

Polynomial Regression (Handwriting Assignment)

Name: 박예감

Student ID: 2023 1226

Instructor: Professor Kyungjae Lee

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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 .

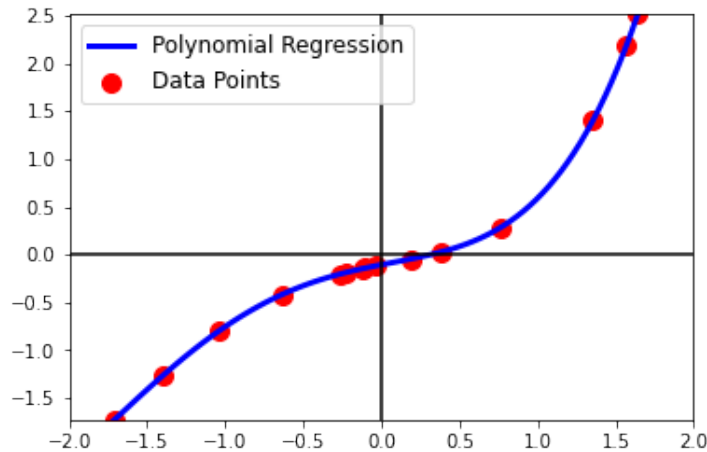


Figure 1: Example of Polynomial Regression

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)

$$\vec{w} = \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_d \end{bmatrix} \text{ the size of vector } w \text{ is } d+1$$

$$\vec{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \text{ the size of vector } y \text{ is } n$$

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

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

size of matrix A is $n \times (d+1)$

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

$d+1 = n$ \Rightarrow A is square matrix of order n

$$A_n = \det(A) = \begin{vmatrix} 1 & x_1 & x_1^2 & \dots & x_1^{n-1} \\ 1 & x_2 & x_2^2 & \dots & x_2^{n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & \dots & x_n^{n-1} \end{vmatrix} = \begin{vmatrix} 1 & x_1-x_1 & x_1^2-x_1^2 & \dots & x_1^{n-1}-x_1^{n-1} \\ 1 & x_2-x_1 & x_2^2-x_1x_2 & \dots & x_2^{n-1}-x_1x_2^{n-2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n-x_1 & x_n^2-x_1x_n & \dots & x_n^{n-1}-x_1x_n^{n-2} \end{vmatrix}$$

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

$$A_n = \det(A) = (x_n-x_1)(x_{n-1}-x_1) \dots (x_2-x_1) \begin{vmatrix} 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & x_2 & \dots & x_2^{n-2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 1 & x_n & \dots & x_n^{n-2} \end{vmatrix}$$

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

$$= (x_n-x_1)(x_{n-1}-x_1) \dots (x_2-x_1) A_{n-1}$$

이러한 과정을 반복하면 answer은 다음과 같다

answer : $\prod_{1 \leq i < j}^n (x_j - x_i)$ for $n \geq 2$

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

$$\det A = \prod_{1 \leq i < j \leq n} (x_j - x_i) \neq 0$$

$$x_j \neq x_i \text{ for } (1 \leq i < j \leq n) \text{ or}$$

determinant of A is non-zero or

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)

$$\text{determinant of } A \text{ is non-zero or } \det \neq 0 \text{ or}$$

or A is invertible or

$$Aw = y \rightarrow A^T A w = A^T y \rightarrow w = A^T y$$

$$\therefore w = A^T y$$

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

$n > d+1$ 이므로 matrix A 는 square matrix 가 아니다. 따라서 matrix A 는 not invertible 하다.

따라서 vector \mathbf{w} 를 계산할 수 없으므로 least square solution $\hat{\mathbf{w}}$ 를 계산할 수 있다.

"matrix $A \in \mathbb{R}^{m \times n}$ $m > n$ 이고 모든 column vectors 가 linearly independent 하면 $A^T = (A^T A)^+ A^T$ 이고 $A^T A$ 는 invertible matrix 이다" 라는 정의를 활용하면 A 의 inverse 대신에 A 의 pseudo inverse 를 사용하며 $\hat{\mathbf{w}}$ 을 계산할 수 있다.

모든 column vector 가 linearly independent 이므로

$$\mathbf{y} = A \hat{\mathbf{w}} \rightarrow A^T \mathbf{y} = A^T A \hat{\mathbf{w}} \rightarrow (A^T A)^+ A^T \mathbf{y} = \hat{\mathbf{w}} = A^+ \mathbf{y}$$

$$\therefore \hat{\mathbf{w}} = A^+ \mathbf{y}$$