Lecture 2

Multiple Linear Regression: Estimation

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Lecture Outline

- 1 Multiple Linear Regression: Estimation
 - Algebraic Properties of LS Estimation
 - Statistical Properties of LS Estimation
 - LS Estimation in Matrix Notations
 - Consequence of Over- and Under-Specification

Linear Specification

In practice, the systematic part of the dependent variable y may be better characterized by a collection of k (k > 1) explanatory variables, such that

$$y = f(x_1, \ldots, x_k) + u,$$

where u is the error term (non-systematic part of y). As in simple linear regression, it is convenient to postulate f as the linear function, and

$$y = \underbrace{\beta_0 + \beta_1 x_1 + \dots + \beta_k x_k}_{\text{systematic part}} + \underbrace{u(\beta_0, \beta_1, \dots, \beta_k)}_{\text{error}},$$

with k+1 unknown parameters β_0 , β_1, \ldots, β_k .

Least-Squares Minimization

Given the sample data $(x_{i1}, \ldots, x_{ik}, y_i)$, $i = 1, \ldots, n$, we have

$$y_i = \beta_0 + \beta_1 x_{i1} + \dots + \beta_k x_{ik} + u_i, \quad i = 1, \dots, n,$$

where $u_i = u_i(\beta_0, \beta_1, \dots, \beta_k)$ is the ith error. Our goal now is to find a hyperplane that "best" fits the sample data. The best fit of data can be obtained by minimizing the sum of squared errors with respect to $\beta_0, \beta_1, \dots, \beta_k$:

$$Q_n(\beta_0, \beta_1, \dots, \beta_k) = \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_{i1} - \dots - \beta_k x_{ik})^2.$$

The FOCs of the LS problem now contain k+1 equations with k+1 unknowns:

$$\frac{\partial Q_n(\beta_0, \beta_1, \dots, \beta_k)}{\partial \beta_0} = -2 \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_{i1} - \dots - \beta_k x_{ik}) = 0,$$

$$\frac{\partial Q_n(\beta_0, \beta_1, \dots, \beta_k)}{\partial \beta_1} = -2 \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_{i1} - \dots - \beta_k x_{ik}) x_{i1} = 0,$$

$$\vdots$$

$$\frac{\partial Q_n(\beta_0, \beta_1, \dots, \beta_k)}{\partial \beta_k} = -2 \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_{i1} - \dots - \beta_k x_{ik}) x_{ik} = 0.$$

The solutions to the FOCs are the OLS estimators: $\hat{\beta}_0, \hat{\beta}_1, \dots, \hat{\beta}_k$. We shall present the analytic forms of these estimators using matrix notations later.

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Remark: The OLS method does not require any assumptions on sample data, except that there should be no exact linear relations among regressors and the constant term. To see this, suppose $x_{i3} = x_{i1} + x_{i2}$ for all i. Then, the following two FOCs:

$$\sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_{i1} - \dots - \beta_k x_{ik}) x_{i1} = 0,$$

$$\sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_{i1} - \dots - \beta_k x_{ik}) x_{i2} = 0,$$

imply that the FOC: $\sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_{i1} - \dots - \beta_k x_{ik}) x_{i3} = 0$ also holds. That is, when there is an exact linear relation among regressors, some FOC must be redundant, and the number of effective FOCs would be less than k+1. As such, he OLS estimators cannot be uniquely solved from the FOCs.

Given $\hat{\beta}_0, \hat{\beta}_1, \dots, \hat{\beta}_k$, the estimated regression hyperplane is:

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \dots + \hat{\beta}_k x_k,$$

with the *i*th fitted value $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_{i1} + \cdots + \hat{\beta}_k x_{ik}$; the *i*th residual is $\hat{u}_i = y_i - \hat{y}_i$.

- $\hat{\beta}_i = d\hat{y}/dx_i$, still known as a "slope" parameter, predicts how much y would change when the jth regressor changes by one unit, while holding other regressors fixed. We usually say $\hat{\beta}_i$ is the marginal effect of x_i after the effects of other regressors are "controlled."
- $\hat{\beta}_i$ is not the same as the OLS estimate of regressing y on x_i only, because the latter is obtained without controlling other regressors; see the following slides.
- $\hat{\beta}_n$ is the intercept and predicts the level of y when $x_1 = \cdots = x_k = 0$.

A "Partialling Out" Interpretation

We shall use the following analytic formula to illustrate the marginal effect of the OLS estimator (we omit the proof):

$$\hat{\beta}_1 = \frac{\sum_{i=1}^n \hat{r}_{i,1} y_i}{\sum_{i=1}^n \hat{r}_{i,1}^2},$$

where $\hat{r}_{i,1}$ are the ith OLS residuals of regressing x_1 on the constant one and x_2, \ldots, x_k .

- This is also the OLS estimator of regressing y on \hat{r}_1 (without the constant term) and represents the marginal effect of \hat{r}_1 on y.
- By definition, \hat{r}_1 is part of x_1 that is **not** linearly related with x_2,\ldots,x_k . Hence, $\hat{\beta}_1$ can be understood as the "pure" effect of x_1 on y, because the effects of x_2,\ldots,x_k on x_1 have been "partialled out" or "purged away".

Note that $\hat{\beta}_1$ is, in general, not the same as the OLS estimator of regressing y on the constant one and x_1 :

$$\hat{b}_1 = \frac{\sum_{i=1}^n (x_{i,1} - \bar{x}_1) y_i}{\sum_{i=1}^n (x_{i,1} - \bar{x}_1)^2},$$

unless $x_{i,1} - \bar{x}_1 = \hat{r}_{i,1}$. These two estimators would coincide when x_2, \ldots, x_k are not linearly related to x_1 , so that regressing x_1 on the constant one and x_2, \ldots, x_k yields:

$$x_{i,1} = \bar{x}_1 + \hat{r}_{i,1}.$$

On the other hand, this equality above fails when x_2, \ldots, x_k are linearly related to x_1 , so that $\hat{\beta}_1 \neq \hat{b}_1$. As \hat{b}_1 is the marginal effect of x_1 on y without controlling other regressors, it involves both the "pure" effect $(\hat{\beta}_1)$ of x_1 on y and the "indirect" effects of x_2, \ldots, x_k on y via x_1 .

