

Consider the vectors $x_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$, $x_2 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$, $x_3 = \begin{bmatrix} 2 \\ 3 \\ 3 \end{bmatrix}$

Let M the set of all linear combinations of x_1, x_2, x_3

$\{x_1, x_2, x_3\}$: spanning set

We can easily check $3x_1 - x_2 = x_3 \Rightarrow x_1, x_2, x_3$ linearly dep.

Any two of x_1, x_2, x_3 form a basis for ~~the space~~ M

M contains vectors with the form $\begin{bmatrix} a \\ b \\ b \end{bmatrix}$, $a, b \in \mathbb{R}$

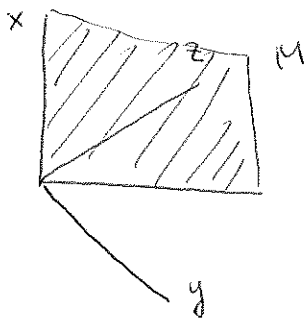
† Def [Rank of a subspace]: The rank of a subspace M is the number of elements in a basis for M . The rank is written $rank(M)$, $r(M)$ or $dim(M)$.

If A is a $m \times n$ matrix, the rank of $C(A)$ is called the rank of A and is written as $r(A)$. $= n$
 $< n$

★ Result: $r(C(A)) = dim(C(A)) = r(A)$: # of linearly independent columns of A (= # of basis vectors for $C(A)$).

\Rightarrow When $r(X) = r$, the r linearly independent columns of X span the r -dimensional estimation space $C(X)$

\Rightarrow The space spanned by $\{x_1, x_2, x_3\}$ has rank 2.



OR consider $A = \begin{bmatrix} 1 & 1 & 2 \\ 1 & 0 & 3 \\ 1 & 0 & 3 \end{bmatrix}$

$$r(A) = 2 = r(C(A))$$

$$\underline{\mathbf{X}^T \mathbf{X}}$$

- **Q:** How to find a solution $\hat{\beta}$ if $r(\mathbf{X}) = r(\mathbf{X}^T \mathbf{X}) < p$ (singular)?

Here is our strategy!

△ There is no unique solution for β when $r(\mathbf{X}) = r(\mathbf{X}^T \mathbf{X}) < p$.

△ Instead we will find $\hat{\mathbf{y}} \in C(\mathbf{X})$ closest to \mathbf{y} in the Euclidean distance.

△ Then we will find $\hat{\beta}$ such that $\hat{\mathbf{y}} = \mathbf{X}\hat{\beta}$.

- **Q:** How to find such $\hat{\mathbf{y}}$?

We will consider the perpendicular projection matrix!



