

Constraints on Solutions to the Normal Equations

If $\text{rank}(\mathbf{X}) = r < p$, there are infinitely many solutions to the NE

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

For $(\mathbf{X}'\mathbf{X})^-$ any GI of $\mathbf{X}'\mathbf{X}$, the set of all solutions is

$$\{(\mathbf{X}'\mathbf{X})^- \mathbf{X}'\mathbf{y} + (\mathbf{I} - (\mathbf{X}'\mathbf{X})^- \mathbf{X}'\mathbf{X})\mathbf{z} : \mathbf{z} \in \mathbb{R}^p\}.$$

It is possible to place additional constraints on a solution to the NE so that \exists a unique solution that satisfies the constraints.

Example:

Suppose

$$y_{ij} = \mu + \tau_i + \varepsilon_{ij} \quad (i = 1, \dots, t; j = 1, \dots, n_i)$$

where

$$E(\varepsilon_{ij}) = 0 \quad \forall i, j.$$

Consider the following constraints on a solution to the NE $\hat{\beta} = \begin{bmatrix} \hat{\mu} \\ \hat{\tau}_1 \\ \vdots \\ \hat{\tau}_2 \end{bmatrix}$.

(Note that constraints are on $\hat{\beta}$ not β .)

Four common choices are

1. $\hat{\tau}_1 = 0$ (set first to zero)

2. $\hat{\tau}_t = 0$ (set last to zero)

3. $\sum_{i=1}^t \hat{\tau}_i = 0$ (sum to zero)

4. $\sum_{i=1}^t n_i \hat{\tau}_i = 0$ (weighted sum to zero)

Any one of these constraints may be imposed by insisting that a solution to the NE $\hat{\beta}$ satisfies $A\hat{\beta} = \mathbf{0}$ for some matrix A whose rows

define linear constraints on $\hat{\beta} = \begin{bmatrix} \hat{\mu} \\ \hat{\tau}_1 \\ \vdots \\ \hat{\tau}_2 \end{bmatrix}$.

For example,

1. $A = [0, 1, 0, \dots, 0]$.

2. $A = [0, 0, 0, \dots, 1]$.

3. $A = [0, 1, 1, \dots, 1]$.

4. $A = [0, n_1, n_2, \dots, n_t]$.

Note that solution $\hat{\beta}$ satisfies both the NE and the constraint equations
 $A\hat{\beta} = \mathbf{0}$ iff

$$\begin{bmatrix} \mathbf{X}'\mathbf{X} \\ \mathbf{A} \end{bmatrix} \hat{\beta} = \begin{bmatrix} \mathbf{X}'\mathbf{y} \\ \mathbf{0} \end{bmatrix}.$$

Furthermore, we know that

$$\mathbf{X}'\mathbf{X}\mathbf{b} = \mathbf{X}'\mathbf{y} \iff \mathbf{X}\mathbf{b} = \mathbf{P}_{\mathbf{X}}\mathbf{y}.$$

Thus, we have $\hat{\boldsymbol{\beta}}$ a solution to NE satisfying the constraints iff

$$\begin{bmatrix} \mathbf{X} \\ \mathbf{A} \end{bmatrix} \hat{\boldsymbol{\beta}} = \begin{bmatrix} \mathbf{P}_{\mathbf{X}}\mathbf{y} \\ \mathbf{0} \end{bmatrix}.$$

We now know that if we want a unique solution to NE and constraint equations, we need $\begin{bmatrix} \mathbf{X} \\ \mathbf{A} \end{bmatrix}$ to be of full-column rank; that is, we need

$$\text{rank} \left(\begin{bmatrix} \mathbf{X} \\ \mathbf{A} \end{bmatrix} \right) = p.$$

$\text{rank}(\mathbf{X}) = r < p$. Thus, we know \mathbf{X} has r LI rows.