Similarly, let $\hat{r}_{i,j}$ denote the ith OLS residuals of regressing x_j on 1 and x_h , $h \neq j$. Then,

$$\hat{\beta}_j = \frac{\sum_{i=1}^n \hat{r}_{i,j} y_i}{\sum_{i=1}^n \hat{r}_{i,j}^2}, \quad j = 2, \dots, k,$$

which represent the "pure" effect of x_j on y when other regressors $(x_h, h \neq j)$ are controlled. In general, $\hat{\beta}_j$ is not the same as \hat{b}_j , the OLS estimator of regressing y on the constant one and x_j only. These results show that including all relevant variables in a multiple linear regression is important because it allows us to identify the "pure" effect of each regressor.

Algebraic Properties

• Plugging $\hat{\beta}_0, \hat{\beta}_1, \dots, \hat{\beta}_k$ into the FOCs we obtain:

$$\sum_{i=1}^{n} (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_{i1} - \dots - \hat{\beta}_k x_{ik}) = \sum_{i=1}^{n} \hat{u}_i = 0,$$

so that the positive and negative residuals cancel out, and

$$\sum_{i=1}^{n} (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_{i1} - \dots - \hat{\beta}_k x_{ik}) x_{ij} = \sum_{i=1}^{n} \hat{u}_i x_{ij} = 0, \quad j = 1, \dots, k,$$

so that the sample covariance between x_{ij} and \hat{u}_i is zero.

• As $\sum_{i=1}^{n} \hat{u}_i = 0$, we can see:

$$\bar{y} = \hat{\beta}_0 + \hat{\beta}_1 \bar{x}_1 + \dots + \hat{\beta}_k \bar{x}_k,$$

which shows the estimated regression hyperplane must pass through $(\bar{x}_1, \dots, \bar{x}_{\nu}, \bar{y})$.



• Knowing that $\sum_{i=1}^n \hat{u}_i = 0$ and $\sum_{i=1}^n \hat{u}_i x_{ii} = 0$, we have

$$\sum_{i=1}^{n} \hat{u}_{i} \hat{y}_{i} = \sum_{i=1}^{n} \hat{u}_{i} (\hat{\beta}_{0} + \hat{\beta}_{1} x_{i1} + \dots + \hat{\beta}_{k} x_{ik})$$

$$= \hat{\beta}_{0} \sum_{i=1}^{n} \hat{u}_{i} + \hat{\beta}_{1} \sum_{i=1}^{n} \hat{u}_{i} x_{i1} + \dots + \hat{\beta}_{k} \sum_{i=1}^{n} \hat{u}_{i} x_{ik}$$

$$= 0,$$

so that the sample covariance between the fitted values and the residuals is also zero.

It follows that

$$\sum_{i=1}^{n} \hat{u}_{i} y_{i} = \sum_{i=1}^{n} \hat{u}_{i} (\hat{y}_{i} + \hat{u}_{i}) = \sum_{i=1}^{n} \hat{u}_{i}^{2}.$$

Goodness of Fit: R^2

We have learned that the total sum of squares (SST) is the sum of the residual sum of squares (SSR) and the explained sum of squares (SSE):

$$\sum_{i=1}^{n} (y_i - \bar{y})^2 = \sum_{i=1}^{n} \hat{u}_i^2 + \sum_{i=1}^{n} (\hat{y}_i - \bar{y})^2.$$

For multiple regressions, we also use the coefficient of determination as a measure of goodness of fit:

$$R^2 = SSE/SST = 1 - SSR/SST,$$

which measures the proportion of the total variation (SST) of y_i due to the variation of \hat{y}_i (SSE). Again, $0 \le R^2 \le 1$, and a specification has a better (worse) fit of data if its R^2 is closer to one (zero).



Drawback: R^2 is non-decreasing in the number of regressors. That is, adding regressors to a regression will result in higher R^2 . As such, one would tend to choose a more complex model if R^2 is the criterion for determining a model. To see this, consider two estimated regressions:

$$y_{i} = \tilde{\beta}_{0} + \tilde{\beta}_{1}x_{i1} + \tilde{\beta}_{2}x_{i2} + \tilde{v}_{i},$$

$$y_{i} = \hat{\beta}_{0} + \hat{\beta}_{1}x_{i1} + \hat{\beta}_{2}x_{i2} + \hat{\beta}_{3}x_{3i} + \hat{u}_{i}.$$

Note that the former can be written as:

$$y_i = \tilde{\beta}_0 + \tilde{\beta}_1 x_{i1} + \tilde{\beta}_2 x_{i2} + 0 \cdot x_{3i} + \tilde{v}_i.$$

Clearly, the estimates $\tilde{\beta}_0, \tilde{\beta}_1, \tilde{\beta}_2, 0$ do not minimize the sum of squared errors in the 3-regressor regression, because the last coefficient is restricted to zero. This shows that R^2 of a 2-regressor regression must be smaller (or no greater) than R^2 of the regression with these two regressors and an additional regressor.

Goodness of Fit: Adjusted R^2

To avoid the problem of non-decreasing R^2 , a modified measure of goodness of fit is usually adopted. This is known as \bar{R}^2 , defined as R^2 adjusted for the degrees of freedom:

$$\bar{R}^2 = 1 - \frac{\text{SSR}/(n-k-1)}{\text{SST}/(n-1)}.$$

It can also be written as the difference between R^2 and a penalty term:

$$\bar{R}^2 = R^2 - \frac{k}{n-k-1}(1-R^2),$$

where the penalty term depends on the trade-off between model complexity (k) and model explanatory ability (R^2). Thus, \bar{R}^2 may be decreasing when the contribution of additional regressors to model fitness does not outweigh the penalty on model complexity. In practice, we compare models based on \bar{R}^2 , rather than R^2 .

