Numerical Methods

DS288 and UMC201

Ratikanta Behera

Department of Computational and Data Sciences,
Indian Institute of Science Bangalore

August-December 2025

Polynomial Least Squares

- Given a set of data $\{x_i, y_i\}_{i=1}^{m}$, to approximate it with an algebraic polynomial of degree $n < m-1$

$$P_n(x) = a_n x^n + a_{n-1}x^{n-1} + \ldots a_1 x + a_0$$

- Choose the constants $a_0, a_1, \ldots, a_n$ to minimize the least squares error $E = E(a_0, a_1, \ldots, a_n)$, where

$$E = \sum_{i=1}^{m}(y_i - P_n(x_i))^2 = \sum_{i=1}^{m} y_i^2 - 2\sum_{i=1}^{m} P_n(x_i)y_i + \sum_{i=1}^{m}(P_n(x_i))^2$$

$$= \sum_{i=1}^{m} y_i^2 - 2\sum_{i=1}^{m}\left(\sum_{j=0}^{n} a_j x_i^j\right) y_i + \sum_{i=1}^{m}\left(\sum_{j=0}^{n} a_j x_i^j\right)^2$$

$$= \sum_{i=1}^{m} y_i^2 - 2\sum_{j=0}^{n} a_j \left(\sum_{i=1}^{m} y_i x_i^j\right) + \sum_{j=0}^{n}\sum_{k=0}^{n} a_j a_k \left(\sum_{i=1}^{m} x_i^{j+k}\right)$$

Polynomial Least Squares

- For E to be minimized, $\frac{\partial E}{\partial a_j} = 0$, for each $j = 0, 1, \ldots, n$, Thus,

$$\frac{\partial E}{\partial a_j} = -2\sum_{i=1}^{m} y_i x_i^j + 2\sum_{k=0}^{n} a_k \sum_{i=1}^{m} x_i^{j+k} = 0$$

- We have $n+1$ normal equations

$$\sum_{k=0}^{n} a_k \sum_{i=1}^{m} x_i^{j+k} = \sum_{i=1}^{m} y_i x_i^j, \quad j = 0, 1, \ldots, n$$

Polynomial Least Squares

- The $n+1$ normal equations can be written as

$$
\begin{aligned}
a_0 \sum_{i=1}^{m} x_i^0 + a_1 \sum_{i=1}^{m} x_i^1 + a_2 \sum_{i=1}^{m} x_i^2 + \cdots + a_n \sum_{i=1}^{m} x_i^n &= \sum_{i=1}^{m} y_i x_i^0 \\
a_0 \sum_{i=1}^{m} x_i^1 + a_1 \sum_{i=1}^{m} x_i^2 + a_2 \sum_{i=1}^{m} x_i^3 + \cdots + a_n \sum_{i=1}^{m} x_i^{n+1} &= \sum_{i=1}^{m} y_i x_i^1 \\
&\vdots \\
a_0 \sum_{i=1}^{m} x_i^n + a_1 \sum_{i=1}^{m} x_i^{n+1} + a_2 \sum_{i=1}^{m} x_i^{n+2} + \cdots + a_n \sum_{i=1}^{m} x_i^{2n} &= \sum_{i=1}^{m} y_i x_i^n.
\end{aligned}
$$

which have a unique solution provided that x_i are distinct.

Example

Example

Fit the following data with a discrete least square polynomial of degree at most 2

i	1	2	3	4	5
x	0	0.25	0.50	0.75	1.00
$f(x)$	1.00	1.2840	1.6487	2.1170	2.7183

Ans: $P_2(x) = 1.0051 + 0.86468x + 0.84316x^2$

Polynomial Least Squares

- Assume that the data are exponentially related, i.e., $y = be^{ax}$.
- The least squares error is

$$E = \sum_{i=1}^{m} (y_i - be^{ax_i})^2.$$

- And the respective normal equations

$$\frac{\partial E}{\partial b} = -2e^{ax_i} \sum_{i=1}^{m} (y_i - be^{ax_i}) = 0,$$

$$\frac{\partial E}{\partial a} = -2bx_i e^{ax_i} \sum_{i=1}^{m} (y_i - bx_i^a) = 0.$$

- In general, exact solutions for the two equations may not get.
- The commonly used method is taking the logarithm of the approximating equation as $ln\ y = ln\ b + ax$.

