Numerical Methods

7/10/25

Numerical Integration

Use interpolating polynomial

error term

$$\int_a^b f(x)\,dx = \int_a^b \sum_{i=0}^{n} f(x_i)\cdot l(x_i) + \int_a^b \prod_{i=0}^{n} \frac{f^{(n+1)}(y(x))\,(x-x_i)}{(n+1)!}$$

$$= \boxed{\sum_{i=0}^{n} a_i\, f(x_i)} + \int_a^b \prod_{i=0}^{n} \frac{f^{(n+1)}(y(x))\,(x-x_i)}{(n+1)!}.$$

where $a_i = \int_a^b l_i(x)\,dx, \quad \forall i = 0 \ldots n$

→ Trapezoidal rule

→ Let $x_0 = a$, $x_1 = b$ & $h = b-a$. Use Lagrange linear polynomial:

$$f(x) \approx P_1(x) = \frac{x-x_1}{x_0-x_1} f(x_0) + \frac{x-x_0}{x_1-x_0} f(x_1)$$

$$\therefore \int_a^b f(x)\,dx \approx \int_a^b P(x)\,dx = \int_a^b \frac{x-x_1}{x_0-x_1} f(x_0) + \frac{x-x_0}{x_1-x_0} f(x_1)\,dx$$

error term

$$= \boxed{\frac{h}{2}\left[f(x_0)+f(x_1)\right]} - \frac{h^3 \cdot f''(y)}{12}$$

Simpson's Rule

→ Use double trapezoid (using quadratic Lagrange polynomial)

→ Integrate over equally spaced nodes:

$x_0 = a$

$x_1 = a + h$

$x_2 = a + 2h = b$

Hence,

$$\int_a^b f(x) \approx \boxed{\frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right]} - \frac{h^5 \cdot f^{(4)}(\eta)}{90}$$

Degree of accuracy : The degree of accuracy of a quadrature formula is the largest +ve integer n s.t. the formula is exact for x^k for each $k = 0, 1 \ldots n$

→ Degree of accuracy of Trapezoid is 1, of Simpson is 3. These methods are called Newton-Cotes formulae.

Newton-Cotes formulae

Because boundary pts. are included

→ The $(n+1)$ point closed Newton-Cotes formula uses nodes $x_i = x_0 + ih$, where $i = 0, 1 \ldots n$ and $h = \frac{b-a}{n}$.

$$\therefore \int_a^b f(x)\, dx = \sum_{i=0}^{n} a_i f(x_i)$$

→ Error: $E(f) = \dfrac{h^{n+3} f^{(n+2)}(\eta)}{(n+2)!} \displaystyle\int_0^n + C.$

Simpson's Three-Eighths Rule

$$\int_a^b f(x)\,dx = \frac{3h}{8}\left[f(x_0)+3f(x_1)+3f(x_2)+f(x_3)\right] - \frac{3h^6 f^{(5)}(\eta)}{80}$$ (For $n=4$)

$$\int_a^b f(x)\,dx = \frac{2h}{45}\left[7f_0+32f_1+12f_2+32f_3+7f_4\right] - \frac{8h^7 f^{(6)}(\eta)}{945}$$ (For $n=5$)

14/10/25

Composite Trapezoidal Rule

$$\int_a^b f(x)\,dx = \frac{h}{2}\left(f(a)+2\sum_{j=1}^{n-1} f(x_j)+f(b)\right) - \frac{b-a}{12}h^2 f''(\mu)$$

error, $\mu \in (a,b)$

Composite Simpson's Rule

$$\int_a^b f(x)\,dx = \frac{h}{3}\left[f(a)+2\sum_{j=1}^{(n/2)-1} f(x_{2j}) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + f(b)\right] - \frac{(b-a)h^4 f^{(4)}(\eta)}{180}$$

→ Composite Simpson's Rule requires n (no. of intervals) to be even. Simpson's $1/3$ rule requires 2 intervals.

Best choice of h

→ Approximation error is of the form ch^p. Hence, error → 0 as $h \to 0$.

