

**“JUST THE MATHS”**

**SLIDES NUMBER**

**14.12**

**PARTIAL DIFFERENTIATION 12**  
**(The principle of least squares)**

**by**

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**14.12.1 The normal equations**

**14.12.2 Simplified calculation of regression lines**

## UNIT 14.12

### PARTIAL DIFFERENTIATION 12

#### THE PRINCIPLE OF LEAST SQUARES

##### 14.12.1 THE NORMAL EQUATIONS

Suppose  $x$  and  $y$ , are known to obey a “**straight line law**” of the form  $y = a + bx$ , where  $a$  and  $b$  are constants to be found.

In an experiment to test this law, let  $n$  pairs of values be  $(x_i, y_i)$ , where  $i = 1, 2, 3, \dots, n$ .

If the values,  $x_i$ , are **assigned** values, they are likely to be free from error.

The **observed** values,  $y_i$ , will be subject to experimental error

For the straight line of “**best fit**”, the sum of the squares of the  $y$ -deviations, from the line, of all observed points is a minimum.

#### The Calculation

The  $y$ -deviation,  $\epsilon_i$ , of the point,  $(x_i, y_i)$ , is given by

$$\epsilon_i = y_i - (a + bx_i).$$

Hence,

$$\sum_{i=1}^n \epsilon_i^2 = \sum_{i=1}^n [y_i - (a + bx_i)]^2 = P \text{ say.}$$

Regarding  $P$  as a function of  $a$  and  $b$ , it will be a minimum when

$$\frac{\partial P}{\partial a} = 0, \quad \frac{\partial P}{\partial b} = 0, \quad \frac{\partial^2 P}{\partial a^2} > 0 \quad \text{or} \quad \frac{\partial^2 P}{\partial b^2} > 0,$$

and

$$\frac{\partial^2 P}{\partial a^2} \cdot \frac{\partial^2 P}{\partial b^2} - \left( \frac{\partial^2 P}{\partial a \partial b} \right)^2 > 0.$$

For these conditions,

$$\frac{\partial P}{\partial a} = -2 \sum_{i=1}^n [y_i - (a + bx_i)] \quad \text{and} \quad \frac{\partial P}{\partial b} = -2 \sum_{i=1}^n x_i [y_i - (a + bx_i)].$$

These will be zero when

$$\sum_{i=1}^n [y_i - (a + bx_i)] = 0 \quad \text{--- (1)}$$

and

$$\sum_{i=1}^n x_i [y_i - (a + bx_i)] = 0 \quad \text{--- (2)}$$

From (1),

$$\sum_{i=1}^n y_i - \sum_{i=1}^n a - \sum_{i=1}^n bx_i = 0.$$

That is,

$$\sum_{i=1}^n y_i = na + b \sum_{i=1}^n x_i \quad \text{--- (3)}.$$

From (2),

$$\sum_{i=1}^n x_i y_i = a \sum_{i=1}^n x_i + b \sum_{i=1}^n x_i^2 \quad \text{--- (4)}.$$

Statements (3) and (4) (which must be solved for  $a$  and  $b$ ) are called the “**normal equations**”.

A simpler notation for the normal equations is

$$\Sigma y = na + b\Sigma x;$$

$$\Sigma xy = a\Sigma x + b\Sigma x^2.$$

Eliminating  $a$  and  $b$  in turn,

$$a = \frac{\Sigma x^2 \cdot \Sigma y - \Sigma x \cdot \Sigma xy}{n\Sigma x^2 - (\Sigma x)^2} \quad \text{and} \quad b = \frac{n\Sigma xy - \Sigma x \cdot \Sigma y}{n\Sigma x^2 - (\Sigma x)^2}.$$

The straight line, with equation  $y = a + bx$ , is called the “**regression line of  $y$  on  $x$** ”.

**Note:**

We also need the results that

$$\frac{\partial^2 P}{\partial a^2} = \sum_{i=1}^n 2 = 2n, \quad \frac{\partial^2 P}{\partial b^2} = \sum_{i=1}^n 2x_i^2, \quad \text{and} \quad \frac{\partial^2 P}{\partial a \partial b} = \sum_{i=1}^n 2x_i.$$

The first two of these are clearly positive.

