Numerical Analysis

Ordinary Differential Equation

목 차

Lecture Note for Numerical Analysis: Ordinary Differential Equation

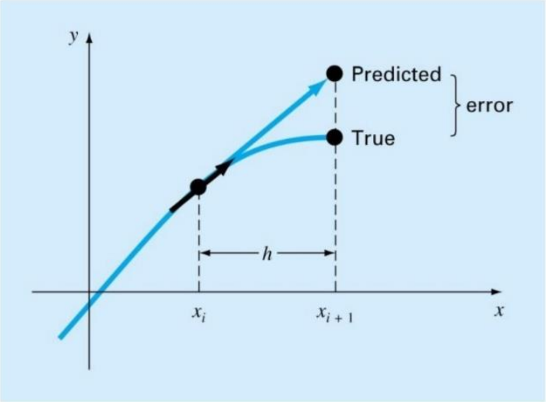
1. Problem Statement of Initial Value Problem

- The 1st order nonlinear ordinary differential equation(ODE)

$$\frac{dy}{dx} = f(x,y), \quad y(x_0) = y_0 \text{ where } x \in R, y \in R, y \in R$$

Solution

$$y(x) = y_0 + \int_{x_0}^{x} f(\tilde{x}, y)d\tilde{x}$$



2. Euler's method: 1st order forward differencing for the 1st function derivative

$$\frac{dy}{dx} = f(x,y), \quad y(x_0) = y_0 \text{ where } x \in R, y \in R, f \in R$$

- 1st function derivative using the 1st order forward difference formula

$$\boxed{\frac{dy}{dx} \approx \frac{y(x_{j+1}) - y(x_j)}{h} \approx f\left(x_j, y(x_j)\right)} \rightarrow \boxed{y(x_{j+1}) = y(x_j) + hf\left(x_j, y(x_j)\right)}$$

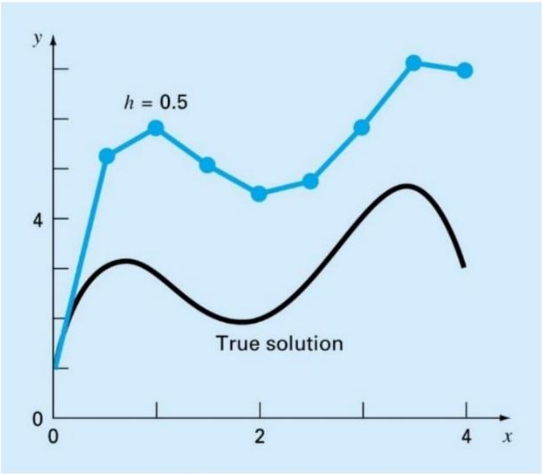
Error in Euler's Method

Problem Statement and Euler Method

- **Error Analysis for Euler's Method/**

  Numerical solutions of ODEs involves two types of error:

  - Truncation error
    - Local truncation error
    - Propagated truncation error
  - The sum of the two is the total or global truncation error
  - Round-off errors



- The Taylor series provides a means of quantifying the error in Euler's method. However;

  ✓ The Taylor series provides only an estimate of the local truncation error-that is, the error created during a single step of the method.

  ✓ In actual problems, the functions are more complicated than simple polynomials. Consequently, the derivatives needed to evaluate the Taylor series expansion would not always be easy to obtain.

- Conclusion,

  ✓ the error can be reduced by reducing the step size

  ✓ If the solution to the differential equation is linear, the method will provide error free predictions as for a straight line the 2nd derivative would be zero.

목 차

Heun's Predictor-Corrector Method

3. Heun's method: Predictor-Corrector Scheme

$$\frac{dy}{dx} = f(x, y), \quad y(x_0) = y_0 \text{ where } x \in R,\ y \in R,\ f \in R$$

- One method to improve the estimate of the slope involves the determination of two derivatives for the interval:
  - ✓ At the initial point
  - ✓ At the end point

  The two derivatives are then averaged to obtain an improved estimate of the slope for the entire interval.

