

Polynomial Regression

Regression task

In regression task, the problem is to approximate an unknown real valued target function, such that:

$$y = f(x) + \varepsilon$$

y : output data.

x : input data.

f : real valued target function.

ε is a centered white noise with $E[\varepsilon] = 0$ and $Var(\varepsilon) = \sigma^2$.

Linear Model

Definition: linear model

A model is said to be linear if it is linear in parameters. Linear model is featured by the following hypothesis:

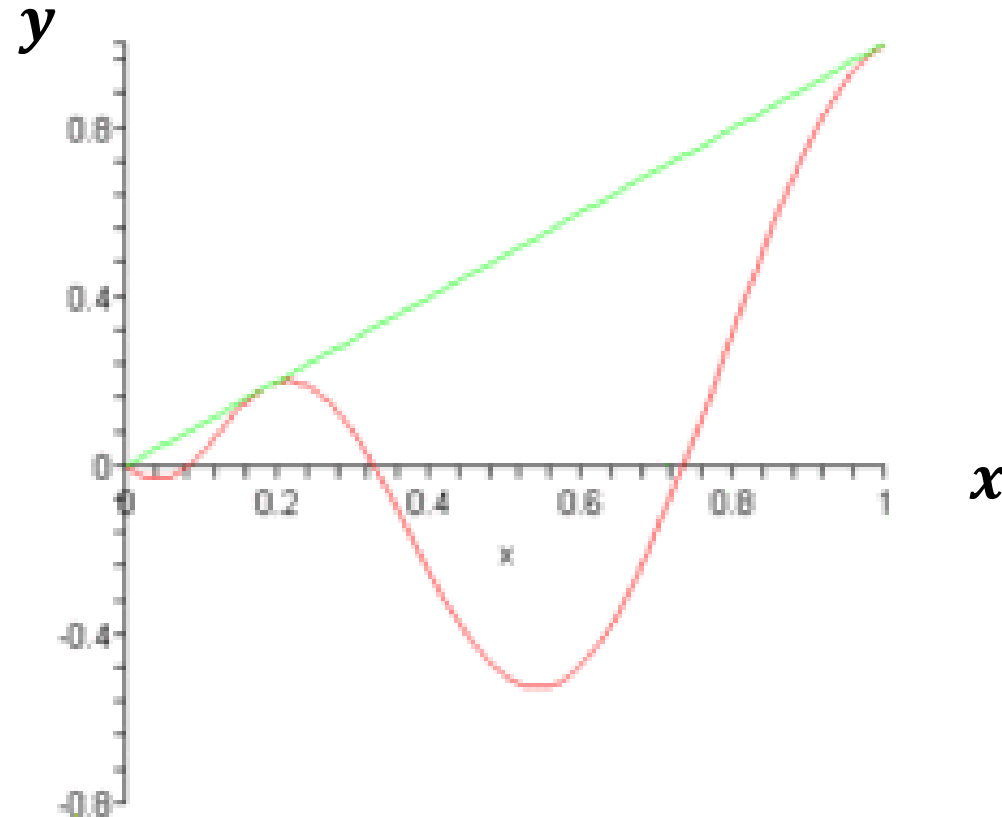
$$h_w(x) = \sum_{i=0}^d w_i x_i$$

Linear model is characterized by a linear class of hypothesis.

Motivation

Objective:

Explain the quantitative variable y by the d variables $x = (x_1, \dots, x_d)$.



Tool:

Polynomial Regression

Polynomial Regression

To approximate f :

- We should define a real-valued hypothesis class H based on prior knowledge.
- We should find the best hypothesis that has small general risk.

Let's consider that the prior knowledge assumes that the relationship between the outputs y and the inputs x is polynomial.

