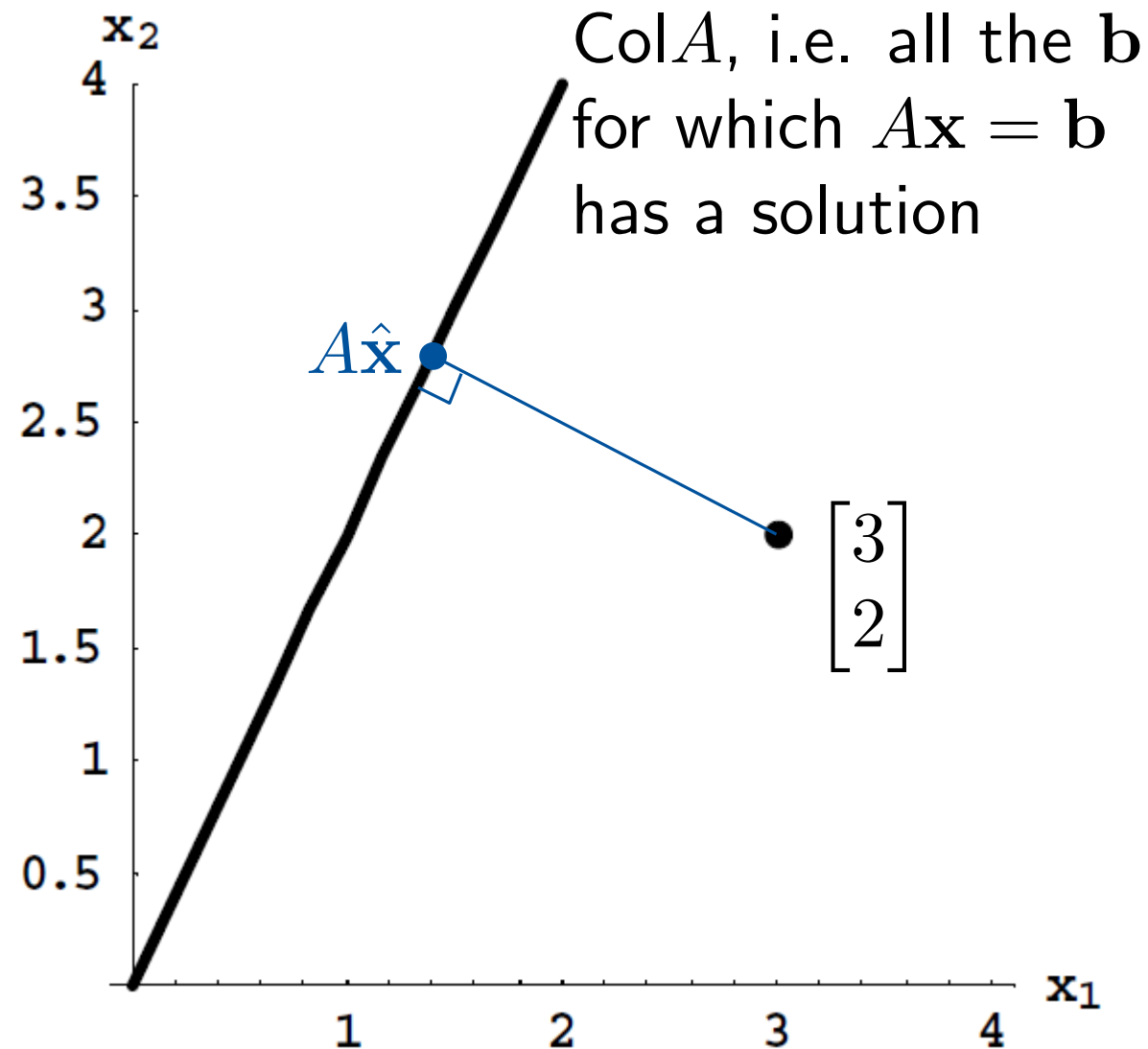


Let  $A = \begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix}$ . The linear system  $A\mathbf{x} = \begin{bmatrix} 3 \\ 2 \end{bmatrix}$  does not have a solution, because

$$\begin{bmatrix} 3 \\ 2 \end{bmatrix} \text{ is not in } \text{Col}A = \text{Span} \left\{ \begin{bmatrix} 1 \\ 2 \end{bmatrix} \right\}.$$