Section-8.2
Orthogonal Polynomials and Least Squares Approximation

Least Squares Approximation of functions

- Let $f \in C[a,b]$, and a polynomial $P_n(x) = \sum_{k=0}^{n} a_k x^k$ of degree at most n is required to minimize the error

$$E = \int_a^b [f(x) - P_n(x)]^2 dx$$

$$\text{Thus, } E = E(a_0, a_1, \ldots, a_n) = \int_a^b \left(f(x) - \sum_{k=0}^{n} a_k x^k \right)^2 dx$$

- A necessary condition to find real coefficients $a_0, a_1, \ldots a_n$, that minimizes E is

$$\frac{\partial E}{\partial a_j} = 0, \text{ for each } j = 0, 1, \ldots, n$$

Least Squares Approximation of functions

- The least squares error is

$$E = \int_a^b [f(x)]^2 dx - 2\sum_{k=0}^{n} a_k \int_a^b x^k f(x) dx + \int_a^b \left(\sum_{k=0}^{n} a_k x^k\right)^2 dx$$

Such that,

$$\frac{\partial E}{\partial a_j} = -2\int_a^b x^j f(x) dx + 2\sum_{k=0}^{n} a_k \int_a^b x^{j+k} dx = 0$$

- To solve the following $n+1$ linear normal equations to find $P_n(x)$

$$\sum_{k=0}^{n} a_k \int_a^b x^{j+k} dx = \int_a^b x^j f(x) dx, \text{ for each } j = 0, 1, \ldots n$$

- A unique solution exists provided that $f \in C[a, b]$.

Example

Example

Find the least squares approximating polynomial of degree 2 for the function $f(x) = \sin \pi x$ on the interval $[0, 1]$.

- Let $f(x) = \sin \pi x, x \in [0, 1]$. We have to find the least squares approximating polynomial of degree 2
- Normal equations for $P_2(x) = a_2 x^2 + a_1 x + a_0$ are

$$
\begin{aligned}
a_0 \int_0^1 1 dx + a_1 \int_0^1 x dx + a_2 \int_0^1 x^2 dx &= \int_0^1 \sin \pi x dx, \\
a_0 \int_0^1 x dx + a_1 \int_0^1 x^2 dx + a_2 \int_0^1 x^3 dx &= \int_0^1 x \sin \pi x dx, \\
a_0 \int_0^1 x^2 dx + a_1 \int_0^1 x^3 dx + a_2 \int_0^1 x^4 dx &= \int_0^1 x^2 \sin \pi x dx.
\end{aligned}
$$

Example

- The above three equations can be simplified to

$$\begin{aligned} a_0 + \frac{1}{2}a_1 + \frac{1}{3}a_2 &= \frac{2}{\pi}, \\ \frac{1}{2}a_0 + \frac{1}{3}a_1 + \frac{1}{4}a_2 &= \frac{1}{\pi}, \\ \frac{1}{3}a_0 + \frac{1}{4}a_1 + \frac{1}{5}a_2 &= \frac{\pi^2 - 4}{\pi^3}. \end{aligned}$$

- The solutions are

$$a_0 = \frac{12\pi^2 - 120}{\pi^3} \approx -0.050465, \text{ and } a_1 = -a_2 = \frac{720 - 60\pi^2}{\pi^3} \approx 4.12251$$

- Hence, the least square approximating polynomial of degree 2 for $f(x) = \sin \pi x, x \in [0, 1]$ is $P_2(x) = -4.12251x^2 + 4.12251x - 0.050465.$

Linearly Independent Function

Definition

The set of functions $\{\phi_0, \cdots \phi_n\}$ is said to be linearly independent on $[a, b]$ if, whenever

$$c_0\phi_0 + c_0\phi_0 + \cdots + c_n\phi_n = 0, \quad \text{for all } x \in [a, b]$$

Otherwise, the set of functions is said to be linearly dependent.

Theorem

Suppose that for each $j = 0, 1, \ldots, n$, $\phi_j(x)$ is a polynomial of degree j. Then $\{\phi_0, \ldots, \phi_n\}$ is linearly independent on any interval $[a, b]$.