→ The approximation $f^{(r)}(x)$ contains h^r in the denominator. As $h \to 0$, truncation error decreases, but round-off error may increase.

Richardson's Extrapolation

→ We know that $f_j' = \dfrac{f_{j+1}-f_{j-1}}{2h} + O(h^2)$ (Central difference formula)

Read lec. notes

Romberg Integration

→ For $f \in C^{\infty}[a,b]$, the composite trapezoidal rule

Read lec. notes

Adaptive Quadrature Methods

→ Composite formulae suffer occasionally, because they require equally-spaced nodes. This may be inappropriate for functions with large value at one point.

→ To approximate $\int_a^b f(x)\,dx$, within a tolerance $\varepsilon > 0$:

$$\int_a^b f(x)\,dx = \frac{h}{3}\left[f(a) + f(a+h) + f(b)\right] - \frac{h^5}{90} f^{(4)}(\xi)$$

Let $S(a,b) = \frac{h}{3}\left[f(a) + f(a+h) + f(b)\right]$

Method of Undetermined Coefficient

Let $\int_a^b f(x)\,dx = A_0 f(a) + A_1 f(b) + \alpha f''(\beta)$

Taking $f(x) = 1 \Rightarrow b - a = A_0 + A_1$

Taking $f(x) = x \Rightarrow \frac{b^2 - a^2}{2} = A_0 a + A_1 b$

Solving, we get $A_0 = A_1 = \frac{b-a}{2}$

Initial Value Problems for Ordinary Differential Eqns.

→ An eqn. involving one dependent variable & ≥ 1 independent variable

→ Ordinary differential eqn is one with single independent variable.

→ Partials " " " " " multiple " "

→ Order of " " : Order of highest derivative

→ General ordinary differential eqn. w/t order n: $F(x, y, y', y'' \dots y^{(n)}) = 0$

→ Well-posed problem: The initial value problem $\frac{dy}{dx} = f(x, y)$, $y(x_0) = y$ is well posed if:

→ A unique soln. $y(x)$ exists for the problem

→ Stability condn:

There exist constants $\varepsilon_0 > 0$ & $k > 0$ s.t., if $|\delta(x)| < \varepsilon_0$ $\forall x \in [a, b]$, the initial value problem:

Perturbed problem $\left\{ \frac{dz}{dx} = f(x, z) + \delta(x) \right.$, $x \in [a, b]$, $z(x_0) = y_0 + \delta_0$,

has a unique soln $z(x)$ s.t.:

$$|y(x) - z(x)| < k\varepsilon \quad \forall x \in [a, b]$$

Example: $\frac{dy}{dx} = \frac{3y}{x}$, $y(0) = 1$

$$\int \frac{1}{3y} dy = \int \frac{1}{x} dx$$

$$\frac{\ln|3y|}{3} = \ln|x| + c$$

$$\boxed{\ln|3y| = 3\ln|x| + c}$$

general soln.

we cannot substitute $x = 0$, hence c cannot be determined.

Hence, this system is not well-posed.

Existence of initial value problem

$$\frac{dy}{dx} = f(x, y)$$

Peano's Theorem: Let $f(x,y)$ be continuous in the closed rectangular domain:

$$R = \{ |x - x_0| \leq a, \ |y - y_0| \leq b \},$$

Then the IVP has atleast one soln in the interval $I = |x - x_0| < h$, where $h = \min\{a, \frac{b}{M}\}$ and $M = \max_{(x,y) \in R} f(x,y)$

→ This theorem is a sufficient condn, not necessary condn.

Ex: $\frac{dy}{dx} = \frac{y}{x}$, $y(0) = 0$

$$\int \frac{1}{y} dy = \int \frac{1}{x} dx$$

Rectangular domain:

$$\{ |x - 0| \leq 1, \ |y - 0| \leq 1 \}$$

$$\ln|y| = \ln|x| + c_1$$

$$y = e^{\ln|x| + c_1}$$

$$= c_2 \cdot x$$

Hence, as per the theorem, soln. does not exist, however, a soln. DOES exist.

Uniqueness of Soln.