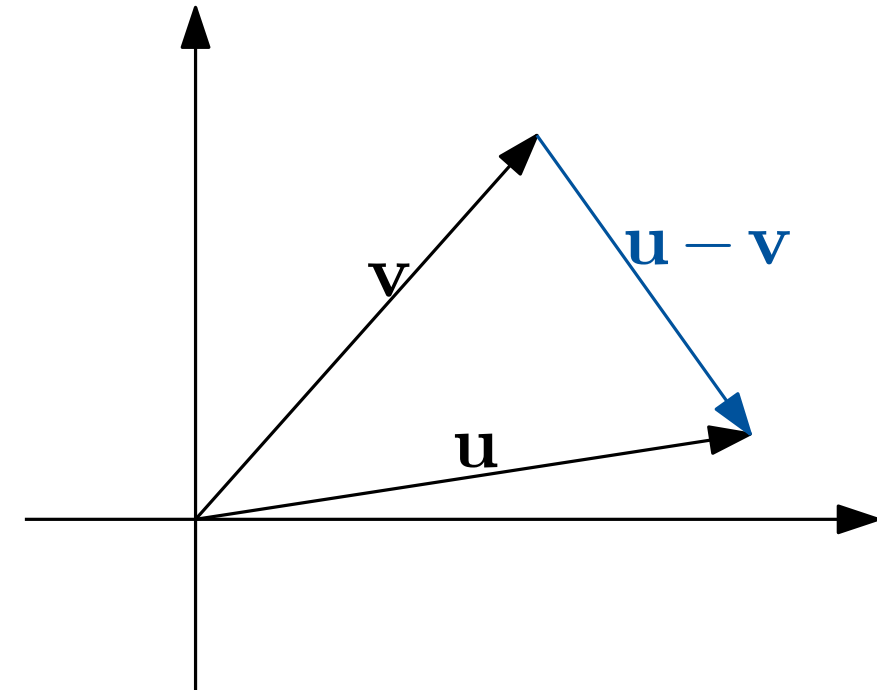


We wish to find a “closest approximate solution”, i.e. a vector  $\hat{\mathbf{x}}$  such that  $A\hat{\mathbf{x}}$  is the unique point in  $\text{Col}A$  that is “closest” to  $\begin{bmatrix} 3 \\ 2 \end{bmatrix}$ . This is called a **least-squares solution** (p17).

To do this, we have to first define what we mean by “closest”, i.e. define the idea of distance.

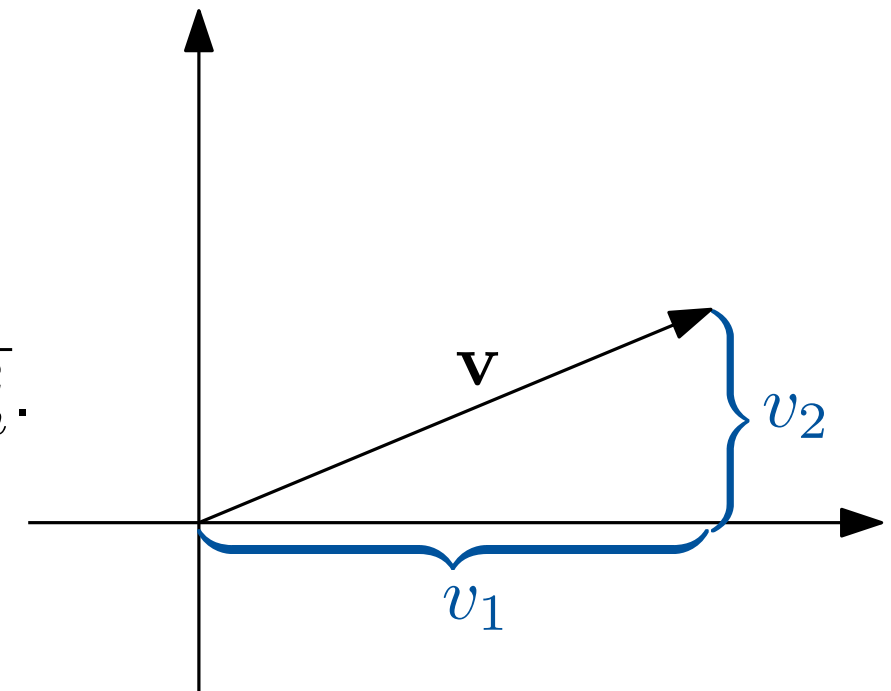
In  $\mathbb{R}^2$ , the distance between  $\mathbf{u}$  and  $\mathbf{v}$  is the length of their difference  $\mathbf{u} - \mathbf{v}$ .

