Runge-Kutta methods

introduction

- recall, we are solving initial value problems of the form

$$\frac{du}{dt} = f(t, u), \quad u(0) = u_0$$

  using numerical methods which determine approximations $u_k \approx u(t_k)$ for some numerical grid $t_0 < t_1 < \cdots < t_n$
- Runge-Kutta (RK) methods are one-step methods with

$$u_{k+1} = u_k + h\phi(t_k, u_k)$$

  - are defined by a special class of functions

$$\phi : [0, T] \times \mathbb{R}^d \to \mathbb{R}^d$$

- The determination of the value of ϕ has two stages:
  1. In the *first stage*, approximations U_k^j of $u(s_j)$ for $s_j \in [t_k, t_{k+1}]$ and $j = 1, \ldots, m$ are determined
  2. In the *second stage*, these values are used to compute the value of ϕ by the formula

$$\phi(t_k, u_k) = \sum_{j=1}^{m} c_j\, f(s_j, U_k^j)$$

    - note that in the RK literature you can often find $k_j = f(s_j, U_k^j)$ (k_j has nothing to do with the index k!)

first stage of RK

- recall that for all $s_i \in [t_k, t_{k+1}]$ the exact solution $u(s_j)$ satisfies

$$u(s_j) = u(t_k) + \int_{t_k}^{s_j} f(r, u(r))\, dr$$

- replacing the integral by numerical quadrature leads to

$$U_k^j = u_k + h \sum_{i=1}^{m} b_{ji}\, f(s_i, U_k^i), \quad j = 1, \ldots, m$$

  where b_{ji} are again quadrature weights
- note however, that the b_{ji} are not necessarily standard quadrature weights and require the solution of systems of polynomial equations

- for *explicit* methods, one chooses the matrix $B = [b_{ji}]$ to be lower diagonal with zero diagonal elements such that $b_{ji} = 0$ for $i \geq j$
- the equation is solved by substitution
- for the first stage often variants of Euler or the midpoint rules are used
- note that the points $s_i \in [t_k, t_{k+1}]$ may contain the same point multiple times so that one may have several approximations of $U_k^i \approx u(s_i)$ with different errors

second stage of RK

- in this stage we determine $u_{k+1} \approx u(t_{k+1})$ from the U_k^i
- the exact value is

$$u(t_{k+1}) = u(t_k) + \int_{t_k}^{t_{k+1}} f(s, u(s))\, ds$$

  so that the formula for ϕ can be interpreted as a quadrature rule for the integral with quadrature points s_j and weights c_j but note that unlike for usual quadrature rules one may have duplicate quadrature points
- for given points s_j the weights c_j are determined such that
  - the quadrature rule is highly accurate
  - lower order (larger) errors in U_k^j are cancelled

design of Runge-Kutta methods

- the determination of the coefficients b_{ij} and c_j and the points $s_i = t_k + a_i h$ defining the Runge-Kunta method are an advanced topic which cannot be covered in more detail here
  - one considers approximation and stability aspects
- Runge-Kutta methods are probably the most widely used solution methods for ODE initial value problems and are also used for intitial value problems for PDEs (partial differential equations)

references

- Peter Henrici, *Discrete Variable Methods in Ordinary Differential Equations*, John Wiley, 1961
- John C. Butcher, *The Numerical Analysis of Ordinary Differential Equations*, John Wiley, 1987
- A. Iserles, *A First Course in the Numerical Analysis of Differential Equations*, Cambridge Uni Press 1996
- E. Hairer, S.P. Norsett, G. Wanner, *Solving Ordinary Differential Equations I – Nonstiff Problems*, Springer 2008, 2nd rev. ed

Butcher tableau

- often the coefficients a_i, b_{ij} and c_j are included in a block matrix

$$T = \begin{vmatrix} a & B \\ 0 & c^T \end{vmatrix}$$

  which is called the *Butcher tableau* after one of the major contributors John Butcher from Auckland

  - note that $a_1 = 0$ and $b_{0j} = 0$ and are sometimes omitted from the tableau

example 1: Euler's method

- many classical one-step methods actually are Runge-Kutta methods
- Stage 1 is trivial for Euler
  - $m = 1$ and $s_1 = t_k$ so that

$$U_k^1 = u_k$$

- Stage 2

$$\phi(t_k, u_k) = f(s_1, U_k^1) = f(t_k, u_k)$$

  - rectangle rule

example 2: Heun's method

- Stage 1
  - $m = 2$, $s_1 = t_k$ and $s_2 = t_{k+1} = t_k + h$

$$
\begin{aligned}
U_k^1 &= u_k \\
U_k^2 &= u_k + hf(s_1, U_k^1)
\end{aligned}
$$

