

# LINEAR REGRESSION AND POLYNOMIAL REGRESSION

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## 1. SIMPLE LINEAR REGRESSION

Simple linear regression is a linear regression of a data which has one independent variable. Suppose that we have  $n$  pairs of data

$$\{(x_i, y_i) \in \mathbb{R}^2 : i = 1, \dots, n\}.$$

We will construct a linear predictor function  $y = \beta_1 x + \beta_0$  from the data, based on the method of least squares.

The *residual*  $r_i$  ( $i = 1, \dots, n$ ) is the difference between an observed value and the fitted value provided by a linear prediction:

$$r_i = y_i - (\beta_1 x_i + \beta_0) \quad (i = 1, \dots, n).$$

The method of least squares provides an approximation of the data by minimizing the sum of the squares of the residuals. In other words, if  $S$  is a function on  $\mathbb{R}^2$  defined by

$$S(b_0, b_1) = \sum_{i=1}^n (y_i - b_1 x_i - b_0)^2,$$

and if the point  $(\beta_0, \beta_1)$  minimizes  $S(b_0, b_1)$ , then the linear predictor function is given by

$$y = \beta_1 x + \beta_0.$$

Intuitively,  $S(b_0, b_1)$  has a global minimum and it has no local maximum or saddle points. Hence, it is enough to find a critical point of  $S$ . To do this, we compute the gradient of  $S$ . By chain rule, we have

$$\nabla S(b_0, b_1) = \left( -2 \sum_{i=1}^n (y_i - b_1 x_i - b_0), -2 \sum_{i=1}^n x_i (y_i - b_1 x_i - b_0) \right).$$

If  $(\beta_0, \beta_1)$  is a critical point of  $S$ , then we have

$$\sum_{i=1}^n (y_i - \beta_1 x_i - \beta_0) = 0 \tag{1.1}$$

$$\sum_{i=1}^n x_i (y_i - \beta_1 x_i - \beta_0) = 0. \tag{1.2}$$

The first equation (1.1) can be written as follows:

$$\sum_{i=1}^n (y_i - \beta_1 x_i) - n\beta_0 = 0.$$

This leads us to

$$\beta_0 = \frac{1}{n} \sum_{i=1}^n (y_i - \beta_1 x_i). \quad (1.3)$$

Substituting (1.3) into (1.2) yields

$$\sum_{i=1}^n x_i (y_i - \beta_1 x_i - \frac{1}{n} \sum_{j=1}^n (y_j - \beta_1 x_j)) = 0.$$

This is equivalent to

$$\beta_1 \left( -\sum_{i=1}^n x_i^2 + \frac{1}{n} \left( \sum_{i=1}^n x_i \right)^2 \right) + \sum_{i=1}^n x_i y_i - \frac{1}{n} \left( \sum_{i=1}^n x_i \right) \left( \sum_{i=1}^n y_i \right) = 0.$$

Thus, we have

$$\beta_1 = \frac{\sum x_i y_i - \frac{1}{n} (\sum x_i) (\sum y_i)}{\sum x_i^2 - \frac{1}{n} (\sum x_i)^2}. \quad (1.4)$$

We denote the means of  $x_i$  and  $y_i$  ( $i = 1, \dots, n$ ) by  $\bar{x}$  and  $\bar{y}$ , respectively. Then (1.3) is equivalent to

$$\beta_0 = \bar{y} - \beta_1 \bar{x}.$$

In the rest of the section, we prove that (1.4) is equivalent to

$$\beta_1 = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sum (x_i - \bar{x})^2}. \quad (1.5)$$

The following calculation shows that the numerator of (1.5) is the same as that of (1.4):

$$\begin{aligned} \sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y}) &= \sum_{i=1}^n \left( x_i - \frac{1}{n} \sum_{j=1}^n x_j \right) \left( y_i - \frac{1}{n} \sum_{j=1}^n y_j \right) \\ &= \sum_{i=1}^n x_i y_i - \frac{2}{n} \left( \sum_{i=1}^n x_i \right) \left( \sum_{i=1}^n y_i \right) + \frac{n}{n^2} \left( \sum_{i=1}^n x_i \right) \left( \sum_{i=1}^n y_i \right) \\ &= \sum_{i=1}^n x_i y_i - \frac{1}{n} \left( \sum_{i=1}^n x_i \right) \left( \sum_{i=1}^n y_i \right). \end{aligned}$$

Replacing  $y_i$  and  $\bar{y}$  with  $x_i$  and  $\bar{x}$  shows that the denominators of (1.4) and (1.5) are the same.

## 2. MULTIVARIATE POLYNOMIAL REGRESSION

Multivariate polynomial regression is a polynomial regression for a data having more than one independent variables. In this section, we only consider the case where a data has two independent variables. Suppose that we have  $n$  triples of data

$$\{(p_i, q_i, y_i) \in \mathbb{R}^2 : i = 1, \dots, n\}.$$

We will establish a polynomial regression of degree 2,

$$y = \beta_0 + \beta_1 p + \beta_2 q + \beta_3 p^2 + \beta_4 pq + \beta_5 q^2$$

from the data, based on the method of least squares.