So, to define distances in  $\mathbb{R}^n$ , it's enough to define the length of vectors.



In  $\mathbb{R}^2$ , the length of  $\begin{bmatrix} v_1 \\ v_2 \end{bmatrix}$  is  $\sqrt{v_1^2 + v_2^2}$ .

So we define the length of  $\begin{bmatrix} v_1 \\ \vdots \\ v_n \end{bmatrix}$  is  $\sqrt{v_1^2 + \cdots + v_n^2}$ .



# §6.1, p368: Length, Orthogonality, Best Approximation

It is more useful to define a more general idea:

**Definition:** The *dot product* of two vectors  $\mathbf{u} = \begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix}$  and  $\mathbf{v} = \begin{bmatrix} v_1 \\ \vdots \\ v_n \end{bmatrix}$  in  $\mathbb{R}^n$  is

the scalar

$$\mathbf{u} \cdot \mathbf{v} = \mathbf{u}^T \mathbf{v} = u_1 v_1 + \cdots + u_n v_n.$$

Warning: do not write  $\mathbf{u}\mathbf{v}$ , which is an undefined matrix-vector product, or  $\mathbf{u} \times \mathbf{v}$ , which has a different meaning.

**Definition:** The *length* or *norm* of  $\mathbf{v}$  is

$$\|\mathbf{v}\| = \sqrt{\mathbf{v} \cdot \mathbf{v}} = \sqrt{v_1^2 + \cdots + v_n^2}.$$

**Definition:** The *distance* between  $\mathbf{u}$  and  $\mathbf{v}$  is  $\|\mathbf{u} - \mathbf{v}\|$ .

$$\mathbf{u} \cdot \mathbf{v} = \mathbf{u}^T \mathbf{v} = u_1 v_1 + \cdots + u_n v_n.$$

$$\|\mathbf{v}\| = \sqrt{\mathbf{v} \cdot \mathbf{v}} = \sqrt{v_1^2 + \cdots + v_n^2}.$$

Distance between  $\mathbf{u}$  and  $\mathbf{v}$  is  $\|\mathbf{u} - \mathbf{v}\|$ .

**Example:**  $\mathbf{u} = \begin{bmatrix} 3 \\ 0 \\ -1 \end{bmatrix}, \mathbf{v} = \begin{bmatrix} 8 \\ 5 \\ -6 \end{bmatrix}.$

$$\mathbf{u} \cdot \mathbf{v} = 3 \cdot 8 + 0 \cdot 5 + (-1) \cdot (-6) = 24 + 0 + 6 = 30.$$

The distance between  $\mathbf{u}$  and  $\mathbf{v}$  is

$$\left\| \begin{bmatrix} 3 \\ 0 \\ -1 \end{bmatrix} - \begin{bmatrix} 8 \\ 5 \\ -6 \end{bmatrix} \right\| = \left\| \begin{bmatrix} -5 \\ -5 \\ 5 \end{bmatrix} \right\| = \sqrt{(-5)^2 + (-5)^2 + 5^2} = \sqrt{75} = 5\sqrt{3}.$$