Statistical Properties

The assumption below is analogous to Classical Assumption I.

Classical Assumption II

The random variables y_i , i = 1, ..., n, are such that:

- (i) $\mathbb{E}(y_i) = b_0 + b_1 x_{i1} + \dots + b_k x_{ik}$ for some b_0, b_1, \dots, b_k , where x_{i1}, \ldots, x_{ik} are non-random;
- (ii) $var(y_i) = \sigma_0^2$, $cov(y_i, y_i) = 0$ for $i \neq j$.

Letting ε_i denote the errors evaluated at b_0, b_1, \ldots, b_k , this assumption is equivalent to: $y_i = b_0 + b_1 x_{i1} + \cdots + b_k x_{ik} + \varepsilon_i$, with x_{i1}, \dots, x_{ik} non-random, $\mathbb{E}(\varepsilon_i) = 0$, $\text{var}(\varepsilon_i) = \sigma_0^2$, and $\text{cov}(\varepsilon_i, \varepsilon_i) = 0$ for $i \neq j$.

Unbiasedness

Unbiasedness of the OLS Estimators

Under Classical Assumption II(i), $\hat{\beta}_j$ are unbiased for b_j , $j=0,1,\ldots,k$.

Proof: Note that $\hat{r}_{i,1}$ are non-random because they are the OLS residuals of regressing x_1 on the constant one and x_2, \ldots, x_k . By Classical Assumption II(i) and the formula for the "partialling out" argument,

$$\mathbb{E}(\hat{\beta}_{1}) = \frac{\sum_{i=1}^{n} \hat{r}_{i,1} \mathbb{E}(y_{i})}{\sum_{i=1}^{n} \hat{r}_{i,1}^{2}}$$

$$= \frac{\sum_{i=1}^{n} \hat{r}_{i,1} (b_{0} + b_{1}x_{i1} + \dots + b_{k}x_{ik})}{\sum_{i=1}^{n} \hat{r}_{i,1}^{2}}$$

$$= \frac{b_{0} \sum_{i=1}^{n} \hat{r}_{i,1} + b_{1} \sum_{i=1}^{n} \hat{r}_{i,1}x_{i1} + \dots + b_{k} \sum_{i=1}^{n} \hat{r}_{i,1}x_{ik}}{\sum_{i=1}^{n} \hat{r}_{i,1}^{2}}.$$

Recall that the FOCs of the LS problem imply: $\sum_{i=1}^{n} \hat{r}_{i,1} = 0$, $\sum_{i=1}^{n} \hat{r}_{i,1} x_{i2} = 0$, ..., $\sum_{i=1}^{n} \hat{r}_{i,1} x_{ik} = 0$. Consequently,

$$\mathbb{E}(\hat{\beta}_1) = \frac{b_1 \sum_{i=1}^n \hat{r}_{i,1} x_{i1}}{\sum_{i=1}^n \hat{r}_{i,1}^2}.$$

By the algebraic properties of OLS regression (Verify!),

$$\sum_{i=1}^{n} \hat{r}_{i,1} x_{i1} = \sum_{i=1}^{n} \hat{r}_{i,1}^{2},$$

so that $\mathbb{E}(\hat{\beta}_1)=b_1$. This proves unbiasedness of $\hat{\beta}_1$. Similarly, we can show $\mathbb{E}(\hat{\beta}_j)=b_j,\,j=2,\ldots,k$.

Variance of the OLS Estimators

Under Classical Assumption II(i) and (ii),

$$\operatorname{var}(\hat{\beta}_j) = \sigma_o^2 \frac{1}{\sum_{i=1}^n (x_{ij} - \bar{x}_j)^2 (1 - R_j^2)}, \quad j = 1, \dots, k,$$

where R_i^2 is R^2 of regressing x_i on 1 and other regressors x_h , $h \neq j$; $var(\hat{\beta}_0)$ has a different form and is omitted.

Remarks

- When x_i is highly linearly related to other regressors, R_i^2 would be high, so that $var(\hat{\beta}_i)$ is large; otherwise, the OLS estimators have a smaller variance and hence are more stable.
- ② When the regressors satisfy an exact linear relation so that $R_i^2 = 1$, the variance would be infinitely large, and the OLS method breaks down, as discussed earlier.



Proof of $var(\hat{\beta}_i)$

To derive $var(\hat{\beta}_1)$, note that under Classical Assumptions,

$$\begin{aligned} \operatorname{var}(\hat{\beta}_{1}) &= \operatorname{var}\left(\frac{\sum_{i=1}^{n} \hat{r}_{i,1} y_{i}}{\sum_{i=1}^{n} \hat{r}_{i,1}^{2}}\right) = \frac{\sum_{i=1}^{n} \hat{r}_{i,1}^{2} \operatorname{var}(y_{i})}{\left(\sum_{i=1}^{n} \hat{r}_{i,1}^{2}\right)^{2}} \\ &= \sigma_{o}^{2} \frac{\sum_{i=1}^{n} \hat{r}_{i,1}^{2}}{\left(\sum_{i=1}^{n} \hat{r}_{i,1}^{2}\right)^{2}} = \sigma_{o}^{2} \frac{1}{\sum_{i=1}^{n} \hat{r}_{i,1}^{2}}. \end{aligned}$$

For the regression of x_1 on the constant one and x_2, \ldots, x_k ,

$$\sum_{i=1}^{n} \hat{r}_{i,1}^{2} = SSR_{1} = SST_{1} - SSE_{1} = SST_{1}(1 - SSE_{1}/SST_{1})$$

$$= \sum_{i=1}^{n} (x_{i1} - \bar{x}_{1})^{2} (1 - R_{1}^{2}),$$

proving the formula for $var(\hat{\beta}_1)$. Other $var(\hat{\beta}_i)$ can be derived similarly.

As \hat{u}_i in multiple linear regression must satisfy k+1 FOCs and hence lose k+1 degrees of freedom, the OLS estimator of σ_0^2 is computed as:

$$\hat{\sigma}^2 = \frac{1}{n-k-1} \sum_{i=1}^n \hat{u}_i^2.$$

This estimator is unbiased for σ_o^2 (proof omitted here).