If we can find $s \equiv p - r$ $p \times 1$ vectors \exists , when these vectors are combined with r LI rows of \mathbf{X} , the set of p vectors is LI, then we can use the s vectors as rows of \mathbf{A} to get

$$\text{rank} \left(\begin{bmatrix} \mathbf{X} \\ \mathbf{A} \end{bmatrix} \right) = p.$$

Suppose $\mathbf{x}_1, \dots, \mathbf{x}_r$ denote r LI rows of X (written as column vectors) or, equivalently, r LI columns of X' .

We seek $\mathbf{a}_1, \dots, \mathbf{a}_s$ ($s = p - r$) so that

$$\{\mathbf{x}_1, \dots, \mathbf{x}_r, \mathbf{a}_1, \dots, \mathbf{a}_s\}$$

is a set of $p = r + s$ LI vectors in \mathbb{R}^p .

Then, with $A' = [\mathbf{a}_1, \dots, \mathbf{a}_s]$, $\begin{bmatrix} X \\ A \end{bmatrix}$ will have full-column rank.

Obviously, $\mathbf{a}_1, \dots, \mathbf{a}_s$ must be LI and $\mathbf{a}_k \notin C(\mathbf{X}') \forall k = 1, \dots, s$.

Show by example that these conditions are not sufficient to guarantee

$$\text{rank} \left(\begin{bmatrix} \mathbf{X} \\ \mathbf{A} \end{bmatrix} \right) = p.$$

Example:

Suppose $r = 1$ and $\mathbf{x}_1 = \mathbf{x}_r = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$.

If $\mathbf{a}_1 = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}$ and $\mathbf{a}_2 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$, then $\mathbf{a}_1, \mathbf{a}_2$ LI, $\mathbf{a}_1 \notin \mathcal{C}(\mathbf{X}')$, and $\mathbf{a}_2 \notin \mathcal{C}(\mathbf{X}')$.

However, $\begin{bmatrix} \mathbf{X} \\ \mathbf{A} \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$ has rank $2 < 3 = p$.

The problem arises because, although neither \mathbf{a}_1 nor \mathbf{a}_2 is in $\mathcal{C}(\mathbf{X}')$, \exists LCs of \mathbf{a}_1 and \mathbf{a}_2 (e.g., $\mathbf{a}_1 + \mathbf{a}_2 = \mathbf{x}_1$) that are in $\mathcal{C}(\mathbf{X}')$.

Prove the following results:

Suppose $\mathbf{x}_1, \dots, \mathbf{x}_r$ LI in \mathbb{R}^p .

Suppose $\mathbf{a}_1, \dots, \mathbf{a}_s$ LI in \mathbb{R}^p .

Suppose $r + s = p$. Then

$$\mathbf{x}_1, \dots, \mathbf{x}_r, \mathbf{a}_1, \dots, \mathbf{a}_s \text{ LI}$$

$$\iff \text{span}\{\mathbf{x}_1, \dots, \mathbf{x}_r\} \cap \text{span}\{\mathbf{a}_1, \dots, \mathbf{a}_s\} = \{\mathbf{0}\}.$$

Proof:

(\implies)

$\mathbf{x}_1, \dots, \mathbf{x}_r, \mathbf{a}_1, \dots, \mathbf{a}_s$ LI iff

$$c_1\mathbf{x}_1 + \dots + c_r\mathbf{x}_r + d_1\mathbf{a}_1 + \dots + d_s\mathbf{a}_s = \mathbf{0}$$

$$\implies c_1 = \dots = c_r = d_1 = \dots = d_s = 0.$$

If $\mathbf{z} \in \text{span}\{\mathbf{x}_1, \dots, \mathbf{x}_r\} \cap \text{span}\{\mathbf{a}_1, \dots, \mathbf{a}_s\}$, then $\exists c_1, \dots, c_r$ and $d_1, \dots, d_s \ni$