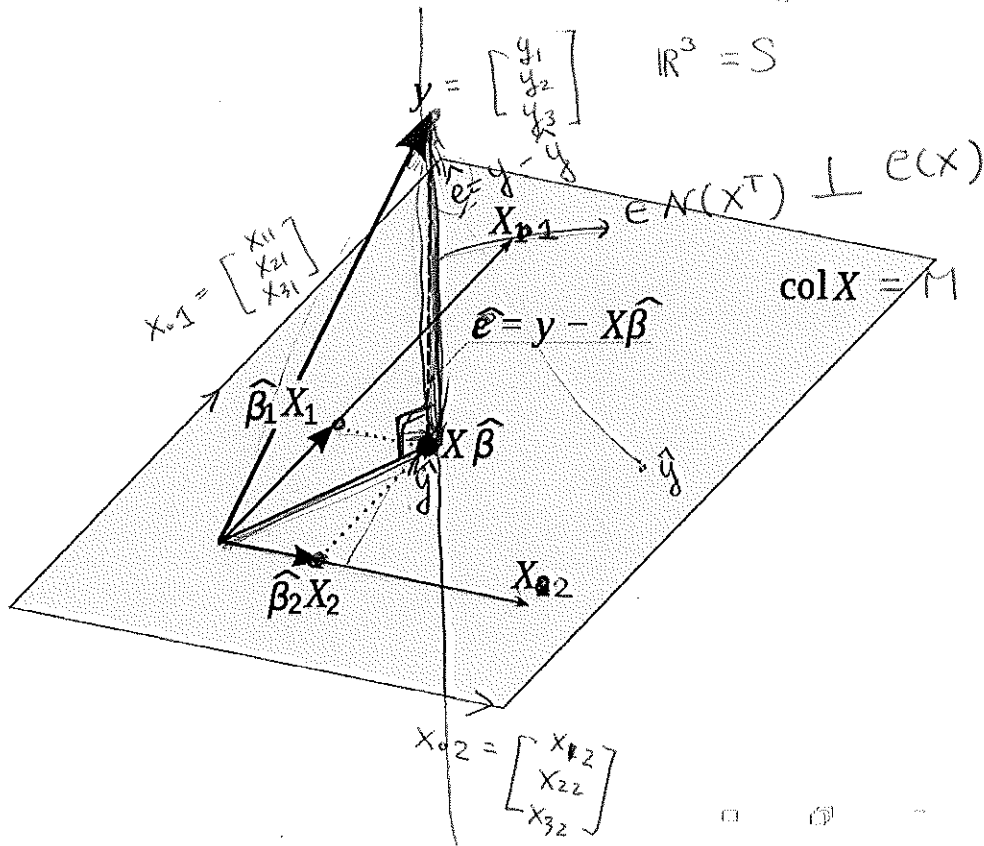
$$\begin{bmatrix} X_{11} \\ X_{21} \\ X_{31} \end{bmatrix} \quad \begin{bmatrix} X_{12} \\ X_{22} \\ X_{32} \end{bmatrix}$$

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} X_{01} \\ X_{02} \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} + \begin{bmatrix} e_1 \\ e_2 \\ e_3 \end{bmatrix}$$

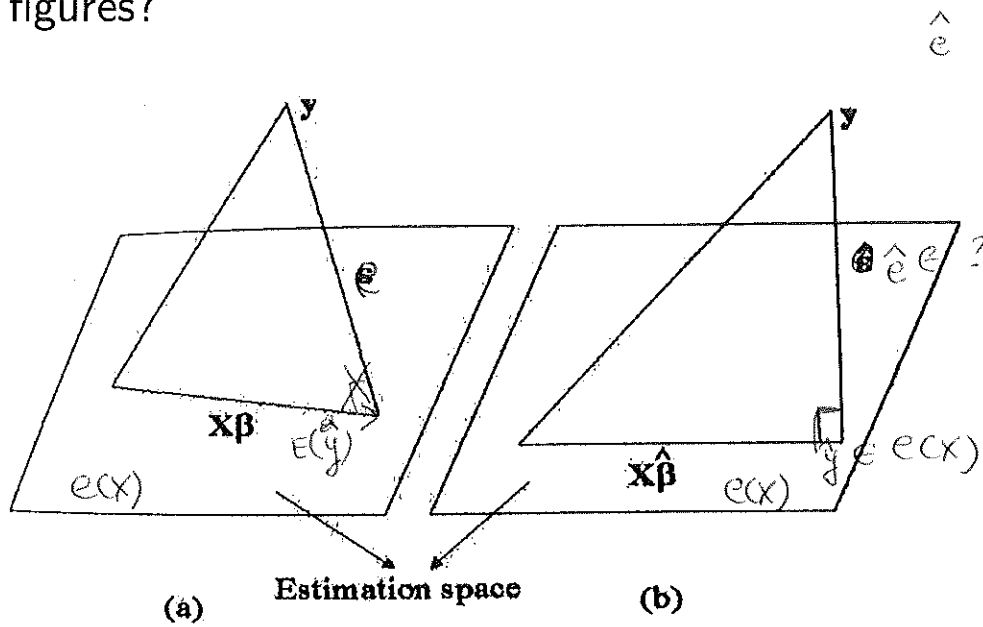
★ Recall the linear models: $y = X\beta + e$ and $X\beta \in C(X)$.