Unbiasedness of $\hat{\sigma}^2$

Under Classical Assumption II(i) and (ii), $\mathbb{E}(\hat{\sigma}^2) = \sigma_{\hat{\sigma}}^2$.

Replacing σ_0^2 with $\hat{\sigma}^2$, we obtain the following variance estimators:

$$\widehat{\text{var}(\hat{\beta}_j)} = \hat{\sigma}^2 \frac{1}{\sum_{i=1}^n (x_{ij} - \bar{x}_j)^2 (1 - R_i^2)}, \quad j = 1, \dots, k,$$

which are also unbiased for $var(\hat{\beta}_i)$. The square root of $var(\hat{\beta}_i)$ is referred to as the standard error of $\hat{\beta}_i$.

Efficiency of the OLS Estimators

From the OLS formula:

$$\hat{\beta}_j = \frac{\sum_{i=1}^n \hat{r}_{i,j} y_i}{\sum_{i=1}^n \hat{r}_{i,j}^2}, \quad j = 1, \dots, k,$$

we can see that $\hat{\beta}_j$ is a linear combination of y_i : $\sum_{i=1}^n a_{i,j} y_i$, with $a_{i,j} = \hat{r}_{i,j} / \sum_{i=1}^n \hat{r}_{i,j}^2$, i.e., an estimator linear in y_i . The result below asserts that, compared with all linear unbiased estimators for b_j , $\hat{\beta}_j$ is the best in the sense that it has the smallest variance or is the most efficient. A proof will be given later using matrix notations.

Gauss-Markov Theorem

Under Classical Assumption II(i) and (ii), $\hat{\beta}_j$ are the best linear unbiased estimators (BLUEs) for b_i , $j=0,1,\ldots,k$.

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Example: Wage Regression with 2 Regressors

The estimated wage model based on Taiwan's 2010 male data (11561 obs): The dependent variable is log(wage), and the estimated parameters are:

$$3.8939 + 0.0800 \, {
m educ} + 0.0166 \, {
m exper}, \quad ar{R}^2 = 0.2893, \ (0.0198) \quad (0.0012) \quad (0.0003) \quad \hat{\sigma} = 0.3595; \ 4.5929 + 0.0494 \, {
m educ}, \qquad ar{R}^2 = 0.1329, \ (0.0156) \quad (0.0012) \qquad \hat{\sigma} = 0.3971; \ 5.1208 \qquad + 0.0059 \, {
m exper}, \quad ar{R}^2 = 0.0263, \ (0.0073) \qquad (0.0003) \qquad \hat{\sigma} = 0.4208;$$

where the numbers in the parentheses are the standard errors. Note that for the regression with two regressors, \bar{R}^2 is much larger than those with only one regressor, and the marginal effect of educ is also larger (8%) when exper is controlled (Why?).

Example: Wage Regression with 3 Regressors

Adding a new regressor exper², the estimated parameters are:

$$3.790 + 0.0779 \, \mathrm{educ} + 0.0365 \, \mathrm{exper} - 0.0005 \, \mathrm{exper}^2,$$
 (0.0199) (0.0012) (0.0009) (0.00002) $\bar{R}^2 = 0.319, \ \hat{\sigma} = 0.3519.$

- The new regressor exper² is a nonlinear function of exper, so that there is no linear relation among regressors. Note that \bar{R}^2 increases.
- The marginal effect of exper is (0.0365 0.001 exper). Setting this effect to zero, we find that the effect of the years of working experience on log(wage) reaches the maximum when exper = 36.5. Thus, log(wage) increases with a decreasing rate (-0.001) before experience reaches 36.5 years.

LS Estimation in Matrix Notations

The specification is: $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{u}(\boldsymbol{\beta})$, where

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, \quad \mathbf{X} = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1k} \\ 1 & x_{21} & x_{22} & \cdots & x_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{nk} \end{bmatrix}, \quad \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_k \end{bmatrix},$$

and $\mathbf{u}(\beta) = (u_1(\beta) \ u_2(\beta) \dots u_n(\beta))'$. The LS problem is to minimize

$$Q_n(\beta) := (\mathbf{y} - \mathbf{X}\beta)'(\mathbf{y} - \mathbf{X}\beta).$$

The FOCs are $-2X'(y - X\beta) = 0$, leading to the normal equations:

$$X'X\beta = X'y,$$

where X'X is $(k+1) \times (k+1)$ and X'y is $(k+1) \times 1$.



The OLS Estimator

Pre-multiplying both sides of the normal equations by $(X'X)^{-1}$ (provided that the inverse exists), we obtain the OLS estimator of β :

$$\hat{\boldsymbol{\beta}} = (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{y}.$$

Remarks:

- The inverse $(X'X)^{-1}$ exists if X is of full column rank k+1, i.e., any column of X is not a linear combination of other columns. As the inverse matrix $(X'X)^{-1}$ is unique, $\hat{\beta}$ is also unique.
- When X is not of full column rank, we say there exists exact
 multicollinearity among regressors. In this case, the matrix X'X is
 not invertible, and the OLS method breaks down.



Given the OLS estimator $\hat{\beta}$, the vector of the OLS fitted values is $\hat{y} = X\hat{\beta}$, and the vector of the OLS residuals is $\hat{u} = y - \hat{y}$. The FOCs yield the following algebraic properties:

$$\boldsymbol{X}'(\boldsymbol{y} - \boldsymbol{X}\hat{\boldsymbol{\beta}}) = \boldsymbol{X}'\hat{\boldsymbol{u}} = \begin{bmatrix} \sum_{i=1}^{n} \hat{u}_{i} \\ \sum_{i=1}^{n} x_{i1} \hat{u}_{i} \\ \vdots \\ \sum_{i=1}^{n} x_{ik} \hat{u}_{i} \end{bmatrix} = \boldsymbol{0},$$
$$\hat{\boldsymbol{y}}'\hat{\boldsymbol{u}} = \sum_{i=1}^{n} \hat{y}_{i} \hat{u}_{i} = \hat{\boldsymbol{\beta}}' \boldsymbol{X}' \hat{\boldsymbol{u}} = 0.$$

These are exactly the algebraic properties we observed earlier.

