LINEAR REGRESSION ANALYSIS

MODULE – II

Lecture - 7

Simple Linear Regression Analysis

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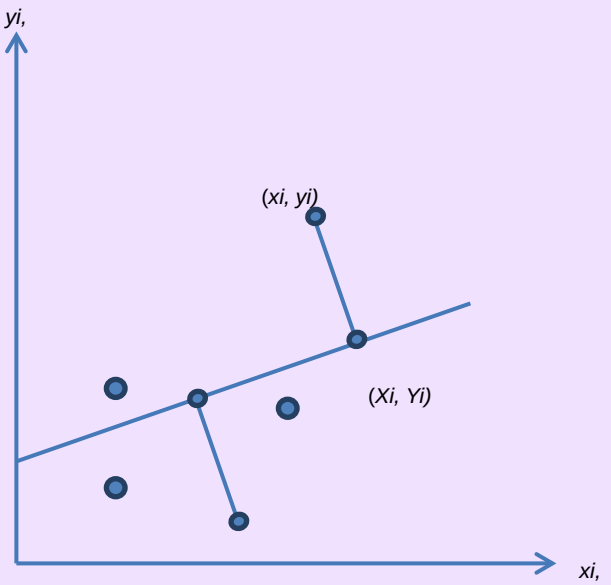
Orthogonal regression method (or major axis regression method)

The direct and reverse regression methods of estimation assume that the errors in the observations are either in *x*-direction or *y*-direction. In other words, the errors can be either in dependent variable or independent variable. There can be situations when uncertainties are involved in dependent and independent variables both. In such situations, the orthogonal regression is more appropriate. In order to take care of errors in both the directions, the least squares principle in orthogonal regression minimizes the squared perpendicular distance between the observed data points and the line in the following scatter diagram to obtain the estimates of regression coefficients. This is also known as **major axis regression method**. The estimates obtained are called as **orthogonal regression estimates** or **major axis regression estimates** of regression coefficients.

If we assume that the regression line to be fitted is $Y_i = \beta_0 + \beta_1 X_i$, then it is expected that all the observations $(x_i, y_i),\ i = 1, 2, ..., n$ lie on this line. But these points deviate from the line and in such a case, the squared perpendicular distance of observed data $(x_i, y_i)(i = 1, 2, ..., n)$ from the line is given by $d_i^2 = (X_i - x_i)^2 + (Y_i - y_i)^2$ where (X_i, Y_i) denotes the i^{th} pair of observation without any error which lie on the line.



Orthogonal or major axis regression method

The objective is to minimize the sum of squared perpendicular distances given by $\sum_{i=1}^{n} d_i^2$ to obtain the estimates of β_0 and β_1.

The observations $(x_i, y_i)(i = 1, 2, ..., n)$ are expected to lie on the line

$$Y_i = \beta_0 + \beta_1 X_i$$

so let

$$E_i = Y_i - \beta_0 - \beta_1 X_i = 0.$$

The regression coefficients are obtained by minimizing $\sum_{i=1}^{n} d_i^2$ under the constraints E_i's using the Lagrangian's multiplier method. The Lagrangian function is

$$L_0 = \sum_{i=1}^{n} d_i^2 - 2\sum_{i=1}^{n} \lambda_i E_i$$

where $\lambda_1, ..., \lambda_n$ are the Lagrangian multipliers.

The set of equations are obtained by setting

$$\frac{\partial L_0}{\partial X_i} = 0, \frac{\partial L_0}{\partial Y_i} = 0, \frac{\partial L_0}{\partial \beta_0} = 0 \text{ and } \frac{\partial L_0}{\partial \beta_1} = 0 \ (i = 1, 2, ..., n).$$

Thus we find

$$\frac{\partial L_0}{\partial X_i} = (X_i - x_i) + \lambda_i \beta_1 = 0$$

$$\frac{\partial L_0}{\partial Y_i} = (Y_i - y_i) - \lambda_i = 0$$

$$\frac{\partial L_0}{\partial \beta_0} = \sum_{i=1}^{n} \lambda_i = 0$$

$$\frac{\partial L_0}{\partial \beta_1} = \sum_{i=1}^{n} \lambda_i X_i = 0.$$

Since

$$X_i = x_i - \lambda_i \beta_1$$

$$Y_i = y_i + \lambda_i$$

so substituting these values in E_i, we obtain

$$E_i = (y_i + \lambda_i) - \beta_0 - \beta_1 (x_i - \lambda_i \beta_1) = 0$$

$$\Rightarrow \lambda_i = \frac{\beta_0 + \beta_1 x_i - y_i}{1 + \beta_1^2}.$$

Also using this λ_i in the equation $\sum_{i=1}^{n} \lambda_i = 0,$ we get

$$\frac{\sum_{i=1}^{n} (\beta_0 + \beta_1 x_i - y_i)}{1 + \beta_1^2} = 0$$

and using $(X_i - x_i) + \lambda_i \beta_1 = 0$ and $\sum_{i=1}^{n} \lambda_i X_i = 0,$ we get

