Runge-Kutta Methods

$$u'(t) = f(u,t) \qquad u \in \mathbb{R}^m$$
$$u(t_0) = \eta$$

$$Y_i = U^n + k \sum_{j=1}^{s} a_{ij} f(Y_j, t_n + c_j k) \qquad 1 \le i \le s$$

$$U^{n+1} = U^n + k \sum_{j=1}^{s} b_j f(Y_j, t_n + c_j k)$$

Butcher Tableau:

$$\begin{array}{c|c} c & A^{s \times s} \\ \hline & b^T \end{array}$$

b: weights

c: abscissas

For example:

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

$$Y_1 = U^n$$
$$Y_2 = U^n + k f(Y_1, t_n)$$
$$U^{n+1} = U^n + \frac{k}{2}\left(f(Y_1, t_n) + f(Y_2, t_n + k)\right)$$

2nd-order $\quad \tau = O(k^2)$

2-stage

$$\begin{array}{c|cccc}
0 & 0 & & & \\
1/2 & 1/2 & 0 & & \\
1/2 & 0 & 1/2 & 0 & \\
1 & 0 & 0 & 1 & 0 \\
\hline
 & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6}
\end{array}$$

$\bigcirc$

RK4

4-stage

4th-order

$$\begin{array}{c|cc}
\frac{1}{2}-\gamma & \frac{1}{4} & \frac{1}{4}-\gamma \\
\frac{1}{2}+\gamma & \frac{1}{4}+\gamma & \frac{1}{4} \\
\hline
 & 1/2 & 1/2
\end{array}$$

$\gamma = \sqrt{3}/6$

Gauss-Legendre

2-stage

4th order

Classes of Runge-Kutta methods

1. Explicit: A is strictly lower-triangular — No need to solve anything

2. Fully implicit: A is a full matrix — Need to solve a system of ms equations

3. Diagonally implicit: A is lower-triangular — Need to solve S systems of m equations

Let's apply a RK method to

$$u'(t) = \lambda u$$

$$Y_i = U^n + \lambda k \sum_j a_{ij} Y_j \qquad 1 \le i \le s$$

$$U^{n+1} = U^n + \lambda k \sum_j b_j Y_j$$

Define:

$$Y = \begin{bmatrix} Y_1 \\ \vdots \\ Y_s \end{bmatrix} \qquad \mathbb{1} = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}$$

$$z = k\lambda$$

$$Y = U^n \mathbb{1} + z A Y$$

$$U^{n+1} = U^n + z b^T Y$$

$$(I - zA) Y = \mathbb{1} U^n$$

$$Y = (I - zA)^{-1} \mathbb{1} U^n$$

$$U^{n+1} = \underbrace{\left(1 + z b^T (I - zA)^{-1} \mathbb{1}\right)}_{R(z)} U^n$$

$R(z)$ (abs. stab. fcn.)

$$U^{n+1} = R(z) U^n$$

$R(z)$ is a rational function

Neumann:

$$\frac{1}{1-x} = 1 + x + x^2 + \cdots = \sum_{j=0}^{\infty} x^j$$

$$(I - zA)^{-1} = \sum_{j=0}^{\infty} z^j A^j$$

$$R(z) = 1 + b^T \sum_{j=0}^{\infty} z^{j+1} A^j \mathbb{1}$$

If A is strictly lower-triangular then $A^s = 0$.

So for explicit methods:

$$R(z) = 1 + b^T \sum_{j=0}^{s-1} z^{j+1} A^j \mathbb{1}$$

(polynomial of degree s)

For instance, for RK4

$$\underline{R(z) = 1 + z + \tfrac{1}{2} z^2 + \tfrac{1}{6} z^3 + \tfrac{1}{24} z^4}$$

Exact solution of $\begin{array}{l} u'(t) = \lambda u \\ u(0) = \eta \end{array}$

is

$$u(t) = e^{\lambda t} \eta$$

$$u(t_n) = e^{\lambda t_n} \eta$$

$$u(t_n + k) = e^{\lambda(t_n + k)} \eta$$

$$u(t_n + k) = e^{\lambda k} u(t_n) = e^{z} u(t_n)$$

So $R(z) \approx e^z$.

To get accuracy of order k^p:

i.e. we want (for explicit methods)

$$\left. 1 + b^T \sum_{j=0}^{p-1} z^{j+1} A^j \mathbb{1} = \sum_{j=0}^{p} \frac{z^j}{j!} \right\}$$

this means

$$b^T z^j A^{j-1} \mathbb{1} = \frac{z^j}{j!}$$

$$b^T A^{j-1} \mathbb{1} = \frac{1}{j!} \quad 1 \le j \le p$$

These conditions are necessary but not sufficient for accuracy of order p on a general ODE $u'(t)=f(u)$.

For instance, to achieve 3rd order we also require

$$\sum_i b_i \left(\sum_j a_{ij}\right)^2 = \frac{1}{3}.$$

How to choose K?

We want both

1. Small enough for stability
2. Small enough to achieve desired accuracy

Bounding the global is very expensive. Instead we focus on bounding local errors.

The LTE depends on derivatives of $u(t)$, which may vary greatly.

So we want to adjust K adaptively, to enforce $\tau^n < \varepsilon \leftarrow$ tolerance

Embedded RK Pairs

$$Y_i = U^n + k\sum_{j=0}^{s} a_{ij} f(Y_j, t_n + c_j k)$$

$$U^{n+1} = U^n + k\sum_{j=0}^{s} b_j f(Y_j, t_n + c_j k)$$

$$\hat{U}^{n+1} = U^n + k\sum_{j=0}^{s} \hat{b}_j f(Y_j, t_n + c_j k)$$

b_j chosen to get order p

$\hat{b}_j$ chosen to get order $p-1$

$$U^{n+1} = u(t_n + k) + \mathcal{O}(k^{p+1})$$

$$\hat{U}^{n+1} = u(t_n + k) + \mathcal{O}(k^{p})$$

So $U^{n+1} - \hat{U}^{n+1} = \mathcal{O}(k^p)$ is an estimate of the error in the second solution.

Step size adaption

1. Take a step and estimate the local error
$$\delta = |U^{n+1} - \hat{U}^{n+1}|$$
2. If $\delta > \varepsilon$, go back and redo step with smaller k.
3. If $\delta < \varepsilon$ continue.
(if δ is significantly smaller than ε, increase k)