Let this be a first-order IVP: $\frac{dy}{dx} = f(x, y)$, $y(x_0) = y_0$

Theorem: (Picard) Let f & $\frac{\delta f}{\delta y}$ be continuous in the closed rectangular space:

← Dependent variable

$$R = \{ |x - x_0| \leq a, \ |y - y_0| \leq b \}$$

Then, the IVP has a unique soln. in the interval:

$$I = |x - x_0| < h, \text{ where } h = \min\{a, \frac{b}{M}\} \ \& \ M = \max_{(x,y)\in R} f(x,y)$$

$\rightarrow$ This theorem is also a sufficient condn.

Picard's iteration for IVP

Picard iteration gives approx soln. to the IVP: $\frac{dy}{dx} = f(x,y)$, $y(x_0) = y_0$

IVP is equivalent to the integral eqn. $y(x) = y_0 + \int_{x_0}^{x} f(t, y(t))\,dt$

We consider $y(x) \approx y_0$ as a soln. of $y(x)$.

Hence, $y_1(x) = y_0 + \int_{x_0}^{x} f(t, y_0)\,dt$

$y_2(x) = y_0 + \int_{x_0}^{x} f(t, y_1)\,dt$

$\vdots$

$y_n(x) = y_0 + \int_{x_0}^{x} f(t, y_{n-1})\,dt$

Ex: $\frac{dy}{dx} = 2x(1-y)$ $\qquad y(0) = 2$

$y_1(x) = y_0 + \int_{x_0}^{x} f(t, y_0)\,dt$

$$= 2 + \int_{x_0}^{x} 2t(1-2)\, dt$$

$$= 2 - 2\int_{x_0}^{x} t\, dx$$

$$= 2 - 2\left[\frac{t^2}{2}\right]_{x_0}^{x}$$

$$= 2 - (x^2 - \cancel{x_0^2})$$

(orange, above the struck term: 0)

$$= 2 - x^2$$

$$y_2(x) = 2 + \int_{x_0}^{x} 2t(t^2-1)\, dt \qquad f(t, y_1(t))$$

$$= f(t, 2-t^2)$$

$$= 2t(1-(2-t^2))$$

$$= 2t(t^2-1)$$

$$= 2 + \int_{x_0}^{x} 2t^3 - 2t\, dt$$

$$= 2 + \left[\frac{t^4}{4} - t^2\right]_{x_0}^{x}$$

$$= 2 + \frac{x^4}{4} - x^2$$

$$\vdots$$

$$y_{(n)}(x) = 2 - x^2 + \frac{x^4}{2} - \frac{x^6}{3!} + \dots = 2 + \sum_{i=1}^{n} (-1)^i \frac{x^{2i}}{i!}$$

$$= 1 + e^{-x^2}$$

By MacLaurin series

Analytical soln: $\frac{dy}{dx} = 2x(1-y)$, $y(0) = 2$

$$\int \frac{1}{1-y}\,dy = \int 2x\,dx$$

$$-\ln|1-y| = x^2 + c_0$$

$$\ln|1-y| = c_1 - x^2 \qquad (c_1 = -c_0)$$

$$1-y = e^{c_1 - x^2}$$

$$1-y = c_2 e^{-x^2} \qquad (c_2 = e^{c_1})$$

$$y = 1 - c_2 e^{-x^2}$$

$$2 = 1 - c_2 e^0$$

$$c_2 = -1 \Rightarrow y = 1 + e^{-x^2} \quad \text{(same as numerical soln.)}$$

Numerical soln. of IVP

→ Let there be a finite no. of sub-intervals bet. a & b:

$$\frac{dy}{dx} = f(x,y), \quad y(x_0) = y_0, \quad a \le x \le b$$

→ Let y_i be the approx. soln. at x_i. Estimate the soln at different points $y_0, y_1, \ldots$ using truncated Taylor series expansion. The set of nos. $\{y_i\}$ is called as numerical soln. of IVP.

