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Lecture 33 Runge-Kutta Method of Numerical Integration # 12

Numerical Integration

$$\begin{aligned} \frac{d\mathbf{r}}{dt} = \mathbf{v} & \implies \frac{d\mathbf{x}}{dt} = \mathbf{y} & \iff \frac{dx^i}{dt} = y^i & i = 1, 2, 3 \\ \frac{d\mathbf{v}}{dt} = \mathbf{g}(\mathbf{r}) & & \frac{dy^i}{dt} = f^i(\mathbf{x}) & \\ & & \mathbf{x}(t_0) = \mathbf{x}_0 \quad \mathbf{y}(t_0) = \mathbf{y}_0 \quad \mathbf{f}(\mathbf{x}_0) = \mathbf{f}_0 & \end{aligned}$$

Taylor Series Expansion

$$\begin{aligned} \mathbf{x}(t+h) &= \mathbf{x}_0 + h \left. \frac{d\mathbf{x}}{dt} \right|_{t=t_0} + \frac{h^2}{2!} \left. \frac{d^2\mathbf{x}}{dt^2} \right|_{t=t_0} + \dots = \mathbf{x}_0 + h\mathbf{y}_0 + \frac{h^2}{2!}\mathbf{f}_0 + \dots \\ \mathbf{y}(t+h) &= \mathbf{y}_0 + h \left. \frac{d\mathbf{y}}{dt} \right|_{t=t_0} + \frac{h^2}{2!} \left. \frac{d^2\mathbf{y}}{dt^2} \right|_{t=t_0} + \dots = \mathbf{y}_0 + h\mathbf{f}_0 + \frac{h^2}{2!}\mathbf{f}'_0 + \dots \\ &= \mathbf{y}_0 + h\mathbf{f}_0 + \underbrace{\frac{h^2}{2!} \left. \frac{\partial \mathbf{f}}{\partial \mathbf{x}} \frac{d\mathbf{x}}{dt} \right|_{t=t_0}}_{= \mathbf{F}_0 \mathbf{y}_0} + \dots \end{aligned}$$

First Order Method

$$\begin{aligned} \mathbf{x} &= \mathbf{x}_0 + h\mathbf{y}_0 + O(h^2) \\ \mathbf{y} &= \mathbf{y}_0 + h\mathbf{f}_0 + O(h^2) \end{aligned}$$

Second Order Method

$$\begin{aligned} \mathbf{x} &= \mathbf{x}_0 + h\mathbf{y}_0 + \frac{1}{2}h^2\mathbf{f}_0 + O(h^3) \\ \mathbf{y} &= \mathbf{y}_0 + h\mathbf{f}_0 + \frac{1}{2}h^2\mathbf{F}_0\mathbf{y}_0 + O(h^3) \end{aligned}$$

How to Avoid Calculating the Matrix \mathbf{F}_0

$$\mathbf{f}(\mathbf{x}_0 + \delta\mathbf{x}) = \mathbf{f}_0 + \left. \frac{\partial \mathbf{f}}{\partial \mathbf{x}} \right|_{t=t_0} \delta\mathbf{x} + O[(\delta x)^2]$$

or for any constant p

$$\mathbf{f}(\mathbf{x}_0 + hpy_0) = \mathbf{f}_0 + \left. \frac{\partial \mathbf{f}}{\partial \mathbf{x}} \right|_{t=t_0} hpy_0 = \mathbf{f}_0 + hp\mathbf{F}_0\mathbf{y}_0 + O(h^2)$$

or

$$\frac{1}{p}[\mathbf{f}(\mathbf{x}_0 + hpy_0) - \mathbf{f}_0] = h\mathbf{F}_0\mathbf{y}_0 + O(h^2)$$

