Notes on the least squares estimator

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The argument leading to the asymptotic variance of the least squares estimator (6.20) requires clarification. This file elaborates on the topic.

Linear regression with one predictor variable

Consider the simple linear regression model

$$y = 1\alpha + \widetilde{X}b + e \tag{1}$$

where y is a vector of observations with n elements, 1 is a vector of 1's with n elements, the scalar α is the intercept, \widetilde{X} is the observed $n \times 1$ full rank matrix containing the values of the covariate across observations, b is the unknown regression parameter (a scalar) and e is the vector of n residuals, independent of \widetilde{X} , with mean 0 and variance $I\sigma^2$. Write (1) as

$$y = X\beta + e \tag{2}$$

where $X = \{X_i\}_{i=1}^n$ has the appended column of 1's in its first column and $\beta = (\alpha, b)$. The least squares estimator is

$$\hat{\beta} = (X'X)^{-1}X'y \tag{3}$$

and its variance is

$$Var(\hat{\beta}|, X, \sigma^2) = (X'X)^{-1}\sigma^2.$$
(4)

It is easy to check that X'X has the following form,

$$X'X = \begin{bmatrix} n & \sum_{i} X_{i} \\ \sum_{i} X_{i} & \sum_{i} X_{i}^{2} \end{bmatrix}$$
$$= n \begin{bmatrix} \frac{1}{X} & \frac{\overline{X}}{n} \sum_{i} X_{i}^{2} \end{bmatrix}$$
(5)

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where \overline{X} is $\sum_{i} X_i/n$, the average value of X. The determinant of (5) is

$$\det(X'X) = n \left(\sum_{i} X_{i}^{2} - n \overline{X}^{2} \right)$$
$$= n \sum_{i} (X_{i} - \overline{X})^{2}.$$

The inverse matrix $(X'X)^{-1}$ is therefore

$$(X'X)^{-1} = \frac{1}{\sum_{i} (X_i - \overline{X})^2} \begin{bmatrix} \frac{1}{n} \sum_{i} X_i^2 & -\overline{X} \\ -\overline{X} & 1 \end{bmatrix}.$$
 (6)

The least squares estimator (3) can be expressed as

$$\begin{bmatrix} \hat{\alpha} \\ \hat{b} \end{bmatrix} = \frac{1}{\sum_{i} (X_{i} - \overline{X})^{2}} \begin{bmatrix} \frac{1}{n} \sum_{i} X_{i}^{2} & -\overline{X} \\ -\overline{X} & 1 \end{bmatrix} \begin{bmatrix} \sum_{i} y_{i} \\ \sum_{i} X_{i} y_{i} \end{bmatrix},$$

and

$$\hat{b} = \frac{\sum_{i} X_{i} y_{i} - n \overline{X} \overline{y}}{\sum_{i} (X_{i} - \overline{X})^{2}} = \frac{\sum_{i} (X_{i} - \overline{X}) (y_{i} - \overline{y})}{\sum_{i} (X_{i} - \overline{X})^{2}}.$$
 (7)

From (4) and (6), multiplying and dividing by n,

$$Var(\hat{b}|X,\sigma^2) = \frac{\sigma^2}{n} \left[\frac{1}{n} \sum_{i} (X_i - \overline{X})^2 \right]^{-1}, \tag{8}$$

where $\frac{1}{n}\sum_{i}(X_{i}-\overline{X})^{2}$ is the sampling variance of X.

If X is allowed to vary, the unconditional (with respect to X) variance of the least squares estimator is

$$Var(\hat{b}|\sigma^{2}) = E_{X}\left[Var(\hat{b}|X,\sigma^{2})\right] + Var_{X}\left[E(\hat{b}|X,\sigma^{2})\right]$$

$$= E_{X}\left[Var(\hat{b}|X,\sigma^{2})\right]$$

$$= \frac{\sigma^{2}}{n}E\left\{\left[\frac{1}{n}\sum_{i}(X_{i}-\overline{X})^{2}\right]^{-1}\right\}.$$
(9)

As n increases, the sampling variance of X converges to the true variance of X, Var(X), the inverse of the sampling variance converges to the inverse of the true variance, and

$$Var(\hat{b}|\sigma^2) \to \frac{\sigma^2}{n} [Var(X)]^{-1}.$$
 (10)

Another line of argument followed in the book that leads to (10) is as follows. Instead of fitting model (1) consider fitting the model to the original data y excluding the intercept and using centred covariates $x_i = (X_i - \overline{X})$. The equation for the mean of y given x is

$$E(y|x) = xb. (11)$$

The least squares estimator is now

$$\hat{b} = (x'x)^{-1}x'y$$

$$= \left[\sum_{i} (X_{i} - \overline{X})^{2}\right]^{-1} \sum_{i} (X_{i} - \overline{X})y_{i}$$

$$= \frac{\sum_{i} (X_{i} - \overline{X})(y_{i} - \overline{y})}{\sum_{i} (X_{i} - \overline{X})^{2}}$$

as in (7) with sampling variance

$$Var(\hat{b}|x,\sigma^2) = (x'x)^{-1}\sigma^2$$

$$= \frac{\sigma^2}{\sum_i (X_i - \overline{X})^2}$$
(12)

as in (8). Arguing as before, the same asymptotic unconditional variance (10) is obtained in the case of (12).

