Lecture 2

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Taylor series

$$y_1 = y(x_1) = y_0 + hy_0' + \frac{h^2}{2!}y_0'' + \frac{h^3}{3!}y_0''' + ... + \frac{h^n}{n!}y_0^{(n)} + ...$$

$$y_2 = y(x_1 + h) = y_1 + hy_1' + \frac{h^2}{2!}y_1'' + \frac{h^3}{3!}y_1''' + ... + \frac{h^n}{n!}y_1^{(n)} + ...$$

If one take proper higher order terms, Taylor series provide desire accuracy faster. However the disadvantage is that one need to evaluate higher derivatives of the function.

Euler Method

$$y_n = y_{n-1} + hf(x_{n-1}, y_{n-1}), \text{ where } x_n = x_{n-1} + h$$

One don't need any higher order derivative and with proper *h*, get reasonable result

What if one can achieve the accuracy of Taylor series without requiring calculation of higher derivatives.

Runge-Kutta Methods

Developed by two German mathmaticians Carl Runge and Wilhelm Kutta

They provide the desirable feature of the Taylor series method, but with replacement of the higher order derivatives with the requirement to evaluate f(x,y) at some points within the step x_i to x_{i+1}.

Most general form

$$y_{i+1} = y_i + \phi(x_i, y_i, h)h$$

$$\phi(x_i, y_i, h) \text{ is called an increment function}$$

This increment function can be written in general form as

$$\phi_i = a_1 k_1 + a_2 k_2 + ... + a_n k_n$$

where the *a*'s are constants and the *k*'s are

$$k_1 = f(x_i, y_i)$$

$$k_2 = f(x_i + p_1 h, y_i + q_{11} k_1 h)$$

$$k_3 = f(x_i + p_2 h, y_i + q_{21} k_1 h + q_{22} k_2 h)$$

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$$k_n = f(x_i + p_{n-1} h, y_i + q_{(n-1)1} k_1 h + q_{(n-1)2} k_2 h) + ... + q_{(n-1)(n-1)} k_{n-1} h)$$

p,*q* are constants

k appears as recurrence

$$y_{i+1} = y_i + \phi(x_i, y_i, h)h$$

$$\phi_i = a_1k_1 + a_2k_2 + ... + a_nk_n$$

$$k_1 = f(x_i, y_i)$$

First order Runge-Kutta is exactly Euler's Method

$$y_{i+1} = y_i + a_1k_1h$$

Second order Runge-Kutta

$$y_{i+1} = y_i + (a_1k_1 + a_2k_2)h$$

$$k_1 = f(x_i, y_i)$$

$$k_2 = f(x_i + p_1h, y_i + q_{11}k_1h)$$

a_1,a_2, p_1 and q_{11} are evaluted by setting the equation equal to a Taylor series expansion to the second-order term

One get three equations to evaluate four unknown constants

$$a_1 + a_2 = 1; \quad a_2p_1 = \frac{1}{2}; \quad a_2q_{11} = \frac{1}{2}$$

$$a_1 = 1 - a_2; \quad p_1 = q_{11} = \frac{1}{2a_2}$$

Must assume one value to determine other three

Second-order RK Method

$$k_1 = f(x_i, y_i) \qquad (1a)$$

$$y_{i+1} = y_i + (a_1 k_1 + a_2 k_2)h \qquad (1)$$

$$k_2 = f(x_i + p_1 h, y_i + q_{11} k_1 h) \qquad (1b)$$

Taylor series $$y_{i+1} = y_i + f(x_i, y_i)h + \frac{f'(x_i, y_i)}{2!}h^2 \qquad (2)$$

$f'(x_i, y_i)$ determined by chain-rule differentiation

$$f'(x_i, y_i) = \frac{\partial f(x,y)}{\partial x} + \frac{\partial f(x,y)}{\partial y}\frac{dy}{dx} (3)$$

substituting in (2), one gets

$$y_{i+1} = y_i + f(x_i, y_i)h + \left(\frac{\partial f(x_i, y_i)}{\partial x} + \frac{\partial f(x_i, y_i)}{\partial y}\frac{dy}{dx}\right)\frac{h^2}{2!} \qquad (4)$$

