Solution of Ordinary Differential Equations (Initial Value Problems) - Lecture 04

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Outline

- Discuss the advantages and disadvantages of the **Runge-Kutta method**
- Derive the 2-Stage Runge-Kutta algorithm
- Discuss the extension to the m-stage Runge-Kutta methods
    - Present the most common 4-stage scheme
- Examine the local truncation error and function evaluations per step

Runge-Kutta Method

Advantages:

1. Easy to program
2. Method is self-starting
3. Relatively good stability characteristics

Disadvantages:

1. Requires more function evaluations per step than methods of comparable accuracy
2. Can be difficult to obtain local error estimates

Two-stage Runge-Kutta Method

The ODE we are studying is:

$$\frac{dy}{dt} = f(t,y) \quad \Rightarrow \quad w' = f(t,w)$$

Exact **Numerical**

The two-stage Runge-Kutta method can be written as:

$$w_{i+1} = w_i + \sum_{j=1}^{m=2} \gamma_j k_j = w_i + \gamma_1 k_1 + \gamma_2 k_2 \tag{1a}$$

where

$$k_1 = \Delta t \, f(t_i, w_i) \tag{1b}$$

$$k_2 = \Delta t \, f(t_i + \alpha \Delta t, w_i + \beta k_1) \tag{1c}$$

We have 4 free parameters, $(\alpha, \beta, \gamma_1, \gamma_2)$. The idea is to choose them such that Eqn. (1) matches a Taylor Series expansion of w in which the time derivatives of w are written in terms of f via the ODE.

Two-stage Runge-Kutta Derivation (1)

Let's start with the Taylor series expansion step.

$$w_{i+1} = w_i + \Delta t\, w_i' + \frac{(\Delta t)^2}{2} w_i'' + \vartheta(\Delta t)^3$$

$$w_{i+1} = w_i + \Delta t\, f_i + \frac{(\Delta t)^2}{2} f_i' + \vartheta(\Delta t)^3$$

$$w_{i+1} = w_i + \Delta t\, f_i + \frac{(\Delta t)^2}{2}\left[\frac{\partial f}{\partial t} + \frac{\partial f}{\partial w}\frac{\partial w}{\partial t}\right]_i + \cdots$$

$$\boxed{w_{i+1} = w_i + \Delta t\, f_i + \frac{\Delta t^2}{2}\left[\left(\frac{\partial f}{\partial t}\right) + f\left(\frac{\partial f}{\partial w}\right)\right]_i + \cdots \qquad (2)}$$

Now, we will write out the algorithm in one step and compare to the above.

Two-stage Runge-Kutta Derivation (2)

Substituting (1b) and (1c) into (1a) yields the 2-Stage RK scheme:

$$w_{i+1} = w_i + \sum_{j=1}^{m=2} \gamma_j k_j = w_i + \gamma_1 k_1 + \gamma_2 k_2$$

$$= w_i + \gamma_1 \Delta t\, f(t_i, w_i) + \gamma_2 \Delta t\, f(t_i + \alpha\Delta t, w_i + \beta k_1) \qquad (3)$$

To compare to (2), we first need to expand $f(t_i + \alpha\Delta t, w_i + \beta k_1)$ in a Taylor series

$$f(t_i + \alpha\Delta t, w_i + \beta k_1) = f(t_i, w_i) + \alpha\Delta t\left(\frac{\partial f}{\partial t}\right)_i + \beta f_i \Delta t\left(\frac{\partial f}{\partial w}\right)_i + \vartheta(\Delta t^2, \Delta w^2) \qquad (4)$$

Substitute (4) into (3) and re-arrange

$$\boxed{w_{i+1} = w_i + \Delta t\,(\gamma_1 + \gamma_2) f_i + \Delta t^2 \left[\alpha\gamma_2 \frac{\partial f}{\partial t} + \beta\gamma_2 f \frac{\partial f}{\partial w}\right]_i} \qquad (5)$$

This is the equivalent 2-Stage Runge-Kutta method written in one-step form.