Example

Let $\phi_0(x) = 2$, $\phi_1(x) = x - 3$, and $\phi_2(x) = x^2 + 2x + 7$, and $Q(x) = a_0 + a_1 x + a_2 x^2$. Show that there exist constants c_0, c_1, and c_2 such that $Q(x) = c_0\phi_0(x) + c_1\phi_1(x) + c_2\phi_2(x)$.

Here $\{\phi_0, \phi_1, \phi_2\}$ is linearly independent on any interval $[a, b]$. First note that

$$1 = \frac{1}{2}\phi_0(x), \quad x = \phi_1(x) + 3 = \phi_1(x) + \frac{3}{2}\phi_0(x), \text{and}$$

$$x^2 = \phi_2(x) - 2x - 7 = \phi_2(x) - 2\left[\phi_1(x) + \frac{3}{2}\phi_0(x)\right] - 7\left[\frac{1}{2}\phi_0(x)\right] \tag{1}$$

$$= \phi_2(x) - 2\phi_1(x) - \frac{13}{2}\phi_0(x). \tag{2}$$

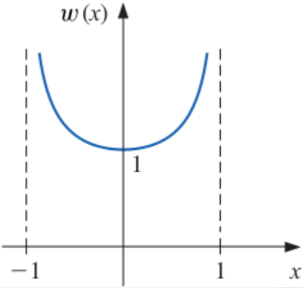
$$Q(x) = a_0\left[\frac{1}{2}\phi_0(x)\right] + a_1\left[\phi_1(x) + \frac{3}{2}\phi_0(x)\right] + a_2\left[\phi_2(x) - 2\phi_1(x) - \frac{13}{2}\phi_0(x)\right] \tag{3}$$

$$= \left(\frac{1}{2}a_0 + \frac{3}{2}a_1 - \frac{13}{2}a_2\right)\phi_0(x) + [a_1 - 2a_2]\phi_1(x) + a_2\phi_2(x). \tag{4}$$

Orthogonal Functions

Definition: An integrable function w is called a **weight function** on the interval I, if $w(x) \geq 0$, for all $x \in I$, but $w(x) \neq 0$ on any subinterval of I.

- Purpose is to assign varying degrees of importance to approximations on certain portions of the interval.
- Example: $w(x) = \frac{1}{\sqrt{1-x^2}}$ places less emphasis near the center of the interval $(-1, 1)$, and more when $|x|$ is near 1



Orthogonal Functions

Definition

$\{\phi_0, \phi_1, \ldots, \phi_n\}$ is an **orthogonal set of functions** for the interval $[a, b]$ with respect to the weight function w if

$$\int_a^b w(x)\phi_k(x)\phi_j(x)dx = \begin{cases} 0, & \text{when } j \neq k, \\ \alpha_j > 0, & \text{when } j = k \end{cases}.$$

If in addition, $\alpha_j = 1$, the set is said to be **orthonormal**.

- Let $\{\phi_0, \phi_1, \ldots, \phi_n\}$ is a set of LI functions on $[a, b]$.
- w is a weight function for $[a, b]$
- Given $f \in C[a, b]$, we need to find a linear combination

$$P(x) = \sum_{k=0}^{n} a_k\phi_k(x) \quad \text{to minimize the error}$$

Orthogonal Functions

- Let $E = E(a_0, a_1, \ldots, a_n) = \int_a^b w(x)\left[f(x) - \sum_{k=0}^{n} a_k \phi_k(x)\right]^2 dx$
- The necessary condition is

$$\frac{\partial E}{\partial a_j} = 2\int_a^b w(x)\left[f(x) - \sum_{k=0}^{n} a_k \phi_k(x)\right]\phi_j(x)dx = 0$$

- The system of normal equations for $j = 0, 1, \ldots, n$ is

$$\int_a^b w(x) f(x)\phi_j(x)dx = \sum_{k=0}^{n} a_k \int_a^b w(x)\phi_k(x)\phi_j(x)dx$$

- Choose the functions $\phi_j(x)$, such that

$$\int_a^b w(x)\phi_k(x)\phi_j(x)dx = \begin{cases} 0, & \text{when } j \neq k \\ \alpha_j > 0, & \text{when } j = k \end{cases}.$$