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

Substituting λ_i in this equation, we get

$$\frac{\sum_{i=1}^{n} (\beta_0 x_i + \beta_1 x_i^2 - y_i x_i)}{(1 + \beta_1^2)} - \frac{\beta_1 \sum_{i=1}^{n} (\beta_0 + \beta_1 x_i - y_i)^2}{(1 + \beta_1^2)^2} = 0. \qquad (1)$$

Using λ_i in the equation and using the equation $\sum_{i=1}^{n} \lambda_i = 0$, we solve

$$\frac{\sum_{i=1}^{n} (\beta_0 + \beta_1 x_i - y_i)}{1 + \beta_1^2} = 0 .$$

The solution provides an orthogonal regression estimate of β_0 as

$$\hat{\beta}_{0OR} = \bar{y} - \hat{\beta}_{1OR}\bar{x}$$

where $\hat{\beta}_{1OR}$ is an orthogonal regression estimate of β_1.

Now, substituting β_{0OR} in equation (1), we get

$$\sum_{i=1}^{n}(1+\beta_1^2)\left[\bar{y}x_i - \beta_1\bar{x}x_i + \beta_1 x_i^2 - x_i y_i\right] - \beta_1\sum_{i=1}^{n}\left(\bar{y} - \beta_1\bar{x} + \beta_1 x_i - y_i\right)^2 = 0$$

or $$(1+\beta_1^2)\sum_{i=1}^{n} x_i\left[y_i - \bar{y} - \beta_1(x_i - \bar{x})\right] + \beta_1\sum_{i=1}^{n}\left[-(y_i - \bar{y}) + \beta_1(x_i - \bar{x})\right]^2 = 0$$

or $$(1+\beta_1^2)\sum_{i=1}^{n}(u_i + \bar{x})(v_i - \beta_1 u_i) + \beta_1\sum_{i=1}^{n}(-v_i + \beta_1 u_i)^2 = 0$$

where

$$u_i = x_i - \bar{x},$$
$$v_i = y_i - \bar{y}.$$

Since $\sum_{i=1}^{n} u_i = \sum_{i=1}^{n} v_i = 0$, so

$$\sum_{i=1}^{n}\left[\beta_1^2 u_i v_i + \beta_1(u_i^2 - v_i^2) - u_i v_i\right] = 0$$

or

$$\beta_1^2 s_{xy} + \beta_1(s_{xx} - s_{yy}) - s_{xy} = 0.$$

Solving this quadratic equation provides the orthogonal regression estimate of β_1 as

$$\hat{\beta}_{1OR} = \frac{\left(s_{yy} - s_{xx}\right) + sign\left(s_{xy}\right)\sqrt{(s_{xx} - s_{yy})^2 + 4s_{xy}^2}}{2s_{xy}}$$

where $sign(s_{xy})$ denotes the sign of s_{xy} which can be positive or negative. So

$$sign(s_{xy}) = \begin{cases} 1 & \text{if } s_{xy} > 0 \\ -1 & \text{if } s_{xy} < 0. \end{cases}$$

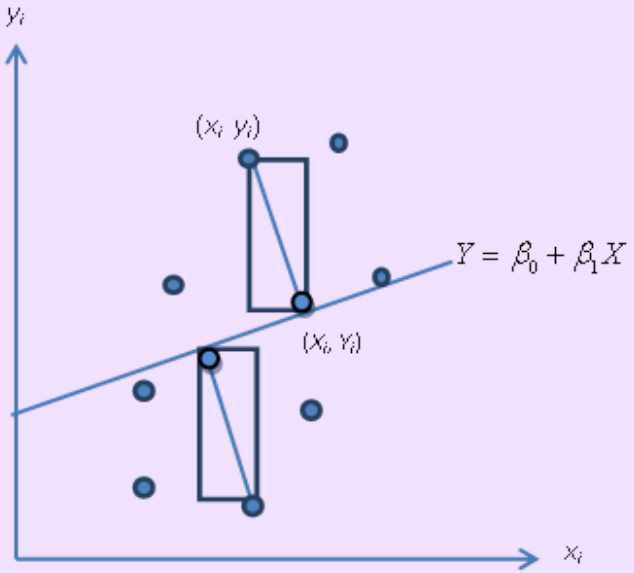
Notice that this gives two solutions for $\hat{\beta}_{1OR}$. We choose the solution which minimizes $\sum_{i=1}^{n} d_i^2$.