Hence, the second-order method is equivalent to

$$\begin{aligned} \mathbf{x} &= \mathbf{x}_0 + h\mathbf{y}_0 + \frac{1}{2}h^2\mathbf{f}(\mathbf{x}_0) + O(h^3) \\ \mathbf{y} &= \mathbf{y}_0 + h\left(1 - \frac{1}{2p}\right)\mathbf{f}(\mathbf{x}_0) + \frac{1}{2p}h\mathbf{f}(\mathbf{x}_0 + hpy_0) + O(h^3) \end{aligned}$$

Choose $p = \frac{1}{2}$ and note that $\mathbf{f}(\mathbf{x}_0) - \mathbf{f}(\mathbf{x}_0 + hpy_0) = O(h)$. Therefore, we have

$$\begin{aligned} \mathbf{x} &= \mathbf{x}_0 + h\mathbf{y}_0 + \frac{1}{2}h^2\mathbf{f}(\mathbf{x}_0 + \frac{1}{2}h\mathbf{y}_0) + O(h^3) \\ \mathbf{y} &= \mathbf{y}_0 + h\mathbf{f}(\mathbf{x}_0 + \frac{1}{2}h\mathbf{y}_0) + O(h^3) \end{aligned}$$

with only one evaluation of the function $\mathbf{f}(\mathbf{x})$ for $\mathbf{x} = \mathbf{x}_0 + \frac{1}{2}h\mathbf{y}_0$.

Formal Derivation of the Second-Order Method

Choose a , b , p so that

$$\begin{aligned} \mathbf{x} &= \mathbf{x}_0 + h\mathbf{y}_0 + h^2 a \mathbf{k} + O(h^3) & \mathbf{x} &= \mathbf{x}_0 + h\mathbf{y}_0 + \frac{1}{2}h^2 \boldsymbol{\alpha}_0 + O(h^3) \\ \mathbf{y} &= \mathbf{y}_0 + hb\mathbf{k} + O(h^3) & \mathbf{y} &= \mathbf{y}_0 + h(\boldsymbol{\alpha}_0 + \frac{1}{2}h\boldsymbol{\alpha}_1) + O(h^3) \\ \mathbf{k} &= \mathbf{f}(\mathbf{x}_0 + hpy_0) & \mathbf{k} &= \boldsymbol{\alpha}_0 + hp\boldsymbol{\alpha}_1 + O(h^2) \end{aligned}$$

where $\boldsymbol{\alpha}_0 = \mathbf{f}_0$ and $\boldsymbol{\alpha}_1 = \mathbf{f}'_0 = \mathbf{F}_0 \mathbf{y}_0$.

Expand $\mathbf{f}(\mathbf{x}_0 + hpy_0)$ in a Taylor series:

$$\mathbf{f}(\mathbf{x} + \delta\mathbf{x}) = \mathbf{f}_0 + \left. \frac{\partial \mathbf{f}}{\partial \mathbf{x}} \right|_{t=t_0} \delta\mathbf{x} + O[(\delta x)^2] \implies \mathbf{f}(\mathbf{x}_0 + hpy_0) = \underbrace{\mathbf{f}_0 + \left. \frac{\partial \mathbf{f}}{\partial \mathbf{x}} \right|_{t=t_0} hpy_0}_{= \boldsymbol{\alpha}_0 + hp\boldsymbol{\alpha}_1} + O(h^2)$$

Then

$$\begin{aligned} \mathbf{x} &= \mathbf{x}_0 + h\mathbf{y}_0 + h^2 a(\boldsymbol{\alpha}_0 + hp\boldsymbol{\alpha}_1) + O(h^3) & \mathbf{x} &= \mathbf{x}_0 + h\mathbf{y}_0 + \frac{1}{2}h^2 \boldsymbol{\alpha}_0 + O(h^3) \\ \mathbf{y} &= \mathbf{y}_0 + hb(\boldsymbol{\alpha}_0 + hp\boldsymbol{\alpha}_1) + O(h^3) & \mathbf{y} &= \mathbf{y}_0 + h(\boldsymbol{\alpha}_0 + \frac{1}{2}h\boldsymbol{\alpha}_1) + O(h^3) \end{aligned}$$