Taylor series for two-variable function

$$g(x + r, y + s) = g(x, y) + r\frac{\partial g}{\partial x} + s\frac{\partial g}{\partial y} + \ldots$$

Use to expand (1b)

$$f(x_i + ph, y_i + q_{11} k_1 h) = f(x_i, y_i) + p_1 h\frac{\partial f}{\partial x} + q_{11} k_1 h\frac{\partial f}{\partial y} + O(h^2) \qquad (5)$$

Put (5) and (1a) in (1)

$$y_{i+1} = y_i + [a_1 f(x_i, y_i) + a_2 h f(x_i, y_i) + a_2 p_1 h^2 \frac{\partial f}{\partial x} + a_2 q_{11} h^2 f(x_i, y_i)\frac{\partial f}{\partial y} + O(h^3)$$

$$y_{i+1} = y_i + [a_1 f(x_i, y_i) + a_2 f(x_i, y_i)]h + \left[a_2 p_1 \frac{\partial f}{\partial x} + a_2 q_{11} f(x_i, y_i)\frac{\partial f}{\partial y}\right] h^2 + O(h^3)$$

$$y_{i+1} = y_i + [a_1 f(x_i, y_i) + a_2 f(x_i, y_i)]h + \left[a_2 p_1 \frac{\partial f}{\partial x} + a_2 q_{11} f(x_i, y_i) \frac{\partial f}{\partial y}\right] h^2 + O(h^3)$$

Compare with

$$y_{i+1} = y_i + f(x_i, y_i)h + \left(\frac{\partial f(x_i, y_i)}{\partial x} + \frac{\partial f(x_i, y_i)}{\partial y}\frac{dy}{dx}\right)\frac{h^2}{2!}$$

$$a_1 + a_2 = 1$$

$$a_2 p_1 = \frac{1}{2}$$

$$a_2 q_{11} = \frac{1}{2}$$

Four unknown constants, three simultaneous equations.

When a_2=1/2

a_1=1/2 and p_1=q_{11}=1

$$y_{i+1} = y_i + (\frac{1}{2}k_1 + \frac{1}{2}k_2)h$$ where $$k_1 = f(x_i, y_i),\ k_2 = f(x_i + h, y_i + k_1 h)$$

Same as Heun’s technique

When a_2=1

a_1=0 and p_1=q_{11}=1/2

$$y_{i+1} = y_i + k_2 h$$ where $$k_1 = f(x_i, y_i),\ k_2 = f(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_1 h)$$

Same as Midpoint method

When a_2=2/3

Ralston and Rabinowitz determined that choosing a_2=2/3 provides a minimum bound on the truncation error for second-order RK algorithms

a_1=1/3 and p_1=q_{11}=3/4

$$y_{i+1} = y_i + (\frac{1}{3}k_1 + \frac{2}{3}k_2)h$$ where $$k_1 = f(x_i, y_i),\ k_2 = f(x_i + \frac{3}{4}h, y_i + \frac{3}{4}k_1 h)$$