The other solution maximizes $\sum_{i=1}^{n} d_i^2$ and is in the direction perpendicular to the optimal solution.

The optimal solution can be chosen with the sign of s_{xy}.

Reduced major axis regression method

The direct, reverse and orthogonal methods of estimation minimize the errors in a particular direction which is usually the distance between the observed data points and the line in the scatter diagram. Alternatively, one can consider the area extended by the data points in certain neighbourhood and instead of distances, the area of rectangles defined between corresponding observed data point and nearest point on the line in the following scatter diagram can also be minimized. Such an approach is more appropriate when the uncertainties are present in study as well as explanatory variables. This approach is termed as reduced major axis regression.



Reduced major axis method

Suppose the regression line is $Y_i = \beta_0 + \beta_1 X_i$ on which all the observed points are expected to lie. Suppose the points $(x_i, y_i),\ i = 1, 2, ..., n$ are observed which lie away from the line.

The area of rectangle extended between the i^{th} observed data point and the line is

$$A_i = (X_i \sim x_i)(Y_i \sim y_i) \quad (i = 1, 2, ..., n)$$

where (X_i, Y_i) denotes the i^{th} pair of observation without any error which lie on the line.

The total area extended by *n* data points is $\sum_{i=1}^{n} A_i = \sum_{i=1}^{n} (X_i \sim x_i)(Y_i \sim y_i).$

All observed data points $(x_i, y_i), (i = 1, 2, ..., n)$ are expected to lie on the line

$$Y_i = \beta_0 + \beta_1 X_i$$

and let

$$E_i^* = Y_i - \beta_0 - \beta_1 X_i = 0.$$

So now the objective is to minimize the sum of areas under the constraints E_i^* to obtain the reduced major axis estimates of regression coefficients. Using the Lagrangian multiplies method, the Lagrangian function is

$$L_R = \sum_{i=1}^{n} A_i - \sum_{i=1}^{n} \mu_i E_i^*$$

$$= \sum_{i=1}^{n} (X_i - x_i)(Y_i - y_i) - \sum_{i=1}^{n} \mu_i E_i^*$$

where $\mu_1, ..., \mu_n$ are the Lagrangian multipliers. The set of equations are obtained by setting

$$\frac{\partial L_R}{\partial X_i} = 0, \frac{\partial L_R}{\partial Y_i} = 0, \frac{\partial L_R}{\partial \beta_0} = 0, \frac{\partial L_R}{\partial \beta_1} = 0 \quad (i = 1, 2, ..., n).$$

Thus

$$\frac{\partial L_R}{\partial X_i} = (Y_i - y_i) + \beta_1 \mu_i = 0$$

$$\frac{\partial L_R}{\partial Y_i} = (X_i - x_i) - \mu_i = 0$$

$$\frac{\partial L_R}{\partial \beta_0} = \sum_{i=1}^{n} \mu_i = 0$$

$$\frac{\partial L_R}{\partial \beta_1} = \sum_{i=1}^{n} \mu_i X_i = 0.$$

Now

$$X_i = x_i + \mu_i$$

$$Y_i = y_i - \beta_1 \mu_i$$

$$\beta_0 + \beta_1 X_i = y_i - \beta_1 \mu_i$$

$$\beta_0 + \beta_1 (x_i + \mu_i) = y_i - \beta_1 \mu_i$$

$$\Rightarrow \mu_i = \frac{y_i - \beta_0 - \beta_1 x_i}{2\beta_1}.$$

Substituting μ_i in $\sum_{i=1}^{n} \mu_i = 0$, we get the reduced major axis regression estimate of β_0 is obtained as

$$\hat{\beta}_{0RM} = \bar{y} - \hat{\beta}_{1RM} \bar{x}$$

where $\hat{\beta}_{1RM}$ is the reduced major axis regression estimate of β_1. Using $X_i = x_i + \mu_i$, μ_i and $\hat{\beta}_{0RM}$ in $\sum_{i=1}^{n} \mu_i X_i = 0$,

we get

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

Let $u_i = x_i - \overline{x}$ and $v_i = y_i - \overline{y}$, then this equation can be re-expressed as $\sum_{i=1}^{n}(v_i - \beta_1 u_i)(v_i + \beta_1 u_i + 2\beta_1 \overline{x}) = 0.$

