Non-Linear Regression: Polynomial Regression

1. Introduction

Polynomial Regression is a form of regression analysis in which the relationship between the independent variable x and the dependent variable y is modeled as an n-th degree polynomial. It extends linear regression by introducing polynomial terms to capture non-linearity.

1.1 Polynomial Regression Equation

The general form of a polynomial regression model of degree n is:

$$y = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + ... + a_n x^n + \varepsilon$$

Where:

- y is the dependent variable.
- x is the independent variable.
- $a_0, a_1, a_2, ..., a_n$ are the coefficients to be determined.
- ε represents the error term.

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2. Polynomial Regression Using the Normal Equation

To determine the polynomial coefficients, we use the **Normal Equation**:

$$A = (X^T X)^{-1} X^T Y$$

Where:

- X is the **design matrix** constructed from the input x values.
- Y is the column vector of y values.
- A is the column vector of polynomial coefficients.

The steps involve:

1. Constructing the **design matrix** X.
2. Computing $X^T X$.
3. Finding the **determinant** of $X^T X$.
4. Computing the **adjoint** and **inverse** of $X^T X$.
5. Multiplying $(X^T X)^{-1}$ by $X^T Y$ to obtain the coefficients.

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3. Example Problem

We will fit a quadratic polynomial regression ($y = a_0 + a_1 x + a_2 x^2$) to the given dataset:

x	y
1	2
2	3
3	5
4	7
5	11

Step 1: Construct the Design Matrix X

For quadratic regression ($n = 2$), the design matrix is:

$$X = \begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ 1 & x_3 & x_3^2 \\ 1 & x_4 & x_4^2 \\ 1 & x_5 & x_5^2 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1^2 \\ 1 & 2 & 2^2 \\ 1 & 3 & 3^2 \\ 1 & 4 & 4^2 \\ 1 & 5 & 5^2 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 4 \\ 1 & 3 & 9 \\ 1 & 4 & 16 \\ 1 & 5 & 25 \end{bmatrix}$$

The response vector Y is:

$$Y = \begin{bmatrix} 2 \\ 3 \\ 5 \\ 7 \\ 11 \end{bmatrix}$$

Step 2: Compute $X^T X$

$$X^T = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & 3 & 4 & 5 \\ 1 & 4 & 9 & 16 & 25 \end{bmatrix}$$

Multiplying X^T by X:

$$X^T X = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & 3 & 4 & 5 \\ 1 & 4 & 9 & 16 & 25 \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 4 \\ 1 & 3 & 9 \\ 1 & 4 & 16 \\ 1 & 5 & 25 \end{bmatrix}$$

$$= \begin{bmatrix} 5 & 15 & 55 \\ 15 & 55 & 225 \\ 55 & 225 & 979 \end{bmatrix}$$

Step 3: Compute Determinant of $X^T X$

$$\text{Det}(X^T X) = \begin{vmatrix} 5 & 15 & 55 \\ 15 & 55 & 225 \\ 55 & 225 & 979 \end{vmatrix}$$

Using determinant formula for a 3×3 matrix:

$$\text{Det} = 5(55 \times 979 - 225 \times 225) - 15(15 \times 979 - 225 \times 55) + 55(15 \times 225 - 55 \times 55)$$

$$= 5(53745 - 50625) - 15(14685 - 12375) + 55(3375 - 3025)$$

$$= 5(3120) - 15(2310) + 55(350)$$

$$= 15600 - 34650 + 19250 = 200$$

Step 4: Compute Adjoint of $X^T X$

Using cofactor expansion, we find the adjoint matrix:

$$\text{Adj}(X^T X) = \begin{bmatrix} ? & ? & ? \\ ? & ? & ? \\ ? & ? & ? \end{bmatrix}$$

(Here, the exact adjoint matrix calculations are tedious, but we would compute each minor and cofactor).

Step 5: Compute Inverse of $X^T X$

$$(X^T X)^{-1} = \frac{1}{\text{Det}} \times \text{Adj}(X^T X)$$

Step 6: Compute $A = (X^T X)^{-1} X^T Y$

By multiplying the inverse matrix with $X^T Y$, we obtain:

$$A = \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} ? \\ ? \\ ? \end{bmatrix}$$

Thus, the polynomial regression model is:

$$y = a_0 + a_1x + a_2x^2$$

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4. Exercise

Fit a **cubic polynomial regression** $y = a_0 + a_1x + a_2x^2 + a_3x^3$ using:

x	y
1	1
2	8
3	27
4	64

Solution Steps:

1. Construct the **design matrix** X.
2. Compute X^TX.
3. Find **Determinant**, **Adjoint**, and **Inverse**.
4. Compute $A = (X^TX)^{-1}X^TY$.
5. Write the final cubic polynomial.