

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 .

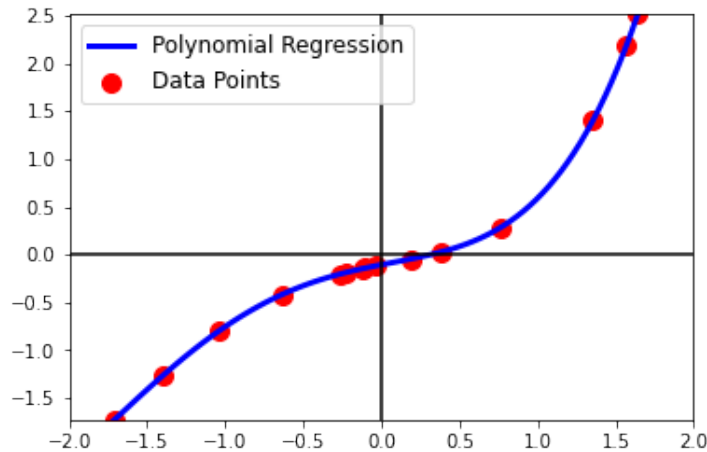


Figure 1: Example of Polynomial Regression

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 \mathbf{w} and \mathbf{y} ? (10pt)

the size of vector \mathbf{w} is $d+1$ and

the size of vector \mathbf{y} is n

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

The size of matrix A is $n \times d$

$$A = \begin{bmatrix} 1 & x_1 & x_1^2 & x_1^3 & \dots & x_1^d \\ 1 & x_2 & x_2^2 & x_2^3 & \dots & x_2^d \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & x_n^3 & \dots & x_n^d \end{bmatrix}$$

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

A_n is $n \times n$ of square matrix and then $d = n$ is given.

Answer: Determinant of A_n is $\prod_{1 \leq i < j \leq n} (x_j - x_i)$

Derivation: Use mathematical induction

$$P(n) = \det A_n = \prod_{1 \leq i < j \leq n} (x_j - x_i) \text{ 라고 하면}$$

basic step: $n=1, 2$ 일 때 성립함을 보인다.

$$P(1) = \det A_1 = |1| = 1 \text{ 이 되며 성립함}$$

$$P(2) = \det A_2 = \begin{vmatrix} 1 & x_1 \\ 1 & x_2 \end{vmatrix} = x_2 - x_1 \text{ 이므로 성립함}$$

induction step: $n=k$ 일 때 성립한다고 가정하면

$$\det A_k = \prod_{1 \leq i < j \leq k} (x_j - x_i) \text{ 가 성립하고 이때 } n=k+1 \text{ 일 때 성립함을 보인다.}$$

$n=k+1$ 일 때는 A_n 의 행이 A_k 와 같고 나머지 행의 변수를 x_{k+1} 라고 하고 그 행을 통해

행렬식을 계산하면 $C_{i,j} = (-1)^{i+j} M_{i,j}$ 라고 하고 (i 번째 row와 j 번째 column을 없애 matrix의 determinant를 $M_{i,j}$ 라고 하면)

$$\det A_{k+1} = |C_{(k+1),1}| + x_{k+1} |C_{(k+1),2}| + x_{k+1}^2 |C_{(k+1),3}| + \dots + x_{k+1}^k |C_{(k+1),k+1}| \text{ 그런데 이때 이 행렬식은 } k \text{ 차 다항함수이고}$$

이 값을 $f(x)$ 라 하면 $f(x_1) = f(x_2) = \dots = f(x_k) = 0$ 이므로 $f(x)$ 는 $C(x-x_1)(x-x_2)\dots(x-x_k)$ (C 는 상수)로 표현할 수 있다.

이때 C 는 $f(x)$ 의 최고차항의 계수와 같으므로 $C = C_{(k+1),k+1}$ 이다. $C_{(k+1),k+1} = \prod_{1 \leq i < j \leq k} (x_j - x_i)$ 이므로 $C_{(k+1),k+1} = (-1)^{k+1+k+1} \cdot M_{(k+1),k+1}$ (071 라면)

$$\text{최종적으로 } f(x) \text{가 } x_{k+1} \text{라고 하면 } f(x) = \left[\prod_{1 \leq i < j \leq k} (x_j - x_i) \right] (x_{k+1} - x_1)(x_{k+1} - x_2) \dots (x_{k+1} - x_k) = \prod_{1 \leq i < j \leq k+1} (x_j - x_i)$$

$$\text{이므로 } \det A_{k+1} = \prod_{1 \leq i < j \leq k+1} (x_j - x_i) \text{ 이므로 } \det A_n \text{는 } \prod_{1 \leq i < j \leq n} (x_j - x_i) \text{ 이다.}$$

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

$x_1 \neq x_2 \neq x_3 \neq \dots \neq x_n$ 이어야 A의 determinant가 0이 되지 않는다.

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)

A^{-1} column은 independent한 동시에 A는 square matrix이기 때문에 invertible하다

따라서 $w = A^{-1}y$ 로 쓸 수 있다.

2. (20pt)

Suppose that $n > d$. 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 $A\mathbf{w} = \mathbf{y}$? (Hint: Pseudo Inverse)

$\lambda_1 \neq \lambda_2 \neq \lambda_3 \neq \dots \neq \lambda_n$ 이기 때문에 A 의 column은 independent 하다.

$$\text{즉 } \begin{bmatrix} 1 & 1 & \dots & 1 \\ \lambda_1 & \lambda_2 & \dots & \lambda_n \\ \lambda_1^2 & \lambda_2^2 & \dots & \lambda_n^2 \\ \vdots & \vdots & \ddots & \vdots \\ \lambda_1^d & \lambda_2^d & \dots & \lambda_n^d \end{bmatrix} \begin{bmatrix} \lambda_1 & \lambda_1^2 & \dots & \lambda_1^d \\ \lambda_2 & \lambda_2^2 & \dots & \lambda_2^d \\ \vdots & \vdots & \ddots & \vdots \\ \lambda_n & \lambda_n^2 & \dots & \lambda_n^d \end{bmatrix} = \begin{bmatrix} 1 \times n & \lambda_1 + \lambda_2 + \dots + \lambda_n & \dots & \lambda_1^d + \lambda_2^d + \dots + \lambda_n^d \\ \lambda_1 + \lambda_2 + \dots + \lambda_n & \lambda_1^2 + \lambda_2^2 + \dots + \lambda_n^2 & \dots & \lambda_1^{d+1} + \lambda_2^{d+1} + \dots + \lambda_n^{d+1} \\ \vdots & \vdots & \ddots & \vdots \\ \lambda_1^d + \lambda_2^d + \dots + \lambda_n^d & \lambda_1^{d+1} + \lambda_2^{d+1} + \dots + \lambda_n^{d+1} & \dots & \lambda_1^{2d} + \lambda_2^{2d} + \dots + \lambda_n^{2d} \end{bmatrix}$$

이 대각선 (diagonal) 이거나 아니라 대각이요 ATA 의 column은 independent 이기 때문에 ATA 는 invertible 하다.

[결과]

$$\begin{aligned} A\mathbf{w} &= \mathbf{y} \\ A^T A \mathbf{w} &= A^T \mathbf{y} \\ \mathbf{w} &= (A^T A)^{-1} A^T \mathbf{y} \quad \text{이러. } ((A^T A)^{-1} A^T = A^+) \\ \mathbf{w} &= A^+ \mathbf{y} \end{aligned}$$