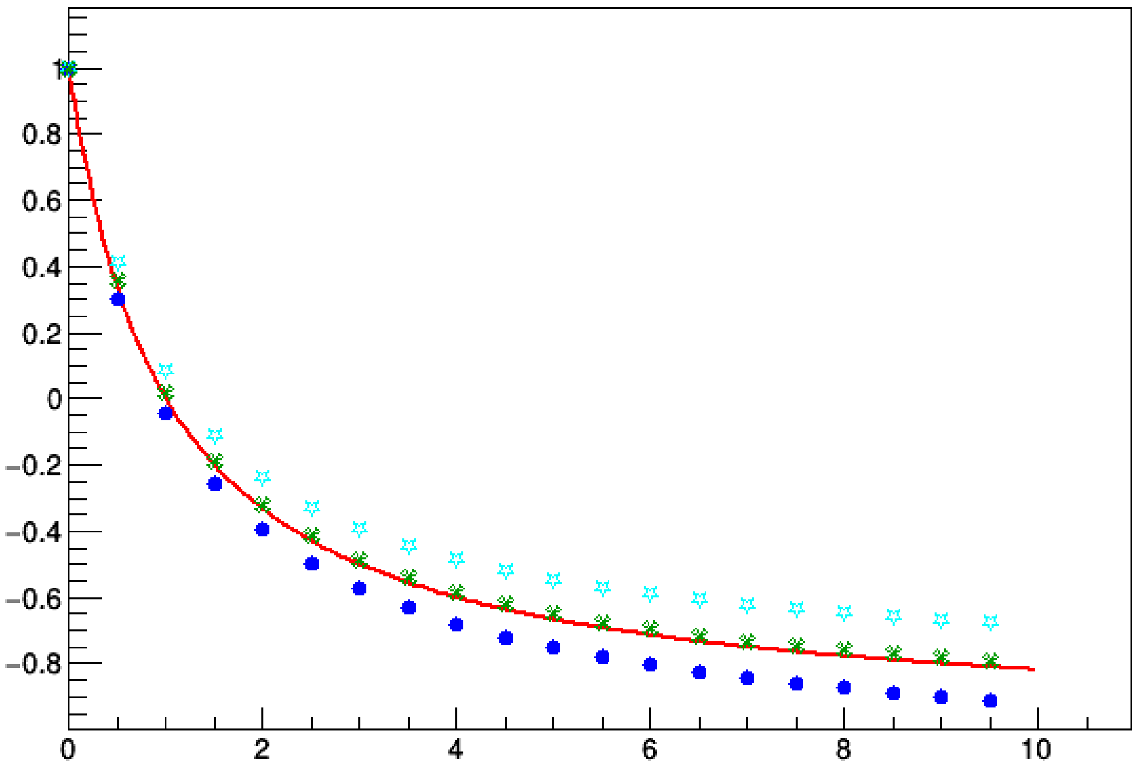
$$\frac{dy}{dx} = -\frac{1+y^2}{1+x^2} \text{ with IC } y(0) = 1$$

$$\text{Solution : } \quad y = \frac{1-x}{1+x}$$

RG2 method with $a_2 = 1/2$, $a_1=1/2$; $p_1=q_{11}=1$ (**Heun's Method**)

RG2 method with $a_2=1$, $a_1=0$, $p_1=q_{11}=1/2$ (**Midpoint Method**)

RG2 method with $a_2 = 2/3$, $a_1=1/3$; $p_1=q_{11}=3/4$ (**Ralston's Method**)



