Estimable Functions and Their Least Squares Estimators

Consider the GLM

$$\underset{n\times 1}{\boldsymbol{y}} = \underset{n\times p}{\boldsymbol{X}}\ \underset{p\times 1}{\boldsymbol{\beta}} + \underset{n\times 1}{\boldsymbol{\varepsilon}}, \quad \text{where} \quad E(\boldsymbol{\varepsilon}) = \mathbf{0}.$$

Suppose we wish to estimate $\boldsymbol{c}'\boldsymbol{\beta}$ for some fixed and known $\boldsymbol{c} \in \mathbb{R}^p$.

An estimator $t(\boldsymbol{y})$ is an unbiased estimator of the function $\boldsymbol{c}'\boldsymbol{\beta}$ iff

$$E[t(\boldsymbol{y})] = \boldsymbol{c}'\boldsymbol{\beta} \quad \forall\, \boldsymbol{\beta} \in \mathbb{R}^p.$$

An estimator $t(\boldsymbol{y})$ is a linear estimator in $\boldsymbol{y}$ iff

$$t(\boldsymbol{y}) = d + \boldsymbol{a}'\boldsymbol{y}$$

for some known constants $d, a_1, \ldots, a_n$.

A function $\boldsymbol{c}'\boldsymbol{\beta}$ is linearly estimable iff $\exists$ a linear estimator that is an unbiased estimator of $\boldsymbol{c}'\boldsymbol{\beta}$.

Henceforth, we will use estimable as a synonym for linearly estimable.

A function $\boldsymbol{c}'\boldsymbol{\beta}$ is said to be nonestimable if there does not exist a linear estimator that is an unbiased estimator of $\boldsymbol{c}'\boldsymbol{\beta}$.

Result 3.1:

Under the GLM, $\boldsymbol{c}'\boldsymbol{\beta}$ is estimable iff the following equivalent conditions hold:

(i) $\exists\, \boldsymbol{a} \ni E(\boldsymbol{a}'\boldsymbol{y}) = \boldsymbol{c}'\boldsymbol{\beta} \quad \forall\, \boldsymbol{\beta} \in \mathbb{R}^p$

(ii) $\exists\, \boldsymbol{a} \ni \boldsymbol{c}' = \boldsymbol{a}'\boldsymbol{X} \quad (\boldsymbol{X}'\boldsymbol{a} = \boldsymbol{c})$

(iii) $\boldsymbol{c} \in \mathcal{C}(\boldsymbol{X}')$.

Show conditions (i), (ii), and (iii) are equivalent.

(i)$\Longleftrightarrow$(ii)$\Longleftrightarrow$(iii):

$$
\begin{aligned}
&\exists\, \boldsymbol{a} \ni E(\boldsymbol{a}'\boldsymbol{y}) = \boldsymbol{c}'\boldsymbol{\beta} \quad \forall\, \boldsymbol{\beta} \in \mathbb{R}^p \\
&\Longleftrightarrow \exists\, \boldsymbol{a} \ni \boldsymbol{a}'E(\boldsymbol{y}) = \boldsymbol{c}'\boldsymbol{\beta} \quad \forall\, \boldsymbol{\beta} \in \mathbb{R}^p \\
&\Longleftrightarrow \exists\, \boldsymbol{a} \ni \boldsymbol{a}'\boldsymbol{X}\boldsymbol{\beta} = \boldsymbol{c}'\boldsymbol{\beta} \quad \forall\, \boldsymbol{\beta} \in \mathbb{R}^p \\
&\Longleftrightarrow \exists\, \boldsymbol{a} \ni \boldsymbol{a}'\boldsymbol{X} = \boldsymbol{c}' \\
&\Longleftrightarrow \exists\, \boldsymbol{a} \ni \boldsymbol{X}'\boldsymbol{a} = \boldsymbol{c} \\
&\Longleftrightarrow \boldsymbol{c} \in \mathcal{C}(\boldsymbol{X}').
\end{aligned}
$$

Show that any of the equivalent conditions is equivalent to $\boldsymbol{c}'\boldsymbol{\beta}$ estimable.

