5. Differentiation & Integration

Derivatives

$$\alpha = \frac{x - x_0}{h}$$

$$\frac{d}{dx} = \frac{d}{d\alpha}\frac{d\alpha}{dx} = \frac{1}{h}\frac{d}{d\alpha}$$

$$h\frac{dy}{dx} = \frac{d}{d\alpha}\left\{ y_0 + \alpha \Delta y_0 + \frac{\alpha(\alpha-1)}{2}\Delta^2 y_0 + \cdots \right\}$$

$$= \Delta y_0 + \frac{2\alpha-1}{2}\Delta^2 y_0 + \cdots$$

At $\alpha = 0 \rightarrow x = x_0$

$$h\left[\frac{dy}{dx}\right]_{x=x_0} = \Delta y_0 - \frac{1}{2}\Delta^2 y_0 + \frac{1}{3}\Delta^3 y_0$$

$$h y_n' = \left(\Delta - \frac{1}{2}\Delta^2 + \frac{1}{3}\Delta^3 + \cdots\right) y_n$$

$$= y_{n+1} - y_n - \frac{1}{2}\left(y_{n+2} - 2y_{n+1} + y_n\right) + \cdots$$

2nd derivative

$$\frac{d^2y}{dx^2} = \frac{1}{h^2}\frac{d^2y}{d\alpha^2}$$

$x^3 - 3x^2$
$3x^2 - 6x$
$6x - 6$

$$h^2\frac{d^2y}{dx^2} = \frac{d^2}{d\alpha^2}\left(y_0 + \alpha\Delta y_0 + \frac{\alpha(\alpha-1)}{2}\Delta^2 y_0 + \frac{\alpha(\alpha-1)(\alpha-2)}{6}\Delta^3 y_0 + \cdots \right)$$

$$= \Delta^2 y_0 + (\alpha - 1)\Delta^3 y_0 + \cdots$$

At $\alpha = 0$

$$h^2 y_n'' = \left(\Delta^2 - \Delta^3 \cdots\right) y_n$$

Integration

$$I = \int_{x_0}^{x_0+h} y(t)\, d\cancel{x}$$

$$= \int_{x_0}^{x_0+h} \left(y_0 + \alpha \Delta y_0 + \frac{\alpha(\alpha-1)}{2} \Delta^2 y_0 + \cdots \right) d\cancel{x}$$

$$= \int_0^1 \left(y_0 + \alpha \Delta y_0 + \frac{\alpha(\alpha-1)}{2} \Delta^2 y_0 + \cdots \right) h\, d\alpha$$

keep linear term

$$\cong y_0 h + \frac{\Delta y_0}{2} h$$

$$= \frac{h}{2} \left[2y_0 + y_1 - y_0 \right]$$

$$= \frac{h}{2} \left[y_0 + y_1 \right] \sim \text{trapezoid rule}$$

$$I = \int_{x_0}^{x_0+2h} \left[y_0 + \alpha \Delta y_0 + \frac{\alpha(\alpha-1)}{2} \Delta^2 y_0 + \frac{\alpha(\alpha-1)(\alpha-2)}{6} \Delta^3 y_0 \right] d\cancel{x}$$

$$= h \int_0^2 \left(y_0 + \alpha \Delta y_0 + \frac{\alpha(\alpha-1)}{2} \Delta^2 y_0 + \frac{\alpha(\alpha-1)(\alpha-2)}{6} \Delta^3 y_0 + \cdots \right) d\alpha$$

keep quadratic term

$$\cong \frac{h}{3} \left(y_0 + 4y_1 + y_2 \right) \sim \text{Simpson's rule}$$

Error Estimates

Look at first neglected term

Trapezoid rule

$$I = \frac{h}{2}(y_1 + y_0) + \left\{ \int_0^1 \frac{\alpha(\alpha-1)}{2}\, d\alpha \right\} h\, \Delta^2 y_0$$

$$\Delta^2 y_0 = h^2 y_0'' + \Delta^3 y_0$$

$$\Delta^3 y_0 = h^3 y_0''' \pm \Delta^4 y_0$$

Assume $h \ll 1$

$$y_0'' = y_0''' = \cdots = O(1)$$

$$I = \frac{h}{2}(y_1 + y_0) + O(h^3)$$

Simpson's rule

$$\int_{x_0}^{x_0+2h} y\, dx = I = \frac{h}{3}(y_0 + 4y_1 + y_2) + O(h^5)$$

$$\int_0^2 \frac{\alpha(\alpha-1)(\alpha-2)}{6} = 0$$

3장 상미분 방정식 — 초기치 문제

1. Explicit Integration Formula

$$\frac{dy}{dt} = f(y), \quad y_0 = y(0)$$

Integrate DE

$$\int_{t_n}^{t_{n+1}} \frac{dy}{dt}\, dt = \int_{t_n}^{t_{n+1}} f(y(t))\, dt$$

$$y_{n+1} = y_n + \int_{t_n}^{t_{n+1}} f(y)\, dt$$

$$= y_n + \int_{t_n}^{t_{n+1}} y'\, dt$$

$$y_{n+1} = y_n + \int_0^1 y'\, h\, d\alpha \qquad \alpha \equiv \frac{t - t_n}{t_{n+1} - t_n}$$

$$y = y_n + \alpha \nabla y_n + \frac{\alpha(\alpha+1)}{2} \nabla^2 y_n + \frac{\alpha(\alpha+1)(\alpha+2)}{6} \nabla^3 y_n + \cdots$$