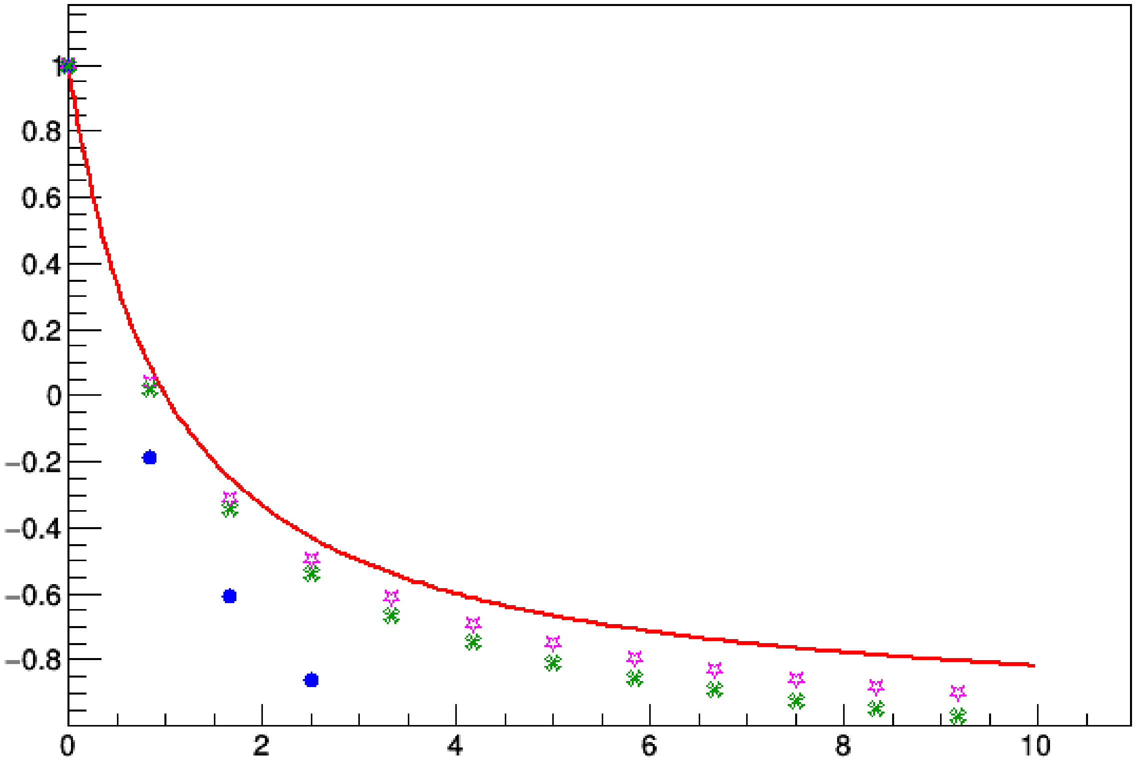
Third-order Runge-Kutta Methods

N=3, result result in six equations with eight unknowns.
Therefore, values of two of the unknowns must be specified a priori

$$y_{i+1} = y_i + \frac{1}{6}(k_1 + 4k_2 + k_3)h$$

One famous version used is

$$k_1 = f(x_i, y_i),\ k_2 = f(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_1 h),\ k_3 = f(x_i + h, y_i - k_1 h + 2k_2 h)$$



$$\frac{dy}{dx} = -\frac{1+y^2}{1+x^2} \text{ with IC } y(0) = 1$$

RG3 method
RG2 method **Ralston's Method**
RG2 method **Heun's Method**

$$\text{Solution}: \ y = \frac{1-x}{1+x}$$

Fourth-order Runge-Kutta Methods

Most famous our of all the order of RK methods.
Commonly used form (Classical fourth-order RK method)

