Polynomial Regression (Handwriting Assignment)

Name: 박민혁

Student ID: 20214241

Instructor: Professor Kyungjae Lee

October 21, 2021

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 nth degree polynomial in x.

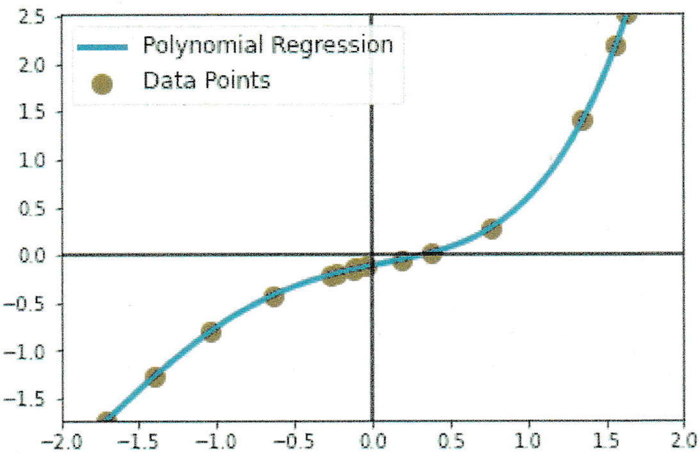


Figure 1: Example of Polynomial Regression

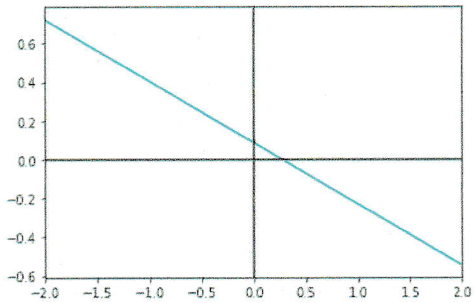
First, what is a regression? we can find a definition from the book as follows: *Regression analysis is a form of predictive modelling technique which investigates the relationship between a dependent and independent variable.* Actually, this definition is a bookish definition, in simple terms the regression 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,

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

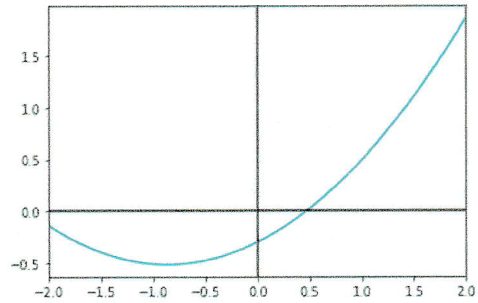
The goal of regression is to find a function $\hat{f}$ such that

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

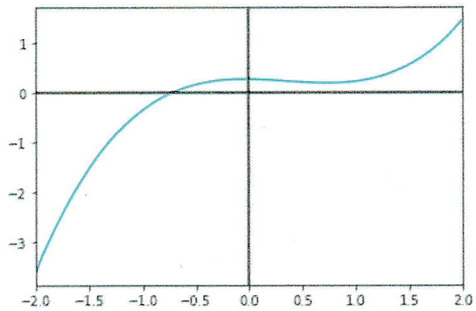
This is the simplest definition of the regression problem. Note that many details about regression analysis are omitted here, but, you will learn more rigorous definition in other courses such as



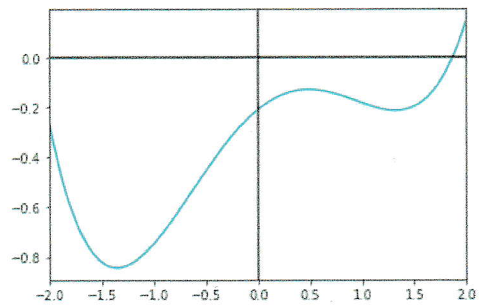
(a) $0.089 - 0.32x$



(b) $-0.29 + 0.50x + 0.29x^2$



(c) $0.28 - 0.03x - 0.34x^2 + 0.32x^3$



(d) $-0.21 + 0.34x - 0.35x^2 - 0.06x^3 + 0.1x^4$

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:

$$
\begin{aligned}
\text{Degree of } 0 &: f(x) = w_0 \\
\text{Degree of } 1 &: f(x) = w_1 \cdot x + w_0 \\
\text{Degree of } 2 &: f(x) = w_2 \cdot x^2 + w_1 \cdot x + w_0 \\
\text{Degree of } 3 &: f(x) = w_3 \cdot x^3 + w_2 \cdot x^2 + w_1 \cdot x + w_0 \\
&\vdots \\
\text{Degree of } d &: f(x) = \sum_{i=0}^{d} w_i \cdot x^i,
\end{aligned}
$$

where $w_0, w_1, \cdots, w_d$ 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 $\{w_0, w_1, \cdots, w_d\}$. 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, $(x_1, y_1), (x_2, y_2), \cdots, (x_n, y_n)$. Let the degree of polynomial be d. Then, we want to find $w_0, w_1, w_2, \cdots, w_d$ of the polynomial such that

