Notation: y_i is a scalar, and x_i is a $K \times 1$ vector. Y is an $n \times 1$ vector, and X is an $n \times K$ matrix.

1 Algebra of Least Squares

1.1 OLS estimator

As we have learned from the linear project model, the parameter β

$$y_i = x_i'\beta + e_i$$
$$E[x_ie_i] = 0$$

can be written as $\beta = (E[x_i x_i'])^{-1} E[x_i y_i]$.

While population is something imaginary, in reality we possess a sample of n observations. We thus replace the population mean $E\left[\cdot\right]$ by the sample mean, and the resulting estimator is

$$\widehat{\beta} = \left(\frac{1}{n} \sum_{i=1}^{n} x_i x_i'\right)^{-1} \frac{1}{n} \sum_{i=1}^{n} x_i y_i = (X'X)^{-1} X'y.$$

This is one way to motivate the OLS estimator.

Alternatively, we can derive the OLS estimator from minimizing the sum of squared residuals $\sum_{i=1}^{n} (y_i - x_i'\beta)^2$. By a routine optimization, we obtain exactly the same $\widehat{\beta}$.

Here we introduce some definitions and properties from OLS estimation.

- Fitted value: $\widehat{Y} = X\widehat{\beta}$.
- Residual: $\hat{e} = Y \hat{Y}$.
- Projector: $P_X = X (X'X)^{-1} X$; Annihilator: $M_X = I_n P_X$.
- $P_X M_X = M_X P_X = 0.$
- Idempotent matrix: $P_X P_X = P_X$, $M_X M_X = M_X$.
- $\hat{e} = Y \hat{Y} = Y X\hat{\beta} = M_X Y = M_X (X\beta + e) = M_X e$.

- $X'\widehat{e} = XM_X e = 0$.
- $\frac{1}{n} \sum_{i=1}^{n} \widehat{e}_i = 0$ if x_i contains a constant.

1.2 Goodness of Fit

The so-called R-square is the most popular measure of goodness-of-fit in the linear regression. R-square is well defined only when a constant is included in the regressors. Let $M_{\iota} = I_n - \frac{1}{n}\iota\iota'$, where ι is an $n \times 1$ vector of 1's. M_{ι} is the demeaner, in the sense that $M_{\iota}(z_1, \ldots, z_n)' = (z_1 - \overline{z}, \ldots, z_n - \overline{z})'$, where $\overline{z} = \frac{1}{n} \sum_{i=1}^{n} z_i$. For any X, we can decompose $Y = P_X Y + M_X Y = \widehat{Y} + \widehat{e}$. The total variation is

$$Y'M_{\iota}Y = \left(\widehat{Y} + \widehat{e}\right)'M_{\iota}\left(\widehat{Y} + \widehat{e}\right) = \widehat{Y}'M_{\iota}\widehat{Y} + 2\widehat{Y}'M_{\iota}\widehat{e} + \widehat{e}'M_{\iota}\widehat{e} = \widehat{Y}'M_{\iota}\widehat{Y} + \widehat{e}'\widehat{e}$$

where the last equality follows by $M_{\iota}\widehat{e} = \widehat{e}$ as $\frac{1}{n}\sum_{i=1}^{n}\widehat{e}_{i} = 0$, and $\widehat{Y}'\widehat{e} = Y'P_{X}M_{X}e = 0$. R-square is defined as $\widehat{Y}'M_{\iota}\widehat{Y}/Y'M_{\iota}Y$.

1.3 Frish-Waugh-Lovell Theorem

If
$$Y = X_1\beta_1 + X_2\beta_2 + e$$
, then $\hat{\beta}_1 = (X_1'M_{X_2}X_1)^{-1}X_1'M_{X_2}Y$.

2 Statistical Properties of Least Squares

To talk about the statistical properties, we impose the following assumptions.

- 1. The data $(y_i, x_i)_{i=1}^n$ is a random sample from the same data generating process $y_i = x_i' \beta + e_i$.
- 2. e_i and x_i are independent.
- 3. $e_i \sim N(0, \sigma^2)$.

2.1 Normal Regression

Under the normality assumption, $y_i|x_i \sim N(x_i'\beta, \gamma)$, where $\gamma = \sigma^2$. The conditional likelihood of observing a sample $(y_i, x_i)_{i=1}^n$ is

$$\prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\gamma}} \exp\left(-\frac{1}{2\gamma} \left(y_i - x_i'\beta\right)^2\right),\,$$

and the (conditional) log-likelihood function is

$$L(\beta, \gamma) = -\frac{n}{2} \log 2\pi - \frac{n}{2} \log \gamma - \frac{1}{2\gamma} \sum_{i=1}^{n} (y_i - x_i'\beta)^2.$$

Therefore, the maximum likelihood estimator (MLE) coincides with the OLS estimator, and $\hat{\gamma}_{\text{MLE}} = \hat{e}'\hat{e}/n$.