$$y_{i+1} = y_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)h$$

where

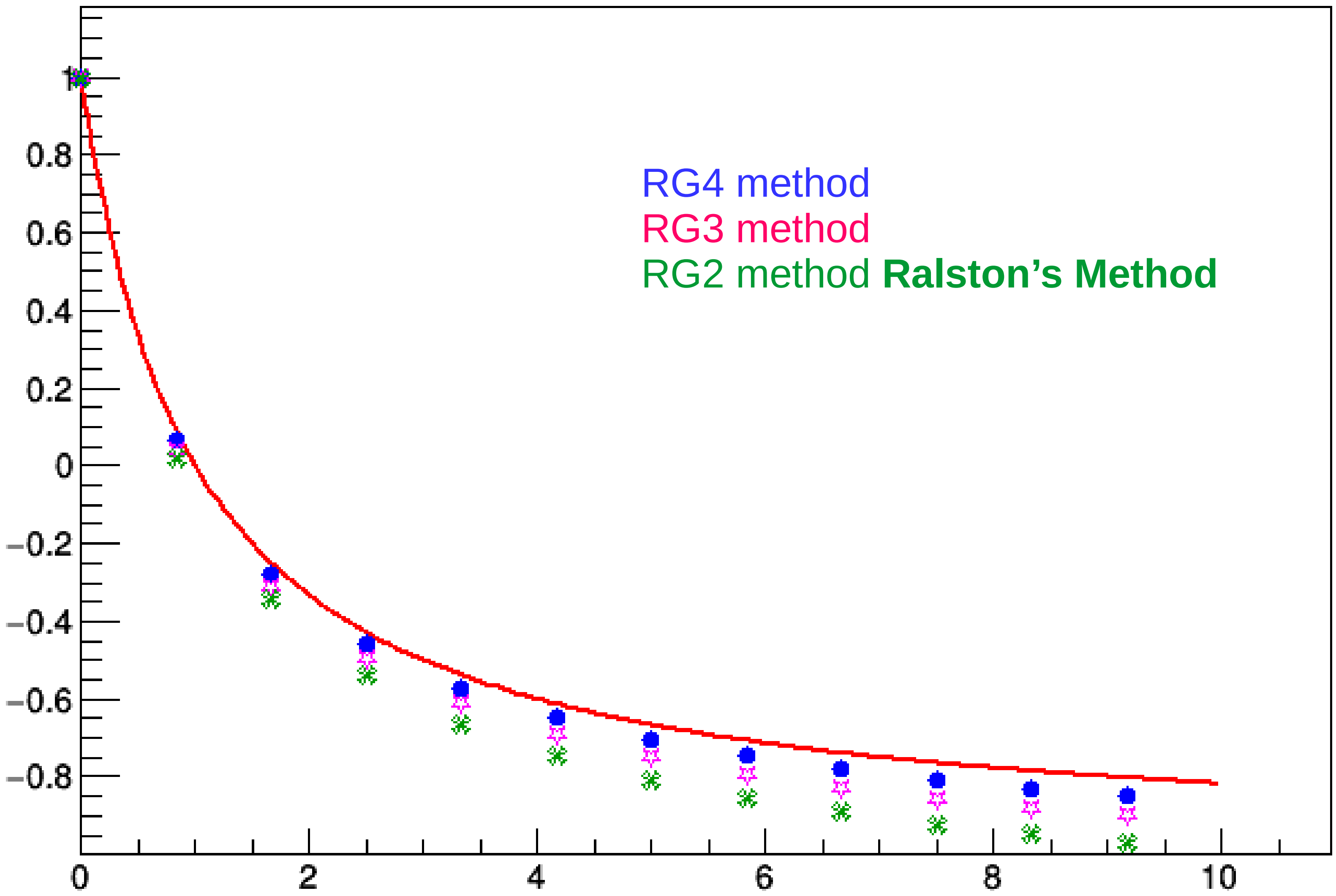
$$k_1 = f(x_i, y_i), \qquad k_2 = f(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_1 h)$$

$$k_3 = f(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_2 h), \qquad k_4 = f(x_i + h, y_i + k_3 h)$$

- Gives greater accuracy and is most widely used for finding the approximate solution of first order ODE.
- Method is well suited for comptuers

$$\frac{dy}{dx} = -\frac{1+y^2}{1+x^2} \text{ with IC } y(0) = 1$$

$$\text{Solution}: \quad y = \frac{1-x}{1+x}$$



Higher-order Runge-Kutta Methods

If more accurate results are requrired, Butcher's fifth-order RK method is recommended

$$y_{i+1} = y_i + \frac{1}{90}(7k_1 + 32k_3 + 12k_4 + 32k_5 + 7k_6)h$$

$$k_1 = f(x_i, y_i), \qquad k_2 = f(x_i + \frac{1}{4}h, y_i + \frac{1}{4}k_1 h)$$

$$k_3 = f(x_i + \frac{1}{4}h, y_i + \frac{1}{8}k_1 h + \frac{1}{8}k_2 h), \qquad k_4 = f(x_i + \frac{1}{2}h, y_i - \frac{1}{2}k_2 h + k_3 h)$$