Availability of \hat{b} leads to the estimator of α

$$\hat{\alpha} = \overline{y} - \hat{b}\overline{X}.\tag{13}$$

These results obtained using a single covariate regression model as an example, extend to a model based on an arbitrary number p of (possibly) correlated covariates, provided p < n and matrix X is of full rank.

Linear regression with multiple predictor variables

The multiple linear regression model takes the standard form

$$y = 1\alpha + Xb + e \tag{14}$$

where y is the vector of records with n elements, as before, 1 is the column vector of 1's with n elements, α is the scalar intercept, $X = \{X_{ij}\}, i = 1, ..., n; j = 1, ..., p$, is the full rank matrix of p covariates of order $n \times p$, p is the vector of p multiple regression coefficients and the random residuals are collected in the vector $e \sim (0, I\sigma^2)$. Given the model, the normal equations are

$$1'1\hat{\alpha} + 1'X\hat{b} = 1'y,$$

$$X'1\hat{\alpha} + X'X\hat{b} = X'y.$$

Absorbing $\hat{\alpha}$ in the second equation results in the system

$$X'(I-P)X\hat{b} = X'(I-P)y \tag{15}$$

where the operator P is given by

$$P = 1(1'1)^{-1}1' = \frac{1}{n}11' \tag{16}$$

and I - P is symmetric and idempotent. It is easy to confirm that the effect of P on the system (15) is such that

$$X'(I - P)X = x'x,$$

$$X'(I - P) = x'$$

where

$$x = X - \overline{X} \tag{17}$$

and the $n \times p$ matrix \overline{X} has the *i*th generic row equal to $(\overline{X}_1, \overline{X}_2, \dots, \overline{X}_p)$, $\overline{X}_i = \frac{1}{n} \sum_{j=1}^n X_{ij}$. Therefore the least squares estimator for b is

$$\hat{b} = (x'x)^{-1}x'y (18)$$

with sampling variance

$$Var(\hat{b}|X,\sigma^2) = \sigma^2(x'x)^{-1}.$$
 (19)

With \hat{b} available, the estimator of α is

$$\hat{\alpha} = \overline{y} - \sum_{i=1}^{p} \overline{X}_i \hat{b}_i. \tag{20}$$

The marginal asymptotic variance of the least squares estimator is obtained arguing as before. Write (19) as

$$Var(\hat{b}|X,\sigma^2) = \frac{\sigma^2}{n} \left(\frac{1}{n}x'x\right)^{-1}.$$
 (21)

The *i*th diagonal element of $\frac{1}{n}x'x$ is

$$\frac{1}{n}\left[\left(X_{1i}-\overline{X}_i\right)^2+\left(X_{2i}-\overline{X}_i\right)^2+\cdots+\left(X_{ni}-\overline{X}_i\right)^2\right]$$

and the element in row i and column j of $\frac{1}{n}x'x$ is

$$\frac{1}{n} \left[\left(X_{1i} - \overline{X}_i \right) \left(X_{1j} - \overline{X}_j \right) + \left(X_{2i} - \overline{X}_i \right) \left(X_{2j} - \overline{X}_j \right) + \dots + \left(X_{ni} - \overline{X}_i \right) \left(X_{nj} - \overline{X}_j \right) \right].$$

These are sampling variances of the ith covariate and sampling covariances between covariates i and j, respectively. As n increases towards infinity, these sample moments converge to the true variances and covariances and

$$\frac{1}{n}x'x \to V$$

the true variance-covariance matrix of X. Therefore the marginal unconditional variance of \hat{b} is

$$Var(\hat{b}|\sigma^{2}) = E_{X} \left[Var(\hat{b}|X, \sigma^{2}) \right] + Var_{X} \left[E(\hat{b}|X, \sigma^{2}) \right]$$

$$= E_{X} \left[Var(\hat{b}|X, \sigma^{2}) \right]$$

$$= \frac{\sigma^{2}}{n} E \left\{ \left[\frac{1}{n} x'x \right]^{-1} \right\}$$

$$\rightarrow \frac{\sigma^{2}}{n} V^{-1}.$$
(22)

The same result (22) is arrived at if a model excluding the intercept and using centred covariates is fitted to the original data y. The model for the mean takes the form

$$E(y|x) = xb,$$

where x is defined in (17). This leads to the least squares estimator (18) and the remaining narrative leading to (22) is the same as before.

References