$$\mathbf{z} = c_1\mathbf{x}_1 + \dots + c_r\mathbf{x}_r = -d_1\mathbf{a}_1 - \dots - d_s\mathbf{a}_s$$

$$\implies c_1\mathbf{x}_1 + \dots + c_r\mathbf{x}_r + d_1\mathbf{a}_1 + \dots + d_s\mathbf{a}_s = \mathbf{0}$$

$$\implies c_1 = \dots = c_r = d_1 = \dots = d_s = 0$$

$$\implies \mathbf{z} = \mathbf{0}.$$

(\Leftarrow)

$$\text{span}\{\mathbf{x}_1, \dots, \mathbf{x}_r\} \cap \text{span}\{\mathbf{a}_1, \dots, \mathbf{a}_s\} = \{\mathbf{0}\} \Rightarrow$$

$$c_1\mathbf{x}_1 + \dots + c_r\mathbf{x}_r = -d_1\mathbf{a}_1 - \dots - d_s\mathbf{a}_s \quad \text{only when}$$

$$\sum_{i=1}^r c_i\mathbf{x}_i = \sum_{j=1}^s (-d_j)\mathbf{a}_j = \mathbf{0}.$$

$\therefore \mathbf{x}_1, \dots, \mathbf{x}_r$ LI and $\mathbf{a}_1, \dots, \mathbf{a}_s$ LI,

$$\sum_{i=1}^r c_i\mathbf{x}_i = \sum_{j=1}^s (-d_j)\mathbf{a}_j = \mathbf{0}$$

$$\iff c_1 = \dots = c_r = d_1 = \dots = d_s = 0.$$

$$\therefore c_1\mathbf{x}_1 + \dots + c_r\mathbf{x}_r + d_1\mathbf{a}_1 + \dots + d_s\mathbf{a}_s = \mathbf{0} \quad \text{only when}$$

$$c_1 = \dots = c_r = d_1 = \dots = d_s = 0.$$

$\therefore \mathbf{x}_1, \dots, \mathbf{x}_r, \mathbf{a}_1, \dots, \mathbf{a}_s$ are LI.

□

Note that the condition

$$\begin{aligned} \text{span}\{\mathbf{x}_1, \dots, \mathbf{x}_r\} \cap \text{span}\{\mathbf{a}_1, \dots, \mathbf{a}_s\} &= \{\mathbf{0}\} \\ \Rightarrow (d_1\mathbf{a}_1 + \dots + d_s\mathbf{a}_s)'\boldsymbol{\beta} &\text{ is not estimable whenever} \\ d_1, \dots, d_s &\text{ are not all 0.} \end{aligned}$$

Thus, the constraints that we add, as well as all nontrivial LCs of those constraints, must correspond to nonestimable functions.

Note that $\mathbf{a}_1, \dots, \mathbf{a}_s$ with the desired properties always exist. Why is that?

We know $\mathcal{C}(\mathbf{X}')^\perp$ has $\dim p - r = s$ and satisfies

$$\mathcal{C}(\mathbf{X}') \cap \mathcal{C}(\mathbf{X}')^\perp = \{\mathbf{0}\}.$$

We can take $\mathbf{a}_1, \dots, \mathbf{a}_s$ to be basis vectors of

$$\mathcal{C}(\mathbf{X}')^\perp = \mathcal{N}(\mathbf{X}).$$

Although choosing basis vectors from $\mathcal{N}(\mathbf{X})$ is one possibility, we don't need $\mathbf{a}_1, \dots, \mathbf{a}_s \in \mathcal{N}(\mathbf{X})$.

Demonstrate this with an example.

Example:

Suppose $\text{rank}(\mathbf{X}) = 1$ and $\mathbf{x}_1 = \mathbf{x}_r = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$.

