $d_i = O(h^2)$

Explicit trapezoidal method

- In the implicit trapezoidal rule, we need to solve for y_{i+1}
- We can approximate $y(t_{i+1})$ first using forward Euler:

$$Y = y_i + hf(t_i, y_i)$$

- Then plug Y into the formula for the implicit trapezoidal method

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

- This is a two-stage explicit Runge-Kutta method
- Local truncation error is

$$d_i = \frac{y(t_{i+1}) - y(t_i)}{h} - \frac{1}{2}[f(t_i, y(t_i)) + f(t_{i+1}, y(t_i) + hf(t_i, y(t_i)))]$$

$d_i = O(h^2)$, a bit involved to derive it

Implicit midpoint

- Use the midpoint quadrature rule:

$$\begin{aligned} y_{i+1} &= y_i + hf\left(t_{i+1/2}, y_{i+1/2}\right) \\ &= y_i + hf\left(t_i + h/2, (y_i + y_{i+1})/2\right) \end{aligned}$$

- That is, we solve for y_{i+1}
- Order is 2

Explicit midpoint method

- Take a step of size $h/2$ with forward Euler

$$Y = y_i + \frac{h}{2} f(t_i, y_i)$$

- Plug into the formula from the midpoint quadrature rule:

$$y_{i+1} = y_i + hf\left(t_i + h/2, Y\right),$$

- This is a two-stage explicit Runge-Kutta method
- Order is 2

Classical 4th order Runge-Kutta

- Based on Simpson's quadrature rule
- 4 stages
- Order 4, $O(h^4)$ accuracy

$$
\begin{aligned}
Y_1 &= y_i \\
Y_2 &= y_i + \frac{h}{2} f(t_i, Y_1) \\
Y_3 &= y_i + \frac{h}{2} f(t_i + h/2, Y_2) \\
Y_4 &= y_i + h f(t_i + h/2, Y_3) \\
y_{i+1} &= y_i + \frac{h}{6} \big[f(t_i, Y_1) + 2f(t_i + h/2, Y_2) + 2f(t_i + h/2, Y_3) + f(t_{i+1}, Y_4) \big]
\end{aligned}
$$

f :: R x R^n -> R^n

Stepsize control

- Estimate the error: Runge-Kutta pair (details omitted)
- Let h be the current stepsize
- Local error is of the form $e_i = ch^{q+1}$
- Assume an estimate for e_i is computed
- We require $e_i = ch^{q+1} \leq$ tol
- If the tolerance is satisfied, we accept the step and predict stepsize for the next step
- Otherwise, reject the step and repeat with smaller $\bar{h}$

- From $ch_i^{q+1} = e_i$,
$$c = \frac{e_i}{h^{q+1}}$$
and
$$ch_{i+1}^{q+1} = \frac{e_i}{h^{q+1}} h_{i+1}^{q+1} = \text{ tol}$$
From which
$$h_{i+1} = h \left(\frac{\text{tol}}{e_i} \right)^{1/(q+1)}$$
- Since tol $\geq e_i$, $h_{i+1} \geq h$

- If $e_i > \text{tol}$, the stepsize is rejected
- Repeat the step with

$$\bar{h} = h \left(\frac{\text{tol}}{e_i} \right)^{1/(q+1)}$$

- For "safety", typically new stepsize is computed by

$$0.9h \left(\frac{0.5\,\text{tol}}{e_i} \right)^{1/(q+1)}$$

Example

Denote $h = t_{i+1} - t_i$. Consider forward Euler and the explicit trapezoid methods

$$
\begin{aligned}
y_{i+1} &= y_i + hf(t_i, y_i), && \text{local error } O(h^2) \\
\widehat{y}_{i+1} &= y_i + \tfrac{1}{2}h[f(t_i, y_i) + f(t_{i+1}, y_{i+1})], && \text{local error } O(h^3)
\end{aligned}
$$

The error in y_{i+1} is $e = \|y_{i+1} - \widehat{y}_{i+1}\|$. Given tolerance tol ,

if $e \leq$ tol
  accept $\widehat{y}_{i+1}$ at t_{i+1}
  predict $\bar{h}$ for the next step
else
  reject the step
  predict $\bar{h} < h$
  repeat the step with $\bar{h}$

Example cont.

The error is $e = ch^2$ for some $c \geq 0$

Suppose $e \leq$ tol. On the next step $\bar{e} = \bar{c}\bar{h}^2$, for some $\bar{c} \geq 0$

Assume $c \approx \bar{c}$. Then

$$\begin{aligned}\bar{e} = \bar{c}\bar{h}^2 \approx c\bar{h}^2 &= \frac{e}{h^2}\bar{h}^2 \\ &= e\left(\frac{\bar{h}}{h}\right)^2\end{aligned}$$

Example cont.

Requiring $\bar{e} = \text{tol}$,

$$\bar{h} = h \left(\frac{\text{tol}}{e} \right)^{1/2}$$

Aim at $0.5\,\text{tol}$ and multiply by 0.9, safety factors:

$$\bar{h} = 0.9h \left(\frac{0.5\,\text{tol}}{e} \right)^{1/2}$$

If $e \geq \text{tol}$, use the same formula

$$\bar{h} \leftarrow \min\{0.5h, \bar{h}\}$$

How to form tol. Assume absolute atol and relative rtol tolerances are given. Then

$$\text{tol} = \text{rtol} \cdot \|y_i\| + \text{atol}$$