It may also be shown that

$$\frac{\partial^2 P}{\partial a^2} \cdot \frac{\partial^2 P}{\partial b^2} - \left( \frac{\partial^2 P}{\partial a \partial b} \right)^2 > 0.$$

**EXAMPLE**

Determine the equation of the regression line of  $y$  on  $x$  for the following data, which shows the Packed Cell Volume,  $x$ mm, and the Red Blood Cell Count,  $y$  millions, of 10 dogs:

$x$	45	42	56	48	42	35	58	40	39	50
$y$	6.53	6.30	9.52	7.50	6.99	5.90	9.49	6.20	6.55	8.72

## Solution

$x$	$y$	$xy$	$x^2$
45	6.53	293.85	2025
42	6.30	264.60	1764
56	9.52	533.12	3136
48	7.50	360.00	2304
42	6.99	293.58	1764
35	5.90	206.50	1225
58	9.49	550.42	3364
40	6.20	248.00	1600
39	6.55	255.45	1521
50	8.72	436.00	2500
455	73.70	3441.52	21203

The regression line of  $y$  on  $x$  has equation  $y = a + bx$ , where

$$a = \frac{(21203)(73.70) - (455)(3441.52)}{(10)(21203) - (455)^2} \simeq -0.645$$

and

$$b = \frac{(10)(3441.52) - (455)(73.70)}{(10)21203 - (455)^2} \simeq 0.176$$

Thus,

$$y = 0.176x - 0.645$$

## 14.12.2 SIMPLIFIED CALCULATION OF REGRESSION LINES

We consider a temporary change of origin to the point  $(\bar{x}, \bar{y})$  where  $\bar{x}$  is the arithmetic mean of the values  $x_i$  and  $\bar{y}$  is the arithmetic mean of the values  $y_i$ .

### RESULT

The regression line of  $y$  on  $x$  contains the point  $(\bar{x}, \bar{y})$ .

### Proof:

From the first of the normal equations,

$$\frac{\Sigma y}{n} = a + b \frac{\Sigma x}{n}$$

That is,

$$\bar{y} = a + b\bar{x}.$$

A change of origin to the point  $(\bar{x}, \bar{y})$ , with new variables  $X$  and  $Y$  is associated with the formulae

$$X = x - \bar{x} \quad \text{and} \quad Y = y - \bar{y}.$$

In this system of reference, the regression line will pass through the origin.

The equation of the regression line is

$$Y = BX,$$

where

$$B = \frac{n\Sigma XY - \Sigma X.\Sigma Y}{n\Sigma X^2 - (\Sigma X)^2}.$$

However,

$$\Sigma X = \Sigma (x - \bar{x}) = \Sigma x - \Sigma \bar{x} = n\bar{x} - n\bar{x} = 0$$

and

$$\Sigma Y = \Sigma (y - \bar{y}) = \Sigma y - \Sigma \bar{y} = n\bar{y} - n\bar{y} = 0.$$

Thus,

$$B = \frac{\Sigma XY}{\Sigma X^2}.$$



**Note:**

In a given problem, we make a table of values of  $x_i$ ,  $y_i$ ,  $X_i$ ,  $Y_i$ ,  $X_iY_i$  and  $X_i^2$ .

The regression line is then

$$y - \bar{y} = B(x - \bar{x}) \quad \text{or} \quad y = BX + (\bar{y} - B\bar{x}).$$

There may be slight differences in the result obtained compared with that from the earlier method.

**EXAMPLE**

Determine the equation of the regression line of  $y$  on  $x$  for the following data which shows the Packed Cell Volume,  $x$ mm, and the Red Blood Cell Count,  $y$  millions, of 10 dogs:

$x$	45	42	56	48	42	35	58	40	39	50
$y$	6.53	6.30	9.52	7.50	6.99	5.90	9.49	6.20	6.55	8.72

**Solution**

The arithmetic mean of the  $x$  values is  $\bar{x} = 45.5$

The arithmetic mean of the  $y$  values is  $\bar{y} = 7.37$

This gives the following table:

$x$	$y$	$X = x - \bar{x}$	$Y = y - \bar{y}$	$XY$	$X^2$
45	6.53	-0.5	-0.84	0.42	0.25
42	6.30	-3.5	-1.07	3.745	12.25
56	9.52	10.5	2.15	22.575	110.25
48	7.50	2.5	0.13	0.325	6.25
42	6.99	-3.5	-0.38	1.33	12.25
35	5.90	-10.5	-1.47	15.435	110.25
58	9.49	12.5	2.12	26.5	156.25
40	6.20	-5.5	-1.17	6.435	30.25
39	6.55	-6.5	-0.82	5.33	42.25
50	8.72	4.5	1.35	6.075	20.25
455	73.70			88.17	500.5

Hence,

$$B = \frac{88.17}{500.5} \simeq 0.176$$

and so the regression line has equation

$$y = 0.176x + (7.37 - 0.176 \times 45.5)$$

That is,

$$y = 0.176x - 0.638$$