$\boldsymbol{c}'\boldsymbol{\beta}$ estimable

$$\iff \exists\, d, \boldsymbol{a} \ni E(d + \boldsymbol{a}'\boldsymbol{y}) = \boldsymbol{c}'\boldsymbol{\beta} \quad \forall\, \boldsymbol{\beta} \in \mathbb{R}^p$$

$$\iff \exists\, d, \boldsymbol{a} \ni d + \boldsymbol{a}'\boldsymbol{X}\boldsymbol{\beta} = \boldsymbol{c}'\boldsymbol{\beta} \quad \forall\, \boldsymbol{\beta} \in \mathbb{R}^p$$

$$\iff \exists\, \boldsymbol{a} \ni \boldsymbol{a}'\boldsymbol{X}\boldsymbol{\beta} = \boldsymbol{c}'\boldsymbol{\beta} \quad \forall\, \boldsymbol{\beta} \in \mathbb{R}^p$$

$$\iff \exists\, \boldsymbol{a} \ni \boldsymbol{a}'\boldsymbol{X} = \boldsymbol{c}'.$$

$\square$

Example:

Suppose that when team i competes against team j, the expected margin of victory for team i over team j is $\mu_i - \mu_j$, where $\mu_1, \ldots, \mu_5$ are unknown parameters.

Suppose we observe the following outcomes.

Team	1	beats Team	2	by	7	points
	3		1		3	
	3		2		14	
	3		5		17	
	4		5		10	
	4		1		1	

Determine $\boldsymbol{y}, \boldsymbol{X}, \boldsymbol{\beta}$.

$$\underset{\boldsymbol{y}}{\begin{bmatrix} 7 \\ 3 \\ 14 \\ 17 \\ 10 \\ 1 \end{bmatrix}}, \quad \underset{\boldsymbol{X}}{\begin{bmatrix} 1 & -1 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 1 & -1 \\ -1 & 0 & 0 & 1 & 0 \end{bmatrix}}, \quad \underset{\boldsymbol{\beta}}{\begin{bmatrix} \mu_1 \\ \mu_2 \\ \mu_3 \\ \mu_4 \\ \mu_5 \end{bmatrix}}$$

Is $\mu_1 - \mu_2$ is estimable?

Yes, $\mu_1 - \mu_2$ is estimable.

$\mu_1 - \mu_2 = \boldsymbol{c}'\boldsymbol{\beta}$, where

$$\begin{aligned}\boldsymbol{c}' &= [1, -1, 0, 0, 0] \\ &= [1, 0, 0, 0, 0, 0] \begin{bmatrix} 1 & -1 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 1 & -1 \\ -1 & 0 & 0 & 1 & 0 \end{bmatrix} \\ &= \boldsymbol{a}'\boldsymbol{X}.\end{aligned}$$

Thus,

$$\boldsymbol{a}'\boldsymbol{y} = [1, 0, 0, 0, 0, 0]\boldsymbol{y} = y_1$$

is an unbiased estimator of $\boldsymbol{c}'\boldsymbol{\beta} = \mu_1 - \mu_2$.

Is $\mu_1 - \mu_3$ is estimable?

Yes, $\mu_1 - \mu_3$ is estimable.

$\mu_1 - \mu_3 = \boldsymbol{c}'\boldsymbol{\beta}$, where

$$
\begin{aligned}
\boldsymbol{c}' &= [1, 0, -1, 0, 0] \\
&= [0, -1, 0, 0, 0, 0] \begin{bmatrix} 1 & -1 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 1 & -1 \\ -1 & 0 & 0 & 1 & 0 \end{bmatrix} \\
&= \boldsymbol{a}'\boldsymbol{X}.
\end{aligned}
$$

$\therefore -y_2$ is unbiased estimator of $\mu_1 - \mu_3$.

Is $\mu_1 - \mu_5$ is estimable?

Yes, $\mu_1 - \mu_5$ is estimable.

$\mu_1 - \mu_5 = \boldsymbol{c}'\boldsymbol{\beta}$, where

$$
\begin{aligned}
\boldsymbol{c}' &= [1, 0, 0, 0, -1] \\
&= [0, -1, 0, 1, 0, 0] \begin{bmatrix} 1 & -1 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 1 & -1 \\ -1 & 0 & 0 & 1 & 0 \end{bmatrix} \\
&= \boldsymbol{a}'\boldsymbol{X}.
\end{aligned}
$$

$\therefore y_4 - y_2$ is unbiased estimator of $\mu_1 - \mu_5$.

Is μ_1 estimable?