★ Suppose $\hat{\beta}$ is a solution for the NEs (that is, minimize $\|y - X\beta\|^2$).

→ Let fitted value $\hat{y} = X\hat{\beta} \in C(X)$ and residual $\hat{e} = y - \hat{y}$.



★ More figures?



Q: Where does \hat{e} lie?

$Ay = 0$: homogeneous linear system

$\Rightarrow y$: a solution

$\Rightarrow N(A) =$ the set of solutions to the homogeneous linear system

† Def [Nullspace]: The null space of a $m \times n$ matrix A , denoted by $\mathcal{N}(A)$,

$$\mathcal{N}(A) = \{y \mid Ay = 0\} \subset \mathbb{R}^n.$$

$m \times n$ $n \times 1$

♣ Th: If A is $m \times n$ and $r(A) = r$, then the rank of the null space of A is $n - r$, that is,

$$\dim(C(A)) + \dim(\mathcal{N}(A)) = n.$$

ex let $A = \begin{bmatrix} 1 & 1 & 1 \\ 2 & 2 & 2 \\ -1 & 1 & -3 \\ 1 & 2 & 0 \end{bmatrix}_{4 \times 3}$

let's find $N(A)$

$$Ay = 0 \Rightarrow \begin{cases} y_1 + y_2 + y_3 = 0 \\ 2y_1 + 2y_2 + 2y_3 = 0 \\ -y_1 + y_2 + 3y_3 = 0 \\ y_1 + 2y_2 + 0 = 0 \end{cases} \Rightarrow \begin{cases} -4y_2 + 2y_2 + 2y_2 = 0 \\ 2y_2 + y_2 - 3y_3 = 0 \Rightarrow y_3 = \frac{3}{2}y_2 \\ y_1 = -2y_2 \end{cases}$$

32/61

$$y = \begin{bmatrix} -2y_2 \\ y_2 \\ y_2 \end{bmatrix} = y_2 \begin{bmatrix} -2 \\ 1 \\ 1 \end{bmatrix}, \quad y_2 \in \mathbb{R}$$

$$N(A) = \left\{ c \begin{bmatrix} -2 \\ 1 \\ 1 \end{bmatrix}, c \in \mathbb{R} \right\} \subset \mathbb{R}^3 \Rightarrow \begin{matrix} \text{dim} \\ \text{dim}(N(A)) = 1 \\ \text{dim}(C(A)) = 2 \end{matrix}$$

★ Result: Recall the NEs:

$$\mathbf{X}^T \mathbf{X} \boldsymbol{\beta} = \mathbf{X}^T \mathbf{y}.$$

Suppose $\hat{\boldsymbol{\beta}}$ is a solution for the NEs.

- $\hat{\mathbf{y}} = \mathbf{X} \hat{\boldsymbol{\beta}} \in C(\mathbf{X}).$

- $\mathbf{X}^T (\mathbf{y} - \mathbf{X} \hat{\boldsymbol{\beta}}) = \mathbf{X}^T \hat{\mathbf{e}} = 0 \Rightarrow \hat{\mathbf{e}} \in \mathcal{N}(\mathbf{X}^T)$

$$\mathbf{X}^T \mathbf{y} - \mathbf{X}^T \mathbf{X} \hat{\boldsymbol{\beta}} = 0 \quad \begin{matrix} \hat{\mathbf{y}} - \hat{\mathbf{y}} \\ \hat{\mathbf{y}} \\ \hat{\mathbf{e}} \end{matrix}$$

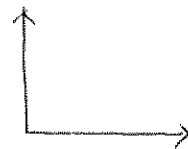
Q: What is the relationship between $C(\mathbf{X})$ and $\mathcal{N}(\mathbf{X}^T)$?