- U_k^2 uses rectangle rule
- Stage 2

$$
\phi(t_k, u_k) = 0.5f(s_1, U_k^1) + 0.5f(s_2, U_k^2)
$$

  - the associated quadrature rule is the trapezoidal rule

example 3: midpoint method

- Stage 1
  - $m = 2$, $s_1 = t_k$ and $s_2 = t_k + h/2$

$$U_k^1 = u_k$$
$$U_k^2 = u_k + 0.5hf(s_1, U_k^1)$$

- U_k^2 uses rectangle rule
- Stage 2

$$\phi(t_k, u_k) = f(s_2, U_k^2)$$

  - the associated quadrature rule is the midpoint rule

example 4: fourth order Runge Kutta method

- Stage 1
  - $m = 4$, $s_1 = t_k$, $s_2 = s_3 = t_k + h/2$ and $s_4 = t_k + h$

$$
\begin{aligned}
U_k^1 &= u_k \\
U_k^2 &= u_k + 0.5hf(s_1, U_k^1) \\
U_k^3 &= u_k + 0.5hf(s_2, U_k^2) \\
U_k^4 &= u_k + hf(s_3, U_k^3)
\end{aligned}
$$

  - U_k^2 uses rectangle rule
  - U_k^3 uses right-handed rectangle rule
  - U_k^4 uses midpoint rule
- Stage 2

$$\phi(t_k, u_k) = \frac{1}{6}(f(s_1, U_k^1) + 2f(s_2, U_k^2) + 2f(s_3, U_k^3) + f(s_4, U_k^4))$$

  - the associated quadrature rule is Simpson's rule

example 5: 3/8-rule fourth-order method

- stage 1
  - $m = 4$, $s_1 = t_k$, $s_2 = t_k + h/3$, $s_3 = t_k + 2h/3$ and $s_4 = t_k + h$

$$
\begin{aligned}
U_k^1 &= u_k \\
U_k^2 &= u_k + h/3 f(s_1, U_k^1) \\
U_k^3 &= u_k + -h/3 f(s_1, U_k^1) + hf(s_2, U_k^2) \\
U_k^4 &= u_k + hf(s_1, U_k^1) - hf(s_2, U_k^2) + hf(s_3, U_k^3)
\end{aligned}
$$

  - U_k^2 uses rectangle rule
  - U_k^3 and U_k^4 do not use standard rules
- stage 2

$$
\phi(t_k, u_k) = \frac{1}{8}(f(s_1, U_k^1) + 3f(s_2, U_k^2) + 3f(s_3, U_k^3) + f(s_4, U_k^4))
$$

  - the associated quadrature rule is Simpson's 3/8 rule

Computing the coefficients in 1D case

computations in ring of polynomials in h modulo h^2

- arithmetic modulo h^2 (more generally h^p)
  - examples – we use $O(h^2)$ in a purely algebraic sense
    $$4h^2 + 2h - 3 = 2h - 3 + O(h^2)$$
    or
    $$\exp(h) = 1 + h + O(h^2)$$
  - the symbol $O(h^2)$ thus denotes the zero in the ring of polynomials modulo h^2
- Taylor series of $u(t+h)$
  $$u(t+h) = u(t) + hf(t, u(t) + O(h^2)$$
- If
  $$s = t + ah + O(h^2), \quad \text{and} \quad U = u(t) + bhf(t, u(t)) + O(h^2)$$
  one gets from the Taylor series of f:
  $$f(s, U) = f(t, u(t)) + (t-s)f_t(t, u(t)) + (U - u(t))f_u(t, u(t)) + O(h^2)$$

a second order general explicit Runge Kutta method

- Stage 1
  - $m = 2$, $s_1 = t_k$ and $s_2 = t_k + ah$

$$
\begin{aligned}
U_k^1 &= u_k \\
U_k^2 &= u_k + bhf(t_k, u_k)
\end{aligned}
$$

- Stage 2 gives then

$$\phi(t_k, u_k) = c_1 f(t_k, u_k) + c_2 f(t_k + ah, u_k + bhf(t_k, u_k))$$

- modulo h^2 one gets

$$\phi(t_k, u_k) = (c_1 + c_2) f(t_k, u_k) + c_2 ahf_t(t_k, u_k) + c_2 bhf_u(t_k, u_k) + O(h^2)$$

the slope of the secant

- note: be careful with division, i.e., do division of Taylor series first then compute remainder mod h^2:

$$\frac{u(t+h)-u(t)}{h} = u'(t) + h\frac{u''(t)}{2} + O(h^2)$$

- second derivative – use gradient and chain rule (exact):

$$u''(t) = f_t(t, u(t)) + f_u(t, u(t))f(t, u(t))$$

- one then gets for the slope of the secant ($t = t_k$ and $u(t) = u_k$):

$$\begin{aligned}\frac{u(t+h)-u(t)}{h} &= f(t_k, u_k) \\ &\quad + h\frac{f_t(t_k, u_k)}{2} + h\frac{f_u(t_k, u_k)f(t_k, u_k)}{2} + O(h^2)\end{aligned}$$

local approximation error or truncation error:

$$L(t,h) = \frac{u(t+h) - u(t)}{h} - \phi(t_k, u_k)$$

where $u_k = u(t)$ and $t = t_k$

- substituting the expressions for the secant slope and ϕ one gets

$$\begin{aligned} L(t_k, h) = &(1 - c_1 - c_2)\, f(t_k, u_k) \\ &+ h(\frac{1}{2} - c_2 a)\, f_t(t_k, u_k) + h(\frac{1}{2} - c_2 b)\, f_u(t_, u_k)\, f(t_k, u_k) + O(h^2) \end{aligned}$$