- Preditor Step: 1st function derivative using the 1st order forward difference formula

$$\boxed{\frac{dy}{dx} \approx \frac{y^p(x_{j+1}) - y(x_j)}{h} \approx f\big(x_j, y(x_j)\big)} \rightarrow \boxed{y^p(x_{j+1}) = y(x_j) + hf\big(x_j, y(x_j)\big)}$$

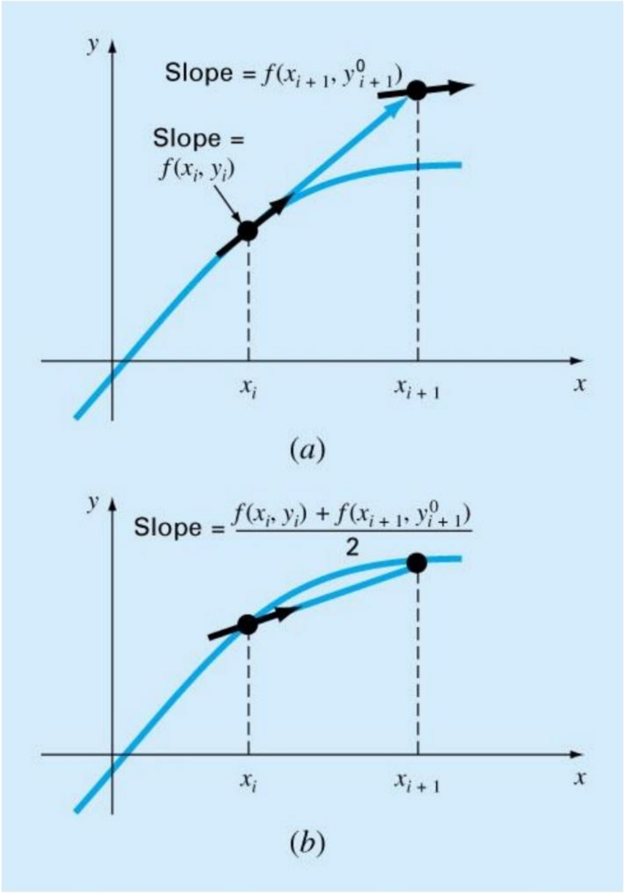
  Prediction of 1st function derivative at $x = x_{j+1}$ using the predicted function value $y^p(x_{j+1})$ as

$$\boxed{\frac{dy(x_{j+1})}{dx} = f(x_{j+1}, y^p(x_{j+1}))}$$

- Corrector Step:

$$\boxed{y(x_{j+1}) = y(x_j) + \frac{h}{2}\left\{f\big(x_j, y(x_j)\big) + f(x_{j+1}, y^p(x_{j+1}))\right\}}$$

Heun's Predictor-Corrector Method



Schematic for Predictor-Corrector Scheme

목 차

Runge-Kutta Method

4. Mid-Point Method

$$\frac{dy}{dx} = f(x, y), \quad y(x_0) = y_0 \ \text{ where } x \in R,\ y \in R,\ f \in R^n$$

- Uses Euler's method t predict a value of y at the midpoint of the interval:

$$\boxed{y(x_{j+1}) = y(x_j) + \frac{h}{2} f\left(x_{j+1/2}, y(x_{j+1/2})\right)}$$

5. Runge-Kutta Method

$$\frac{dy}{dx} = f(x, y), \quad y(x_0) = y_0 \ \text{ where } x \in R,\ y \in R,\ f \in R$$

- Runge-Kutta methods achieve the accuracy of a Taylor series approach without requiring the calculation of higher derivatives.

$$y_{j+1} = y_j + h\left(a_1 k_1 + a_2 k_2 + \cdots + a_n k_n\right)$$

$$\begin{aligned}
k_1 &= f(x_j, y_j) \\
k_2 &= f(x_j + p_1 h, y_j + q_{11} k_1 h) \\
k_3 &= f(x_j + p_2 h, y_j + q_{21} k_1 h + q_{22} k_2 h) \\
&\vdots \\
k_n &= f(x_j + p_{n-1} h, k_j + q_{n-1} k_1 h + q_{n-1,2} k_2 h + \cdots + q_{n-1,n-1} k_{n-1} h)
\end{aligned}$$

Runge-Kutta Method

- k's are recurrence functions. Because each k is a functional evaluation, this recurrence makes RK methods efficient for computer calculations.
- Various types of RK methods can be devised by employing different number of terms in the increment function as specified by n.
- First order RK method with $n=1$ is in fact Euler's method.
- Once n is chosen, values of a's, p's, and q's are evaluated by setting general equation equal to terms in a Taylor series expansion.