† Def [**Orthogonal**]:

- ▶ (Inner Product) The *inner product* between two vectors, \mathbf{x} and \mathbf{y} is $\mathbf{x}^T \mathbf{y}$
- ▶ (Orthogonal Vectors) Two vectors \mathbf{x} and \mathbf{y} are *orthogonal* (or *perpendicular*) (written $\mathbf{x} \perp \mathbf{y}$) if $\mathbf{x}^T \mathbf{y} = 0$.
- ▶ (Orthogonal Spaces) Two subspaces \mathcal{M}_1 and \mathcal{M}_2 are *orthogonal* if $\mathbf{x} \in \mathcal{M}_1$ and $\mathbf{y} \in \mathcal{M}_2$ implies $\mathbf{x}^T \mathbf{y} = 0$
- ▶ (Orthogonal Basis) $\{\mathbf{x}_1, \dots, \mathbf{x}_r\}$ is an *orthogonal basis* for \mathcal{M} if $\{\mathbf{x}_1, \dots, \mathbf{x}_r\}$ is a basis of \mathcal{M} and for $i \neq j$, $\mathbf{x}_i^T \mathbf{x}_j = 0$.

$$\begin{bmatrix} 1 \\ 2 \end{bmatrix} \quad \begin{bmatrix} 3 \\ 2 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$



† Def [**Orthogonal**]: — Contd

- ▶ (Orthonormal Basis) $\{\mathbf{x}_1, \dots, \mathbf{x}_r\}$ is an *orthonormal basis* for \mathcal{M} if $\{\mathbf{x}_1, \dots, \mathbf{x}_r\}$ is an orthogonal basis and $\mathbf{x}_i^T \mathbf{x}_i = 1$ for $i = 1, \dots, r$

• Note:

- \mathbf{Q} has orthogonal columns $\Rightarrow \mathbf{Q}^T \mathbf{Q} = \mathbf{D}$ (diagonal matrix)
- \mathbf{Q} has orthonormal columns $\Rightarrow \mathbf{Q}^T \mathbf{Q} = \mathbf{I}$

||

$$M_S^\perp \cap M = \{0\}$$

† Def [**Orthogonal Complement**]: Let \mathcal{S} be a vector space, and let \mathcal{M} be a subspace of \mathcal{S} . Let $\mathcal{M}_S^\perp = \{\mathbf{y} \in \mathcal{S} \mid \mathbf{y} \perp \mathcal{M}\}$. \mathcal{M}_S^\perp is called the *orthogonal complement* of \mathcal{M} with respect to \mathcal{S} .
such that

If \mathcal{S} is taken as \mathbb{R}^n , then $\mathcal{M}_S^\perp \equiv \mathcal{M}^\perp$ is simply referred to as the orthogonal complements of \mathcal{M} .

In layman's terms, every vector in $\mathcal{M} \subset \mathcal{S}$ is orthogonal to every vector in \mathcal{M}_S^\perp .

♣ Th: Let \mathcal{S} be a vector space, and let \mathcal{M} be a subspace of \mathcal{S} .

► The orthogonal complement of \mathcal{M} with respect to \mathcal{S} is a subspace of \mathcal{S} ;

► If $x \in \mathcal{S}$, x can be written uniquely as $x = x_0 + x_1$ with $x_0 \in \mathcal{M}$ and $x_1 \in \mathcal{M}_S^\perp$.
 \mathbb{R}^n $\hat{y} = \hat{y} + \hat{e}$ $e(A)$

► The ranks of these spaces satisfy the relation, $r(\mathcal{S}) = r(\mathcal{M}) + r(\mathcal{M}_S^\perp)$.

$$S = \mathbb{R}^3 \quad A = \begin{bmatrix} 1 & 1 & 2 \\ 1 & 0 & 3 \\ 1 & 0 & 3 \end{bmatrix} \quad M = \text{e}(A)$$

$$\Leftrightarrow M = \left\{ \text{all the vectors with the form } \begin{bmatrix} a \\ b \\ b \end{bmatrix}, a, b \in \mathbb{R} \right\}$$

What is M^\perp ?

$$M^\perp = \left\{ \text{all the vectors with the form } \begin{bmatrix} 0 \\ 0 \\ -a \end{bmatrix}, a \in \mathbb{R} \right\}$$