Equate corresponding coefficients of $\boldsymbol{\alpha}_0$ and $\boldsymbol{\alpha}_1$

$$a = \frac{1}{2} \quad \begin{bmatrix} 1 \\ p \end{bmatrix} b = \begin{bmatrix} 1 \\ \frac{1}{2} \end{bmatrix} \implies a = p = \frac{1}{2} \quad b = 1$$

In summary:

$$\begin{aligned} \mathbf{x} &= \mathbf{x}_0 + h\mathbf{y}_0 + \frac{1}{2}h^2 \mathbf{k} + O(h^3) \\ \mathbf{y} &= \mathbf{y}_0 + h\mathbf{k} + O(h^3) \\ \mathbf{k} &= \mathbf{f}(\mathbf{x}_0 + \frac{1}{2}h\mathbf{y}_0) \end{aligned}$$

Taylor Expansion using Indicial Notation and Summation Convention

$$\begin{aligned} x^i(t+h) &= x^i + h \frac{dx^i}{dt} + \frac{h^2}{2!} \frac{d^2 x^i}{dt^2} + \frac{h^3}{3!} \frac{d^3 x^i}{dt^3} + \frac{h^4}{4!} \frac{d^4 x^i}{dt^4} + \dots \\ &= x^i + hy^i + \frac{h^2}{2!} f^i + \frac{h^3}{3!} \frac{df^i}{dt} + \frac{h^4}{4!} \frac{d^2 f^i}{dt^2} + \dots \\ &= x^i + hy^i + \frac{h^2}{2!} f^i + \frac{h^3}{3!} \sum_{j=1}^3 \frac{\partial f^i}{\partial x^j} \frac{dx^j}{dt} + \frac{h^4}{4!} \sum_{j=1}^3 \frac{d}{dt} \left(\frac{\partial f^i}{\partial x^j} \frac{dx^j}{dt} \right) + \dots \\ &= x^i + hy^i + \frac{h^2}{2!} f^i + \frac{h^3}{3!} f_j^i y^j + \frac{h^4}{4!} (f_{jk}^i y^j y^k + f_j^i f^j) + \dots \end{aligned}$$

Taylor Expansion of a Vector Function of a Vector

$$f^i(x^i + \delta^i) = f^i + f_j^i \delta^j + \frac{1}{2} f_{jk}^i \delta^j \delta^k + \frac{1}{6} f_{jkl}^i \delta^j \delta^k \delta^l + \dots$$

$$\begin{aligned} \mathbf{x} &= \mathbf{x}_0 + h\mathbf{y}_0 + h^2(a_0\mathbf{k}_0 + a_1\mathbf{k}_1) + O(h^4) \\ \mathbf{y} &= \mathbf{y}_0 + h(b_0\mathbf{k}_0 + b_1\mathbf{k}_1) + O(h^4) \\ \mathbf{k}_0 &= \mathbf{f}(\mathbf{x}_0 + hp_0\mathbf{y}_0) \\ \mathbf{k}_1 &= \mathbf{f}(\mathbf{x}_0 + hp_1\mathbf{y}_0 + h^2q_1\mathbf{k}_0) \end{aligned}$$

Series Expansion Using Indicical Notation

$$\begin{aligned} x^i(t+h) &= x^i + hy^i + \frac{1}{2}h^2f^i + \frac{1}{6}h^3f_j^iy^j + O(h^4) \\ y^i(t+h) &= y^i + hf^i + \frac{1}{2}h^2f_j^iy^j + \frac{1}{6}h^3(f_{jk}^iy^jy^k + f_j^if^j) + O(h^4) \\ k_0^i &= f^i(x^i + \underbrace{hp_0y^i}_{\delta_0^i}) = f^i + f_j^ihp_0y^j + \frac{1}{2}f_{jk}^i(hp_0y^j)(hp_0y^k) + O(h^3) \\ k_1^i &= f^i(x^i + \underbrace{hp_1y^i + h^2q_1k_0^i}_{\delta_1^i}) = f^i[x^i + hp_1y^i + h^2q_1f^i + O(h^3)] \\ &= f^i + f_j^i(hp_1y^j + h^2q_1f^j) + \frac{1}{2}f_{jk}^i(hp_1y^j)(hp_1y^k) + O(h^3) \end{aligned}$$