$\mu_1 = \boldsymbol{c}'\boldsymbol{\beta}$, where

$$\boldsymbol{c}' = [1, 0, 0, 0, 0].$$

So, does $\exists\ \boldsymbol{a} \ni \boldsymbol{a}'\boldsymbol{X} = [1, 0, 0, 0, 0]$?

$$
\boldsymbol{a}'\boldsymbol{X} = [a_1, a_2, a_3, a_4, a_5, a_6] \begin{bmatrix} 1 & -1 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 1 & -1 \\ -1 & 0 & 0 & 1 & 0 \end{bmatrix}
$$

$$
= [a_1 - a_2 - a_6, -a_1 - a_3, a_2 + a_3 + a_4, a_5 + a_6, -a_4 - a_5]
$$

$$
\stackrel{?}{=} [1, 0, 0, 0, 0].
$$

$$a_1 - a_2 - a_6 = 1 \quad (1)$$

$$-a_1 - a_3 = 0 \quad (2)$$

$$a_2 + a_3 + a_4 = 0 \quad (3)$$

$$a_5 + a_6 = 0 \quad (4)$$

$$-a_4 - a_5 = 0 \quad (5)$$

(1) and (2) imply $-a_2 - a_3 - a_6 = 1$.

(4) and (5) imply $a_4 = a_6$, which together with (3) implies $a_2 + a_3 + a_6 = 0$.

$\therefore$ There does not exist $\boldsymbol{a} \ni \boldsymbol{a}'\boldsymbol{X} = [1, 0, 0, 0, 0] \Rightarrow \mu_1$ is nonestimable.

Result 3.1 tells us that $\boldsymbol{c}'\boldsymbol{\beta}$ is estimable iff $\exists\ \boldsymbol{a} \ni \boldsymbol{c}'\boldsymbol{\beta} = \boldsymbol{a}'\boldsymbol{X}\boldsymbol{\beta} \quad \forall\ \boldsymbol{\beta} \in \mathbb{R}^p$.

Recall that $E(\boldsymbol{y}) = \boldsymbol{X}\boldsymbol{\beta}$.

Thus, $\boldsymbol{c}'\boldsymbol{\beta}$ is estimable iff it is a LC of the elements of $E(\boldsymbol{y})$.

This leads to Method 3.1:

LCs of expected values of observations are estimable.

$\boldsymbol{c}'\boldsymbol{\beta}$ is estimable iff $\boldsymbol{c}'\boldsymbol{\beta}$ is a LC of the elements of $E(\boldsymbol{y})$; i.e.,

$$\boldsymbol{c}'\boldsymbol{\beta} = \sum_{i=1}^{n} a_i E(y_i) \quad \text{for some} \quad a_1, \ldots, a_n.$$

Use Method 3.1 to show that $\mu_2 - \mu_4$ is estimable in our previous example.

$$E(\boldsymbol{y}) = \boldsymbol{X\beta} = \begin{bmatrix} \mu_1 - \mu_2 \\ \mu_3 - \mu_1 \\ \mu_3 - \mu_2 \\ \mu_3 - \mu_5 \\ \mu_4 - \mu_5 \\ \mu_4 - \mu_1 \end{bmatrix}.$$

$$\mu_2 - \mu_4 = -(\mu_1 - \mu_2) - (\mu_4 - \mu_1) = -E(y_1) - E(y_6).$$

Method 3.2:

$\boldsymbol{c}'\boldsymbol{\beta}$ is estimable iff $\boldsymbol{c} \in \mathcal{C}(\boldsymbol{X}')$.

Thus, find a basis for $\mathcal{C}(\boldsymbol{X}')$, say $\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_r\}$, and determine if

$$\boldsymbol{c} = \sum_{i=1}^{r} d_i \boldsymbol{v}_i \quad \text{for some} \quad d_1, \ldots, d_r.$$

Method 3.3:

By Result A.5, we know that $\mathcal{C}(\boldsymbol{X}')$ and $\mathcal{N}(\boldsymbol{X})$ are orthogonal complements in $\mathbb{R}^p$.

Thus,

$$\boldsymbol{c} \in \mathcal{C}(\boldsymbol{X}') \quad \text{iff} \quad \boldsymbol{c}'\boldsymbol{d} = 0 \quad \forall\, \boldsymbol{d} \in \mathcal{N}(\boldsymbol{X}),$$

which is equivalent to

$$\boldsymbol{X}\boldsymbol{d} = \boldsymbol{0} \Rightarrow \boldsymbol{c}'\boldsymbol{d} = 0.$$

Reconsider our previous example.

Use Method 3.3 to show that μ_1 is nonestimable.

$$
\begin{aligned}
\boldsymbol{Xd} = \boldsymbol{0} \Rightarrow d_1 - d_2 &= 0 \\
d_3 - d_1 &= 0 \\
d_3 - d_2 &= 0 \\
d_3 - d_5 &= 0 \\
d_4 - d_5 &= 0 \\
d_4 - d_1 &= 0.
\end{aligned}
$$

$\Rightarrow d_1 = d_2 = d_3 = d_4 = d_5$.