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x \\ \frac{y+z}{2} \\ \frac{y+z}{2} \end{bmatrix} + \begin{bmatrix} 0 \\ \frac{y-z}{2} \\ -\frac{y-z}{2} \end{bmatrix}$$

$$C(\mathbf{X}) \quad N(\mathbf{X}^T)$$

$$\hat{\mathbf{y}} \quad \hat{\mathbf{e}}$$

$$\hat{\mathbf{y}}^T \hat{\mathbf{e}} = 0$$

vector spaces w/ vectors

in \mathbb{R}^m
 $\mathbf{x} \in C(\mathbf{A})$

$$\mathbf{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_m \end{bmatrix}$$

★ Result: For any matrix \mathbf{A} ($m \times n$), $C(\mathbf{A})$ and $N(\mathbf{A}^T)$ are orthogonal complements in \mathbb{R}^m .

$$\text{Let } r(\mathbf{A}) = r(\mathbf{A}^T) = r \quad \Rightarrow \quad \dim(C(\mathbf{A})) = r$$

$$\dim(N(\mathbf{A}^T)) = m - r$$

Ⓐ Suppose $v \in C(\mathbf{A})$ & $v \in N(\mathbf{A}^T) \Rightarrow$ want to show $v = 0$

$$v \in C(\mathbf{A}) \Rightarrow \exists c (c \neq 0) \text{ s.t. } v = \mathbf{A}c$$

$$v \in N(\mathbf{A}^T) \Rightarrow \mathbf{A}^T v = 0 = \mathbf{A}^T \mathbf{A}c$$

$$\Rightarrow \text{consider } v^T v = (\mathbf{A}c)^T (\mathbf{A}c) = c^T \underbrace{\mathbf{A}^T \mathbf{A}}_{=0} c = 0$$

$$\mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix}$$

• Bottom Line: $C(\mathbf{X})$ and $N(\mathbf{X}^T)$ are orthogonal complements in \mathbb{R}^n . So, $\hat{\mathbf{y}} \perp \hat{\mathbf{e}}$ and $\mathbf{y} = \hat{\mathbf{y}} + \hat{\mathbf{e}}$ is the unique decomposition.

Ⓑ Suppose $v \in C(\mathbf{A})$ and $w \in N(\mathbf{A}^T) \Rightarrow$ want to show $v \perp w$

$$v \in C(\mathbf{A}) \Rightarrow \exists c (c \neq 0) \text{ s.t. } v = \mathbf{A}c$$

$$\Rightarrow v^T w = (\mathbf{A}c)^T w = c^T \mathbf{A}^T w = 0$$

By Ⓐ & Ⓑ, $C(\mathbf{A})$ and $N(\mathbf{A}^T)$ are orthogonal complements in \mathbb{R}^m

★ Summary! Recall the NEs:

$$\mathbf{X}^T \mathbf{X} \boldsymbol{\beta} = \mathbf{X}^T \mathbf{y}.$$

Suppose $\hat{\boldsymbol{\beta}}$ is a solution for the NEs.

- $\mathbf{y} \in \mathbb{R}^n$.
 - $\hat{\mathbf{y}} = \mathbf{X} \hat{\boldsymbol{\beta}} \in C(\mathbf{X})$.
 - $\mathbf{X}^T (\mathbf{y} - \mathbf{X} \hat{\boldsymbol{\beta}}) = \mathbf{X}^T \hat{\mathbf{e}} = 0 \Rightarrow \hat{\mathbf{e}} \in \mathcal{N}(\mathbf{X}^T)$ \perp
- (
- $\hat{\mathbf{y}} \perp \hat{\mathbf{e}}$
 - $\mathbf{y} = \hat{\mathbf{y}} + \hat{\mathbf{e}}$ is the unique decomposition.

- $\mathbf{y} = \hat{\mathbf{y}} + \hat{\mathbf{e}}$ is the unique decomposition.