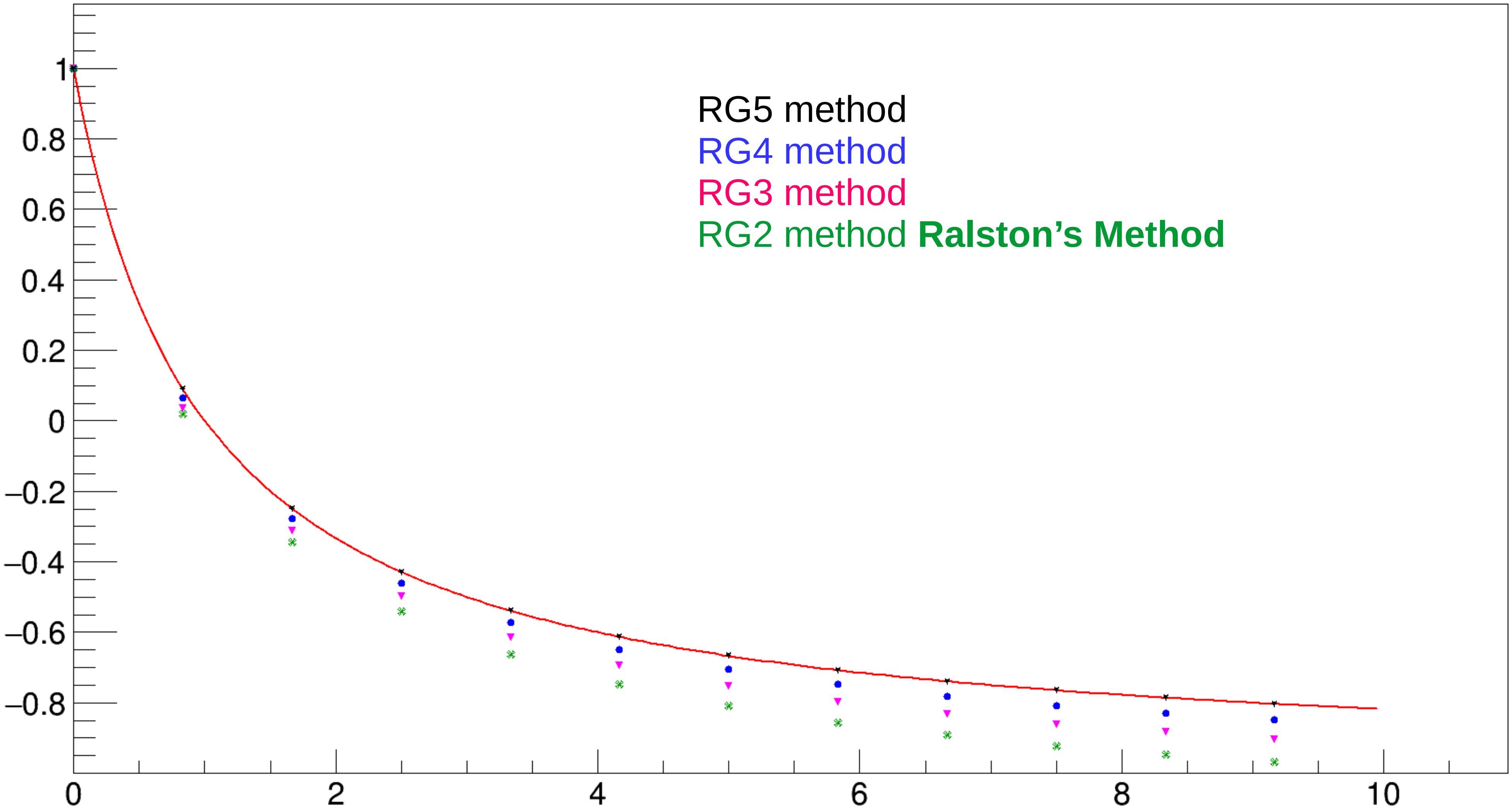
$$k_5 = f(x_i + \frac{3}{4}h, y_i + \frac{3}{16}k_1 h + \frac{9}{16}k_4 h),$$

$$k_6 = f(x_i + h, y_i - \frac{3}{7}k_1 h + \frac{2}{7}k_2 h + \frac{12}{7}k_3 h - \frac{12}{7}k_4 h + \frac{8}{7}k_5 h)$$

Above fourth order method, the gain is accuracy is unfavored by the complexity and added computational effort.

$$\frac{dy}{dx} = -\frac{1+y^2}{1+x^2} \text{ with IC } y(0) = 1$$

$$\text{Solution : } y = \frac{1-x}{1+x}$$



Adaptive Runga-Kutta Methods

If the solution is gradually changing, then RK methods works perfectly.
In case the solution changes abruptly then one will need very small steps in order to solve.

