Moving toward Higher Order Methods

- From the Fundamental Theorem of Calculus, we know

$$y(x+h) = y(x) + \int_x^{x+h} f(t, y(t))dt.$$

  - ◇ If we can improve the approximation of $f(t, y(t))$, then we can improve the integrator.
  - ◇ There are many ways to improve the approximation and, hence, result in different numerical schemes:
    - ▷ Runge-Kutta methods: This class of methods involve *one step* but usually *multiple function evaluations*.
    - ▷ Linear Multi-Step methods: This class of method involve *multiple steps* but usually *one or two function evaluations*.

- An example:
  - ◇ Consider using the midpoint, instead of the endpoint, to approximate the integrand:

$$f(t, y(t)) \approx f\left(x + \frac{h}{2}, y(x + \frac{h}{2})\right).$$

  - ◇ An Euler-type shooting ends with

$$y_{n+1} = y_n + hf\left(x_n + \frac{h}{2}, y(x_n + \frac{h}{2})\right).$$

  - ◇ Since the midpoint is still unknown to us, we do a further approximation:

$$\begin{aligned} y(x_n + \frac{h}{2}) &\approx y(x_n) + \frac{h}{2} f(x_n, y(x_n)) \\ y_{n+1} &= y_n + hf\left(x_n + \frac{h}{2}, \mathbf{y_n} + \frac{\mathbf{h}}{\mathbf{2}}\mathbf{f}(\mathbf{x_n}, \mathbf{y_n}))\right) \end{aligned}$$

- ▷ Note that there are two function evaluations involved.
- ▷ An Euler step is used to estimate the solution at the midpoint, at which the slope is used again as an Euler step to re-shoot from (x_n, y_n).
- ▷ This is a 2-stage method.

- It is curious to know the order of accuracy and the property of stability of this new method. (Students, Try to answer this question.)

  - ◇ Recall that the exact solution y at $x+h$ would satisfy

$$y(x+h) = y(x) + hf(x,y) + \frac{h^2}{2}(f_x(x,y) + f_y(x,y)f(x,y) + O(h^3).$$

  - ◇ Exam the LTE of the new 2-stage method:

$$f(x+\frac{h}{2}, y+\frac{h}{2}f(x,y)) = f(x,y)+\frac{h}{2}f_x(x,y)+\frac{h}{2}f_y(x,y)f(x,y)+O(h^2).$$

$$\begin{aligned} T_{n+1} &= y(x+h) - y(x) - h\left(f(x,y) + \frac{h}{2}f_x(x,y) + \frac{h}{2}f_y(x,y)f(x,y) + O(h^2)\right) \\ &= O(h^3). \end{aligned}$$

Runge-Kutta Formulas

- A general R-stage Runge-Kutta method is defined by the one-step method:

$$y_{n+1} = y_n + h\phi(x_n, y_n, h) \tag{1}$$

where

$$\begin{aligned} \phi(x_n, y_n, h) &= \sum_{r=1}^{R} c_r k_r && (2) \\ \sum_{r=1}^{R} c_r &= 1 \\ k_r &= f(x_n + a_r h, y_n + h\sum_{s=1}^{R} b_{rs} k_s) && (3) \\ \sum_{s=1}^{R} b_{rs} &= a_r. \end{aligned}$$

- It is convenient to display the coefficients occurring in (**??**) and (**??**) in the following form, known as a *Butcher array*:

$$\begin{array}{c|cccc} a_1 & b_{11} & b_{12} & \dots & b_{1R} \\ a_2 & b_{21} & b_{22} & \dots & b_{2R} \\ \vdots & \vdots & & & \vdots \\ a_R & b_{R1} & b_{R2} & \dots & b_{RR} \\ \hline & c_1 & c_2 & \dots & c_R \end{array}$$

- Lots of research has been done in the past few decades to find out the *best* combinations of these coefficients. (If you like to know more about these, join the graduate school and be a scholar!)