

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 .

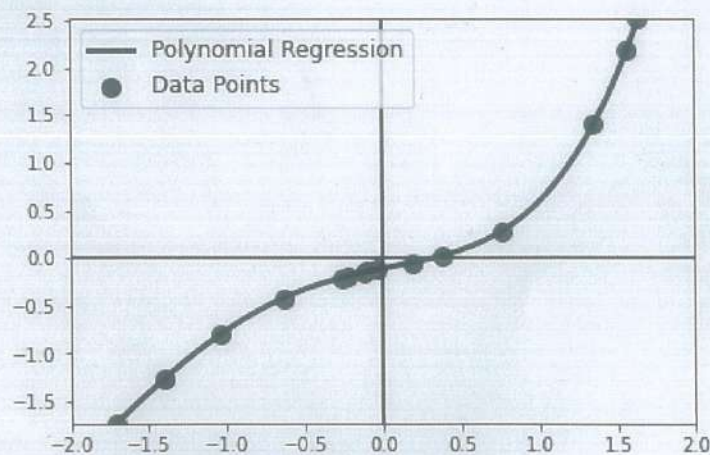


Figure 1: Example of Polynomial Regression

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

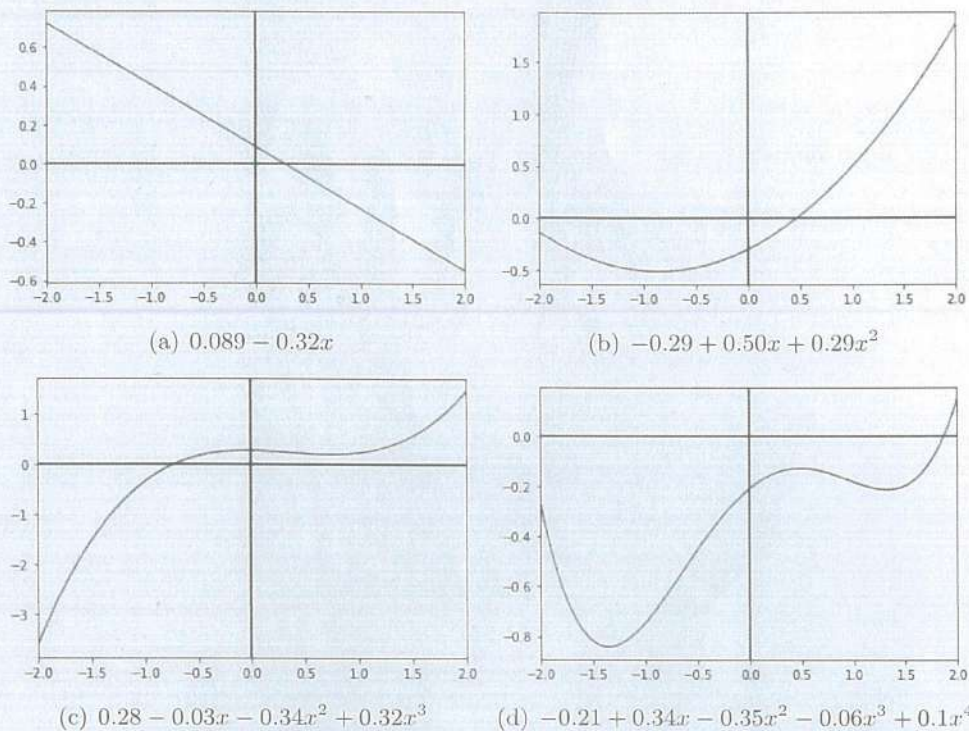


Figure 2: Examples of polynomial functions

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

$$\hat{f}(x_1) = w_0 + w_1x_1 + w_2x_1^2 + \dots + w_dx_1^d = y_1,$$

$$\hat{f}(x_2) = w_0 + w_1x_2 + w_2x_2^2 + \dots + w_dx_2^d = y_2,$$

$$\hat{f}(x_3) = w_0 + w_1x_3 + w_2x_3^2 + \dots + w_dx_3^d = y_3,$$

$$\hat{f}(x_4) = w_0 + w_1x_4 + w_2x_4^2 + \dots + w_dx_4^d = y_4,$$

$$\hat{f}(x_5) = w_0 + w_1x_5 + w_2x_5^2 + \dots + w_dx_5^d = y_5,$$

\vdots

$$\hat{f}(x_n) = w_0 + w_1x_n + w_2x_n^2 + \dots + w_dx_n^d = y_n.$$

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,

$$[1, x_2, x_2^2, x_2^3, \dots, x_2^d] \mathbf{w} = y_2,$$

$$[1, x_3, x_3^2, x_3^3, \dots, x_3^d] \mathbf{w} = y_3,$$

$$[1, x_4, x_4^2, x_4^3, \dots, x_4^d] \mathbf{w} = y_4,$$

$$[1, x_5, x_5^2, x_5^3, \dots, x_5^d] \mathbf{w} = y_5,$$

\vdots

$$[1, x_n, x_n^2, x_n^3, \dots, x_n^d] \mathbf{w} = y_n.$$

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)

Since w represents the coefficients of the polynomial of degree d , there are $d+1$ coefficients in total.

The vector y captures the y values of the n data points. Therefore, the size of y is n .

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)

The size of matrix A is determined by the number of data points n and the degree of the polynomial d .

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

The matrix A can be written as:

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

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

if $d+1 = n$, then A becomes a square $n \times n$ Vandermonde matrix. The determinant of a Vandermonde matrix is:

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

Derivation:

consider the $n \times n$ Vandermonde matrix:

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

1. Subtract the $(i-1)^{\text{th}}$ row from the i^{th} row for $i=2, 3, \dots, n$. this operation won't change the determinant.