Runge-Kutta Method

(5-1) 1st order Runge-Kutta Method

$$\begin{aligned} y_{j+1} &= y_j + a_1 k_1 h \\ &= y_j + f(x_j, y_i)h \end{aligned} \leftarrow \begin{array}{l} a_1 = 1 \\ \text{Since Talor Expnasion of } y_{j+1} = y_j + f(x_j, y_j)h + O(h) \end{array}$$

- 1st order Runge-Kutta Method is the same as Euler's method

Runge-Kutta Method

(5-2) 2nd order Runge-Kutta Method

$$y_{j+1} = y_j + h\left(a_1 k_1 + a_2 k_2\right) \quad \text{where} \quad \begin{aligned} k_1 &= f(x_j, y_j) \\ k_2 &= f(x_j + p_1 h, y_j + q_{11} k_1 h) \end{aligned}$$

The 2nd order approximation $y_{j+1} = y_j + f(x_j, y_j)h + \dfrac{f'(x_j, y_j)}{2}h^2$

Using the chain rule,

$$f'(x,y) = \frac{df(x,y)}{dx} = \frac{\partial f(x,y)}{\partial x} + \frac{\partial f(x,y)}{\partial y}\frac{\partial y}{\partial x} \quad \rightarrow \quad \begin{aligned} y_{j+1} &= y_j + f(x_j, y_j)h + \frac{1}{2}\left(\frac{\partial f}{\partial x} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial x}\right)_{x=x_j} h^2 \\ y_{j+1} &= y_j + f(x_j, y_j)h + \frac{1}{2}\left(\frac{\partial f}{\partial x} + \frac{\partial f}{\partial y} f\right)_{x=x_j} h^2 \end{aligned}$$

Taylor series expansion of $f(x_j + p_1 h, y_j + q_{11} k_1 h)$

$$\begin{aligned} f(x_j + p_1 h, y_j + q_{11} k_1 h) &\approx f(x_j, y_j) + \left(\frac{\partial f}{\partial x}\right) p_1 h + \left(\frac{\partial f}{\partial y}\right) q_{11} k_1 h \\ &\approx f(x_j, y_j) + \left(\frac{\partial f}{\partial x}\right) p_1 h + \left(\frac{\partial f}{\partial y}\right) f q_{11} h \\ &\approx f(x_j, y_j) + \left[\left(\frac{\partial f}{\partial x}\right) p_1 + \left(\frac{\partial f}{\partial y}\right) f q_{11}\right] h \end{aligned}$$

Runge-Kutta Method

Taylor series expansion of the 2nd order RK-formula

$$
\begin{aligned}
y_{j+1} &= y_j + h\{a_1 f(x_j, y_j) + a_2 f(x_j + p_1 h, y_j + q_{11} k_1 h)\} \\
&\approx y_j + a_1 f(x_j, y_j)h + a_2\left\{ f(x_j, y_j) + \left[\left(\frac{\partial f}{\partial x}\right)p_1 + \left(\frac{\partial f}{\partial y}\right) f q_{11}\right] h\right\} h \\
&\approx y_j + (a_1 + a_2) f(x_j, y_j) h + a_2\left[\left(\frac{\partial f}{\partial x}\right)p_1 + \left(\frac{\partial f}{\partial y}\right) f q_{11}\right] h^2
\end{aligned}
$$