Euler's method

step length

$$y_{n+1} = y_n + h \cdot f(x_n, y_n)$$

Proof:

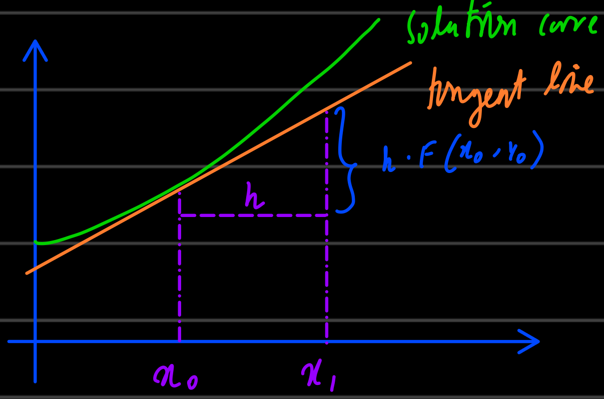
By Taylor series:

error term

$$y(x_{n+1}) = y(x_n) + h\,y'(x_n) + \frac{h^2}{2} y''(\xi_n) \qquad x_n \le \xi_n \le x$$

$y(x_{n+1}) \simeq y(x_n) + h \cdot y'(x_n)$

$y_{n+1} = y_n + h \cdot f(x_n, y_n)$



Ex. Find the values of y corresponding to $x = 0.5$, $h = 0.1$:

$$\frac{dy}{dx} = x + y \quad , \quad y(0) = 1$$

x	x_i	y_i	$y_n = y_{n-1} + hf(x_{n-1}, y_{n-1})$
x_0	0	1.	$1 + 0.1\, f(0,1) = 1 + 0.1(1) = 1.1$
x_1	0.1	1.1	$1.1 + 0.1 \cdot f(0.1, 1.1) = 1.22$
x_2	0.2	1.22	$1.22 + 0.1 \cdot f(0.2, 1.22) = 1.362$
x_3	0.3	1.362	$1.362 + 0.1 \cdot f(0.3, 1.362) = 1.5282$
x_4	0.4	1.5282	$1.5282 + 0.1\, f(0.4, 1.582) = 1.721$
x_5	0.5	1.721	

numerical soln.

Modified Euler (Predictor - Corrector) method

→ Euler method is easy, but solns. are not very accurate

→ A very small step size is reqd. for any meaningful result.

→ Improvement:

→ Take the arithmetic avg. of the slopes at x_n and x_{n+1}

Modified Euler's method:

$$y_{n+1,p} = y_n + h \cdot f(x_n, y_n)$$

Avg. slope = $\dfrac{f(x_n, y_n) + f(x_{n+1}, y_{n+1})}{2}$

Correct the predicted value: $y_{n+1,c} = h \cdot \dfrac{f(x_n + y_n) + f(x_{n+1}, y_{n+1,p})}{2} + y_n$

Hence the modified Euler method is:

$$y_{n+1} = y_n + \frac{h}{2}\left(\text{< fill this >} \right)$$

Lemma 1: $\forall\, x \geq 1$, and any $m \geq 0$, $0 \leq (1+x)^{mx} \leq e^{mx}$

Lemma 2: If s & t are +ve real nos, and $\{a_i\}_{i=0}^{k}$ is a sequence satisfying $a_0 \geq -t/s$ and

$$a_{i+1} \leq (1+s)\, a_i + t \quad \forall\, i = 0, 1, \ldots, k-1$$

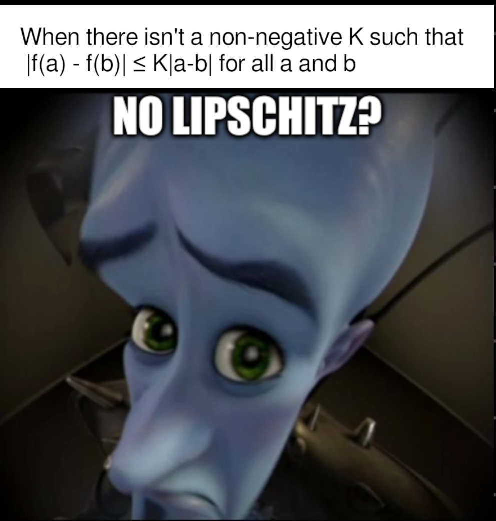
then $a_i =$

Add from slide

Lipschitz Condition

→ A function $f(x,y)$ is said to satisfy a Lipschitz condn. in the variable y on R if a constant $L \geq 0$ exists with

$$|f(x,y_1) - f(x,y_2)| \leq K|y_1 - y_2|$$



lec. slide

Global error of Euler's method

① $f(x,y)$ is continuous and satisfies Lipschitz condn. with constant L. Let $y = y(x)$ be the unique soln. of IVP.