Some Matrix Results

- Given two $n \times 1$ vectors, \mathbf{z} and \mathbf{z} , their inner product is defined as $\mathbf{z}'\mathbf{z} = \sum_{i=1}^{n} x_i z_i$.
- The Euclidean norm of x is

$$\|\mathbf{x}\| = (\mathbf{x}'\mathbf{x})^{1/2} = \Big(\sum_{i=1}^n x_i^2\Big)^{1/2}.$$

- The inner product $x'z = ||x|| ||z|| \cos \theta$, where θ is the angle between x and z. Thus, x and z are said to be orthogonal if x'z = 0.
- The matrix A is said to be a projection matrix if it is idempotent (AA = A). That is, given the projection of x, Ax, projecting it again will not alter the projection: AAx = Ax.



• The projection matrix \mathbf{A} is the orthogonal projection matrix if it is also symmetric $(\mathbf{A} = \mathbf{A}')$. To see this, write $\mathbf{x} = \mathbf{A}\mathbf{x} + (\mathbf{I} - \mathbf{A})\mathbf{x}$. Then, provided that $\mathbf{A} = \mathbf{A}'$, we have

$$(\mathbf{A}\mathbf{x})'(\mathbf{I}-\mathbf{A})\mathbf{x}=\mathbf{x}'\mathbf{A}'(\mathbf{I}-\mathbf{A})\mathbf{x}=\mathbf{x}'(\mathbf{A}-\mathbf{A}\mathbf{A})\mathbf{x}=0.$$

This shows that Ax is orthogonal to (I - A)x, so that Ax is the orthogonal projection of x. Note that when A is an orthogonal projection matrix, so is I - A.

• For two $n \times n$ matrices \boldsymbol{A} and \boldsymbol{B} , $\boldsymbol{A} - \boldsymbol{B}$ is positive semi-definite (p.s.d.) if $x'(\boldsymbol{A} - \boldsymbol{B})x \ge 0$ for all x such that $\|x\| = 1$; $\boldsymbol{A} - \boldsymbol{B}$ is positive definite (p.d.) if the inequality above holds strictly.

Geometric Illustration

Let $P = X(X'X)^{-1}X'$. It can be seen that P is symmetric and idempotent, and hence an orthogonal projection matrix. Note that P projects vectors onto the space spanned by the column vectors of X, span(X). Similarly, I - P is the orthogonal projection matrix that projects vectors onto the orthogonal complement of span(X), span $(X)^{\perp}$. Thus, PX = X, and (I - P)X = 0.

• The vector of the OLS fitted values is

$$\hat{\mathbf{y}} = \mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y} = \mathbf{P}\mathbf{y},$$

the orthogonal projection of y onto span(X).

• The residual vector is $\hat{\boldsymbol{u}} = \boldsymbol{y} - \hat{\boldsymbol{y}} = (\boldsymbol{I} - \boldsymbol{P})\boldsymbol{y}$, the orthogonal projection of \boldsymbol{y} onto span $(\boldsymbol{X})^{\perp}$, and must be orthogonal to $\hat{\boldsymbol{y}}$. That is, $\hat{\boldsymbol{y}}'\hat{\boldsymbol{u}} = 0$.



• Compared with any other projection of y (say, Ay), the orthogonal projection Py provides the "best approximation" to y. Indeed, it is easily verified that the Euclidean norm of $y - Py = \hat{u}$ is the smallest possible:

$$\|\hat{\pmb{u}}\| = \|\pmb{y} - \pmb{P}\pmb{y}\| \le \|\pmb{y} - \pmb{A}\pmb{y}\|,$$

for any other projection matrix **A**. This is precisely what the LS minimization problem does.

• The algebraic property $X'\hat{u} = 0$ holds because \hat{u} is in span $(X)^{\perp}$ and hence must be orthogonal to every column vector of X.

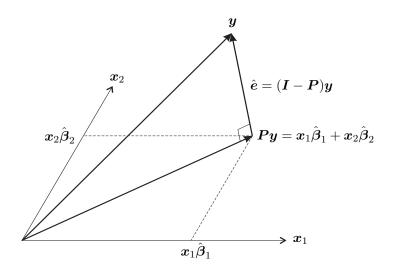


Figure: The orthogonal projection of y onto span (x_1, x_2) .

Example: Simple Linear Regression

The simple linear regression in matrix notations: $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{u}$, with $\boldsymbol{\beta} = (\beta_0 \ \beta_1)'$,

$$\mathbf{X} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}, \quad \mathbf{X}'\mathbf{X} = \begin{bmatrix} n & \sum_{i=1}^n x_i \\ \sum_{i=1}^n x_i & \sum_{i=1}^n x_i^2 \end{bmatrix},$$
$$\mathbf{X}'\mathbf{y} = \begin{bmatrix} \sum_{i=1}^n y_i \\ \sum_{i=1}^n x_i y_i \end{bmatrix}.$$

In this case, X has rank 2 (full column rank) provided that x_i are not a constant. For if x_i are a constant, the second column of X would be a multiple of the first column, so that the rank of X is 1.

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When **X** has full column rank, $(X'X)^{-1}$ exists and reads:

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

Noting that $n \sum_{i=1}^n x_i^2 - (\sum_{i=1}^n x_i)^2 = n \sum_{i=1}^n (x_i - \bar{x})^2$, it is readily verified that

$$(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y} = \left[\begin{array}{c} \bar{y} - \frac{\sum_{i=1}^{n} (x_{i} - \bar{x})y_{i}}{\sum_{i=1}^{n} (x_{i} - \bar{x})^{2}} \bar{x} \\ \frac{\sum_{i=1}^{n} (x_{i} - \bar{x})y_{i}}{\sum_{i=1}^{n} (x_{i} - \bar{x})^{2}} \end{array} \right],$$

which are exactly the OLS estimators $\hat{\beta}_0$ and $\hat{\beta}_1$ obtained earlier in the simple linear regression.