$$y' = y_n' + \alpha \nabla y_n' + \frac{\alpha(\alpha+1)}{2} \nabla^2 y_n' + \frac{\alpha(\alpha+1)(\alpha+2)}{6} \nabla^3 y_n' + \cdots$$

$$y_{n+1} = y_n + h \sum_{i=0}^{q} a_i \nabla^i y_n'$$

$$a_i = \int_0^1 \frac{\alpha(\alpha+1)\cdots(\alpha+i-1)}{i!}\, d\alpha$$

$$a_0 = 1$$

$$a_1 = \int_0^1 \alpha\, d\alpha = \frac{1}{2}$$

$$a_2 = \int_0^1 \frac{\alpha(\alpha+1)}{2}\, d\alpha = \frac{1}{6} + \frac{1}{4} = \frac{5}{12}$$

$$y_{n+1} = y_n + h\left(1 + \frac{1}{2}\nabla + \frac{5}{12}\nabla^2 + \cdots\right) y_n'$$

(1) Euler, (Forward Euler, Explicit Euler)

$q = 0$

$$y_{n+1} = y_n + h f(y_n)$$

$$\frac{y_{n+1} - y_n}{h} = f(y_n)$$

Errors in Euler's method

$$y_{n+1} = y_n + h y_n' + \frac{1}{2} h \nabla y_n' + \cdots$$

$$= y_n + h y_n' + \frac{h^2}{2} y_n'' + \cdots$$

$$= y_n + h y_n' + O(h^2)$$

$$y_{n+1} = y_n + h f(y_n) + O(h^2) \qquad \text{soln}$$

$$\frac{y_{n+1} - y_n}{h} = f(y_n) + O(h) \qquad \text{derivative}$$

(2) Second-order Adams-Bashforth method

$q = 1$

$$y_{n+1} = y_n + h\left[y_n' + \frac{1}{2}\nabla y_n'\right] + O(h^3)$$

$$= y_n + \frac{h}{2}\left[2y_n' + y_n' - y_{n-1}'\right] + O(h^3)$$

$$= y_n + \frac{h}{2}\left[3y_n' - y_{n-1}'\right] + O(h^3)$$

(3) Fourth-order Adams-Bashforth

$q = 3$

$$y_{n+1} = y_n + h\left(y_n' + \tfrac{1}{2}\nabla y_n' + \tfrac{5}{12}\nabla^2 y_n' + \tfrac{3}{8}\nabla^3 y_n'\right) + O(h^5)$$

$$= y_n + \frac{h}{24}\left(55y_n' - 59y_{n-1}' + 37y_{n-2}' - 9y_{n-3}'\right) + O(h^5)$$

* Euler method can start with initial condition only.
* Higher order method must start with small Euler steps

(4) Stability of Explicit Method

Stability : error at any time stays bounded

$$\frac{d\bar{y}}{dt} = f(\bar{y})$$

$$\bar{y}(t) = \underbrace{y_e(t)}_{\text{exact}} + \epsilon(t) \qquad |\epsilon(t)| \ll 1$$

$$\frac{dy_e}{dt} + \frac{d\epsilon}{dt} = f(y_e+\epsilon) = f(y_e) + \left(\frac{\partial f}{\partial y}\right)_{y_e}\epsilon + O(\epsilon^2)$$

$$\frac{d\epsilon}{dt} = \left[\frac{\partial f}{\partial y}\right]_{y_e}\epsilon(t) \qquad \text{ODE for error}$$

* Error controlled by linearized eq.

Assume $\left(\frac{\partial f}{\partial y}\right)_{y_e} = -\lambda$

$$\frac{d\epsilon}{dt} = -\lambda\epsilon$$

Physical instability

$$\lambda < 0 \rightarrow \epsilon(t) = e^{-\lambda t}$$

Numerical instability

$$\lambda > 0, \quad \left|\frac{\epsilon_{n+1}}{\epsilon_n}\right| > 1$$

Euler's method

$$\frac{d\epsilon}{dt} = -\lambda\epsilon \rightarrow \frac{\epsilon_{n+1} - \epsilon_n}{h} = -\lambda\epsilon_n$$

$$\epsilon_{n+1} = \epsilon_n(1 - h\lambda)$$

$$\left|\frac{\epsilon_{n+1}}{\epsilon_n}\right| = |1 - \lambda h| \leq 1 \quad \text{for stability}$$

For stability

$$0 \leq \lambda h \leq 2$$

$\lambda h = 4$: unstable

$\lambda h = 1$: stable

$\lambda < 0$ never stable

$1 < \lambda h \leq 2$ Error oscillates. Oscillation does not mean ~~the~~ instability.

$$\frac{d\underline{y}}{dt} = \begin{bmatrix} -\lambda_1 & 0 \\ 0 & -\lambda_2 \end{bmatrix} \underline{y}(t) \qquad 0 < \lambda_1 \ll \lambda_2$$

$$\kappa(\underline{\underline{A}}) \gg 1.$$

$$y_e(t) = a_1 e^{-\lambda_1 t} \underline{z}_1 + a_2 e^{-\lambda_2 t} \underline{z}_2$$

a_1, a_2: initial condition

<u>Error</u> $\quad \underline{\bar{y}}(t) = \underline{y_e}(t) + \underline{\epsilon}(t)$

$$\frac{d\epsilon}{dt} = \underline{\underline{A}}\,\epsilon(t)$$

Explicit Euler.

$h\lambda_1 < 2$, $\underbrace{h\lambda_2 < 2}_{\text{controls step size.}}$: stiff problem.