Comparing two equations

$$(1) \quad y_{j+1} = y_j + f(x_j, y_j)h + \frac{1}{2}\left(\frac{\partial f}{\partial x} + \frac{\partial f}{\partial y} f\right)_{x=x_j} h^2$$

$$(2) \quad y_{j+1} \approx y_j + (a_1 + a_2) f(x_j, y_j) h + a_2\left[\left(\frac{\partial f}{\partial x}\right)p_1 + \left(\frac{\partial f}{\partial y}\right) f q_{11}\right] h^2$$

$$
\begin{aligned}
a_1 + a_2 &= 1 \\
a_2 p_1 &= \frac{1}{2} \\
a_2 q_{11} &= \frac{1}{2}
\end{aligned}
$$

→ **Four unknowns with three relations, which means the infinite number of RK scheme**

Runge-Kutta Method

(5-2-1) Heun's method with a single corrector (a_2=1/2)

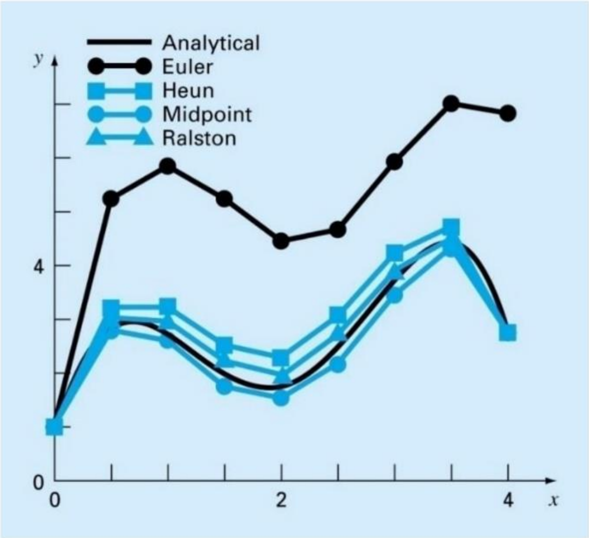
$$a_1 = a_2 = \frac{1}{2}, \quad p_1 = 1, \quad q_{11} = 1 \quad \rightarrow \quad y_{j+1} = y_j + \frac{1}{2}h(k_1 + k_2), \quad k_1 = f(x_j, y_j), \quad k_2 = f(x_j + h, y_j + k_1 h)$$

(5-2-2) Midpoint method (a_2=1)

$$a_1 = 0, \quad a_2 = 1, \quad p_1 = \frac{1}{2}, \quad q_{11} = \frac{1}{2} \quad \rightarrow \quad y_{j+1} = y_j + hk_2, \quad k_1 = f(x_j, y_j), \quad k_2 = f(x_j + \frac{1}{2}h, y_j + \frac{1}{2}k_1 h)$$

(5-2-3) Ralston's method (a_2=2/3)

$$a_1 = \frac{1}{3}, \quad a_2 = \frac{2}{3}, \quad p_1 = \frac{3}{4}, \quad q_{11} = \frac{3}{4} \quad \rightarrow \quad y_{j+1} = y_j + \frac{1}{3}h(k_1 + 2k_2), \quad k_1 = f(x_j, y_j), \quad k_2 = f(x_j + \frac{3}{4}h, y_j + \frac{3}{4}k_1 h)$$



Runge-Kutta Method

(5-3) 3rd order Runge-Kutta Method

→ **Eight unknowns with six relations, which again means the infinite number of RK scheme and two parameters should be specified**

One common version:

$$y_{j+1} = y_j + \frac{1}{6}h(k_1 + 4k_2 + k_3)$$
$$k_1 = f(x_j, y_j)$$
$$k_2 = f(x_j + \frac{1}{2}h, y_j + \frac{1}{2}k_1 h)$$
$$k_3 = f(x_j + h, y_j - k_1 h + 2k_2 h)$$

(5-4) 4th order Runge-Kutta Method

One common version:

$$y_{j+1} = y_j + \frac{1}{6}h(k_1 + 2k_2 + 2k_3 + k_4)$$
$$k_1 = f(x_j, y_j)$$
$$k_2 = f(x_j + \frac{1}{2}h, y_j + \frac{1}{2}k_1 h)$$
$$k_3 = f(x_j + \frac{1}{2}h, y_j + \frac{1}{2}k_2 h)$$
$$k_4 = f(x_j + h, y_j + k_3 h)$$

