

Polynomial Regression (Handwriting Assignment)

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Introduction

In the mid-term project, we will look at a polynomial regression algorithm which can be used to fit non-linear data by using a polynomial function. The 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 in x .

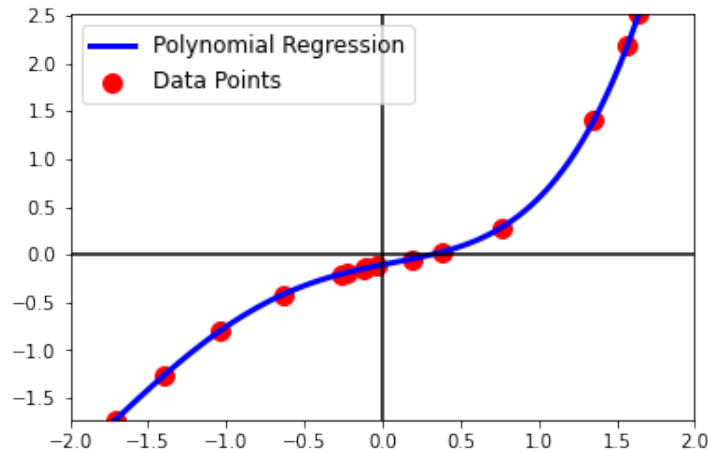


Figure 1: Example of Polynomial Regression

First, what is a regression? we can find a definition from the book as follows: *Regression analysis is a form of predictive modelling technique which investigates the relationship between a dependent and independent variable.* Actually, this definition is a bookish definition, in simple terms the regression can be defined as *finding a function that best explain data which consists of input and output pairs.* Let assume that we have 100 data points,

$$(x_1, y_1), (x_2, y_2), (x_3, y_3), \dots, (x_{98}, y_{98}), (x_{99}, y_{99}), (x_{100}, y_{100}).$$

The goal of regression is to find a function \hat{f} such that

$$\hat{f}(x_1) = y_1, \hat{f}(x_2) = y_2, \hat{f}(x_3) = y_3, \dots, \hat{f}(x_{99}) = y_{99}, \hat{f}(x_{100}) = y_{100}.$$

This is the simplest definition of the regression problem. Note that many details about regression analysis are omitted here, but, you will learn more rigorous definition in other courses such as



Figure 2: Examples of polynomial functions

machine learning or statistics. Then, the polynomial regression is the regression framework that employs the polynomial function to fit the data.

So, what is the polynomial function? I guess you may remember, from high school, the following functions:

$$\text{Degree of 0 : } f(x) = w_0$$

$$\text{Degree of 1 : } f(x) = w_1 \cdot x + w_0$$

$$\text{Degree of 2 : } f(x) = w_2 \cdot x^2 + w_1 \cdot x + w_0$$

$$\text{Degree of 3 : } f(x) = w_3 \cdot x^3 + w_2 \cdot x^2 + w_1 \cdot x + w_0$$

$$\vdots$$

$$\text{Degree of } d : f(x) = \sum_{i=0}^d w_i \cdot x^i,$$

where w_0, w_1, \dots, w_d are a coefficient of polynomial and d is called a degree of a polynomial. So, we can determine a polynomial function $f(x)$ by deciding its degree d and corresponding coefficients $\{w_0, w_1, \dots, w_d\}$. Figure 2 illustrates some examples of polynomial functions.

Then, the polynomial regression is a regression problem to find the best polynomial function to fit the given data points. Especially, the polynomial function is determined by coefficients (let just assume that d is fixed). We can restate the polynomial regression as *finding coefficients of polynomials such that, for all data point, (x_i, y_i) , $y_i = \hat{f}(x_i)$ holds* (if we have noise free data). Figure 1 shows the example of polynomial regression. In the following problems, you have to study how to compute the coefficients of the polynomial to fit the data points.

Problems

1. (80 pt. in total)

Assume that we have n data points, $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$. Let the degree of polynomial be d . Then, we want to find $w_0, w_1, w_2, \dots, w_d$ of the polynomial such that

$$\begin{aligned}\hat{f}(x_1) &= w_0 + w_1x_1 + w_2x_1^2 + \dots + w_dx_1^d = y_1, \\ \hat{f}(x_2) &= w_0 + w_1x_2 + w_2x_2^2 + \dots + w_dx_2^d = y_2, \\ \hat{f}(x_3) &= w_0 + w_1x_3 + w_2x_3^2 + \dots + w_dx_3^d = y_3, \\ \hat{f}(x_4) &= w_0 + w_1x_4 + w_2x_4^2 + \dots + w_dx_4^d = y_4, \\ \hat{f}(x_5) &= w_0 + w_1x_5 + w_2x_5^2 + \dots + w_dx_5^d = y_5, \\ &\vdots \\ \hat{f}(x_n) &= w_0 + w_1x_n + w_2x_n^2 + \dots + w_dx_n^d = y_n.\end{aligned}$$