② There exists a constant M s.t. $|y''(x)| \leq M \quad \forall\, x \in [x_0, b]$

③ Let $w_0, \dots, w_N$, be approximations generated by Euler method. Then

$$|e_i| = |y(x_i) - w_i| \leq \frac{MH}{2L}\left(e^{(x_i - x_0)L} - 1\right), \quad i = 0, 1, \dots, N$$

Runge-Kutta methods

28/10/25

→ Taylor series requires partial derivatives, which may not be possible.

→ Taylor series in two variables:

$$P_n(t,y) = \sum_{i=0}^{\infty}\left[\frac{1}{i!}\sum_{j=0}^{n} {}^{n}C_j\,(t-t_0)^{n-j}\,(y-y_0)^{j}\right]$$ < Lec. slides >

2nd Order Runge-Kutta method:

We have I.V.P. $\frac{dy}{dx} = f(x,y)$, $y(x_0) = y_0$

2nd order Runge-Kutta method states that:

$$y_{n+1} = y_n + \text{Avg. slope}\,(x_{n+1} - x_n)$$

$$= y_n + h\left[\frac{f(x_n,y_n) - f(x_{n+1},y_{n+1})}{2}\right]$$

$$= y_n + \tfrac{1}{2}(k_1+k_2)$$, where:

$$k_1 = hf(x_n,y_n) \quad \text{and} \quad k_2 = hf(x_n+h,\, y_n+k_1)$$

E.g. $\frac{dy}{dx} = x+y$, $y(0)=1$, $h=0.2$

$$k_1 = hf(x_0,y_0) = 0.2$$

$$k_2 = hf\left(x_0+\tfrac{h}{2},\, y_0+\tfrac{k_1}{2}\right) = 0.2\,f(0.1,\,1.1) = 0.2(1.2) = 0.24$$

⋮

Runge - Kutta - 4 method :

We have IVP : $\frac{dy}{dx} = f(x, y)$, $y(x_0) = y_0$,

$$y_{n+1} = y_n + w_1 k_1 + w_2 k_2 + w_3 k_3 + w_4 k_4,$$

where: $k_1 = hf(x_n, y_n)$

$$k_2 = hf(x_n + \alpha h, y_n + \beta k_1)$$

$$k_3 = hf(x_n + \gamma h$$

Lec. slides

System of first-order IVPs.

$$\frac{dy_1}{dx} = f_1(x, y_1, \ldots y_m) \qquad y_1(a) = \alpha_1$$

$$\vdots$$

$$\frac{dy_m}{dx} = f_m(x, y_1, \ldots y_m) \qquad y_m(a) = \alpha_m$$

The objective is to find m functions s.t. $y_1, \ldots y_m$ satisfy the differential equations:

Read lec. slides

Single Step Method

Single step method : The soln. at any point is obtained using the soln. at prev. point. Hence, a general single step method can be written as follows:

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

Increment function

This function can be implicit or explicit.
If y_{n+1} does not depend on x_{n+1} & y_{n+1}, it is known as explicit. In such a case, the single step method can be written as follows:

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

Boundary Value Problem (BVP) 4/11/25

$$y''(x) = f(x, y, y') \quad , \quad y(a) = \alpha, \quad y(b) = \beta, \quad a \le x \le b$$

→ Shooting method
 → Reduces BVP to IVP

Theorem: Suppose f is continuous on the set

$$D = \{(x, y, y') \mid a \le x \le b, \text{ with } -\infty < y < \infty, -\infty < y' < \infty\}$$

and $\frac{\delta y}{\delta x}$ and $\frac{\delta y'}{\delta x}$ are continuous on the set D.