목 차

Handling System of ODEs

6. Systems of the ordinary differential equations

$$\begin{aligned}
\frac{dy_1}{dx} &= f_1(x, y_1, y_2, \cdots, y_n) \\
\frac{dy_2}{dx} &= f_2(x, y_1, y_2, \cdots, y_n) \\
\frac{dy_3}{dx} &= f_3(x, y_1, y_2, \cdots, y_n) \\
&\vdots \\
\frac{dy_n}{dx} &= f_n(x, y_1, y_2, \cdots, y_n)
\end{aligned}$$

which requires n-initial conditions such as

$$\begin{aligned}
y_1(0) &= (y_1)_0 \\
y_2(0) &= (y_2)_0 \\
y_3(0) &= (y_3)_0 \\
&\vdots \\
y_n(0) &= (y_n)_0
\end{aligned}$$

The equations above can be represented as a vector form as

$$\frac{d\mathbf{y}}{dx} = f(x, \mathbf{y}), \quad \text{with } \mathbf{y}(0) = \mathbf{y}_0$$

$$\mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}, \quad \frac{d\mathbf{y}}{dx} = \begin{pmatrix} \frac{dy_1}{dx} \\ \frac{dy_2}{dx} \\ \vdots \\ \frac{dy_n}{dx} \end{pmatrix}, \quad \mathbf{f} = \begin{pmatrix} f_1(x, y_1, y_2, \cdots, y_n) \\ f_2(x, y_1, y_2, \cdots, y_n) \\ \vdots \\ f_n(x, y_1, y_2, \cdots, y_n) \end{pmatrix}, \quad \mathbf{y}(0) = \begin{pmatrix} y_1(0) \\ y_2(0)_0 \\ \vdots \\ y_n(0) \end{pmatrix}, \quad \mathbf{y}_0 = \begin{pmatrix} (y_1)_0 \\ (y_2)_0 \\ \vdots \\ (y_n)_0 \end{pmatrix}$$

Handling System of ODEs

The we can apply the same formula as in the ordinary differential equation as

(6-1) 1st order Euler's method
$$\boxed{\mathbf{y}(x_{j+1}) = \mathbf{y}(x_j) + h\mathbf{f}\left(x_j, \mathbf{y}(x_j)\right)}$$

(6-2) Heun's preditor-corrector method

Predictor step:
$$\boxed{\mathbf{y}^P(x_{j+1}) = \mathbf{y}(x_j) + h\mathbf{f}\left(x_j, \mathbf{y}(x_j)\right)}$$

Corrector step:
$$\boxed{\mathbf{y}(x_{j+1}) = \mathbf{y}(x_j) + \frac{h}{2}\left\{\mathbf{f}\left(x_j, \mathbf{y}(x_j)\right) + \mathbf{f}(x_{j+1}, \mathbf{y}^P(x_{j+1}))\right\}}$$

(6-3) Mid point method
$$\boxed{\mathbf{y}(x_{j+1}) = \mathbf{y}(x_j) + \frac{h}{2}\mathbf{f}\left(x_{j+1/2}, \mathbf{y}(x_{j+1/2})\right)}$$

(6-4) 4-th order Runge-Kutta method
$$\boxed{\begin{aligned}
&\mathbf{y}_{j+1} = \mathbf{y}_j + \frac{1}{6}h\left(\mathbf{k}_1 + 2\mathbf{k}_2 + 2\mathbf{k}_3 + \mathbf{k}_4\right) \\
&\mathbf{k}_1 = \mathbf{f}(x_j, \mathbf{y}_j) \\
&\mathbf{k}_2 = \mathbf{f}(x_j + \frac{1}{2}h, \mathbf{y}_j + \frac{1}{2}\mathbf{k}_1 h) \\
&\mathbf{k}_3 = \mathbf{f}(x_j + \frac{1}{2}h, \mathbf{y}_j + \frac{1}{2}\mathbf{k}_2 h) \\
&\mathbf{k}_4 = \mathbf{f}(x_j + h, \mathbf{y}_j + \mathbf{k}_3 h)
\end{aligned}}$$

