

Polynomial Regression (Handwriting Assignment)

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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 n th degree polynomial in x .

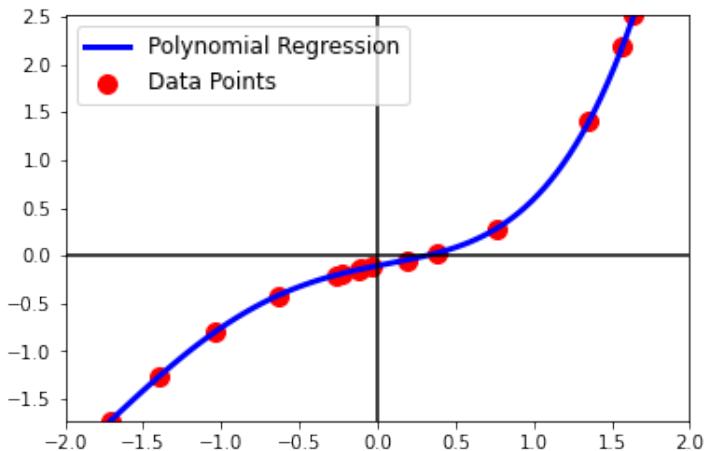


Figure 1: Example of Polynomial Regression

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

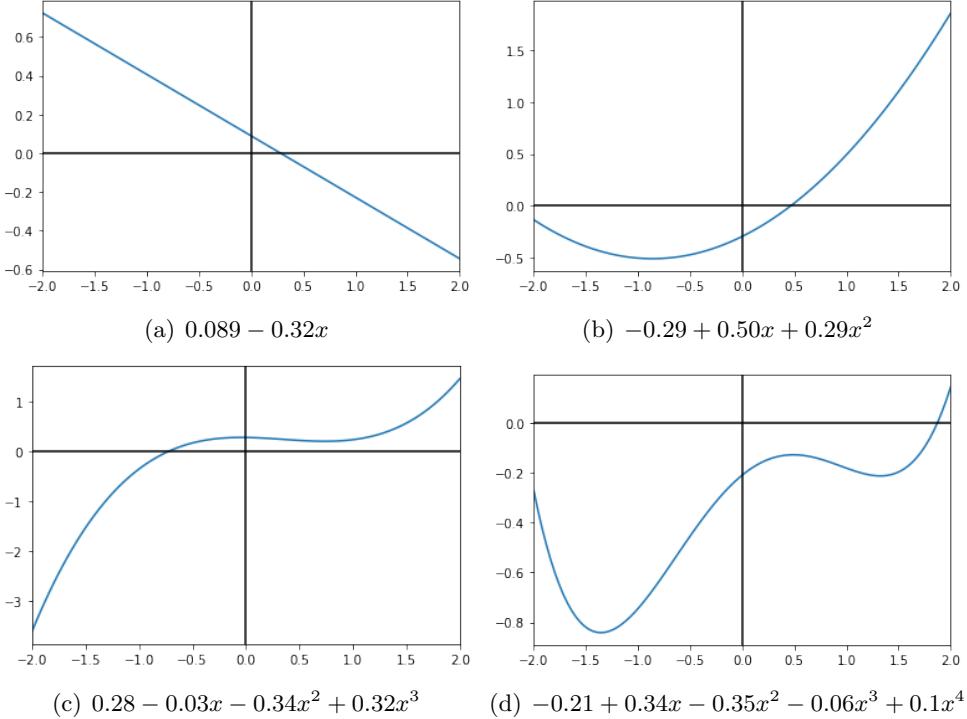


Figure 2: Examples of polynomial functions

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:

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

where w_0, w_1, \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

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

Now, we reformulate the equations into the vector and matrix form. First, let $\mathbf{w} = [w_0, w_1, \dots, w_d]^T$ 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)