## Properties of the dot product:

Let  $\mathbf{u}, \mathbf{v}$  and  $\mathbf{w}$  be vectors in  $\mathbf{R}^n$ , and let  $c$  be any scalar. Then

a.  $\mathbf{u} \cdot \mathbf{v} = \mathbf{v} \cdot \mathbf{u}$

symmetry

b.  $(\mathbf{u} + \mathbf{v}) \cdot \mathbf{w} = \mathbf{u} \cdot \mathbf{w} + \mathbf{v} \cdot \mathbf{w}$

c.  $(c\mathbf{u}) \cdot \mathbf{v} = c(\mathbf{u} \cdot \mathbf{v}) = \mathbf{u} \cdot (c\mathbf{v})$

} linearity in each input  
separately

d.  $\mathbf{u} \cdot \mathbf{u} \geq 0$ , and  $\mathbf{u} \cdot \mathbf{u} = 0$  if and only if  $\mathbf{u} = \mathbf{0}$ . positivity; and the only vector with length 0 is  $\mathbf{0}$

Combining parts b and c, one can show

$$(c_1 \mathbf{u}_1 + \cdots + c_p \mathbf{u}_p) \cdot \mathbf{w} = c_1(\mathbf{u}_1 \cdot \mathbf{w}) + \cdots + c_p(\mathbf{u}_p \cdot \mathbf{w})$$

So b and c together says that, for fixed  $\mathbf{w}$ , the function  $\mathbf{x} \mapsto \mathbf{x} \cdot \mathbf{w}$  is linear - this is true because  $\mathbf{x} \cdot \mathbf{w} = \mathbf{w} \cdot \mathbf{x} = \mathbf{w}^T \mathbf{x}$  and matrix multiplication by  $\mathbf{w}^T$  is linear.

From property c:

$$\|c\mathbf{v}\|^2 = (c\mathbf{v}) \cdot (c\mathbf{v}) = c^2 \mathbf{v} \cdot \mathbf{v} = c^2 \|\mathbf{v}\|^2,$$

so (squareroot both sides)

$$\|c\mathbf{v}\| = |c| \|\mathbf{v}\|.$$

For many applications, we are interested in vectors of length 1.

**Definition:** A **unit vector** is a vector whose **length is 1**.

Given  $\mathbf{v}$ , to create a unit vector in the same direction as  $\mathbf{v}$ , we divide  $\mathbf{v}$  by its length  $\|\mathbf{v}\|$  (i.e. take  $c = \frac{1}{\|\mathbf{v}\|}$  in the equation above). This process is called **normalising**.

**Example:** Find a unit vector in the same direction as  $\mathbf{v} = \begin{bmatrix} 8 \\ 5 \\ -6 \end{bmatrix}$ .

**Answer:**  $\mathbf{v} \cdot \mathbf{v} = 8^2 + 5^2 + (-6)^2 = 125$ .

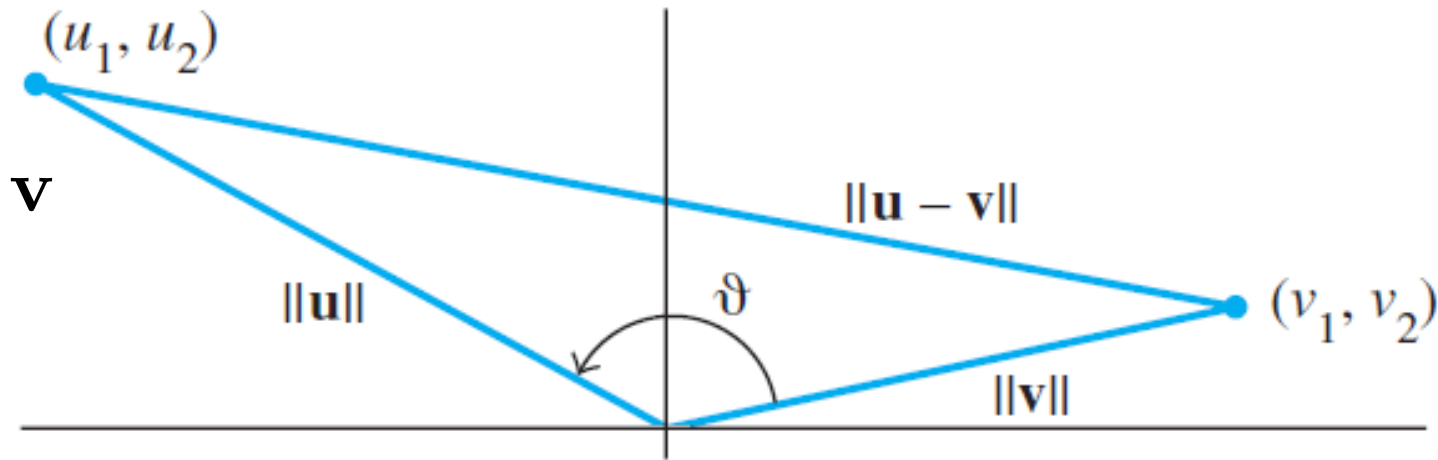
So a unit vector in the same direction as  $\mathbf{v}$  is  $\frac{\mathbf{v}}{\|\mathbf{v}\|} = \frac{1}{\sqrt{125}} \begin{bmatrix} 8 \\ 5 \\ -6 \end{bmatrix}$ .