For example, $\boldsymbol{X1} = \boldsymbol{0}$. Note $[1, 0, 0, 0, 0]\boldsymbol{1} = 1 \neq 0$. Thus, μ_1 is not estimable.

Now use method 3.3 to establish that

$$\boldsymbol{c}'\boldsymbol{\beta} = c_1\mu_1 + c_2\mu_2 + c_3\mu_3 + c_4\mu_4 + c_5\mu_5$$

is estimable iff

$$\sum_{i=1}^{5} c_i = 0.$$

$\{\boldsymbol{d} \in \mathbb{R}^5 : \boldsymbol{X}\boldsymbol{d} = \boldsymbol{0}\} = \{d \underset{5\times 1}{\boldsymbol{1}} : d \in \mathbb{R}\}$. Thus

$$
\begin{aligned}
&\boldsymbol{c}'\boldsymbol{d} = 0 \quad \forall\, \boldsymbol{d} \in \mathcal{N}(\boldsymbol{X}) \\
&\iff \boldsymbol{c}'(d\boldsymbol{1}) = 0 \quad \forall\, d \in \mathbb{R} \\
&\iff d\boldsymbol{c}'\boldsymbol{1} = 0 \quad \forall\, d \in \mathbb{R} \\
&\iff d\sum_{i=1}^{5} c_i = 0 \quad \forall\, d \in \mathbb{R} \\
&\iff \sum_{i=1}^{5} c_i = 0.
\end{aligned}
$$

□

The <u>least squares estimator</u> of an estimable function $\boldsymbol{c}'\boldsymbol{\beta}$ is $\boldsymbol{c}'\hat{\boldsymbol{\beta}}$, where $\hat{\boldsymbol{\beta}}$ is any solution to the NE $(\boldsymbol{X}'\boldsymbol{X}\boldsymbol{b} = \boldsymbol{X}'\boldsymbol{y})$.

Result 3.2:

If $\boldsymbol{c}'\boldsymbol{\beta}$ is estimable, then $\boldsymbol{c}'\hat{\boldsymbol{\beta}}$ is the same for all solutions $\hat{\boldsymbol{\beta}}$ to the NE.

Proof of Result 3.2:

Suppose $\hat{\boldsymbol{\beta}}_1$, and $\hat{\boldsymbol{\beta}}_2$ are any two solutions to the NE.

From Corollary 2.3, we know $\boldsymbol{X}\hat{\boldsymbol{\beta}}_1 = \boldsymbol{X}\hat{\boldsymbol{\beta}}_2$.

Now $\boldsymbol{c}'\boldsymbol{\beta}$ is estimable $\Rightarrow \exists\ \boldsymbol{a} \ni \boldsymbol{c}' = \boldsymbol{a}'\boldsymbol{X}$.

Thus,

$$\boldsymbol{c}'\hat{\boldsymbol{\beta}}_1 = \boldsymbol{a}'\boldsymbol{X}\hat{\boldsymbol{\beta}}_1 = \boldsymbol{a}'\boldsymbol{X}\hat{\boldsymbol{\beta}}_2 = \boldsymbol{c}'\hat{\boldsymbol{\beta}}_2.$$

□

Result 3.3:

The least squares estimator of an estimable function $\boldsymbol{c}'\boldsymbol{\beta}$ is a linear unbiased estimator of $\boldsymbol{c}'\boldsymbol{\beta}$.

Proof of Result 3.3:

From Result 3.2, we know $\boldsymbol{c}'\hat{\boldsymbol{\beta}}$ is the same $\forall$ solution to NE.

We know $(\boldsymbol{X}'\boldsymbol{X})^{-}\boldsymbol{X}'\boldsymbol{y}$ is a solution to NE.

Thus, $\boldsymbol{c}'\hat{\boldsymbol{\beta}} = \boldsymbol{c}'(\boldsymbol{X}'\boldsymbol{X})^{-}\boldsymbol{X}'\boldsymbol{y}$. This is a linear estimator.

Furthermore, $\boldsymbol{c}'\boldsymbol{\beta}$ estimable $\Rightarrow \exists\ \boldsymbol{a} \ni \boldsymbol{c}' = \boldsymbol{a}'\boldsymbol{X}$. Thus,

$$\begin{aligned} E(\boldsymbol{c}'\hat{\boldsymbol{\beta}}) &= E(\boldsymbol{c}'(\boldsymbol{X}'\boldsymbol{X})^{-}\boldsymbol{X}'\boldsymbol{y}) \\ &= \boldsymbol{c}'(\boldsymbol{X}'\boldsymbol{X})^{-}\boldsymbol{X}'E(\boldsymbol{y}) \\ &= \boldsymbol{c}'(\boldsymbol{X}'\boldsymbol{X})^{-}\boldsymbol{X}'\boldsymbol{X}\boldsymbol{\beta} \\ &= \boldsymbol{a}'\boldsymbol{X}(\boldsymbol{X}'\boldsymbol{X})^{-}\boldsymbol{X}'\boldsymbol{X}\boldsymbol{\beta} \\ &= \boldsymbol{a}'\boldsymbol{X}\boldsymbol{\beta} \\ &= \boldsymbol{c}'\boldsymbol{\beta}. \end{aligned}$$

$\square$

Consider again our previous example.