$$\begin{aligned}
\hat{f}(x_1) &= w_0 + w_1 x_1 + w_2 x_1^2 + \cdots + w_d x_1^d = y_1, \\
\hat{f}(x_2) &= w_0 + w_1 x_2 + w_2 x_2^2 + \cdots + w_d x_2^d = y_2, \\
\hat{f}(x_3) &= w_0 + w_1 x_3 + w_2 x_3^2 + \cdots + w_d x_3^d = y_3, \\
\hat{f}(x_4) &= w_0 + w_1 x_4 + w_2 x_4^2 + \cdots + w_d x_4^d = y_4, \\
\hat{f}(x_5) &= w_0 + w_1 x_5 + w_2 x_5^2 + \cdots + w_d x_5^d = y_5, \\
&\vdots \\
\hat{f}(x_n) &= w_0 + w_1 x_n + w_2 x_n^2 + \cdots + w_d x_n^d = y_n.
\end{aligned}$$

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

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

Similarly, we have,

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

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

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

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

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

the size of vector w is d+1

the size of vector y is n

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

$$A = \underbrace{\begin{bmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^d \\ \vdots & \vdots & \vdots & \ddots & \\ 1 & x_n & x_n^2 & & x_n^d \end{bmatrix}}_{d+1} \Big\} n$$

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

ok

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

$$A = \begin{bmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^{n-1} \\ 1 & x_2 & x_2 & \cdots & x_2^{n-1} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_n & x_n^2 & \cdots & x_n^{n-1} \end{bmatrix}$$

elementary row operation을 통해 (어떠한 행의 스칼라를 곱해 다른 행에 더해주는 연산) 새로운 Matrix를 만들더라도 det은 변하지 않음.

$$A' = \begin{bmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^{n-1} \\ 0 & x_2-x_1 & x_2-x_1^2 & \cdots & x_2^{n-1}-x_1^{n-1} \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & x_n-x_1 & x_n^2-x_1^2 & \cdots & x_n^{n-1}-x_1^{n-1} \end{bmatrix}$$

1행 x(-1)을 다른 각 행에 더해줌.

이때 $\det A = \det A'$ 이때 첫번째 column을 기준으로 det을 구하면

$$\det A = \det A' = 1 \cdot \det \begin{bmatrix} x_2-x_1 & x_2^2-x_1^2 & \cdots & x_2^{n-1}-x_1^{n-1} \\ \vdots & & & \vdots \\ x_n-x_1 & x_n^2-x_1^2 & \cdots & x_n^{n-1}-x_1^{n-1} \end{bmatrix}$$

각 행을 보면 $x_i - x_1$이 (i는 2부터 n) 인수임을 알 수 있다.

det의 성질에 의해 인수(스칼라)는 앞으로 빼서 계산가능.

$$= \prod_{i=2}^{n}(x_i - x_1) \det \begin{bmatrix} 1 & x_2+x_1 & \cdots & \sum_{k=0}^{n-2} x_2^k x_1^{n-2-k} \\ \vdots & \vdots & & \vdots \\ 1 & x_n+x_1 & \cdots & \sum_{k=0}^{n-2} x_n^k x_1^{n-2-k} \end{bmatrix}$$

이 되고 j번째 열에서 $-x_1$을 곱하여 j+1 열에 더해주면 (기본열 연산 det에 영향X)

$$= \prod_{i=2}^{n}(x_i - x_1) \det \begin{bmatrix} 1 & x_2 & \cdots & x_2^{n-2} \\ \vdots & \vdots & & \vdots \\ 1 & x_n & \cdots & x_n^{n-2} \end{bmatrix}$$

이 된다. 뒤에 행렬도 Vandermonde Matrix 이므로 상술한 과정을 반복하면

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

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

$1 \le i < j \le n$ 이며 (i,j = integers) 일때 x_j와 x_i가 같지 않아야 한다.

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

det A가 0이 아닐 경우 A^{-1} 가 존재한다는 의미 이므로. ($n \times n$ 일때)

$Aw = y$

$A^{-1}Aw = A^{-1}y$

$w = A^{-1}y$ 이다.

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 $A\mathbf{w} = \mathbf{y}$? (Hint: Pseudo Inverse)

A가 square Matrix 가 아닐 경우 A^{-1}를 찾을 수 없다. 즉 $w = A^{-1}y$ 를 통해 w 값을 구할 수 없으므로 다른 방법을 이용한다. 이때 이용할 것이 Pseudo Inverse 이다.

A^+를 A의 Psedo Inverse 라고 하자 이때 A^+는 정의에의해 $AA^+A = A$, $A^+AA^+ = A^+$가 성립하고 $A^+ = (A^TA)^{-1}A^T$로 계산된다 (A^TA가 invertible)

$$y = Aw$$

$$A^Ty = A^TAw$$

$$(A^TA)^{-1}A^Ty = w$$

$A^+y = w$ 이므로 A^+y의 계산을 통해 w를 구할 수 있다