The residual  $r_i$  is given by

$$r_i = y_i - (\beta_0 + \beta_1 p_i + \beta_2 q_i + \beta_3 p_i^2 + \beta_4 p_i q_i + \beta_5 q_i^2) \quad (i = 1, \dots, n).$$

The sum of the squares of the residuals is given by

$$S = \sum_{i=1}^n [y_i - (\beta_0 + \beta_1 p_i + \beta_2 q_i + \beta_3 p_i^2 + \beta_4 p_i q_i + \beta_5 q_i^2)]^2.$$

We regard  $S$  as a function of  $b_0, b_1, \dots, b_5$  and find the point  $(\beta_0, \dots, \beta_5)$  at which  $S(b_0, \dots, b_5)$  has the global minimum. Intuitively,  $S(b_0, \dots, b_5)$  has a global minimum and it has no local maximum or saddle points. Hence it suffices to find a critical point of  $S$ . To do this, we compute the gradient of  $S$  at the critical point  $(\beta_0, \dots, \beta_5)$ . By chain rule, we have

$$\nabla S = -2 \sum_{i=1}^n (r_i, p_i r_i, q_i r_i, 2p_i r_i, p_i q_i r_i, 2q_i r_i).$$

Since  $\nabla S(\beta_0, \dots, \beta_5) = 0$ , it follows that

$$\begin{aligned} \sum_{i=1}^n r_i &= 0, & \sum_{i=1}^n p_i r_i &= 0, & \sum_{i=1}^n q_i r_i &= 0, \\ \sum_{i=1}^n p_i r_i &= 0, & \sum_{i=1}^n p_i q_i r_i &= 0, & \sum_{i=1}^n q_i r_i &= 0. \end{aligned}$$

### 3. MATRIX REPRESENTATION FOR MULTIVARIATE LINEAR REGRESSION

Suppose that we have  $m$  training datasets consisting of  $n$  features.

$x^{(1)}$	$x^{(2)}$	$\dots$	$x^{(n)}$	$y$
$x_{11}$	$x_{12}$	$\dots$	$x_{1n}$	$y_1$
$x_{21}$	$x_{22}$	$\dots$	$x_{2n}$	$y_2$
$\vdots$		$\dots$		
$x_{m1}$	$x_{m2}$	$\dots$	$x_{mn}$	$y_m$

For instance, if we have the list of  $m$  restaurants, then  $y$  can be the ranks of the restaurants and  $x^{(1)}, x^{(2)}, \dots, x^{(n)}$  can be the quality of food, cleanliness, the price, the area of the restaurant, etc. In this article, we establish a linear predictor function with more than one independent variables. As in the case of a simple linear regression, the multivariate linear regression is given by

$$y = \beta_0 + x^{(1)}\beta_1 + x^{(2)}\beta_2 + \dots + x^{(n)}\beta_n \quad (3.1)$$

and the method of least squares will determine the coefficients  $\beta_0, \dots, \beta_n$ . In other words, if  $S$  is a function of  $b_0, b_1, \dots, b_n$ ,

$$S(b_0, b_1, \dots, b_n) = \sum_{i=1}^m \left( y_i - b_0 - \sum_{j=1}^n x_{ij} b_j \right)^2,$$

then we need to find the minimum point  $\beta_0, \beta_1, \dots, \beta_n$  to determine the coefficients in (3.1). We set  $x_{i0} = 1$  for each  $i = 1, \dots, m$  and let

$$y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix}, \quad X = \begin{bmatrix} x_{10} & x_{11} & x_{12} & \cdots & x_{1n} \\ x_{20} & x_{21} & x_{22} & \cdots & x_{2n} \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ x_{m0} & x_{m1} & x_{m2} & \cdots & x_{mn} \end{bmatrix}, \quad \beta = \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_n \end{bmatrix}$$

so that

$$S(b_0, b_1, \dots, b_n) = \sum_{i=1}^m \left( y_i - \sum_{j=0}^n x_{ij} \beta_j \right)^2 = \sum_{i=1}^m ((y - X\beta)_i)^2 = (y - X\beta)^\top (y - X\beta).$$

To obtain the gradient of  $S$ , we compute the partial derivatives of  $S$ . From

$$S(b_0, b_1, \dots, b_n) = \sum_{i=1}^m \left( y_i - \sum_{j=0}^n x_{ij} b_j \right)^2,$$

it follows that

$$\frac{\partial S}{\partial b_k} = -2 \sum_{i=1}^m x_{ik} \left( y_i - \sum_{j=0}^n x_{ij} b_j \right) \quad (k = 0, \dots, n).$$

Hence we obtain

$$\sum_{i=1}^m \sum_{j=0}^n x_{ik} x_{ij} \beta_j = \sum_{i=1}^m x_{ik} y_i$$

for each  $k = 0, \dots, n$ . We note that this is equivalent to  $X^\top X \beta = X^\top y$ . Thus, we have

$$\beta = (X^\top X)^{-1} X^\top y.$$

The size of  $X^\top X$  is  $(n+1) \times (n+1)$ . If  $n$  is a very large number, then it takes long to compute the inverse of  $X^\top X$ . In that case, it would be better to find the global minimum by *gradient descent*. We first choose  $(b_0, \dots, b_n) \in \mathbb{R}^{n+1}$  and set

$$b_j^{(0)} = b_j$$

and

$$b_j^{(r)} = b_j^{(r-1)} - \alpha \frac{\partial S}{\partial b_j^{(r-1)}} \quad (r = 1, 2, \dots)$$

for each  $j = 0, 1, \dots, n$ . For suitable  $\alpha$ ,  $(b_0^{(r)}, b_1^{(r)}, \dots, b_n^{(r)})$  converges to the minimum point as  $r$  goes to the infinity.

## REFERENCES

- [1] Linear regression on Wikipedia
- [2] Simple linear regression on Wikipedia
- [3] Least squares on Wikipedia