"Partialling Out" Interpretation in Matrix Notations

Frisch-Waugh-Lovell Theorem

For $\mathbf{v} = \mathbf{X}_1 \beta_1 + \mathbf{X}_2 \beta_2 + \mathbf{u}$, the OLS estimators of β_1 and β_2 are:

$$\begin{split} \hat{\boldsymbol{\beta}}_1 &= [\boldsymbol{X}_1'(\boldsymbol{I} - \boldsymbol{P}_2)\boldsymbol{X}_1]^{-1}\boldsymbol{X}_1'(\boldsymbol{I} - \boldsymbol{P}_2)\boldsymbol{y}, \\ \hat{\boldsymbol{\beta}}_2 &= [\boldsymbol{X}_2'(\boldsymbol{I} - \boldsymbol{P}_1)\boldsymbol{X}_2]^{-1}\boldsymbol{X}_2'(\boldsymbol{I} - \boldsymbol{P}_1)\boldsymbol{y}, \end{split}$$

where
$$P_1 = X_1(X_1'X_1)^{-1}X_1'$$
 and $P_2 = X_2(X_2'X_2)^{-1}X_2'$.

Remark: Let $X_1 = (I - P_2)X_1$, the matrix of residuals from regressing X_1 on X_2 . As $I - P_2$ is idempotent, we have

$$\hat{\boldsymbol{\beta}}_1 = [\tilde{\boldsymbol{X}}_1' \tilde{\boldsymbol{X}}_1]^{-1} \tilde{\boldsymbol{X}}_1' \boldsymbol{y},$$

the "pure" marginal effect of X_1 on y, where the effect of X_2 on y (via X_1) has been "partialled out". The interpretation of $\hat{\beta}_2$ is similar.

Proof: Letting $X = [X_1, X_2]$ and $P = X(X'X)^{-1}X'$, we can write

$$\mathbf{y} = \mathbf{X}_1 \hat{\boldsymbol{\beta}}_1 + \mathbf{X}_2 \hat{\boldsymbol{\beta}}_2 + (\mathbf{I} - \mathbf{P})\mathbf{y}.$$

Pre-multiplying both sides by $X'_1(I - P_2)$, we have

$$X'_1(I - P_2)y$$

= $X'_1(I - P_2)X_1\hat{\beta}_1 + X'_1(I - P_2)X_2\hat{\beta}_2 + X'_1(I - P_2)(I - P)y$.

Clearly, $(I - P_2)X_2 = 0$, so that the second term vanishes. As $\operatorname{span}(\boldsymbol{X}_2) \subseteq \operatorname{span}(\boldsymbol{X})$, we have $\operatorname{span}(\boldsymbol{X})^{\perp} \subseteq \operatorname{span}(\boldsymbol{X}_2)^{\perp}$, and hence $(I - P_2)(I - P) = I - P$. It follows that the third term also vanishes because $X_1'(I-P_2)(I-P) = X_1'(I-P) = 0$. Consequently,

$$\boldsymbol{X}_1'(\boldsymbol{I}-\boldsymbol{P}_2)\boldsymbol{y} = \boldsymbol{X}_1'(\boldsymbol{I}-\boldsymbol{P}_2)\boldsymbol{X}_1\hat{\boldsymbol{\beta}}_1,$$

from which we obtain the expression for $\hat{\beta}_1$.

Statistical Properties

Classical Assumption II in Matrix Notations

The random vector \mathbf{y} is such that:

- (i) $\mathbb{E}(y) = X b_o$ for some b_o , where X is non-random;
- (ii) $var(y) = \sigma_o^2 I$.

This assumption is equivalent to: $\mathbf{y} = \mathbf{X} \mathbf{b}_o + \boldsymbol{\varepsilon}$, with \mathbf{X} non-random, $\mathbb{E}(\boldsymbol{\varepsilon}) = \mathbf{0}$, $\mathrm{var}(\boldsymbol{\varepsilon}) = \sigma_o^2 \mathbf{I}$.

• Unbiasedness: By Classical Assumption II(i),

$$\mathbb{E}(\hat{\boldsymbol{\beta}}) = (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\mathbb{E}(\boldsymbol{y}) = (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{X}\boldsymbol{b}_o = \boldsymbol{b}_o.$$

Variance: By Classical Assumption II(i) and (ii),

$$\operatorname{var}(\hat{\boldsymbol{\beta}}) = \operatorname{var}[(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{y}]$$
$$= (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'[\operatorname{var}(\boldsymbol{y})]\boldsymbol{X}(\boldsymbol{X}'\boldsymbol{X})^{-1} = \sigma_o^2(\boldsymbol{X}'\boldsymbol{X})^{-1}.$$



Gauss-Markov Theorem

Under Classical Assumption II(i) and (ii), $\hat{\boldsymbol{\beta}}$ is the BLUE for \boldsymbol{b}_o .