Orthogonal Functions

- The above chosen $\phi_j(x), j = 0, 1, \ldots, n$, the normal equations reduce to

$$\int_a^b w(x)f(x)\phi_j(x)dx = a_j \int_a^b w(x)[\phi_j(x)]^2 dx = a_j\alpha_j$$

- Solving the above equations, we get

$$a_j = \frac{1}{\alpha_j}\int_a^b w(x)f(x)\phi_j(x)dx$$

Least Squares Approximation

- If functions whose values are given at $n+1$ points $x_0, \cdots x_n$

$$E = E(a_0, \ldots, a_n) = \sum_{k=0}^{n} w(x_k) \left[f(x_k) - \sum_{k=0}^{n} a_k \phi_k(x_k) \right]^2 dx \text{ minimum}$$

- If functions are continuous on $[a, b]$ then

$$E = E(a_0, \ldots, a_n) = \int_a^b w(x) \left[f(x) - \sum_{k=0}^{n} a_k \phi_k(x) \right]^2 dx \text{ minimum}$$

Example

- Find a linear polynomial approximation to $f(x) = x^3$ on the interval $[0, 1]$ using the least squares approximation with $w(x) = 1$.
- Find the least squares approximation of second degree for the descrite data

x	-2	-1	0	1	2
$f(x)$	15	1	1	3	19

Chapter-4
Numerical Differentiation and Integration

Numerical Differentiation

- The derivative represents the rate of change of a dependent variable with respect to an independent variable.
- Integration is the inverse of differentiation
- Looking for ways to approximate function derivatives with combinations of function evaluations at discrete points.

Recall: Secant Method and Taylor series

➢ Secant Method

$$f'(x_n) = \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}}$$

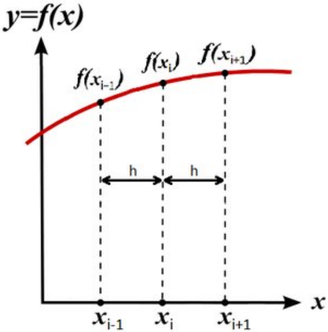
➢ Expand $f(x)$ about x_j, the point where derivative is needed

$$f(x) = f(x_j) + f'(x_j)(x - x_j) + \frac{f''(x_j)}{2!}(x - x_j)^2 + \cdots \tag{5}$$

Numerical Differentiation

- Define $h = x_{j+1} - x_j$, use notation $f_j = f(x_j)$
- Let $x = x_{j+1}$ in the above equation (5)

$$\begin{aligned} f(x_{j+1}) &= f(x_j) + f'(x_j)(x_{j+1} - x_j) + \frac{f''(x_j)}{2!}(x_{j+1} - x_j)^2 + \cdots \\ f_{j+1} &= f_j + hf'_j + h^2\frac{f''(x_j)}{2!} + h^3\frac{f'''(x_j)}{3!} + \cdots \end{aligned}$$



Numerical Differentiation

- If h is small, then higher order terms $(f_j'', f_j''' \cdots)$ will diminish faster.
- $f_j' = \dfrac{f_{j+1} - f_j}{h} + O(h)$, where $O(h)$ error term
- Indeed, $f_j' = \dfrac{f_{j+1} - f_j}{h} - \dfrac{hf''(\zeta)}{2!}$, where $\zeta \in [x_j, x_{j+1}]$
- Define: $\Delta f_j = f_{j+1} - f_j$ (First Forward Difference)

Backward

- Use $x = x_{j-1}$ for the equation (5) and $h = x_j - x_{j-1}$
- $f_j' = \dfrac{f_j - f_{j-1}}{h} - \dfrac{hf''(\zeta)}{2!}$, where $\zeta \in [x_{j-1}, x_j]$
- Define: $\nabla f_j = f_{j+1} - f_j$ (First Backward Difference)

Thus we can write $f_j' = \dfrac{\Delta f_j}{h}$ and $f_j' = \dfrac{\nabla f_j}{h}$

Central Difference

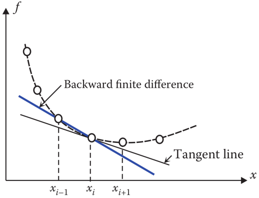
- The quadratic term in the Taylor series.