Series Expansion Using Vector Notation

$$\begin{aligned} \mathbf{x} &= \mathbf{x}_0 + h\mathbf{y}_0 + h^2(\frac{1}{2}\boldsymbol{\alpha}_0 + \frac{1}{6}h\boldsymbol{\alpha}_1) + O(h^4) \\ \mathbf{y} &= \mathbf{y}_0 + h[\boldsymbol{\alpha}_0 + \frac{1}{2}h\boldsymbol{\alpha}_1 + \frac{1}{6}h^2(\boldsymbol{\alpha}_2 + \boldsymbol{\beta}_2)] + O(h^4) \\ \mathbf{k}_0 &= \mathbf{f}(\mathbf{x}_0 + hp_0\mathbf{y}_0) = \boldsymbol{\alpha}_0 + hp_0\boldsymbol{\alpha}_1 + \frac{1}{2}h^2p_0^2\boldsymbol{\alpha}_2 + O(h^3) \\ \mathbf{k}_1 &= \mathbf{f}(\mathbf{x}_0 + hp_1\mathbf{y}_0 + h^2q_1\mathbf{k}_0) = \boldsymbol{\alpha}_0 + hp_1\boldsymbol{\alpha}_1 + h^2(\frac{1}{2}p_1^2\boldsymbol{\alpha}_2 + q_1\boldsymbol{\beta}_2) + O(h^3) \end{aligned}$$

Determine $a_0, a_1, b_0, b_1, p_0, p_1, q_1$

$$\begin{aligned} h^2(a_0\mathbf{k}_0 + a_1\mathbf{k}_1) &\equiv h^2(\frac{1}{2}\boldsymbol{\alpha}_0 + \frac{1}{6}h\boldsymbol{\alpha}_1) \quad \text{to terms of order } h^3 \\ h(b_0\mathbf{k}_0 + b_1\mathbf{k}_1) &\equiv h[\boldsymbol{\alpha}_0 + \frac{1}{2}h\boldsymbol{\alpha}_1 + \frac{1}{6}h^2(\boldsymbol{\alpha}_2 + \boldsymbol{\beta}_2)] \quad \text{to terms of order } h^3 \end{aligned}$$

Condition Equations

$$\begin{aligned} (\boldsymbol{\alpha}) \quad \begin{bmatrix} 1 & 1 \\ p_0 & p_1 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \end{bmatrix} &= \begin{bmatrix} \frac{1}{2} \\ \frac{1}{6} \end{bmatrix} & \begin{bmatrix} 1 & 1 \\ p_0 & p_1 \\ p_0^2 & p_1^2 \end{bmatrix} \begin{bmatrix} b_0 \\ b_1 \end{bmatrix} &= \begin{bmatrix} 1 \\ \frac{1}{2} \\ \frac{1}{3} \end{bmatrix} \\ (\boldsymbol{\beta}) & & & q_1b_1 = \frac{1}{2}(\frac{1}{3}) \end{aligned}$$

Solving the Condition Equations

First

$$\begin{aligned} b_0 + b_1 &= 1 \\ p_0 b_0 + p_1 b_1 &= \frac{1}{2} \\ p_0^2 b_0 + p_1^2 b_1 &= \frac{1}{3} \end{aligned} \implies \begin{aligned} (1-p_0)b_0 + (1-p_1)b_1 &= \frac{1}{2} \\ p_0(1-p_0)b_0 + p_1(1-p_1)b_1 &= \frac{1}{6} \end{aligned} \iff \begin{aligned} a_0 + a_1 &= \frac{1}{2} \\ p_0 a_0 + p_1 a_1 &= \frac{1}{6} \end{aligned}$$

Hence $a_0 = (1-p_0)b_0$ and $a_1 = (1-p_1)b_1$.