⇒ The unique orthogonal decomposition of sums of squares from the Pythagorean Theorem,

$$\|\mathbf{y}\|^2 = \|\hat{\mathbf{y}} + \hat{\mathbf{e}}\|^2 = \|\hat{\mathbf{y}}\|^2 + \|\hat{\mathbf{e}}\|^2$$

- $SST = \|\mathbf{y}\|^2$: the total sum of squares
- $SSR = \|\hat{\mathbf{y}}\|^2 = \|\mathbf{X}^T \hat{\boldsymbol{\beta}}\|^2$: the regression sum of squares
- $SSE = \|\hat{\mathbf{e}}\|^2$: the error sum of squares

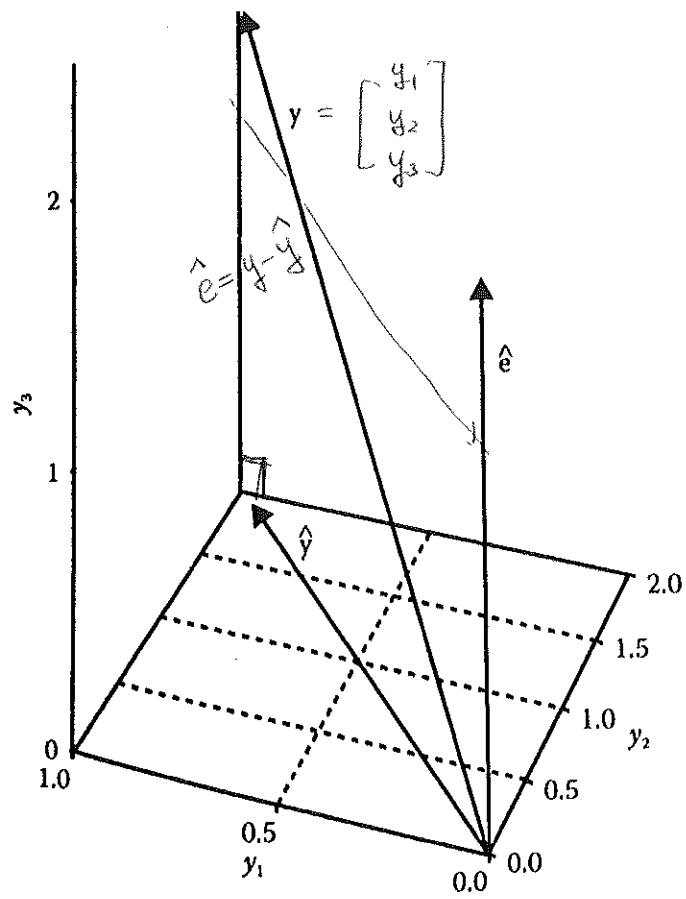
† Geometry of Least Squares:

$$(\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}})^T (\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}) = \min_{\boldsymbol{\beta}} (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$

† Fact:

- Decomposition of $\mathbf{y} = \hat{\mathbf{y}} + \mathbf{y} - \hat{\mathbf{y}}$ into $\hat{\mathbf{y}} = \mathbf{X}\hat{\boldsymbol{\beta}}$ (fitted value) and $\hat{\mathbf{e}} = \mathbf{y} - \hat{\mathbf{y}}$ (residuals)
- $\hat{\mathbf{y}} \in C(\mathbf{X})$
- $\hat{\mathbf{e}}$ is orthogonal to $\hat{\mathbf{y}}$ (that is, $\hat{\mathbf{e}} \in \mathcal{N}(\mathbf{X}^T)$)
- $\hat{\mathbf{y}}$ is the orthogonal projection of \mathbf{y} onto $C(\mathbf{X})$
- $\hat{\mathbf{e}}$ is the orthogonal projection onto the orthogonal complement of $C(\mathbf{X})$. $= \mathcal{N}(\mathbf{X}^T)$

†: The geometry provides good intuition for n -dimensional problems (but hard to visualize for $n > 3$).