If we take $\mathbf{a}_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$ and $\mathbf{a}_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$, then $\mathbf{a}_1 \notin \mathcal{N}(\mathbf{X})$, $\mathbf{a}_2 \notin \mathcal{N}(\mathbf{X})$ and

$$\text{rank} \left(\begin{bmatrix} 1 & 1 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \right) = 3 = p.$$

The result that we proved can be alternatively stated as follows:

Suppose $\text{rank}(\mathbf{X}) = r < p$. Suppose $\text{rank}(\mathbf{A}) = s$ where $s = p - r$. Then

$$\mathcal{C}(\mathbf{X}') \cap \mathcal{C}(\mathbf{A}') = \{\mathbf{0}\} \iff \text{rank} \left(\begin{bmatrix} \mathbf{X} \\ \mathbf{A} \end{bmatrix} \right) = p.$$

Lemma 3.1:

For $\mathbf{A} \in \mathbb{R}^{s \times p}$ $\exists \text{rank}(\mathbf{A}) = s = p - \text{rank}(\mathbf{X})$ and $\mathcal{C}(\mathbf{X}') \cap \mathcal{C}(\mathbf{A}') = \{\mathbf{0}\}$,

$$\begin{bmatrix} \mathbf{X}'\mathbf{X} \\ \mathbf{A} \end{bmatrix} \mathbf{b} = \begin{bmatrix} \mathbf{X}'\mathbf{y} \\ \mathbf{0} \end{bmatrix} \quad \text{is equivalent to}$$

$$\begin{bmatrix} \mathbf{X}'\mathbf{X} \\ \mathbf{A}'\mathbf{A} \end{bmatrix} \mathbf{b} = \begin{bmatrix} \mathbf{X}'\mathbf{y} \\ \mathbf{0} \end{bmatrix}, \quad \text{which is equivalent to}$$

$$(\mathbf{X}'\mathbf{X} + \mathbf{A}'\mathbf{A})\mathbf{b} = \mathbf{X}'\mathbf{y}.$$

Proof of Lemma 3.1:

$$\begin{aligned} \mathbf{Ab} = \mathbf{0} &\Rightarrow \mathbf{A}'\mathbf{Ab} = \mathbf{0} \quad \text{and} \\ \mathbf{A}'\mathbf{Ab} = \mathbf{0} &\Rightarrow \mathbf{b}'\mathbf{A}'\mathbf{Ab} = 0 \\ &\Rightarrow \mathbf{Ab} = \mathbf{0}. \end{aligned}$$

Thus, the first equivalence holds.

Now

$$\begin{bmatrix} X'X \\ A'A \end{bmatrix} \mathbf{b} = \begin{bmatrix} X'y \\ \mathbf{0} \end{bmatrix} \Rightarrow X'X\mathbf{b} = X'y \quad \text{and} \quad A'A\mathbf{b} = \mathbf{0}$$

$$\Rightarrow X'X\mathbf{b} + A'A\mathbf{b} = X'y$$

$$\Rightarrow (X'X + A'A)\mathbf{b} = X'y.$$

Now note that

$$\begin{aligned}(\mathbf{X}'\mathbf{X} + \mathbf{A}'\mathbf{A})\mathbf{b} &= \mathbf{X}'\mathbf{y} \\ \Rightarrow \mathbf{X}'\mathbf{X}\mathbf{b} - \mathbf{X}'\mathbf{y} &= -\mathbf{A}'\mathbf{A}\mathbf{b} \\ \Rightarrow \mathbf{X}'(\mathbf{X}\mathbf{b} - \mathbf{y}) &= \mathbf{A}'(-\mathbf{A}\mathbf{b}).\end{aligned}$$

Now note that $\mathbf{X}'(\mathbf{X}\mathbf{b} - \mathbf{y}) \in \mathcal{C}(\mathbf{X}')$ and $\mathbf{A}'(-\mathbf{A}\mathbf{b}) \in \mathcal{C}(\mathbf{A}')$.