Two-stage Runge-Kutta Derivation (3)

Compare Equations (2) and (5) repeated here.

$$w_{i+1} = w_i + \Delta t\ f_i + \frac{\Delta t^2}{2}\left[\left(\frac{\partial f}{\partial t}\right) + f\left(\frac{\partial f}{\partial w}\right)\right]_i + \cdots \qquad (2)$$

$$w_{i+1} = w_i + \Delta t\,(\gamma_1 + \gamma_2) f_i + \Delta t^2\left[\alpha\gamma_2 \frac{\partial f}{\partial t} + \beta\gamma_2 f\,\frac{\partial f}{\partial w}\right]_i \qquad (5)$$

To match the Taylor series, we need to choose:

$$\boxed{\gamma_1 + \gamma_2 = 1 \qquad \alpha\gamma_2 = \frac{1}{2} \qquad \beta\gamma_2 = \frac{1}{2}}$$

Three equations in four unknowns, i.e., we have a 1-parameter family of second-order accurate methods.

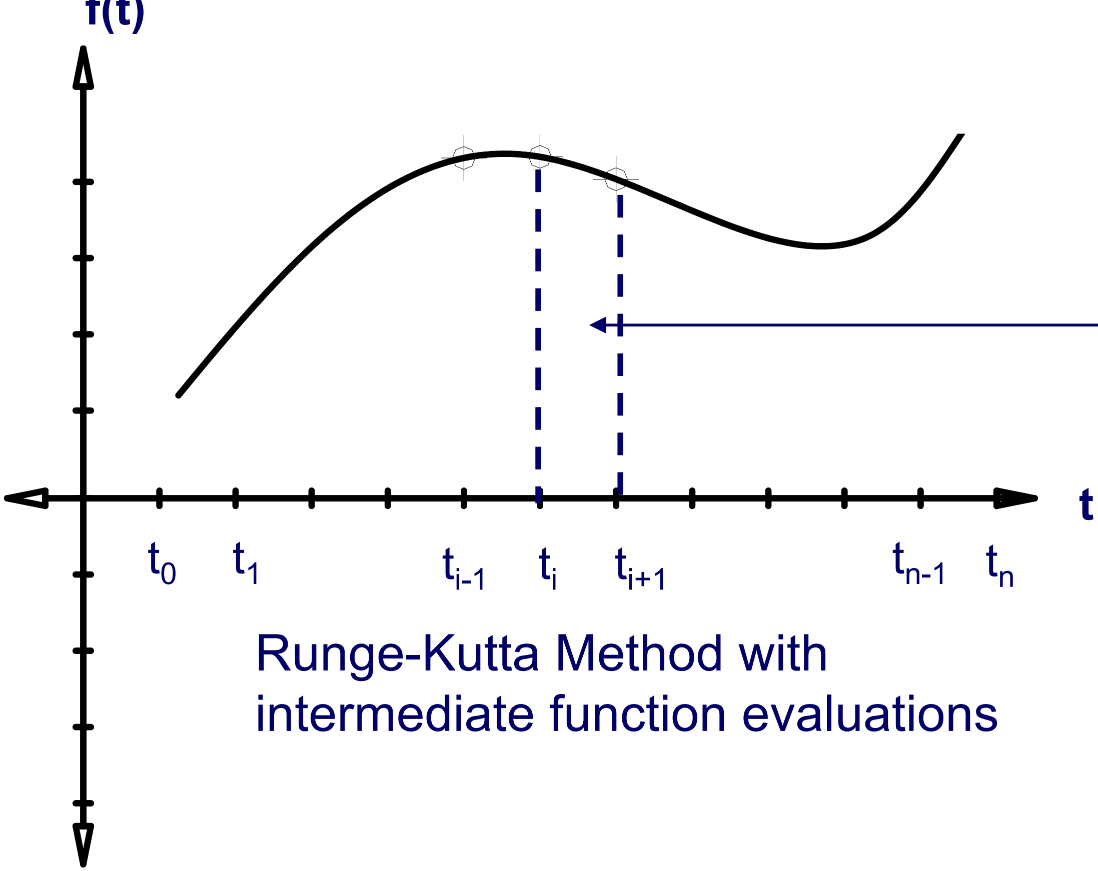
Common Two-Stage Choices

Some of the common choices for the parameters are:

$$\text{Modified Euler's method: } \gamma_1 = \gamma_2 = \tfrac{1}{2}; \alpha = \beta = 1$$

$$\text{Mid-Point Euler method: } \gamma_1 = 0; \gamma_2 = 1; \alpha = \beta = \tfrac{1}{2}$$

$$\textit{Heun's}\text{ Method: } \gamma_1 = \tfrac{1}{4}; \gamma_2 = \tfrac{3}{4}; \alpha = \beta = \tfrac{2}{3}$$



In general, this process leads to the evaluation of the function f at intermediate points between t_i and t_{i+1}.

Runge-Kutta Method with intermediate function evaluations

Common Two-Stage RK schemes

Modified-Euler's Method:

$$w_{i+1} = w_i + \frac{\Delta t}{2}\left[f\left(t_i, w_i\right) + f\left(t_i + \Delta t, w_i + \Delta t\, f\left(t_i, w_i\right)\right)\right]$$

Mid-Point Euler:

$$w_{i+1} = w_i + \Delta t\, f\left[t_i + \frac{\Delta t}{2}, w_i + \frac{\Delta t}{2} f\left(t_i, w_i\right)\right]$$

Heun's Method:

$$w_{i+1} = w_i + \frac{\Delta t}{4}\left[f\left(t_i, w_i\right) + 3 f\left(t_i + \frac{2}{3}\Delta t, w_i + \frac{2}{3}\Delta t\, f\left(t_i, w_i\right)\right)\right]$$

Four-Stage Runge-Kutta

The 4-Stage Runge-Kutta method are the most popular. This involves comparing terms to fourth order and results in 11 equations in 13 unknowns. This leads to a 2-parameter family of schemes that yield 4^{th} order accuracy.

$$\boxed{\begin{aligned} w_{i+1} &= w_i + \frac{1}{6}\left[k_1 + 2k_2 + 2k_3 + k_4\right] \\ k_1 &= \Delta t\ f(t_i, w_i) \\ k_2 &= \Delta t\ f\left(t_i + \frac{\Delta t}{2}, w_i + \frac{k_1}{2}\right) \\ k_3 &= \Delta t\ f\left(t_i + \frac{\Delta t}{2}, w_i + \frac{k_2}{2}\right) \\ k_4 &= \Delta t\ f\left(t_i + \Delta t, w_i + k_3\right) \end{aligned}}$$

The most common choice of parameters is shown on the right. Note that intermediate function evaluations are required.

Runge-Kutta Local Truncation Error

Butcher et. al. established the relationship between the order of the local truncation error and the number of function evaluations per step.

Evaluations Per step	2	3	4	$5 \le n \le 7$	$8 \le n \le 9$	$10 \le n$
Best possible local T.E.	$\vartheta(\Delta t^2)$	$\vartheta(\Delta t^3)$	$\vartheta(\Delta t^4)$	$\vartheta(\Delta t^{n-1})$	$\vartheta(\Delta t^{n-2})$	$\vartheta(\Delta t^{n-3})$

Note that the high order methods (n>4) have poorer relative performance. This favors lower order (n<5) methods with smaller step sizes to achieve an accuracy goal. The fourth order methods are widely used. Note that all of the **Runge-Kutta methods are self-starting**.

Summary

In this lecture we have

- Discussed the relative advantages and disadvantages of the Runge-Kutta method
- Derived the 1-parameter family of 2-stage RK schemes
- Presented the parameters for the most common 4-stage scheme
- Discussed the local truncation error and function evaluations per step