† Geometry of Least Squares:

$$(\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}})^T (\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}) = \min_{\boldsymbol{\beta}} (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$

⇒ LSE $\hat{\boldsymbol{\beta}}$ is the vector that makes $\hat{\mathbf{y}} = \mathbf{X}\hat{\boldsymbol{\beta}} \in C(\mathbf{X})$ closest to \mathbf{y} .

⇒ The vector in $C(\mathbf{X})$ that is closest to \mathbf{y} is the perpendicular projection of \mathbf{y} onto $C(\mathbf{X})$.

$$\hat{\mathbf{y}} = \mathbb{P}_{\mathbf{y}} \in C(\mathbf{X})$$

⇒ Then how to find orthogonal projection matrices?

★ Two ways to find the perpendicular projection matrix onto $C(\mathbf{X})$.

△ A generalized inverse

△ The Gram-Schmidt theorem

* Road map:

- Discuss the perpendicular projection matrix
- Discuss how to find perpendicular projection matrix

Consider $x = \begin{bmatrix} 2 \\ 1 \end{bmatrix} \in \mathbb{R}^2$, $r(x) = 1$

$$e(x) = \left\{ \begin{bmatrix} 2a \\ a \end{bmatrix}, a \in \mathbb{R} \right\}$$

$$\begin{bmatrix} b \\ -2b \end{bmatrix} \perp e(x) \quad \text{for } b \in \mathbb{R}$$

Now consider $M = \begin{bmatrix} 0.8 & 0.4 \\ 0.4 & 0.2 \end{bmatrix}$.

* claim: M is a perpendicular projection matrix onto $e(x)$

Let's check (i) & (ii)

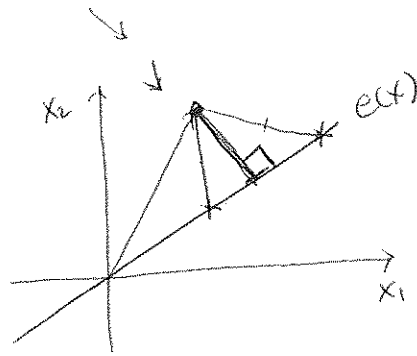
$$\begin{aligned} \text{(i)} \quad v = \begin{bmatrix} 2a \\ a \end{bmatrix} \in e(x), \quad Mv &= \begin{bmatrix} 0.8 & 0.4 \\ 0.4 & 0.2 \end{bmatrix} \begin{bmatrix} 2a \\ a \end{bmatrix} \\ &= \begin{bmatrix} 1.6a + 0.4a \\ 0.8a + 0.2a \end{bmatrix} = \begin{bmatrix} 2a \\ a \end{bmatrix} = v \end{aligned}$$

$$\begin{aligned} \text{(ii)} \quad w = \begin{bmatrix} b \\ -2b \end{bmatrix} \perp e(x), \quad Mw &= \begin{bmatrix} 0.8 & 0.4 \\ 0.4 & 0.2 \end{bmatrix} \begin{bmatrix} b \\ -2b \end{bmatrix} \\ &= \begin{bmatrix} 0.8b - 0.8b \\ 0.4b - 0.4b \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \end{aligned}$$

* Check prop! $e(x) = e(M)$

$$\begin{aligned} \text{(i)} \quad MM &= \begin{bmatrix} 0.8 & 0.4 \\ 0.4 & 0.2 \end{bmatrix} \begin{bmatrix} 0.8 & 0.4 \\ 0.4 & 0.2 \end{bmatrix} = \begin{bmatrix} 0.64 + 0.16 & 0.32 + 0.08 \\ 0.32 + 0.08 & 0.16 + 0.04 \end{bmatrix} \\ &= \begin{bmatrix} 0.8 & 0.4 \\ 0.4 & 0.2 \end{bmatrix} = M \quad \checkmark \end{aligned}$$

(ii) M is symmetric!