Recall that y_1 is a linear unbiased estimator of $\mu_1 - \mu_2$.

Is this the least squares estimator?

It can be shown that the least squares estimator of $\mu_1 - \mu_2$ is

$$\frac{7}{11}y_1 - \frac{3}{11}y_2 + \frac{4}{11}y_3 - \frac{1}{11}y_4 + \frac{1}{11}y_5 - \frac{1}{11}y_6.$$

Based on the observed $\boldsymbol{y}$, the least squares estimate is 8.0.

One of infinitely many solutions to the NE is

$$\hat{\boldsymbol{\beta}} = (\boldsymbol{X}'\boldsymbol{X})^{-}\boldsymbol{X}'\boldsymbol{y} = \begin{bmatrix} 2.8 \\ -5.2 \\ 7.8 \\ 2.8 \\ -8.2 \end{bmatrix}.$$

Which team is best?

Suppose $\boldsymbol{y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$, where $E(\boldsymbol{\varepsilon}) = \mathbf{0}$ and $rank(\underset{n \times p}{\boldsymbol{X}}) = p$.

Show that $\boldsymbol{c}'\boldsymbol{\beta}$ is estimable $\forall\, \boldsymbol{c} \in \mathbb{R}^p$.

Proof:

$rank(\underset{n \times p}{\boldsymbol{X}}) = p \Rightarrow \boldsymbol{X}'$ has p LI columns and each column is an element of $\mathbb{R}^p$.

Thus, by Fact V4, p LI columns of $\boldsymbol{X}'$ form a basis for $\mathbb{R}^p$.

$\therefore \mathcal{C}(\boldsymbol{X}') = \mathbb{R}^p$. This also follows from Result A.7:

$$\mathcal{C}(\boldsymbol{X}') \subseteq \mathbb{R}^p, dim(\mathcal{C}(\boldsymbol{X}')) = dim(\mathbb{R}^p) = p \Rightarrow \mathcal{C}(\boldsymbol{X}') = \mathbb{R}^p.$$

Now from Result 3.1, we know $\boldsymbol{c}'\boldsymbol{\beta}$ is estimable iff $\boldsymbol{c} \in \mathcal{C}(\boldsymbol{X}')$.

$\because \mathcal{C}(\boldsymbol{X}') = \mathbb{R}^p$, $\boldsymbol{c}'\boldsymbol{\beta}$ is estimable $\forall\, \boldsymbol{c} \in \mathbb{R}^p$. $\square$

Alternatively, we can prove the result by noting the following

$$rank(\underset{n\times p}{\boldsymbol{X}}) = p \Rightarrow rank(\boldsymbol{X}'\boldsymbol{X}) = p \text{ by Corollary 2.2.}$$

Now $\boldsymbol{X}'\boldsymbol{X}$ is $p \times p$ of rank p and $\therefore$ $(\boldsymbol{X}'\boldsymbol{X})^{-1}$ exists.

Thus, $\hat{\boldsymbol{\beta}} = (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{y}$ is the unique solution to NE

$$\boldsymbol{X}'\boldsymbol{X}\boldsymbol{b} = \boldsymbol{X}'\boldsymbol{y}.$$

Note that $\forall\, \boldsymbol{c} \in \mathbb{R}^p$

$$\begin{aligned} E(\boldsymbol{c}'\hat{\boldsymbol{\beta}}) &= \boldsymbol{c}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}E(\boldsymbol{y}) \\ &= \boldsymbol{c}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{X}\boldsymbol{\beta} \\ &= \boldsymbol{c}'\boldsymbol{\beta}. \end{aligned}$$

Thus, $\boldsymbol{c}'\hat{\boldsymbol{\beta}} = \boldsymbol{c}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{y}$ is a linear unbiased estimator of $\boldsymbol{c}'\boldsymbol{\beta} \quad \forall\, \boldsymbol{c} \in \mathbb{R}^p$. $\therefore\ \boldsymbol{c}'\boldsymbol{\beta}$ is estimable $\forall\, \boldsymbol{c} \in \mathbb{R}^p$.