Proof: Consider an arbitrary linear estimator $\mathring{\boldsymbol{\beta}} = \boldsymbol{A}\boldsymbol{y}$, where \boldsymbol{A} is a non-random matrix, say, $\boldsymbol{A} = (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}' + \boldsymbol{C}$. Then, $\mathring{\boldsymbol{\beta}} = \hat{\boldsymbol{\beta}} + \boldsymbol{C}\boldsymbol{y}$, and

$$\operatorname{var}(\check{oldsymbol{eta}}) = \operatorname{var}(\hat{oldsymbol{eta}}) + \operatorname{var}(oldsymbol{\mathcal{C}} oldsymbol{y}) + 2 \operatorname{cov}(\hat{oldsymbol{eta}}, oldsymbol{\mathcal{C}} oldsymbol{y}).$$

By Classical Assumption II(i) and (ii), $\mathbb{E}(\check{\beta}) = b_o + CXb_o$, which is unbiased if, and only if, CX = 0. The condition CX = 0 implies

$$\begin{aligned} \operatorname{cov}(\hat{\boldsymbol{\beta}}, \boldsymbol{C} \boldsymbol{y}) &= \mathbb{E}[(\hat{\boldsymbol{\beta}} - \boldsymbol{b}_o) \boldsymbol{y}' \boldsymbol{C}'] = \mathbb{E}[(\boldsymbol{X}' \boldsymbol{X})^{-1} \boldsymbol{X}' (\boldsymbol{y} - \boldsymbol{X} \boldsymbol{b}_o) \boldsymbol{y}' \boldsymbol{C}'] \\ &= (\boldsymbol{X}' \boldsymbol{X})^{-1} \boldsymbol{X}' \mathbb{E}[(\boldsymbol{y} - \boldsymbol{X} \boldsymbol{b}_o) \boldsymbol{y}'] \boldsymbol{C}' \\ &= (\boldsymbol{X}' \boldsymbol{X})^{-1} \boldsymbol{X}' \operatorname{var}(\boldsymbol{y}) \boldsymbol{C}' \\ &= \sigma_o^2 (\boldsymbol{X}' \boldsymbol{X})^{-1} \boldsymbol{X}' \boldsymbol{C}' = \boldsymbol{0}. \end{aligned}$$

Proof (Cont'd): It follows that

$$\operatorname{var}(\check{oldsymbol{eta}}) = \operatorname{var}(\hat{oldsymbol{eta}}) + \operatorname{var}(oldsymbol{\mathcal{C}} oldsymbol{y}) = \operatorname{var}(\hat{oldsymbol{eta}}) + \sigma_o^2 oldsymbol{\mathcal{C}} oldsymbol{\mathcal{C}}';$$

that is, $var(\mathring{\beta}) - var(\mathring{\beta}) = \sigma_0^2 CC'$, a p.s.d. matrix (Verify!). This shows that $\hat{\beta}$ must be more efficient than any linear unbiased estimator $\check{\beta}$. \Box

Note that the estimator $\hat{\sigma}^2$ can be expressed as:

$$\hat{\sigma}^2 = \frac{1}{n-k-1} \sum_{i=1}^n \hat{u}_i^2 = \frac{\hat{u}'\hat{u}}{n-k-1}.$$

It can be shown that, under Classical Assumption II.

$$\mathbb{E}(\hat{\boldsymbol{u}}'\hat{\boldsymbol{u}}) = \sigma_o^2(n-k-1).$$

Hence, $\hat{\sigma}^2$ is unbiased for σ_0^2 .

Inclusion of Irrelevant Variables

For a specification that includes irrelevant variables, we will show the OLS estimators remain unbiased but are not the most efficient.

Suppose we estimate the specification A below:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + u, \quad (A)$$

and obtain the OLS estimators $\tilde{\beta}_i$, j=0,1,2,3. Assume that Classical Assumption II(i) holds with

$$\mathbb{E}(y) = b_0 + b_1 x_1 + b_2 x_2 = b_0 + b_1 x_1 + b_2 x_2 + 0 \cdot x_3;$$

this suggests that the specification A includes an irrelevant regressor x_3 . As Classical Assumption II(i) still holds for b_0 , b_1 , b_2 , and 0, we have $\mathbb{E}(\tilde{\beta}_i) = b_i$, i = 0, 1, 2, and $\mathbb{E}(\tilde{\beta}_3) = 0$.

To examine efficiency of $\tilde{\beta}_i$, note that

$$\operatorname{var}(\tilde{\beta}_1) = \sigma_o^2 \frac{1}{\sum_{i=1}^n (x_{i1} - \bar{x}_1)^2 [1 - R_1^2(A)]},$$

where $R_1^2(A)$ is R^2 of regressing x_1 on 1, x_2 and x_3 . Suppose we estimate the specification B instead:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + u,$$
 (B)

the resulting OLS estimators $\hat{\beta}_i$, j = 0, 1, 2, are such that $\mathbb{E}(\hat{\beta}_i) = b_i$, and

$$\operatorname{var}(\hat{\beta}_1) = \sigma_o^2 \frac{1}{\sum_{i=1}^n (x_{i1} - \bar{x}_1)^2 [1 - R_1^2(B)]},$$

where $R_1^2(B)$ is R^2 of regressing x_1 on 1 and x_2 . Clearly, $R_1^2(B) \le R_1^2(A)$ (Why?), and hence $var(\hat{\beta}_1) \leq var(\tilde{\beta}_1)$. That is, $\tilde{\beta}_1$ is less efficient than $\hat{\beta}_1$. Similarly, $\tilde{\beta}_2$ is less efficient than $\hat{\beta}_2$.

General Case

Suppose we estimate the specification

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{u} = \mathbf{X}_1\boldsymbol{\beta}_1 + \mathbf{X}_2\boldsymbol{\beta}_2 + \mathbf{u},$$

where $\boldsymbol{X} = [\boldsymbol{X}_1 \ \boldsymbol{X}_2]$ with \boldsymbol{X}_1 an $n \times k_1$ matrix and \boldsymbol{X}_2 an $n \times k_2$ matrix, and the OLS estimator is $\tilde{\beta} = (\tilde{\beta}'_1 \ \tilde{\beta}'_2)'$. When the mean function of \mathbf{y} is

$$\mathbb{E}(y) = X_1 b_1 + X_2 0 = X b_0, \quad b_o = (b_1' \ 0')',$$

our specification in fact includes k_2 irrelevant regressors X_2 . Then,

$$\mathbb{E}(\tilde{\boldsymbol{\beta}}) = (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\mathbb{E}(\boldsymbol{y}) = (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{X}\boldsymbol{b}_o = (\boldsymbol{b}_1'\ \boldsymbol{0}')',$$

showing that $\tilde{\beta}_1$ is unbiased for \boldsymbol{b}_1 and $\tilde{\beta}_2$ is unbiased for $\boldsymbol{0}$.