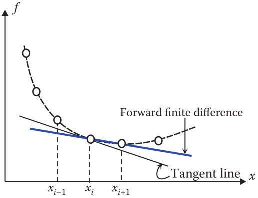
$$\begin{aligned} f_{j-1} &= f_j - hf_j' + h^2\frac{f''}{2!} - h^3\frac{f'''(\zeta)}{3!} \quad \text{where } \zeta \in [x_{j-1}, x_j] \\ f_{j+1} &= f_j + hf_j' + h^2\frac{f''}{2!} + h^3\frac{f'''(\eta)}{3!} \quad \text{where } \zeta \in [x_{j-1}, x_j] \end{aligned}$$

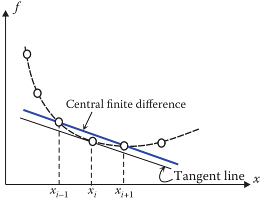
- Subtracting the first equation from the second

$$f_{j+1} - f_{j-1} = 2hf_j' + \frac{1}{3!}h^3[f'''(\zeta) + f'''(\eta)]$$

- Solving for f_j' gives: $f_j' = \dfrac{f_{j+1} - f_{i-1}}{2h} + O(h^2)$







Second Derivatives

- Consider $x = x_{j+2}$

$$f_{j+1} = f_j + hf'_j + h^2\frac{f''}{2!} + h^3\frac{f'''(\eta)}{3!} \quad \text{where } \zeta \in [x_{j-1}, x_j]$$

$$f_{j+2} = f_j + 2hf'_j + (2h)^2\frac{f''}{2!} + (2h)^3\frac{f'''(\zeta)}{3!}, \quad \text{here } x_{j+2} - x_j = 2h$$

- Solve for f_j'', we get

$$\begin{aligned} f_{j+2} - f_{j+1} &= -f_j + h^2 f_j'' + \cdots \\ \Rightarrow f_j'' &= \frac{f_{j+2} - 2f_{j+1} + f_j}{h^2} + O(h) \quad \text{where } \zeta \in [x_j, x_{j+2}] \end{aligned}$$

- On the other hand

$$\begin{aligned} \Delta^2 f_j &= \Delta(\Delta f_j) = \Delta(f_{j+1} - f_j) = \Delta(f_{j+1}) - \Delta(f_j) \\ &= f_{j+2} - f_{j+1} - (f_{j+1} - f_j) = f_{j+2} - 2f_{j+1} + f_j \end{aligned}$$

Thus $\quad f_j'' = \dfrac{\Delta^2 f_j}{h^2}$

Second Derivatives

- Similarly, backward approximation $f_j^{''} = \frac{\nabla^2 f_j}{h^2}$
- Further, we need 3 term Taylor expansions to evaluate $f_j^{'''}$

$$f_j^{'''} = \frac{f_{j+3} - 3f_{j+2} + 3f_{j+1} - f_j}{h^3} + O(h)$$

- In general, one can construct approximation to n^{th} order derivative of f at x_j.
- To accuracy $O(h)$ using the weighted sum of n Taylor expansions requiring $n+1$ function evaluations to $O(h)$ [true for both forward and backward.]
- We can conclude the higher order h means higher accuracy

Higher Order Accuracy

- The three-point forward difference formula approximates the first derivative at x_i by using the values at the points x_i, x_{i+1}, and x_{i+2}

$$f_j' = \frac{-3f_j + 4f_{i+1} - f_{i+2}}{2h} + O(h^2)$$

Example

Consider the data generated by the function $f(x) = e^{-x}\sin(x/2)$ at $x = 1.2, 1.4, 1.6, 1.8.$. Calculate approximate $f'(1.4)$ using the backward, forward, and central difference formula and their relative error.

Difference Formula	**Approximate** $f'(1.4)$	**% Relative Error**
Two-point backward	$\frac{f(1.4)-f(1.2)}{0.2} = -0.0560$	13.22
Two-point forward	$\frac{f(1.6)-f(1.4)}{0.2} = -0.0702$	8.66
Two-point central	$\frac{f(1.6)-f(1.2)}{2(0.2)} = -0.0631$	2.28
Three-point forward	$\frac{-3f(1.4)+4f(1.6)-f(1.8)}{2(0.2)} = -0.0669$	3.56


ANY
QUESTIONS?