Now, we reformulate the equations into the vector and matrix form. First, let $\mathbf{w} = [w_0, w_1, \dots, w_d]^T$ and $\mathbf{y} = [y_1, y_2, \dots, y_n]^T$. Then, the above equations can be rewritten as

$$\hat{f}(x_1) = [1, x_1, x_1^2, x_1^3, \dots, x_1^d] \cdot \begin{bmatrix} w_0 \\ w_1 \\ w_2 \\ w_3 \\ \vdots \\ w_d \end{bmatrix} = [1, x_1, x_1^2, x_1^3, \dots, x_1^d] \mathbf{w} = y_1$$

Similarly, we have,

$$\begin{aligned}[1, x_2, x_2^2, x_2^3, \dots, x_2^d] \mathbf{w} &= y_2, \\ [1, x_3, x_3^2, x_3^3, \dots, x_3^d] \mathbf{w} &= y_3, \\ [1, x_4, x_4^2, x_4^3, \dots, x_4^d] \mathbf{w} &= y_4, \\ [1, x_5, x_5^2, x_5^3, \dots, x_5^d] \mathbf{w} &= y_5, \\ &\vdots \\ [1, x_n, x_n^2, x_n^3, \dots, x_n^d] \mathbf{w} &= y_n.\end{aligned}$$

Then, all equations can be written as the form of linear equation,

$$A\mathbf{w} = \mathbf{y},$$

where A is the stack of $[1, x_i, x_i^2, x_i^3, \dots, x_i^d]$ for $i = 1, \dots, n$. Under this setting, answer the following questions.

1-(a) What is the size of vector w and y ? (10pt)

$$w = \begin{bmatrix} w_0 \\ w_1 \\ w_2 \\ \vdots \\ w_d \end{bmatrix} \quad y = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_d \end{bmatrix}$$

size: $(d+1) \times 1$ size: $n \times 1$

1-(b) What is the size of matrix A ? Write A . (10pt)

size: $n \times (d+1)$

$$A = \begin{bmatrix} 1 & x_1 & x_1^2 & \dots & x_1^d \\ 1 & x_2 & x_2^2 & \dots & x_2^d \\ 1 & x_3 & x_3^2 & \dots & x_3^d \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & \dots & x_n^d \end{bmatrix}$$

1-(c) Let $d+1 = n$, then, A becomes a square matrix. Compute the determinant of A . (40pt in total, Derivation: 30pt, Answer: 10pt)

$$\det A = \begin{vmatrix} 1 & x_1 & x_1^2 & \dots & x_1^{n-1} \\ 1 & x_2 & x_2^2 & \dots & x_2^{n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & \dots & \dots & x_n^{n-1} \end{vmatrix}_{n \times n}$$

여기서 row operation을 하면 (2~n행에 1번째 행을 빼면)

$$= \begin{vmatrix} 1 & x_1 & x_1^2 & \dots & x_1^{n-2} & x_1^{n-1} \\ 0 & x_2 - x_1 & x_2^2 - x_1^2 & \dots & x_2^{n-2} - x_1^{n-2} & x_2^{n-1} - x_1^{n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & x_n - x_1 & x_n^2 - x_1^2 & \dots & x_n^{n-2} - x_1^{n-2} & x_n^{n-1} - x_1^{n-1} \end{vmatrix}_{n \times n}$$

여기서 첫번째 열은 cofactor expansion을 진행 한다.

$$= \begin{vmatrix} x_2 - x_1 & x_2^2 - x_1^2 & \dots & x_2^{n-2} - x_1^{n-2} & x_2^{n-1} - x_1^{n-1} \\ x_3 - x_1 & x_3^2 - x_1^2 & \dots & x_3^{n-2} - x_1^{n-2} & x_3^{n-1} - x_1^{n-1} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ x_n - x_1 & x_n^2 - x_1^2 & \dots & x_n^{n-2} - x_1^{n-2} & x_n^{n-1} - x_1^{n-1} \end{vmatrix}_{(n-1) \times (n-1)}$$