Recall that $\tilde{\boldsymbol{\beta}}_1 = [\boldsymbol{X}_1'(\boldsymbol{I} - \boldsymbol{P}_2)\boldsymbol{X}_1]^{-1}[\boldsymbol{X}_1'(\boldsymbol{I} - \boldsymbol{P}_2)\boldsymbol{y}]$ by the Frisch-Waugh-Lovell Theorem. It is easy to see that, given $var(y) = \sigma_0^2 I$,

$$\begin{split} & \operatorname{var}(\tilde{\boldsymbol{\beta}}_1) \\ &= [\boldsymbol{X}_1'(\boldsymbol{I} - \boldsymbol{P}_2)\boldsymbol{X}_1]^{-1}\boldsymbol{X}_1'(\boldsymbol{I} - \boldsymbol{P}_2)\operatorname{var}(\boldsymbol{y})(\boldsymbol{I} - \boldsymbol{P}_2)\boldsymbol{X}_1[\boldsymbol{X}_1'(\boldsymbol{I} - \boldsymbol{P}_2)\boldsymbol{X}_1]^{-1} \\ &= \sigma_o^2[\boldsymbol{X}_1'(\boldsymbol{I} - \boldsymbol{P}_2)\boldsymbol{X}_1]^{-1}\boldsymbol{X}_1'(\boldsymbol{I} - \boldsymbol{P}_2)(\boldsymbol{I} - \boldsymbol{P}_2)\boldsymbol{X}_1[\boldsymbol{X}_1'(\boldsymbol{I} - \boldsymbol{P}_2)\boldsymbol{X}_1]^{-1} \\ &= \sigma_o^2[\boldsymbol{X}_1'(\boldsymbol{I} - \boldsymbol{P}_2)\boldsymbol{X}_1]^{-1}. \end{split}$$

If we estimate $\mathbf{y} = \mathbf{X}_1 \boldsymbol{\beta}_1 + \mathbf{u}$ without irrelevant regressors \mathbf{X}_2 , the OLS estimator $\hat{\boldsymbol{\beta}}_1 = (\boldsymbol{X}_1' \boldsymbol{X}_1)^{-1} \boldsymbol{X}_1' \boldsymbol{y}$ has variance: $\sigma_2^2 (\boldsymbol{X}_1' \boldsymbol{X}_1)^{-1}$. As

$$\label{eq:control_equation} \mathbf{X}_1'\mathbf{X}_1 - \mathbf{X}_1'(\mathbf{I} - \mathbf{P}_2)\mathbf{X}_1 = \mathbf{X}_1'\mathbf{P}_2\mathbf{X}_1,$$

which is a p.s.d. matrix (Why?),

$$[X_1'(I - P_2)X_1]^{-1} - (X_1'X_1)^{-1}$$

is a p.s.d. matrix. This shows that $\tilde{\beta}_1$ is less efficient than $\hat{\beta}_1$.

Exclusion of Important Variables

For a specification that excludes important variables, the OLS estimators become biased in general. Suppose that we estimate the specification: $y = \beta_0 + \beta_1 x_1 + u$, and obtain the OLS estimators $\tilde{\beta}_0$ and $\tilde{\beta}_1$. Assume $\mathbb{E}(y) = b_0 + b_1 x_1 + b_2 x_2$; this suggests that our specification excludes an important variable x_2 . Then,

$$\mathbb{E}(\tilde{\beta}_{1}) = \frac{\sum_{i=1}^{n} (x_{i1} - \bar{x}_{1}) \mathbb{E}(y_{i})}{\sum_{i=1}^{n} (x_{i1} - \bar{x}_{1})^{2}}$$

$$= \frac{\sum_{i=1}^{n} (x_{i1} - \bar{x}_{1}) (b_{0} + b_{1}x_{i1} + b_{2}x_{i2})}{\sum_{i=1}^{n} (x_{i1} - \bar{x}_{1})^{2}}$$

$$= b_{1} + b_{2} \frac{\sum_{i=1}^{n} (x_{i1} - \bar{x}_{1})x_{i2}}{\sum_{i=1}^{n} (x_{i1} - \bar{x}_{1})^{2}}.$$

Thus, $\ddot{\beta}_1$ is no longer unbiased for b_1 , unless $\sum_{i=1}^n (x_{i1} - \bar{x}_1) x_{i2} = 0$, i.e., the sample covariance of x_{i1} and x_{i2} is zero.

General Case

Suppose we estimate the specification $y = X_1\beta_1 + u$ and obtain the OLS estimator $\tilde{\boldsymbol{\beta}}_1$. If

$$\mathbb{E}(\mathbf{y}) = \mathbf{X}_1 \mathbf{b}_1 + \mathbf{X}_2 \mathbf{b}_2, \quad \mathbf{b}_2 \neq \mathbf{0},$$

so that our specification excludes relevant regressors X_2 , we then have

$$\begin{split} \mathbb{E}(\tilde{\boldsymbol{\beta}}_{1}) &= (\boldsymbol{X}_{1}'\boldsymbol{X}_{1})^{-1}\boldsymbol{X}_{1}'\mathbb{E}(\boldsymbol{y}) \\ &= (\boldsymbol{X}_{1}'\boldsymbol{X}_{1})^{-1}\boldsymbol{X}_{1}'(\boldsymbol{X}_{1}\boldsymbol{b}_{1} + \boldsymbol{X}_{2}\boldsymbol{b}_{2}) \\ &= \boldsymbol{b}_{1} + (\boldsymbol{X}_{1}'\boldsymbol{X}_{1})^{-1}\boldsymbol{X}_{1}'\boldsymbol{X}_{2}\boldsymbol{b}_{2}. \end{split}$$

That is, the OLS estimator $\tilde{\boldsymbol{\beta}}_1$ is biased for \boldsymbol{b}_1 , unless $\boldsymbol{X}_1'\boldsymbol{X}_2 = \boldsymbol{0}$, i.e., every column of X_1 is orthogonal to the columns of X_2 .