If one uses much smaller step size than necessary, one waste computer resources.

Building an algorithm which automatically adjusting the step stize can help in avoiding such an overkill and be of great advantage.

As they adapt to solution’s trajectory, they are said to have adaptive step-size.

Adaptive RK or Step-Halving Method

Estimate y at same point by two methods:

$y_{1(1)}$ → single -step prediction

$y_{1(1/2,1/2)}$ → two half step prediction

$$\Delta = y_{1(1/2,1/2)} - y_{1(1)}$$

Then use the correction to modify the y value

For fourth-order RK

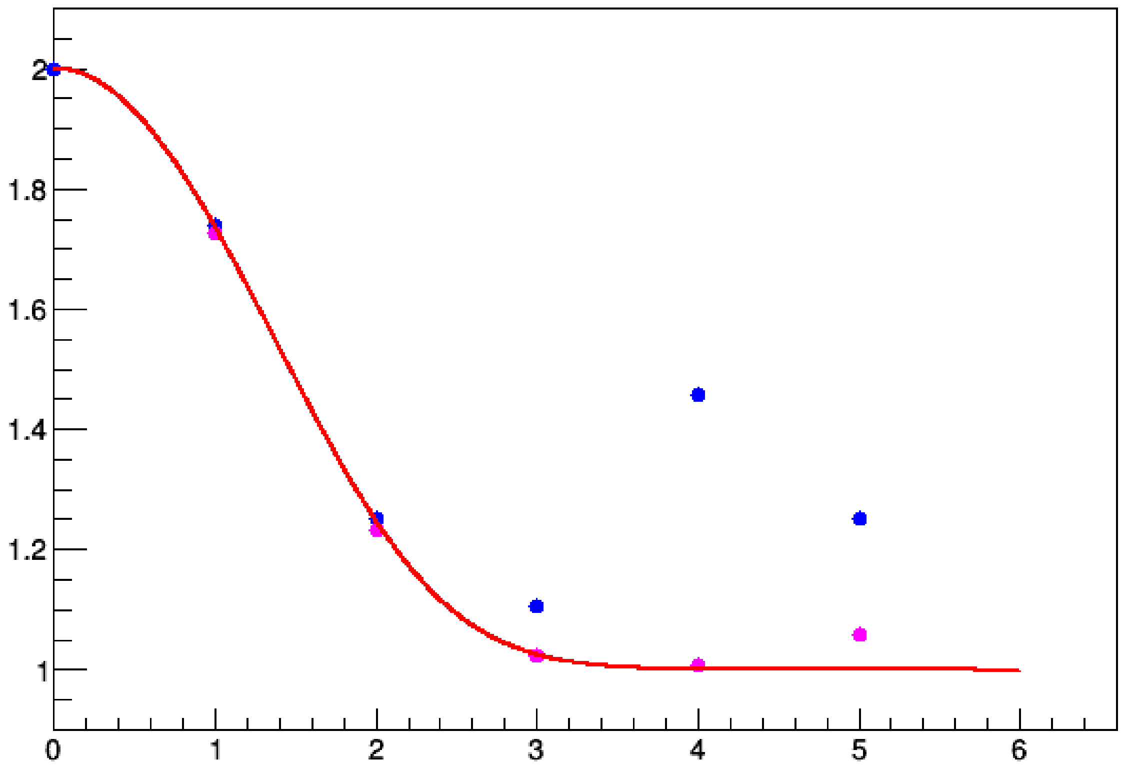
$$y_1 \sim y_{1(1/2,1/2)} + \frac{\Delta}{15}$$

$$\frac{dy}{dx} = \frac{x}{3y^2}(1 - y^3)$$ With IC, x=0, y=2

$$y = \sqrt[3]{1 + 7\exp^{-0.5x^2}}$$

RG 4^{th} order

RG 4^{th} order with Step-Halving Method



What one observe till now

1) Smaller *h*, gives smaller error
2) Higher order RK, gives smaller error
3) Uniform grid, gives varying local error