$$= \det \left(\begin{bmatrix} x_2 - x_1 & 0 & \dots & 0 \\ 0 & x_3 - x_1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & x_n - x_1 \end{bmatrix} \begin{bmatrix} 1 & x_2 + x_1 & \dots & \sum_{i=0}^{n-2} x_2^{n-2-i} x_1^i \\ \vdots & x_3 + x_1 & \dots & \sum_{i=0}^{n-2} x_3^{n-2-i} x_1^i \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_n + x_1 & \dots & \sum_{i=0}^{n-2} x_n^{n-2-i} x_1^i \end{bmatrix} \right)$$

$$= \prod_{j=2}^n (x_j - x_1) \det \left(\begin{bmatrix} 1 & x_2 + x_1 & \dots & \sum_{i=0}^{n-2} x_2^{n-2-i} x_1^i \\ \vdots & x_3 + x_1 & \dots & \sum_{i=0}^{n-2} x_3^{n-2-i} x_1^i \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_n + x_1 & \dots & \sum_{i=0}^{n-2} x_n^{n-2-i} x_1^i \end{bmatrix} \right)$$

$$= \prod_{j=2}^n (x_j - x_1) \det \left(\begin{bmatrix} 1 & x_2 & x_2^2 & \dots & x_2^{n-2} \\ \vdots & x_3 & x_3^2 & \dots & x_3^{n-2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & \dots & x_n^{n-2} \end{bmatrix} \begin{bmatrix} 1 & x_1 & x_1^2 & \dots & x_1^{n-2} \\ 0 & 1 & x_1 & \dots & x_1^{n-3} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 1 \end{bmatrix} \right)$$

$$= \prod_{j=2}^n (x_j - x_1) \begin{vmatrix} 1 & x_2 & x_2^2 & \dots & x_2^{n-2} \\ \vdots & x_3 & x_3^2 & \dots & x_3^{n-2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & \dots & x_n^{n-2} \end{vmatrix}_{(n-1) \times (n-1)} = \prod_{j=2}^n (x_j - x_1) \left(\prod_{i=2}^{n-1} (x_i - x_2) \begin{vmatrix} 1 & x_3 & x_3^2 & \dots & x_3^{n-3} \\ \vdots & x_4 & x_4^2 & \dots & x_4^{n-4} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & \dots & x_n^{n-3} \end{vmatrix}_{(n-2) \times (n-2)} \right)$$

→ 첫번째 행렬식과 형태가 같음 ⇒ 반복

$$= \prod_{j=2}^n (x_j - x_1) \prod_{2 \leq i < j \leq n} (x_j - x_i)$$

$$= \prod_{1 \leq i < j \leq n} (x_j - x_i)$$

1-(d) What is the condition that makes the determinant of A non-zero? (10pt)

$$\det A = \prod_{1 \leq i < j \leq n} (\lambda_j - \lambda_i) \neq 0 \text{ 가 되는 조건은 } 1 \leq i < j \leq n \text{ 인 모든 } i, j \text{ 에 대해}$$

$$(\lambda_j - \lambda_i) \neq 0 \iff \lambda_j \neq \lambda_i \text{ 이어야 한다.}$$

1-(e) Assume that the determinant of A is non-zero, then, what is the solution of linear equation, $Aw = y$, with respect to w ? (10pt)

$\det A \neq 0$ 이므로 A 는 nonsingular 이므로 역행렬이 존재한다.

$$\therefore w = A^{-1}y$$

2. (20pt)

Suppose that $n > d + 1$. Then, we cannot compute the inverse of A since A is not a square matrix. In this case, how can we solve the linear equation $A\mathbf{w} = \mathbf{y}$?

$n > d+1$ 일때 행렬 A 는 정방행렬이 아니기 때문에 다음과 같이 나타낸다.

$$A_{n \times (d+1)} = U \sum_{n \times n} V^T_{n \times (d+1)} \quad (U, V : 직교행렬, \Sigma = 대각행렬).$$

SVD를 사용해 행렬 A 의 특이값분해를 하면 의사역행렬 A^+ 는 다음과 같이 나타낸다.

$$A^+ = V \Sigma^+ U^T \quad (\Sigma^+ : \Sigma \text{의 유사역행렬})$$

$$\text{따라서, } A^+ = (A^T A)^{-1} A^T \text{ 이므로}$$

$$\begin{aligned} & \begin{cases} A\mathbf{w} = \mathbf{y} \\ \mathbf{w} = A^+ \mathbf{y} \end{cases} \text{ 이거나 } A^+ \text{ 대신 } (A^T A)^{-1} A^T \text{ 을 대입하면 } \mathbf{w} = (A^T A)^{-1} A^T \mathbf{y} \text{ 로 구할 수 있다.} \end{aligned}$$