$$\begin{bmatrix} 1 & x_1 & x_1^2 & \dots & x_1^{n-1} \\ 0 & x_2 - x_1 & x_2^2 - x_1^2 & \dots & x_2^{n-1} - x_1^{n-1} \\ 0 & x_3 - x_1 & x_3^2 - x_1^2 & \dots & x_3^{n-1} - x_1^{n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \end{bmatrix}$$

2. Factor out $x_2 - x_1$ from the second row, $x_3 - x_1$ from the third row, and so on up to $x_n - x_1$ from the n^{th} row.

After this operation, the second row becomes:

$$0, 1, x_2 + x_1, x_2^2 + x_1 x_2 + x_1^2, \dots$$

3. This process can be recursively applied. On the next step the determinant of the matrix is the product of differences of the form $(x_j - x_i)$ for $j > 2$

By continuing in this manner, the determinant of the original Vandermonde matrix A is given by:

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

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

1. the matrix A must be square, implying $n = d+1$.
2. none of its rows can be linearly dependent on the others.

Given the determinant formula: $\det(A) = \prod_{1 \leq i < j \leq n} (x_j - x_i)$

The determinant is non-zero if and only if all products $(x_j - x_i)$ are non-zero.

This implies that no x_i and x_j can be the same, ~~note~~

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)

When the determinant of a square matrix A is non-zero, it implies that A is invertible.

Given the linear equation:

$$Aw = y$$

The solution for w can be found by multiplying both sides of the equation by the inverse of A .

Multiply both sides by A^{-1} :

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

Since $A^{-1}A$ is the identity matrix, the equation simplifies to:

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

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

When $n > d + 1$, the Matrix A is an over-determined system. Since this kind of system typically does not have an exact solution, we can seek an approximate solution that minimizes the error between the predicted and actual outputs, by using the method of least squares:

$$E(\mathbf{w}) = \|A\mathbf{w} - \mathbf{y}\|^2$$

To find the \mathbf{w} that minimizes $E(\mathbf{w})$, we can differentiate $E(\mathbf{w})$ with respect to \mathbf{w} and set it to zero.

The solution to this minimization problem would be found to be:

$$\mathbf{w} = (A^T A)^{-1} A^T \mathbf{y}$$