Polynomial Regression

The hypothesis class for polynomial regression model:

Therefore, H will be defined as a class of polynomial hypotheses.

$$H = \{h_W: X \rightarrow \mathbb{R} \text{ , } W \in \mathbb{R}^{D+1}\}$$

$$h_W(x) = w_0 + w_1x_1 + \cdots + w_dx_d + w_{d+1}x_1^2 + w_{d+2}x_1x_2 + \cdots + w_rx_d^2 + \\ \cdots + w_sx_1^Q + w_{s+1}x_1^{Q-1}x_2 + \cdots + w_Dx_d^Q$$

This is a multi-dimensional polynomial regression of order Q .

Polynomial Regression

Indeed, h_w appears to be nonlinear, however, it is linear in parameters W .

Let's take:

$$\begin{aligned} z_1 &= 1 \\ z_2 &= x_1 \\ &\vdots \\ z_d &= x_d \\ z_{d+1} &= x_1^2 \\ &\vdots \\ z_{d+2} &= x_1 x_2 \\ &\vdots \end{aligned}$$

$$\begin{aligned} z_r &= x_d^2 \\ &\vdots \\ z_s &= x_1^Q \\ z_{s+1} &= x_1^{Q+1} x_2 \\ &\vdots \\ z_D &= x_d^Q \end{aligned}$$

Polynomial Regression

So, the hypothesis becomes:

$$h_W(z) = w_0z_0 + w_1z_1 + \cdots + w_dz_d + \cdots + w_rz_r + \cdots + w_sz_s + \cdots + w_Dz_D$$

Which is linear in parameters W .

Definition: Polynomial regression model

It is a linear model used to capture curvature in data by using higher-order values of inputs. It is a linear combination of higher-ordered inputs:

$$h_W(x) = w_0 + w_1x_1 + \cdots + w_dx_d + w_{d+1}x_1^2 + w_{d+2}x_1x_2 + \cdots + w_Dx_d^Q$$

It is also called **curvilinear** regression.

Parameter Estimation

To estimate the parameters of polynomial regression, we should minimize the following loss function:

$$L_S(w) = \frac{1}{m} \sum_{i=1}^m (y^{(i)} - h_w(x^{(i)}))^2$$

Which implies:

$$L_S(w) = \frac{1}{m} \sum_{i=1}^m \left(y^{(i)} - \sum_{j=0}^D w_j z_j^{(i)} \right)^2$$

Parameter Estimation

So, the loss function becomes:

$$L_S(w) = \frac{1}{m} \sum_{i=1}^m (y^{(i)} - w^T \cdot z^{(i)})^2$$

To optimize this function, we can use an iterative algorithm named Gradient Descent:

$$\nabla L_S(w_j) = \frac{-2}{m} \sum_{i=1}^m (y^{(i)} - w^T \cdot z^{(i)}) z_j^{(i)}$$

$$w_j \leftarrow w_j - \alpha \nabla L_S(w_j)$$

Gradient Descent Algorithm for Polynomial Regression

Input: The training data: $S = \{(x^{(1)}, y^{(1)}), \dots, (x^{(m)}, y^{(m)})\}$

The polynomial order Q , The estimation parameter ε

The initial vector of parameters $w^{(0)}$ and the learning rate α

Output: w^* , t and $L_S(w^*)$

Start: $w \leftarrow w^{(0)}$

Compute the value of the hypothesis for each observation x :

$$\begin{aligned} h_W(x) &= w_0 + w_1x_1 + \dots + w_dx_d + w_{d+1}x_1^2 + w_{d+2}x_1x_2 + \dots + w_Dx_d^Q \\ &= \sum_{j=0}^D w_j z_j \end{aligned}$$

Compute the cost function: $L_S(w^{(0)}) = \frac{1}{m} \sum_{i=1}^m (y^{(i)} - (w^{(0)})^T \cdot z^{(i)})^2$

$t = 0$

While $(L_S(w^{(t)}) > \varepsilon)$ {

$$w^{(t+1)} \leftarrow w^{(t)} - \alpha \nabla L_S(w^{(t)})$$

$t \leftarrow t + 1$ }

$$w^* \leftarrow w^{(t)}$$

Return: w^* , t and $L_S(w^*)$

End