Visualising the dot product:

In  $\mathbb{R}^2$ , the cosine law says  $\|\mathbf{u} - \mathbf{v}\|^2 = \|\mathbf{u}\|^2 + \|\mathbf{v}\|^2 - 2 \|\mathbf{u}\| \|\mathbf{v}\| \cos \theta$ .

We can “expand” the left hand side using dot products:

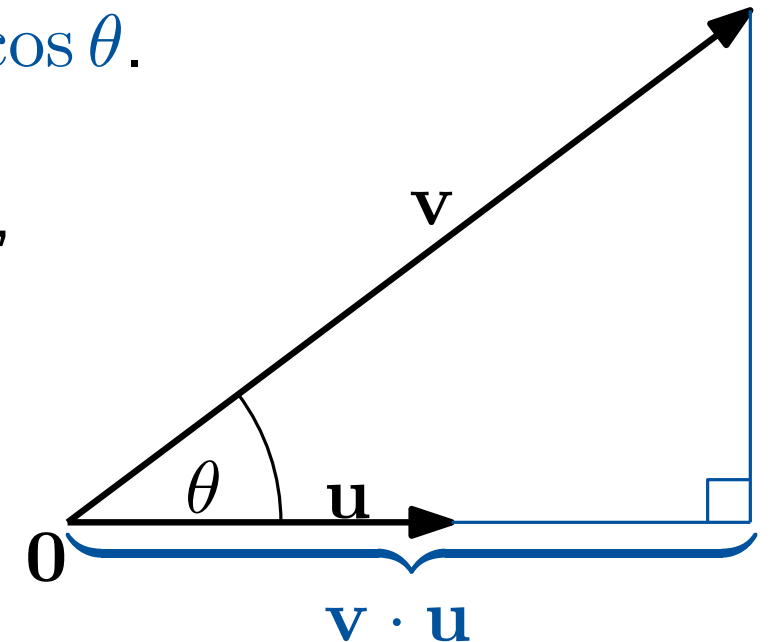
$$\begin{aligned}\|\mathbf{u} - \mathbf{v}\|^2 &= (\mathbf{u} - \mathbf{v}) \cdot (\mathbf{u} - \mathbf{v}) \\ &= \mathbf{u} \cdot \mathbf{u} - \mathbf{u} \cdot \mathbf{v} - \mathbf{v} \cdot \mathbf{u} + \mathbf{v} \cdot \mathbf{v} \\ &= \|\mathbf{u}\|^2 - 2\mathbf{u} \cdot \mathbf{v} + \|\mathbf{v}\|^2.\end{aligned}$$



Comparing with the cosine law, we see  $\mathbf{u} \cdot \mathbf{v} = \|\mathbf{u}\| \|\mathbf{v}\| \cos \theta$ .

In particular, if  $\mathbf{u}$  is a unit vector, then  $\mathbf{v} \cdot \mathbf{u} = \|\mathbf{v}\| \cos \theta$ , as shown in the bottom picture.