Using $\sum_{i=1}^{n} u_i = \sum_{i=1}^{n} v_i = 0,$ we get

$$\sum_{i=1}^{n} v_i^2 - \beta_1^2 \sum_{i=1}^{n} u_i^2 = 0.$$

Solving this equation, the reduced major axis regression estimate of β_1 is obtained as

$$\hat{\beta}_{1RM} = sign(s_{xy})\sqrt{\frac{s_{yy}}{s_{xx}}}$$

where

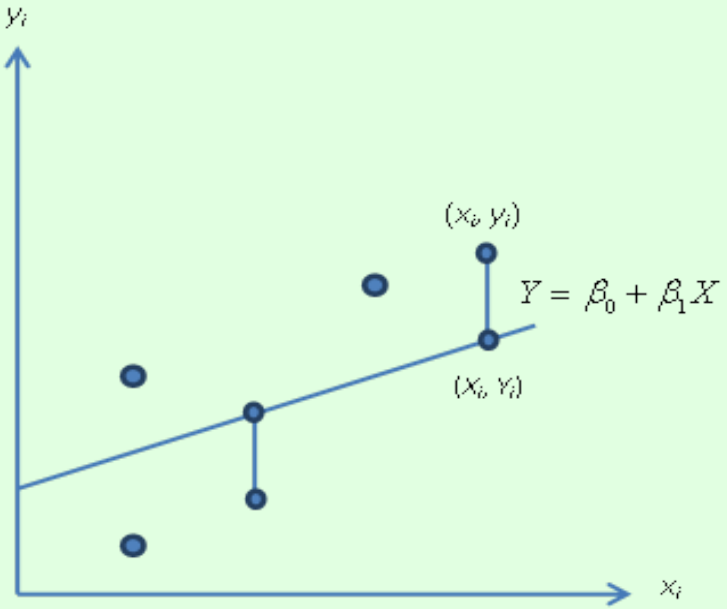
$$sign(s_{xy}) = \begin{cases} 1 & \text{if } s_{xy} > 0 \\ -1 & \text{if } s_{xy} < 0. \end{cases}$$

We choose the regression estimator which has same sign as that of $s_{xy.}$

Least absolute deviation regression method

The least squares principle advocates the minimization of sum of squared errors. The idea of squaring the errors is useful in place of simple errors because the random errors can be positive as well as negative. So consequently their sum can be close to zero indicating that there is no error in the model which can be misleading. Instead of the sum of random errors, the sum of absolute random errors can be considered which avoids the problem due to positive and negative random errors.

In the method of least squares, the estimates of the parameters β_0 and β_1 in the model $y_i = \beta_0 + \beta_1 x_i + \varepsilon_i . (i = 1, 2, ..., n)$ are chosen such that the sum of squares of deviations $\sum_{i=1}^{n} \varepsilon_i^2$ is minimum. In the method of least absolute deviation (LAD) regression, the parameters β_0 and β_1 are estimated such that the sum of absolute deviations $\sum_{i=1}^{n} |\varepsilon_i|$ is minimum. It minimizes the absolute vertical sum of errors as in the following scatter diagram:



Least absolute deviation regression

The LAD estimates $\hat{\beta}_{0L}$ and $\hat{\beta}_{1L}$ are the values β_0 and β_1, respectively which minimize $LAD(\beta_0, \beta_1) = \sum_{i=1}^{n} |y_i - \beta_0 - \beta_1 x_i|$ for the given observations $(x_i, y_i)(i = 1, 2, ..., n)$.