목 차

Handling Higher-Order System of ODEs

7. Handling higher order nonlinear ordinary differential equation

(7-1) 2nd order ODE

$$\frac{d^2\mathbf{y}}{dx^2}=\mathbf{f}(x,\mathbf{y},\mathbf{y}') \text{ where } x\in R,\ \mathbf{y}'=\frac{d\mathbf{y}}{dx}$$

$$\mathbf{y}_1=\mathbf{y}$$

$$\mathbf{y}_2=\mathbf{y}'=\frac{d\mathbf{y}}{dx}$$

Then we can transform above 2nd order system into the 1st order nonlinear ODE as

$$\boxed{\begin{aligned}\frac{d\mathbf{y}_1}{dx}&=\frac{d\mathbf{y}}{dx}=\mathbf{y}'=\mathbf{y}_2\\ \frac{d\mathbf{y}_2}{dx}&=\frac{d^2\mathbf{y}}{dx^2}=\mathbf{f}(x,\mathbf{y},\mathbf{y}')=\mathbf{f}(x,\mathbf{y}_1,\mathbf{y}_2)\end{aligned}} \rightarrow \boxed{\begin{aligned}\frac{d}{dx}\begin{pmatrix}\mathbf{y}_1\\ \mathbf{y}_2\end{pmatrix}&=\begin{pmatrix}\mathbf{y}_2\\ \mathbf{f}(x,\mathbf{y}_1,\mathbf{y}_2)\end{pmatrix}\\ &=\begin{pmatrix}0&1\\0&0\end{pmatrix}\begin{pmatrix}\mathbf{y}_1\\ \mathbf{y}_2\end{pmatrix}+\begin{pmatrix}0\\ \mathbf{f}(x,\mathbf{y}_1,\mathbf{y}_2)\end{pmatrix}\end{aligned}}$$

Handling Higher-Order System of ODEs

(7-2) 3rd order ODE

$$\frac{d^3\mathbf{y}}{dx^3} = \mathbf{f}(x, \mathbf{y}, \mathbf{y}', \mathbf{y}'') \quad \text{where } x \in R,\ \mathbf{y}' = \frac{d\mathbf{y}}{dx},\ \mathbf{y}'' = \frac{d^2\mathbf{y}}{dx^2}$$

$$\mathbf{y}_1 = \mathbf{y}$$

$$\mathbf{y}_2 = \mathbf{y}' = \frac{d\mathbf{y}}{dx}$$

$$\mathbf{y}_3 = \mathbf{y}'' = \frac{d^2\mathbf{y}}{dx^2}$$

Then we can transform above 3rd order system into the 1st order nonlinear ODE as

$$\boxed{\begin{aligned} \frac{d\mathbf{y}_1}{dx} &= \frac{d\mathbf{y}}{dx} = \mathbf{y}_2 \\ \frac{d\mathbf{y}_2}{dx} &= \frac{d^2\mathbf{y}}{dx^2} = \mathbf{y}_3 \\ \frac{d\mathbf{y}_3}{dx} &= \frac{d^3\mathbf{y}}{dx^3} = \mathbf{f}(x, \mathbf{y}, \mathbf{y}', \mathbf{y}'') = \mathbf{f}(x, \mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_3) \end{aligned}} \rightarrow \boxed{\begin{aligned} \frac{d}{dx}\begin{pmatrix} \mathbf{y}_1 \\ \mathbf{y}_2 \\ \mathbf{y}_3 \end{pmatrix} &= \begin{pmatrix} \mathbf{y}_2 \\ \mathbf{y}_3 \\ \mathbf{f}(x, \mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_3) \end{pmatrix} \\ &= \begin{pmatrix} 0 & I & 0 \\ 0 & 0 & I \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \mathbf{y}_1 \\ \mathbf{y}_2 \\ \mathbf{y}_3 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ \mathbf{f}(x, \mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_3) \end{pmatrix} \end{aligned}}$$

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End of Lecture