Thus, $\mathbf{X}'(\mathbf{X}\mathbf{b} - \mathbf{y}) = \mathbf{A}'(-\mathbf{A}\mathbf{b}) \in \mathcal{C}(\mathbf{X}') \cap \mathcal{C}(\mathbf{A}')$, which implies
 $\mathbf{X}'(\mathbf{X}\mathbf{b} - \mathbf{y}) = \mathbf{A}'(-\mathbf{A}\mathbf{b}) = \mathbf{0}$.

Therefore, we have

$$X'(Xb - y) = \mathbf{0} \Rightarrow X'Xb = X'y$$

$$-A'Ab = \mathbf{0} \Rightarrow A'Ab = \mathbf{0}.$$

$$\therefore \begin{bmatrix} X'X \\ A'A \end{bmatrix} b = \begin{bmatrix} X'y \\ \mathbf{0} \end{bmatrix}.$$



Result 3.6:

Suppose $\text{rank}_{n \times p}(\mathbf{X}) = r$, $\text{rank}_{s \times p}(\mathbf{A}) = s = p - r$, and $\mathcal{C}(\mathbf{X}') \cap \mathcal{C}(\mathbf{A}') = \{\mathbf{0}\}$.

Then

(i) $\mathbf{X}'\mathbf{X} + \mathbf{A}'\mathbf{A}$ is nonsingular.

(ii) $(\mathbf{X}'\mathbf{X} + \mathbf{A}'\mathbf{A})^{-1}\mathbf{X}'\mathbf{y}$ is unique solution to $\mathbf{X}'\mathbf{X}\mathbf{b} = \mathbf{X}'\mathbf{y}$ and $\mathbf{A}\mathbf{b} = \mathbf{0}$.

(iii) $(\mathbf{X}'\mathbf{X} + \mathbf{A}'\mathbf{A})^{-1}$ is GI of $\mathbf{X}'\mathbf{X}$.

(iv) $\mathbf{A}(\mathbf{X}'\mathbf{X} + \mathbf{A}'\mathbf{A})^{-1}\mathbf{X}' = \mathbf{0}$.

(v) $\mathbf{A}(\mathbf{X}'\mathbf{X} + \mathbf{A}'\mathbf{A})^{-1}\mathbf{A}' = \mathbf{I}$.

Proof of Result 3.6:

(i)

$$\begin{aligned} p &= \text{rank} \left(\begin{bmatrix} \mathbf{X} \\ \mathbf{A} \end{bmatrix} \right) \\ &= \text{rank} \left(\begin{bmatrix} \mathbf{X}' & \mathbf{A}' \end{bmatrix} \begin{bmatrix} \mathbf{X} \\ \mathbf{A} \end{bmatrix} \right) \quad (\text{By Corollary 2.2}) \\ &= \text{rank}(\mathbf{X}'\mathbf{X} + \mathbf{A}'\mathbf{A}). \end{aligned}$$

Thus, $\mathbf{X}'\mathbf{X} + \mathbf{A}'\mathbf{A}$ is full rank $p \times p$ matrix and is \therefore nonsingular.

(ii) By Lemma 3.1, solution to $(X'X + A'A)\mathbf{b} = X'y$ satisfies $X'X\mathbf{b} = X'y$ and $A\mathbf{b} = \mathbf{0}$ and vice versa.

$\therefore X'X + A'A$ is nonsingular, the unique solution is $(X'X + A'A)^{-1}X'y$, which is obtained by multiplying $(X'X + A'A)\mathbf{b} = X'y$ on the left by $(X'X + A'A)^{-1}$.