We can show the finite-sample exact distribution of $\widehat{\beta}$. Since

$$\widehat{\beta} = (X'X)^{-1} X'y = (X'X)^{-1} X' (X'\beta + e) = \beta + (X'X)^{-1} X'e,$$

we have the estimator $\widehat{\beta}|X \sim N\left(\beta, \sigma^2 \left(X'X\right)^{-1}\right)$, and

$$\widehat{\beta}_k | X \sim N\left(\beta_k, \eta_k' \sigma^2 \left(X'X\right)^{-1} \eta_k\right) \sim N\left(\beta_k, \sigma^2 \left(X'X\right)_{kk}^{-1}\right),$$

where $\eta_k = (1\{l=k\})_{l=1,\dots,K}$ is the selector of the k-th element. Consider the T-statistic

$$T_{k} = \frac{\widehat{\beta}_{k} - \beta_{k}}{\sqrt{s^{2} (X'X)_{kk}^{-1}}} = \frac{\left(\widehat{\beta}_{k} - \beta_{k}\right) / \sqrt{\sigma^{2} (X'X)_{kk}^{-1}}}{\sqrt{s^{2} / \sigma^{2}}}.$$

The numerator follows a standard normal, and the denominator follows $\chi^2(n-K)$. Moreover, the numerator and the denominator are independent. As a result, $T_k \sim t \, (n-K)$.

2.2 Gauss-Markov Theorem

Now we relax the normality assumption and statistical independence. Instead, we assume a random sample and

$$y_i = x_i'\beta + e_i$$

$$E[e_i|x_i] = 0$$

$$E[e_i^2|x_i] = \sigma^2.$$
(1)

- (1) is called the mean independence assumption, and (2) is the homoskedasticity assumption.
 - Unbiasedness: $E\left[\widehat{\beta}|X\right] = E\left[\left(X'X\right)^{-1}XY|X\right] = E\left[\left(X'X\right)^{-1}X\left(X'\beta + e\right)|X\right] = \beta$. Unbiasedness does not rely on the homoskedasticity assumption.
 - Variance:

$$\operatorname{var}\left(\widehat{\beta}|X\right) = E\left[\left(\widehat{\beta} - E\widehat{\beta}\right)\left(\widehat{\beta} - E\widehat{\beta}\right)'|X\right]$$

$$= E\left[\left(X'X\right)^{-1}X'ee'X\left(X'X\right)^{-1}|X\right]$$

$$= \left(X'X\right)^{-1}X'E\left[ee'|X\right]X\left(X'X\right)^{-1}$$

$$= \left(X'X\right)^{-1}X'\left(\sigma^{2}I_{n}\right)X\left(X'X\right)^{-1}$$

$$= \sigma^{2}\left(X'X\right)^{-1}.$$

Gauss-Markov theorem justifies the OLS estimator as the efficient estimator among all linear unbiased ones. Efficient here means that it enjoys the smallest variance in a family of estimators.

There are numerous linearly unbiased estimators. For example, $(Z'X)^{-1}Z'y$ for $z_i = x_i^2$ is unbiased because $E\left[(Z'X)^{-1}Z'y\right] = E\left[(Z'X)^{-1}Z'(X\beta + e)\right] = \beta$.

Let $\tilde{\beta}=A'y$ be a generic linear estimator, where A is any $n\times K$ functions of X. As

$$E\left[A^{\prime}y|X\right]=E\left[A^{\prime}\left(X\beta+e\right)|X\right]=A^{\prime}X\beta.$$

So the linearity and unbiasedness of $\tilde{\beta}$ implies $A'X = I_n$. Moreover, the

variance

$$\operatorname{var}(A'y|X) = E\left[(A'y - \beta) (A'y - \beta)' | X \right] = E\left[A'ee'A|X \right] = \sigma^2 A'A.$$
Let $C = A - X (X'X)^{-1}$.
$$A'A - (X'X)^{-1}$$

$$= \left(C + X (X'X)^{-1} \right)' \left(C + X (X'X)^{-1} \right) - (X'X)^{-1}$$

$$= C'C + (X'X)^{-1} X'C + C'X (X'X)^{-1} = C'C,$$

where the last equality follows as

$$(X'X)^{-1}X'C = (X'X)^{-1}X'(A - X(X'X)^{-1}) = (X'X)^{-1} - (X'X)^{-1} = 0.$$

Therefore $A'A - (X'X)^{-1}$ is a positive semi-definite matrix. The variance of any $\tilde{\beta}$ is no smaller than the OLS estimator $\hat{\beta}$.

Homoskedasticity is a restrictive assumption. Under homoskedasticity, $\operatorname{var}\left(\widehat{\beta}\right) = \sigma^2 \left(X'X\right)^{-1}$. Popular estimator of σ^2 is the sample mean of the residuals $\widehat{\sigma}^2 = \frac{1}{n}\widehat{e}'\widehat{e}$ or the unbiased one $s^2 = \frac{1}{n-K}\widehat{e}'\widehat{e}$. Under heteroskedasticity, Gauss-Markov theorem does not apply.