Next, for consistency,

$$\begin{aligned} b_0 + b_1 &= 1 \\ p_0 b_0 + p_1 b_1 &= \frac{1}{2} \\ p_0^2 b_0 + p_1^2 b_1 &= \frac{1}{3} \end{aligned} \iff D_3 = \begin{vmatrix} 1 & 1 & 1 \\ p_0 & p_1 & \frac{1}{2} \\ p_0^2 & p_1^2 & \frac{1}{3} \end{vmatrix} = 0$$

Expand the determinant

$$D_3 = \begin{vmatrix} 1 & 1 & 1 \\ p_0 & p_1 & \frac{1}{2} \\ p_0^2 & p_1^2 & \frac{1}{3} \end{vmatrix} = \overbrace{\begin{vmatrix} 1 & 1 & 1 \\ p_0 & p_1 & \frac{1}{2} \\ p_0^2 & p_1^2 & \frac{1}{3} \end{vmatrix}}^{\text{Vandermonde determinant}} = \underbrace{(p_1 - p_0)}_{\text{Constraint function}} \left[\frac{1}{3} - \frac{1}{2}(p_0 + p_1) + p_0 p_1 \right] = V_2 \underbrace{L_3(p_0, p_1)}_{=0}$$

Complete solution

$$b_0 = \frac{\frac{1}{2} - p_1}{p_0 - p_1} \quad b_1 = \frac{\frac{1}{2} - p_0}{p_1 - p_0} \quad q_1 = \frac{1}{6} \frac{p_1 - p_0}{\frac{1}{2} - p_0} \quad a_0 = (1-p_0)b_0 \quad a_1 = (1-p_1)b_1$$

with p_0 and p_1 chosen arbitrarily subject to

$$L_3(p_0, p_1) = \frac{1}{3} - \frac{1}{2}(p_0 + p_1) + p_0 p_1 = 0$$

Nyström's Third Order Algorithm with $p_0 = 0$

$$\begin{aligned} \mathbf{x} &= \mathbf{x}_0 + h\mathbf{y}_0 + \frac{1}{4}h^2(\mathbf{k}_0 + \mathbf{k}_1) + O(h^4) \\ \mathbf{y} &= \mathbf{y}_0 + \frac{1}{4}h(\mathbf{k}_0 + 3\mathbf{k}_1) + O(h^4) \\ \mathbf{k}_0 &= \mathbf{f}(\mathbf{x}_0) \\ \mathbf{k}_1 &= \mathbf{f}\left(\mathbf{x}_0 + \frac{2}{3}h\mathbf{y}_0 + \frac{2}{9}h^2\mathbf{k}_0\right) \end{aligned}$$

Note: In the book *Discrete Variable Methods in Ordinary Differential Equations* by Peter Henrici published by John Wiley & Sons, Inc. in 1962, there is a mistake. In his book, Henrici didn't derive the algorithm. He simply stated it. The factor $\frac{2}{9}$ was erroneously written as $\frac{1}{3}$. This error would be difficult to find since the algorithm would not exhibit any particular problem. It just would not be as accurate as it should be.

