Simple cases for $f(x,y)$

(1) $f(x)$ only (not a function of y)

$$y(x_{j+1}) - y(x_j) = \underbrace{\int_{x_j}^{x_{j+1}} f(x)\,dx}$$

last chapter $\Rightarrow$ use Simpson's rule

$$y_{j+1} = y_j + \frac{h}{6}\left[f(x_j) + 4 f(x_j + \tfrac{h}{2}) + f(x_{j+1}) \right]$$

(split double panel $\overset{h}{\underset{x_j}{\bullet}\!\!\longrightarrow}\!\!\underset{x_{j+1}}{\bullet}\!\!\overset{h}{\longrightarrow}\!\!\underset{x_{j+2}}{\bullet}$ into single $\overset{\longleftarrow h \longrightarrow}{\underset{x_j}{\circ} - \underset{x_j+\frac{h}{2}}{+} - \underset{x_{j+1}}{\circ}}$)

For RK4 with $f(x)$ only $K_1 = K_2 = f(x_j + h/2)$

RK4 $y_{j+1} = y_j + \frac{1}{6} h \left[f(x_j) + (2+2) f(x_j + \tfrac{h}{2}) + f(x_j + h) \right]$

RK4 $\Longleftrightarrow$ Simpson's rule when $f(x)$

(2) $f(y)$ only (called autonomous ODE)

test eqn: $y'(x) = \mu y(x)$

$$K_0 = h f(x_j, y_j) = \mu h y_j$$

$$K_1 = h f\left(x_j + \tfrac{h}{2}, y_j + \tfrac{K_0}{2}\right) = h\mu \left[y_j + K_0/2 \right]$$

$$= \left[\mu h + \tfrac{1}{2}(\mu h)^2 \right] y_j$$

$$K_2 = h f\left(x_j + \tfrac{h}{2}, y_j + \tfrac{K_1}{2}\right) = h\mu \left[y_j + K_1/2 \right]$$

$$= \left[\mu h + \tfrac{1}{2}(\mu h)^2 + \tfrac{1}{4}(\mu h)^3 \right] y_j$$

$k_3 = hf(x_j + h, y_j + k_2) =$

$$\left[\mu h + \tfrac{1}{2}(\mu h)^2 + \tfrac{1}{3}(\mu h)^3 + \tfrac{1}{4}(\mu h)^4\right] y_j$$

$$y_{j+1} = y_j + \tfrac{1}{6}(k_0 + 2k_1 + 2k_2 + k_3)$$

$$= \left[1 + \mu h + \tfrac{1}{2}(\mu h)^2 + \tfrac{1}{6}(\mu h)^3 + \tfrac{1}{24}(\mu h)^4\right] y_j$$

exact: $y(x) = ce^{\mu x}$

$y(x_j) = ce^{\mu x_j}$ $\quad y(x_{j+1}) = ce^{\mu(x_j + h)}$

$$\frac{y(x_{j+1})}{y(x_j)} = e^{\mu h} = 1 + \mu h + \tfrac{1}{2}(\mu h)^2 + \tfrac{1}{6}(\mu h)^3 + \tfrac{1}{24}(\mu h)^4 + \tfrac{1}{120}(\mu h)^5 + O(h^6)$$

exact ratio matches y_{j+1}/y_j to $O(h^4)$

[See code IVP Riccati equation RK4]

"Stiffness" describes ill-conditioning of a DE

stiff ODE $\Rightarrow$ unstable in general

Try $y'(x) = 501e^x - 500\,y(x)$ $\quad y(0) = 0$

exact $y(x) = e^x - e^{-500x}$

Large difference in RK4 for 28 or 30 points

(use more points if necessary)

Read about Global adaptive stepping

<u>Local stepping</u> Try to adjust h on the fly

Let's step from x_j to $x_j + h$

$$y(x_j+h) = \underbrace{\hat{y}_{j+1}} + Kh^5 + O(h^6) \qquad (a)$$

Start at x_j, y_j and use RK4 to get $\tilde{y}_{j+1}$

Now step twice : $x_j \to x_j + h/2$, $x_j + \frac{h}{2} \to x_j + h$

$$y(x_j + \tfrac{h}{2}) = \hat{\hat{y}}_{j+1/2} + K(\tfrac{h}{2})^5 + O(h^6)$$

~ 2 steps

$$y(x_j+h) = \hat{\hat{y}}_{j+1} + 2K(\tfrac{h}{2})^5 + O(h^6) \qquad (b)$$

(a), (b) $\hat{\hat{y}}_{j+1} - \hat{y}_{j+1} = \frac{15}{16} K h^5$

[use in (b) $y(x_j+h) = \hat{\hat{y}}_{j+1} + \frac{1}{15}(\hat{\hat{y}}_{j+1} - \hat{y}_{j+1}) + O(h^6)$]

What size h_* should you use to get an acceptable abs. tolerance Δ ?

$$\frac{|\hat{\hat{y}}_{j+1} - \hat{y}_{j+1}|}{\Delta} = \left(\frac{h}{h_*}\right)^5$$

used to make approx to get $\hat{\hat{y}}$, $\hat{y}$ both at $j+1$

-or- $h_* = \alpha h \left| \frac{\Delta}{\hat{\hat{y}}_{j+1} - \hat{y}_{j+1}} \right|^{1/5}$