(iii) By (ii), $(X'X + A'A)^{-1}X'y$ is a solution to $X'Xb = X'y \quad \forall y \in \mathbb{R}^n$.

$$\therefore X'X(X'X + A'A)^{-1}X'y = X'y \quad \forall y \in \mathbb{R}^n$$

$$\Rightarrow X'X(X'X + A'A)^{-1}X' = X'$$

$$\Rightarrow X'X(X'X + A'A)^{-1}X'X = X'X$$

$$\Rightarrow (X'X + A'A)^{-1} \text{ is GI of } X'X.$$

(iv) By (ii), $(X'X + A'A)^{-1}X'y$ solves $Ab = \mathbf{0} \quad \forall y \in \mathbb{R}^n$.

$$\therefore A(X'X + A'A)^{-1}X'y = \mathbf{0} \quad \forall y \in \mathbb{R}^n.$$

$$\therefore A(X'X + A'A)^{-1}X' = \mathbf{0}.$$

(v) HW Problem. See exercise 3.22. □

Returning to our example,

$$y_{ij} = \mu + \tau_i + \varepsilon_{ij} \quad (i = 1, \dots, t; j = 1, \dots, n_i)$$

where

$$E(\varepsilon_{ij}) = 0 \quad \forall i, j.$$

$$\beta = \begin{bmatrix} \mu \\ \tau_1 \\ \vdots \\ \tau_t \end{bmatrix}. \text{ Let's consider the constraint}$$

$$\sum_{i=1}^t n_i \hat{\tau}_i = 0.$$

Find $\hat{\beta}$ that satisfies NE and the constraint.

$$\mathbf{X} = \begin{bmatrix} \mathbf{1}_{n_1} & \mathbf{1}_{n_1} & \mathbf{0}_{n_1} & \cdots & \mathbf{0}_{n_1} \\ \mathbf{1}_{n_2} & \mathbf{0}_{n_2} & \mathbf{1}_{n_2} & \cdots & \mathbf{0}_{n_2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{1}_{n_t} & \mathbf{0}_{n_t} & \mathbf{0}_{n_t} & \cdots & \mathbf{1}_{n_t} \end{bmatrix}$$

$$\mathbf{X}'\mathbf{X} = \begin{bmatrix} n & n_1 & n_2 & \cdots & n_t \\ n_1 & n_1 & 0 & \cdots & 0 \\ n_2 & 0 & n_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ n_t & 0 & 0 & \cdots & n_t \end{bmatrix} .$$

$$\mathbf{X}'\mathbf{X}\hat{\boldsymbol{\beta}} = \begin{bmatrix} n\hat{\mu} + n_1\hat{\tau}_1 + \cdots + n_t\hat{\tau}_t \\ n_1\hat{\mu} + n_1\hat{\tau}_1 \\ \vdots \\ n_t\hat{\mu} + n_t\hat{\tau}_t \end{bmatrix}$$

$$\mathbf{X}'\mathbf{y} = \begin{bmatrix} y_{..} \\ y_{1.} \\ \vdots \\ y_{t.} \end{bmatrix} .$$

Equating $\mathbf{X}'\mathbf{X}\hat{\boldsymbol{\beta}}$ and $\mathbf{X}'\mathbf{y}$ leads to

$$\begin{aligned}
 n\hat{\mu} + n_1\hat{\tau}_1 + \cdots + n_t\hat{\tau}_t &= y_{..} \\
 n_1\hat{\mu} + n_1\hat{\tau}_1 &= y_{1.} \\
 &\vdots \\
 n_t\hat{\mu} + n_t\hat{\tau}_t &= y_{t..}
 \end{aligned}$$

This system of equations has an infinite number of solutions.

However, if we insist that

$$n_1\hat{\tau}_1 + \cdots + n_t\hat{\tau}_t = 0,$$

the first equation becomes

$$n\hat{\mu} = y_{..} \iff \hat{\mu} = \bar{y}_{..}$$

Substituting $\hat{\mu} = \bar{y}_{..}$ in the other equations yields

$$n_i\bar{y}_{..} + n_i\hat{\tau}_i = y_{i.} \iff$$

$$\bar{y}_{..} + \hat{\tau}_i = \bar{y}_{i.} \iff$$

$$\hat{\tau}_i = \bar{y}_{i.} - \bar{y}_{..}$$

For the general case, we can compute

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