What if one set *h* not globally but locally.

One can use 2) to set 1) and control 3)

One compare two different order of RK
Ideally the result should be same.
In case the result, differs. one can make the size of *h* smaller

$$|y_i^{\text{higher order}} - y_i| : \text{Error Measurement}$$

Runge-Kutta-Fehlberg Method (RKF45)

It has a procedure to determine if the proper step size h is being use. At each step, two different approximations for solution are made and compared. If the two answers are in close agreement, the approximation is accepted.
If the two answers do not agree to a specified accuracy, step size is reduced.If answers agree to more significant step size is increased.

$$k_1 = hf(x_i, y_i), \qquad k_2 = hf(x_i + \frac{1}{4}h, y_i + \frac{1}{4}k_1)$$

$$k_3 = hf(x_i + \frac{3}{8}h, y_i + \frac{3}{32}k_1 + \frac{9}{32}k_2), \qquad k_4 = hf(x_i + \frac{12}{13}h, y_i + \frac{1932}{2197}k_1 - \frac{7200}{2197}k_2 + \frac{7296}{2197}k_3)$$

$$k_5 = hf(x_i + h, y_i + \frac{439}{216}k_1 - 8k_2 + \frac{3680}{513}k_3 - \frac{845}{4104}k_4)$$

$$k_6 = hf(x_i + \frac{1}{2}h, y_i - \frac{8}{27}k_1 + 2k_2 - \frac{3544}{2565}k_3 + \frac{1859}{4104}k_4 - \frac{11}{40}k_5)$$

RK order 4

$$y_{i+1}^{4\mathrm{RK}} = y_i + \frac{25}{216}k_1 + \frac{1408}{2565}k_3 + \frac{2197}{4101}k_4 - \frac{1}{5}k_5$$

$$y_{i+1}^{5\mathrm{RK}} = y_i + \frac{16}{135}k_1 + \frac{6656}{12825}k_3 + \frac{28561}{56430}k_4 - \frac{9}{50}k_5 + \frac{2}{55}k_6$$

$$|y_{i+1}^{5\mathrm{RK}} - y_{i+1}^{4\mathrm{RK}}| \ : \ \text{Error measurement}$$

$|y_{i+1}^{\mathrm{5RK}} - y_{i+1}^{\mathrm{4RK}}|$: Error measurement

RKF45

If Error > Tolerance

reject the solution and half the step size there

If Error < Tolerance

accept the solution and double the step size

If Error ~ Tolerance

accept the solution and keep *h* same

Step-halving

One can also use same method for RK4 only case also
Take RK4 two steps and then compare the answer.

If Error > Tolerance

reject the solution and half the step size there

If Error < Tolerance

accept the solution and double the step size

If Error ~ Tolerance

accept the solution and keep *h* same

For RK3

$$a_1 + a_2 + a_3 = 1$$

$$p_1 a_2 + p_2 a_3 = 1/2$$

$$q_{11} a_2 + a_3 (q_{21} + q_{22}) = 1/2$$

$$a_2 p_1^2 + a_3 p_2^2 = 1/3$$

$$a_2 p_1 q_{11} + a_3 p_2 (q_{21} + q_{22}) = 1/3$$

$$a_3 q_{22} p_1 = 1/6$$

$$a_2 q_{11}^2 + a_3 (q_{21} + q_{22})^2 = 1/3$$

$$a_3 q_{22} q_{11} = 1/6$$