Read slides

→ Linear BVP

→ Linear BVP is s.t. the dependent variables & their product is not exist.

e.g. $y \cdot \frac{dy}{dx}$ must not exist

→ Also, degree of dependent variable must at most be 1.

→ Dependent variable must not be transcendental function.

i.e. $f(x, y, y') = p(x)y' + q(x)y + r(x)$

For soln. to be unique, $y'' = p(x)y' + q(x)y + r(x)$ for $a \le x \le b$

→ $p(x)$, $q(x)$ & $r(x)$ are continuous on $[a, b]$

→ $q(x) > 0$ on $[a, b]$

→ Shooting Method for Non-linear problems

→ Approximate the soln. to BVP by using the solns. to a sequence of IVPs involving a parameter t.

→ Choose $t = t_k$ s.t.

$$\lim_{k \to \infty} y(b, t_k) = y(b) = \beta,$$

where $y(x, t_k)$ denotes the soln. to the IVP

$$y'' = f(x, y, y'), \quad x \in [a, b], \text{ with } y(a) = \alpha \text{ \& } y'(a) = t_k$$

We start with a parameter t_0 s.t. $y'(a) = t_0$.

→ If $y(b, t_0)$ is not sufficiently close to β, we correct our approximation in $t_1, t_2, \ldots,$ until $y(b, t_k)$ is sufficiently close to β

→ Do this using Newton's iteration :

$$t_k = t_{k-1} - \frac{y(b, t_{k-1}) - \beta}{\frac{d}{dt} y(b, t_{k-1})}$$

E.g. $y'' = \frac{1}{8}(32 + 2x^3 - yy')$, $x \in [1, 3]$, $f(1) = 17$ $f(3) = 43/3$

Slides

Partial Differential equations

→ Second order linear P.D.E. :

$$A \frac{\partial^2 u}{\partial x^2} + B \frac{\partial^2 u}{\partial x \partial y} + C \frac{\partial^2 u}{\partial y^2} + D \frac{\partial u}{\partial x} + E \frac{\partial u}{\partial y} + Fy = 0$$

If $B^2 - 4AC < 0$, elliptical

Slides

Single Step & Runge - Kutta methods

→ Single step methods : $y_{n+1} = y_n + h\,\phi(x_n, y_n, h)$

→ Used to solve first order O.D.E.s

→ Runge Kutta method :

$$y_{n+1} = y_n + \sum_{i=1}^{s} w_i k_i$$

$$k_i = f\left(x_n + c_i h,\ y_n + h\sum_{j=1}^{s} a_{ij} k_j\right)$$

→ Butcher tableau

$$\begin{array}{c|c} \underset{\sim}{c} & \underset{\sim}{A} \\ \hline & \underset{\sim}{w}^T \end{array}$$

$\underset{\sim}{c}$: node vector

$\underset{\sim}{w}$: weight vector

$\underset{\sim}{A}$: coefficient matrix ← Runge Kutta matrix

→ Consistency condition of RK method :

$$\sum_{i=1}^{s} w_i = 1 \quad \text{and} \quad c_i = \sum_{j=1}^{s} a_{ij}$$

→ If $\underset{\sim}{A}$ is strictly lower triangular,

$$k_i = f\left(x_n + c_i h + \right.$$

→ RK-2 method

0	0	0
1/2	1/2	0
	0	1

$$k_1 = h \cdot f(x_n, y_n)$$

$$k_2 = h \cdot f\left(x_n + \frac{h}{2}, y_n + \frac{k_1}{2}\right)$$

$$y_{n+1} = y_n + k_2$$

→ RK-3 method

0	0	0	0
1/2	1/2	0	0
1	-1	2	0
	1/6	2/3	1/6

$$k_1 = h \cdot f(x_n, y_n)$$

$$k_2 = h \cdot f\left(x_n + \frac{h}{2}, y_n + \frac{k_1}{2}\right)$$

$$k_3 = h \cdot f(x_n + h, y_n - k_1 + k_2)$$

$$y_n =$$