Computational Physics

Notes on Fourth-order Runge-Kutta with Adaptive Stepsize

Imagine we implement the solution to the first order ODE

$$\frac{dx}{dt} = f(x,t)$$

using the RK4 method.

RK4 is accurate to fourth order and has an error at fifth order.
The size of the error on a single step h is ch^5 for some constant c.

If we know $x(t)$ and want to estimate $x(t+2h)$ there are two ways to proceed.

* Single step of size $2h$ with error $c(2h)^5 = 32ch^5$

* Two steps of size h with total error $ch^5 + ch^5 = 2ch^5$

Notes on Adaptive RK4 cont.

The later gives us the estimate

$$x(t+2h) = x_1 + 2ch^5$$

error from 2 h steps

The former gives us the estimate

$$x(t+2h) = x_2 + 32ch^5$$

error from 1 2h step

If $\epsilon_x = ch^5$ is the error on a single step of size h we can see that these two estimates can be used to estimate ϵ.

$$\epsilon_x \simeq \frac{1}{30}(x_1 - x_2)$$

The plan with adaptive stepsize is to make this error equal to a target accuracy we specify by adjusting h.

Notes on Adaptive RK4 cont.

Typically we will find that if are target accuracy is δ that either

$$\epsilon < \delta h \quad \text{(stepsize too small, wasting time)}$$

$$\epsilon > \delta h \quad \text{(stepsize too large, error too large)}$$

If we take a step of size h' then:

$$\epsilon' = c(h')^5 = ch^5\left(\frac{h'}{h}\right)^5 = \frac{1}{3}(x_1 - x_2)\left(\frac{h'}{h}\right)^5$$

We want $\frac{1}{30}\|x_1 - x_2\|\left(\frac{h'}{h}\right)^5 = h'\delta$ for fixed δ

Solving for $h' = h\left(\frac{h\delta}{\frac{1}{30}\|x_1-x_2\|}\right)^{1/4} = h\left(\frac{30h\delta}{\|x_1-x_2\|}\right)^{1/4}$

$$h' = h\rho^{1/4} \qquad \rho \equiv \frac{30h\delta}{\|x_1-x_2\|}$$

Notes on Adaptive RK4 cont.

$$\rho = \frac{h\delta}{\frac{1}{30}\|x_1 - x_2\|} = \frac{30 h \delta}{\|x_1 - x_2\|}$$

is ratio of desired accuracy and the actual accuracy for a step h

Method:

If $\rho > 1$ we know the actual accuracy is better than we require, so our last step was fine but wasteful. We move to the next step of the calculation but use a larger step $h' = h\rho^{1/4}$

If $\rho < 1$ we have missed our target accuracy. Repeat the current step again with step size $h' = h\rho^{1/4}$

Notes on Adaptive RK4 cont.

Note that we always use X_1 to advance the solution as the error on X_1 is smaller than the error on X_2.

It is possible, by chance, that $X_2 - X_1 \simeq 0$ such that $\rho^{1/4}$ becomes unreasonably large, and breaks the algorithm. To stabalize this we can enforce that the stepsize does not increase by more than a fixed amount. A good rule of thumb is that $h'/h \leq 2$.

So
$$h' = \begin{cases} \rho^{1/4}\, h & \text{if} \quad \rho^{1/4} < 2 \\ 2\, h & \text{if} \quad \rho^{1/4} > 2 \end{cases}$$

Notes on Adaptive RK4 cont.

This generalizes to multidimentional RK4 with the caveat that the criteria for setting the target accuracy will depend on the problem.

You may have a problem

$$\frac{dx}{dt} = f_x(x, y, t) \qquad \frac{dy}{dt} = f_y(x, y, t)$$

Where you primarily care about x and thus take

$$\rho = \frac{h\delta}{\epsilon_x} = \frac{30h\delta}{\|x_1 - x_2\|}$$

or maybe you care more about $\sqrt{x^2+y^2}$ and take

$$\rho = \frac{h\delta}{\sqrt{\epsilon_x^2+\epsilon_y^2}} = \frac{30h\delta}{(\|x_1-x_2\|^2+\|y_1-y_2\|^2)^{1/2}}$$