The moral is **Never copy somebody's algorithm!!** *Always derive it for yourself.*

Nyström's Fourth Order Algorithm

Used in the Apollo Guidance Computer

$$\mathbf{x} = \mathbf{x}_0 + h\mathbf{y}_0 + \frac{1}{6}h^2(\mathbf{k}_0 + 2\mathbf{k}_1) + O(h^5)$$

$$\mathbf{y} = \mathbf{y}_0 + \frac{1}{6}h(\mathbf{k}_0 + 4\mathbf{k}_1 + \mathbf{k}_2) + O(h^5)$$

where

$$\mathbf{k}_0 = \mathbf{f}(t_0, \mathbf{x}_0)$$

$$\mathbf{k}_1 = \mathbf{f}(t_0 + \frac{1}{2}h, \mathbf{x}_0 + \frac{1}{2}h\mathbf{y}_0 + \frac{1}{8}h^2\mathbf{k}_0)$$

$$\mathbf{k}_2 = \mathbf{f}(t_0 + h, \mathbf{x}_0 + h\mathbf{y}_0 + \frac{1}{2}h^2\mathbf{k}_1)$$

Nyström's Fifth Order Algorithm

$$\mathbf{x} = \mathbf{x}_0 + h\mathbf{y}_0 + \frac{1}{192}h^2(23\mathbf{k}_0 + 75\mathbf{k}_1 - 27\mathbf{k}_2 + 25\mathbf{k}_3) + O(h^6)$$

$$\mathbf{y} = \mathbf{y}_0 + \frac{1}{192}h(23\mathbf{k}_0 + 125\mathbf{k}_1 - 81\mathbf{k}_2 + 125\mathbf{k}_3) + O(h^6)$$

where

$$\mathbf{k}_0 = \mathbf{f}(t_0, \mathbf{x}_0)$$

$$\mathbf{k}_1 = \mathbf{f}(t_0 + \frac{2}{5}h, \mathbf{x}_0 + \frac{2}{5}h\mathbf{y}_0 + \frac{2}{25}h^2\mathbf{k}_0)$$

$$\mathbf{k}_2 = \mathbf{f}(t_0 + \frac{2}{3}h, \mathbf{x}_0 + \frac{2}{3}h\mathbf{y}_0 + \frac{2}{9}h^2\mathbf{k}_0)$$

$$\mathbf{k}_3 = \mathbf{f}[t_0 + \frac{4}{5}h, \mathbf{x}_0 + \frac{4}{5}h\mathbf{y}_0 + \frac{4}{25}h^2(\mathbf{k}_0 + \mathbf{k}_1)]$$

R-K-N Sixth Order Algorithm

$$\mathbf{x} = \mathbf{x}_0 + h\mathbf{y}_0 + \frac{1}{90}h^2(7\mathbf{k}_0 + 24\mathbf{k}_1 + 6\mathbf{k}_2 + 8\mathbf{k}_3) + O(h^7)$$

$$\mathbf{y} = \mathbf{y}_0 + \frac{1}{90}h(7\mathbf{k}_0 + 32\mathbf{k}_1 + 12\mathbf{k}_2 + 32\mathbf{k}_3 + 7\mathbf{k}_4) + O(h^7)$$

where

$$\mathbf{k}_0 = \mathbf{f}(t_0, \mathbf{x}_0)$$

$$\mathbf{k}_1 = \mathbf{f}(t_0 + \frac{1}{4}h, \mathbf{x}_0 + \frac{1}{4}h\mathbf{y}_0 + \frac{1}{32}h^2\mathbf{k}_0)$$

$$\mathbf{k}_2 = \mathbf{f}[t_0 + \frac{1}{2}h, \mathbf{x}_0 + \frac{1}{2}h\mathbf{y}_0 - \frac{1}{24}h^2(\mathbf{k}_0 - 4\mathbf{k}_1)]$$

$$\mathbf{k}_3 = \mathbf{f}[t_0 + \frac{3}{4}h, \mathbf{x}_0 + \frac{3}{4}h\mathbf{y}_0 + \frac{1}{32}h^2(3\mathbf{k}_0 + 4\mathbf{k}_1 + 2\mathbf{k}_2)]$$

$$\mathbf{k}_4 = \mathbf{f}[t_0 + h, \mathbf{x}_0 + h\mathbf{y}_0 + \frac{1}{14}h^2(6\mathbf{k}_1 - \mathbf{k}_2 + 2\mathbf{k}_3)]$$