As explained in the equations we can write the equation as

$$\underbrace{\begin{bmatrix} 1 & x_1 & x_1^2 & x_1^3 & \cdots & x_1^d \\ 1 & x_2 & x_2^2 & x_2^3 & \cdots & x_2^d \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & x_n^3 & \cdots & x_n^d \end{bmatrix}}_A \underbrace{\begin{bmatrix} w_0 \\ w_1 \\ w_2 \\ w_3 \\ \vdots \\ w_d \end{bmatrix}}_{\mathbf{w}} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_n \end{bmatrix}$$

i.e. \mathbf{W} is a $(d+1) \times 1$ matrix, i.e. a vector of size $d+1$
and \mathbf{y} is a $n \times 1$ matrix, i.e. a vector of size n

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

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

i.e. A is a $n \times (d+1)$ matrix

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.)

The answer is on the back page of question 2

1-(d) What is the condition that makes the determinant of A non-zero? (10pt)
 $A_s \det(A) = \prod_{1 \leq i < j \leq n} (x_j - x_i)$

we have

$$\det A \neq 0 \Leftrightarrow x_j \neq x_i \text{ for all } 1 \leq i < j \leq n$$

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)

If $\det A \neq 0$, then we have A^{-1} exists and hence

$$Aw = y \Rightarrow w = A^{-1}y$$

i.e. the solution is given by

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

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

Given $d+1=n$

Hence we have

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

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

We prove the result by induction on n

$n=2$, In this case

$$A = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \end{bmatrix}$$

Thus, $\det(A) = (x_2 - x_1)$

Let the result hold for $n=k$,

Then we prove the result for $n=k+1$

$$A = \begin{bmatrix} 1 & x_1 & x_1^2 & x_1^3 & \cdots & x_1^n \\ 1 & x_2 & x_2^2 & x_2^3 & \cdots & x_2^n \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{k+1} & x_{k+1}^2 & x_{k+1}^3 & \cdots & x_{k+1}^{k+1} \end{bmatrix}$$

As the determinant of matrix is not affected by elementary column operations we have denoting the i -th column by C_i

$C_{k+1} - x_1 C_1$ implies

$$A = \begin{bmatrix} 1 & x_1 & x_1^2 & x_1^3 & \cdots & 0 \\ 1 & x_2 & x_2^2 & x_2^3 & \cdots & x_2^{k+1} - x_1 x_2^k \\ 1 & x_3 & x_3^2 & x_3^3 & \cdots & x_3^{k+1} - x_1 x_3^k \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{k+1} & x_{k+1}^2 & x_{k+1}^3 & \cdots & x_{k+1}^{k+1} - x_1 x_{k+1}^k \end{bmatrix} = \begin{bmatrix} 1 & x_1 & x_1^2 & x_1^3 & \cdots & 0 \\ 1 & x_2 & x_2^2 & x_2^3 & \cdots & (x_2 - x_1)x_2^k \\ 1 & x_3 & x_3^2 & x_3^3 & \cdots & (x_3 - x_1)x_3^k \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{k+1} & x_{k+1}^2 & x_{k+1}^3 & \cdots & (x_{k+1} - x_1)x_{k+1}^k \end{bmatrix}$$

Similarly,

$$C_k - x_1 C_{k-1}$$

$$C_{k-1} - x_1 C_{k-2}$$

⋮

$$C_3 - x_1 C_2$$

$$C_2 - x_1 C_1$$

implies

$$A = \begin{bmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ 1 & x_2 - x_1 & (x_2 - x_1)x_2 & (x_2 - x_1)x_2^2 & \cdots & (x_2 - x_1)x_2^k \\ 1 & x_3 - x_1 & (x_3 - x_1)x_3 & (x_3 - x_1)x_3^2 & \cdots & (x_3 - x_1)x_3^k \\ & \vdots & & & & \\ 1 & x_{k+1} - x_1 & (x_{k+1} - x_1)x_{k+1} & (x_{k+1} - x_1)x_{k+1}^2 & \cdots & (x_{k+1} - x_1)x_{k+1}^k \end{bmatrix}$$