- we want a method of second order, i.e., $L(t,h) = O(h^2)$
- from this it follows

$$c_1 = 1 - \frac{1}{2a}, \quad c_2 = \frac{1}{2a}, \quad \text{and} \quad b = a$$

- one obtains Heun's method with $a = 1$

Computational exploration

Example

Consider the IVP

$$\frac{du(t)}{dt} = -4t(1+t^2)\,u(t)^2, \quad u(0) = 1.$$

You can check that the exact solution is

$$u(t) = \frac{1}{(t^2+1)^2}.$$

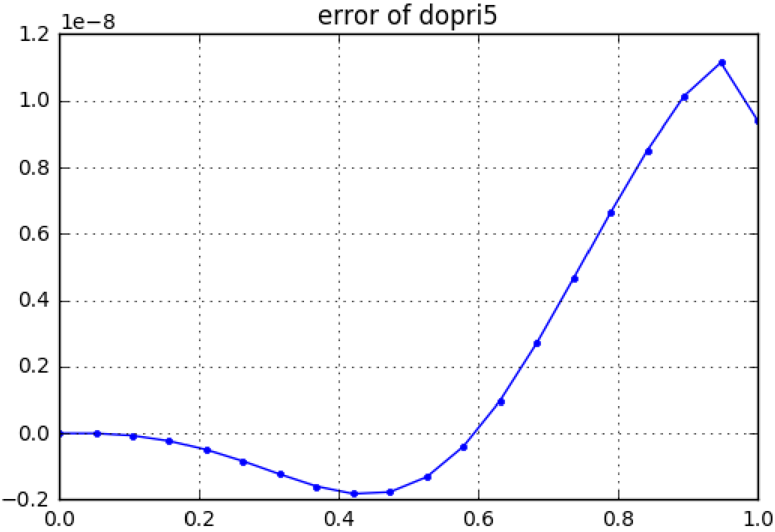
```
# example run of library RK routine DOPRI5 from odepack, se

# set the ode and integrator
f = lambda t,u : -4*t*(1.0+t**2)*u**2   # rhs of ODE
solver = scint.ode(f)
solver.set_integrator('dopri5')

# initial conditions
t0 = 0.0; u0 = 1.0
solver.set_initial_value(u0, t0)

# compute solution
n = 20
tn = np.linspace(0,1.0,n)
uex = 1.0/(tn**2+1.0)**2      # exact solution
unum = [u0,]
for t in tn[1:]:
    unum.append(solver.integrate(t)[0])
```

```
plt.title('error of dopri5')
plt.plot(tn, unum-uex,'.-');
plt.grid('on')
```



study accuracy vs cost (number of integration steps) of dopri5

```
# set the ode and integrator
f = lambda t,u : -4*t*(1.0+t**2)*u**2

def solout(t,u):
    ts.append(t)

t0 = 0.0; u0 = 1.0    # initial conditions
tn = 1.0
uex = 1.0/(tn**2+1.0)**2      # exact solution
```

```python
for itol in range(5,15):
    atol = 10**(-itol); solver = scint.ode(f)
    solver.set_integrator('dopri5',atol=atol,rtol=0)
    ts = []; solver.set_solout(solout)  # store results
    solver.set_initial_value(u0, t0)
    unum = solver.integrate(t)[0]
    print(len(ts), atol, (unum-uex)/atol)
```

```
11 1e-05 0.519207076399
14 1e-06 0.33133525329
19 1e-07 0.297607787858
27 1e-08 0.270854844109
39 1e-09 0.246938580695
60 1e-10 0.210362283148
92 1e-11 0.198763228099
144 1e-12 0.198230321047
226 1e-13 0.194289029309
355 1e-14 0.210942374679
```

documentation for the ode solvers

```
help(solver)

Help on ode in module scipy.integrate._ode object:

class ode(builtins.object)
 |  A generic interface class to numeric integrators.
 |
 |  Solve an equation system :math:`y'(t) = f(t,y)` with (o
 |
 |  *Note*: The first two arguments of ``f(t, y, ...)`` are
 |  opposite order of the arguments in the system definitio
 |  by `scipy.integrate.odeint`.
 |
 |  Parameters
 |  ----------
 |  f : callable ``f(t, y, *f_args)``
 |      Right-hand side of the differential equation. t is
 |      ``y.shape == (n,)``
```

Reference

A. C. Hindmarsh, *ODEPACK, A Systematized Collection of ODE Solvers,* in vol. 1 of IMACS Transactions on Scientific Computation), pp. 55-64, 1983.