† Def [**Projection**]: A square matrix \mathbf{M} is a *perpendicular projection operator* (matrix) onto $C(\mathbf{X})$ if and only if

- (i) $\mathbf{v} \in C(\mathbf{X})$ implies $\mathbf{M}\mathbf{v} = \mathbf{v}$ (projection)
- (ii) $\mathbf{w} \perp C(\mathbf{X})$ implies $\mathbf{M}\mathbf{w} = \mathbf{0}$ (perpendicularity)

★ Note: Any projection that is not a perpendicular projection is called an *oblique projection operator*.

★ Prop If \mathbf{M} is a *perpendicular projection operator* onto $C(\mathbf{X})$, then $C(\mathbf{M}) = C(\mathbf{X})$.

♣ Th: \mathbf{M} is a perpendicular projection operator on $C(\mathbf{M})$ if and only if (i) $\mathbf{M}\mathbf{M} = \mathbf{M}$ (idempotent) and (ii) $\mathbf{M}^T = \mathbf{M}$ (symmetric).

♣ Th: Perpendicular projection operators are unique.

$$y = \hat{y} + \hat{e}$$

$$Iy = P_1 y + P_2 y$$

$$I = P_1 + P_2$$

$$P_2 = I - P_1$$

♣ Th: Let \mathbf{M}_1 and \mathbf{M}_2 are perpendicular projection matrices on \mathbb{R}^n . $(\mathbf{M}_1 + \mathbf{M}_2)$ is the perpendicular projection matrix onto $C(\mathbf{M}_1, \mathbf{M}_2)$ if and only if $C(\mathbf{M}_1) \perp C(\mathbf{M}_2)$.

♣ Th: If \mathbf{M}_1 and \mathbf{M}_2 are symmetric, $C(\mathbf{M}_1) \perp C(\mathbf{M}_2)$, and $(\mathbf{M}_1 + \mathbf{M}_2)$ is the perpendicular projection matrix, then \mathbf{M}_1 and \mathbf{M}_2 are perpendicular projection matrices.

♣ Th: \mathbf{M} and \mathbf{M}_0 are perpendicular projection matrices with $C(\mathbf{M}_0) \subset C(\mathbf{M})$. Then $\mathbf{M} - \mathbf{M}_0$ is a perpendicular projection matrix.

♣ Th: \mathbf{M} and \mathbf{M}_0 are perpendicular projection matrices with $C(\mathbf{M}_0) \subset C(\mathbf{M})$. Then $C(\mathbf{M} - \mathbf{M}_0)$ is the orthogonal complement of $C(\mathbf{M}_0)$ with respect to $C(\mathbf{M})$. If $\mathbf{x} \in C(\mathbf{M})$ and $\mathbf{x} \perp C(\mathbf{M}_0)$, then $\mathbf{x} = \mathbf{M}\mathbf{x} = (\mathbf{M} - \mathbf{M}_0)\mathbf{x} + \mathbf{M}_0\mathbf{x} = (\mathbf{M} - \mathbf{M}_0)\mathbf{x}$. Thus, $\mathbf{x} \in C(\mathbf{M} - \mathbf{M}_0)$, so the orthogonal complement of $C(\mathbf{M}_0)$ with respect to $C(\mathbf{M})$ is contained in $C(\mathbf{M} - \mathbf{M}_0)$.

★ Cor: $r(\mathbf{M}) = r(\mathbf{M}_0) + r(\mathbf{M} - \mathbf{M}_0)$

★ Summary!

- Say \mathbf{P} is the perpendicular projection matrix onto $C(\mathbf{X})$.
- I is the perpendicular projection operator onto \mathbb{R}^n .
- $(I - \mathbf{P})$: the perpendicular projection matrix onto the orthogonal complement of $C(\mathbf{X})$ with respect to \mathbb{R}^n .
- $r(I) = r(\mathbf{P}) + r(I - \mathbf{P}) = r + (n - r)$ where $r(C(\mathbf{X})) = r$.
- Decompose \mathbf{y} into

$$\mathbf{y} = \mathbf{P}\mathbf{y} + (I - \mathbf{P})\mathbf{y} = \hat{\mathbf{y}} + \hat{\mathbf{e}}$$