Now opening the determinant along the first row we have

$$\det \begin{bmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ 1 & x_2 - x_1 & (x_2 - x_1)x_2 & (x_2 - x_1)x_2^2 & \cdots & (x_2 - x_1)x_2^k \\ 1 & x_3 - x_1 & (x_3 - x_1)x_3 & (x_3 - x_1)x_3^2 & \cdots & (x_3 - x_1)x_3^k \\ & \vdots & & & & \\ 1 & x_{k+1} - x_1 & (x_{k+1} - x_1)x_{k+1} & (x_{k+1} - x_1)x_{k+1}^2 & \cdots & (x_{k+1} - x_1)x_{k+1}^k \end{bmatrix}$$

$$= \det \begin{bmatrix} 1 & x_2 - x_1 & (x_2 - x_1)x_2 & (x_2 - x_1)x_2^2 & \cdots & (x_2 - x_1)x_2^k \\ 1 & x_3 - x_1 & (x_3 - x_1)x_3 & (x_3 - x_1)x_3^2 & \cdots & (x_3 - x_1)x_3^k \\ & \vdots & & & & \\ 1 & x_{k+1} - x_1 & (x_{k+1} - x_1)x_{k+1} & (x_{k+1} - x_1)x_{k+1}^2 & \cdots & (x_{k+1} - x_1)x_{k+1}^k \end{bmatrix}$$

$$= \prod_{\substack{2 \leq j \leq (k+1)}} (x_j - x_1) \det \begin{bmatrix} 1 & x_2 & x_2^2 & \cdots & x_2^k \\ 1 & x_3 & x_3^2 & \cdots & x_3^k \\ & \vdots & & & \\ 1 & x_{k+1} & x_{k+1}^2 & \cdots & x_{k+1}^k \end{bmatrix}$$

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But we have

$$\det \begin{bmatrix} 1 & x_2 & x_2^2 & \cdots & x_2^k \\ 1 & x_3 & x_3^2 & \cdots & x_3^k \\ \vdots & & & & \\ 1 & x_{k+1} & x_{k+1}^2 & \cdots & x_{k+1}^k \end{bmatrix} = \prod_{1 \leq i < j \leq (k+1)} (x_j - x_i)$$

by induction hypothesis

Hence we have

$$\begin{aligned} \det & \begin{bmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ 1 & x_2 - x_1 & (x_2 - x_1)x_2 & (x_2 - x_1)x_2^2 & \cdots & (x_2 - x_1)x_2^k \\ 1 & x_3 - x_1 & (x_3 - x_1)x_3 & (x_3 - x_1)x_3^2 & \cdots & (x_3 - x_1)x_3^k \\ \vdots & & & & & \\ 1 & x_{k+1} - x_1 & (x_{k+1} - x_1)x_{k+1} & (x_{k+1} - x_1)x_{k+1}^2 & \cdots & (x_{k+1} - x_1)x_{k+1}^k \end{bmatrix} \\ & \stackrel{\text{II}}{=} \prod_{2 \leq j \leq (k+1)} (x_j - x_1) \det \begin{bmatrix} 1 & x_2 & x_2^2 & \cdots & x_2^k \\ 1 & x_3 & x_3^2 & \cdots & x_3^k \\ \vdots & & & & \\ 1 & x_{k+1} & x_{k+1}^2 & \cdots & x_{k+1}^k \end{bmatrix} \\ & = \left(\prod_{2 \leq j \leq (k+1)} (x_j - x_1) \right) \left(\prod_{2 \leq i < j \leq (k+1)} (x_j - x_i) \right) \\ & = \prod_{1 \leq i < j \leq (k+1)} (x_j - x_i) \end{aligned}$$

i.e. we have proved by induction that

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