Conceptually, LAD procedure is simpler than OLS procedure because |*e*| (absolute residuals) is a more straightforward measure of the size of the residual than e^2 (squared residuals). The LAD regression estimates of β_0 and β_1 are not available in closed form. Rather they can be obtained numerically based on algorithms. Moreover, this creates the problems of non-uniqueness and degeneracy in the estimates. The concept of non-uniqueness relates to more than one best lines passing through a data point. The degeneracy concept describes that the best line through a data point also passes through more than one other data points. The non-uniqueness and degeneracy concepts are used in algorithms to judge the quality of the estimates. The algorithm for finding the estimators generally proceeds in steps. At each step, the best line is found that passes through a given data point. The best line always passes through another data point, and this data point is used in the next step. When there is non-uniqueness, then there are more than one best lines. When there is degeneracy, then the best line passes through more than one other data point. When either of the problem is present, then there is more than one choice for the data point to be used in the next step and the algorithm may go around in circles or make a wrong choice of the LAD regression line. The exact tests of hypothesis and confidence intervals for the LAD regression estimates can not be derived analytically. Instead they are derived analogous to the tests of hypothesis and confidence intervals related to ordinary least squares estimates.

Estimation of parameters when *X* is stochastic

In a usual linear regression model, the study variable is supped to be random and explanatory variables are assumed to be fixed. In practice, there may be situations in which the explanatory variable also becomes random.

Suppose both dependent and independent variables are stochastic in the simple linear regression model

$$y = \beta_0 + \beta_1 X + \varepsilon$$

where ε is the associated random error component. The observations (x_i, y_i), $i = 1, 2, ..., n$ are assumed to be jointly distributed. Then the statistical inferences can be drawn in such cases which are conditional on *X*.

Assume the joint distribution of *X* and *y* to be bivariate normal $N(\mu_x, \mu_y, \sigma_x^2, \sigma_y^2, \rho)$ where μ_x and μ_y are the means of *X* and $y; \sigma_x^2$ and σ_y^2 are the variances of *X* and *y*, and ρ is the correlation coefficient between *X* and *y*. Then the conditional distribution of *y* given *X* = *x* is univariate normal conditional mean

$$E(y \mid X = x) = \mu_{y|x} = \beta_0 + \beta_1 x$$

and conditional variance of *y* given *X* = *x* is

$$Var(y|X = x) = \sigma_{y|x}^2 = \sigma_y^2(1 - \rho^2)$$

where

$$\beta_0 = \mu_y - \mu_x \beta_1$$

and

$$\beta_1 = \frac{\sigma_y}{\sigma_x} \rho.$$

When both *X* and *y* are stochastic, then the problem of estimation of parameters can be reformulated as follows. Consider a conditional random variable *y*|*X* = *x* having a normal distribution with mean as conditional mean $\mu_{y|x}$ and variance as conditional variance $Var(y|X=x)=\sigma^2_{y|x}$. Obtain *n* independently distributed observation $y_i|x_i,\ i=1,2,...,n$ from $N(\mu_{y|x},\sigma^2_{y|x})$ with nonstochastic *X*. Now the method of maximum likelihood can be used to estimate the parameters which yields the estimates of β_0 and β_1 as earlier in the case of nonstochastic *X* as

$$\tilde{b}=\overline{y}-\tilde{b}_1\overline{x}$$

and

$$\tilde{b}_1=\frac{s_{xy}}{s_{xx}}$$

respectively.

Moreover, the correlation coefficient

$$\rho=\frac{E(y-\mu_y)(X-\mu_x)}{\sigma_y\sigma_x}$$

can be estimated by the sample correlation coefficient

$$\begin{aligned}\hat{\rho}&=\frac{\sum_{i=1}^{n}(y_i-\overline{y})(x_i-\overline{x})}{\sqrt{\sum_{i=1}^{n}(x_i-\overline{x})^2}\sqrt{\sum_{i=1}^{n}(y_i-\overline{y})^2}}\\&=\frac{s_{xy}}{\sqrt{s_{xx}}\sqrt{s_{yy}}}\\&=\tilde{b}_1\sqrt{\frac{s_{xx}}{s_{yy}}}.\end{aligned}$$

Thus

$$\hat{\rho}^2 = \tilde{b}_1^2 \frac{s_{xx}}{s_{yy}}$$

$$= \tilde{b}_1 \frac{s_{xy}}{s_{yy}}$$

$$= \frac{s_{yy} - \sum_{i=1}^{n} \hat{\varepsilon}_i^2}{s_{yy}}$$

$$= R^2$$

which is same as the coefficient of determination.

Thus R^2 has the same expression as in the case when X is fixed.

Thus R^2 again measures the goodness of fitted model even when X is stochastic.