$\alpha \sim 4/5$ for safety

Two Equations

Often in physics we solve coupled ODEs

$$y_0'(x) = f_0(x, y_0(x), y_1(x)) \qquad y_0(a) = c_0$$
$$y_1'(x) = f_1(x, y_0(x), y_1(x)) \qquad y_1(a) = c_1$$

$y_0(x)$ and $y_1(x)$ are dep. variables

Note that we can have a single 2^{nd} order IVP

$$w''(x) = f(x, w, w') \quad w(a) = c \quad w'(a) = d$$

and transform it to

$$y_0(x) = w(x)$$
$$y_1(x) = w'(x) = y_0'(x)$$

So that

$$y_0'(x) = y_1(x) \qquad y_0(a) = c$$
$$y_1'(x) = f(x, y_0(x), y_1(x)) \qquad y_1(a) = d$$

Even more generally for $y_0(x), y_1(x), \dots y_{\nu-1}(x)$

$$\vec{y}\,'(x) = \vec{f}(x, \vec{y}(x))$$

ν functions

$$\vec{y}(a) = \vec{c}$$

$\vec{c}$ is vector of ν dim

We discretize with n grid points and carry over results

BW Euler: $\vec{y}_{j+1} = \vec{y}_j + h\vec{f}(x_{j+1}, \vec{y}_{j+1})$ $\quad j=0,1,\ldots n-2$

$\vec{y}_0 = \vec{c}$

RK4 $\quad \vec{k}_0 = h\vec{f}(x_j, \vec{y}_j)$

$$\vec{k}_1 = h\vec{f}\left(x_j + \frac{h}{2}, \vec{y}_j + \frac{\vec{k}_0}{2}\right)$$

$$\vec{k}_2 = h\vec{f}\left(x_j + \frac{h}{2}, \vec{y}_j + \frac{\vec{k}_1}{2}\right)$$

$$\vec{k}_3 = h\vec{f}\left(x_j + h, \vec{y}_j + \vec{k}_2\right)$$

$$\vec{y}_{j+1} = \vec{y}_j + \frac{1}{6}\left(\vec{k}_0 + 2\vec{k}_1 + 2\vec{k}_2 + \vec{k}_3\right)$$

Just to be clear $\vec{y}_0$ is each $y(x)$ function evaluated at index $\emptyset$ $\quad (y_0)_0, (y_1)_0, (y_2)_0, \ldots$ (at x_0)

Recall Riccati eqn: $\quad y'(x) = \dfrac{-30}{1-x^2} + \dfrac{2x}{1-x^2}y(x) - y^2(x)$

$$y(0.05) = 19.53$$

Let $\quad y(x) = w'(x)/w(x)$

$$y' = \frac{w''}{w} - \frac{(w')^2}{w^2} = \frac{w''}{w} - y^2$$

$$\frac{w''}{w} = -\frac{30}{1-x^2} + \frac{2x}{1-x^2}y(x)$$

$$w''(x) = \frac{-30}{1-x^2} w(x) + \frac{2x}{1-x^2} w'(x)$$

Since $w'(x) = y(x) w(x)$

$w(0.05) = 0.0927\ldots \quad w'(0.05) = 1.8096\ldots$

[know $y(0.05) \rightarrow \frac{w'(.05)}{w(.05)}$ know $y'(.05) \rightarrow \frac{w''(.05)}{w(.05)}$

and above equation relating w'', w', w]

And our new way of writing 2nd order as 2 first orders

$$y_0'(x) = y_1(x)$$

$$y_1'(x) = \frac{-30}{1-x^2} y_0(x) + \frac{2x}{1-x^2} y_1(x)$$

[see code]

Boundary Value Problems (BVP)

We will address 2nd order ODE

$$w''(x) = f(x, w, w') \quad \underbrace{w(a) = c \quad w(b) = d}_{\text{boundary conditions (Dirichlet)}}$$

$w'(a)$ is not known $\Rightarrow$ can't step though w/ RK4

Shooting method: guess $w'(a)$ and see if it can take you from $w(a) \rightarrow w(b)$

iterate based on where you 'land'

method: $w_0 = c \quad w_{n-1} = d$

trial value $w'(a) = \sigma$

Use RK4 to get w_{n-1}. Call effect of RK4 (or other integrator) g so $g(\sigma) = w_{n-1} = d$

g is a method but we can treat it as unknown fcn

So we need root of equation $g(\sigma) = d$

Ex: $w''(x) = \frac{-30}{1-x^2} w(x) + \frac{2x}{1-x^2} w'(x)$

[$w(x) = P_5(x)$ 5^{th} legendre poly $\frac{1}{8}(63x^5 - 70x^3 + 15x)$]

$w(0.05) = 0.0926\ldots \quad w(0.49) = 0.11177\ldots$

Recall that secant method found roots without needing $f'(x)$, just used $f(x)$ to find $f(x)=0$

[See code]

Summary: start with 2^{nd} order BVP

write it as 2 coupled ODEs

guess an initial value

use IVP solver and root finder to find correct initial value

use IVP solver w/ good initial values