Notice that  $\mathbf{u}$  and  $\mathbf{v}$  are **perpendicular** if and only if  $\theta = \frac{\pi}{2}$ , i.e. when  $\cos \theta = 0$ . This is equivalent to  $\mathbf{u} \cdot \mathbf{v} = 0$ .



So, to generalise the idea of perpendicularity to  $\mathbb{R}^n$  for  $n > 2$ , we make the following definition:

**Definition:** Two vectors  $\mathbf{u}$  and  $\mathbf{v}$  are **orthogonal** if  $\mathbf{u} \cdot \mathbf{v} = 0$ .

We also say  **$\mathbf{u}$  is orthogonal to  $\mathbf{v}$** .

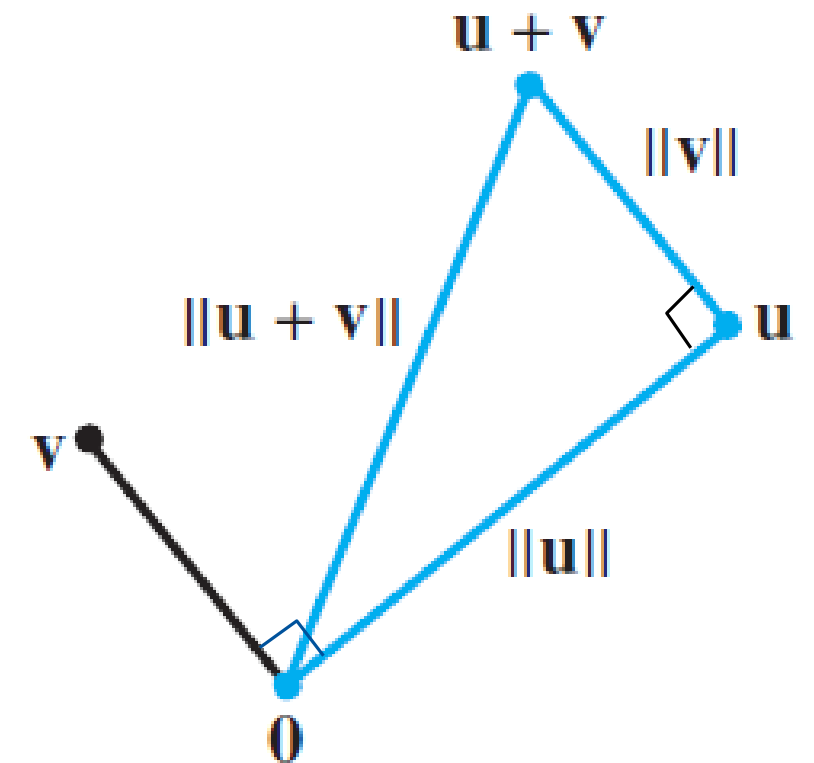
Another way to see that orthogonality generalises perpendicularity:

**Theorem 2: Pythagorean Theorem:** Two vectors  $\mathbf{u}$  and  $\mathbf{v}$  are **orthogonal** if and only if  $\|\mathbf{u} + \mathbf{v}\|^2 = \|\mathbf{u}\|^2 + \|\mathbf{v}\|^2$ .

**Proof:**

$$\begin{aligned}\|\mathbf{u} + \mathbf{v}\|^2 &= (\mathbf{u} + \mathbf{v}) \cdot (\mathbf{u} + \mathbf{v}) \\ &= \mathbf{u} \cdot \mathbf{u} + \mathbf{u} \cdot \mathbf{v} + \mathbf{v} \cdot \mathbf{u} + \mathbf{v} \cdot \mathbf{v} \\ &= \|\mathbf{u}\|^2 + 2\mathbf{u} \cdot \mathbf{v} + \|\mathbf{v}\|^2.\end{aligned}$$

So  $\|\mathbf{u} + \mathbf{v}\|^2 = \|\mathbf{u}\|^2 + \|\mathbf{v}\|^2$  if and only if  $\mathbf{u} \cdot \mathbf{v} = 0$ .





Instead of  $\mathbf{v}$  being orthogonal to just a single vector  $\mathbf{u}$ , we can consider orthogonality to a set of vectors:

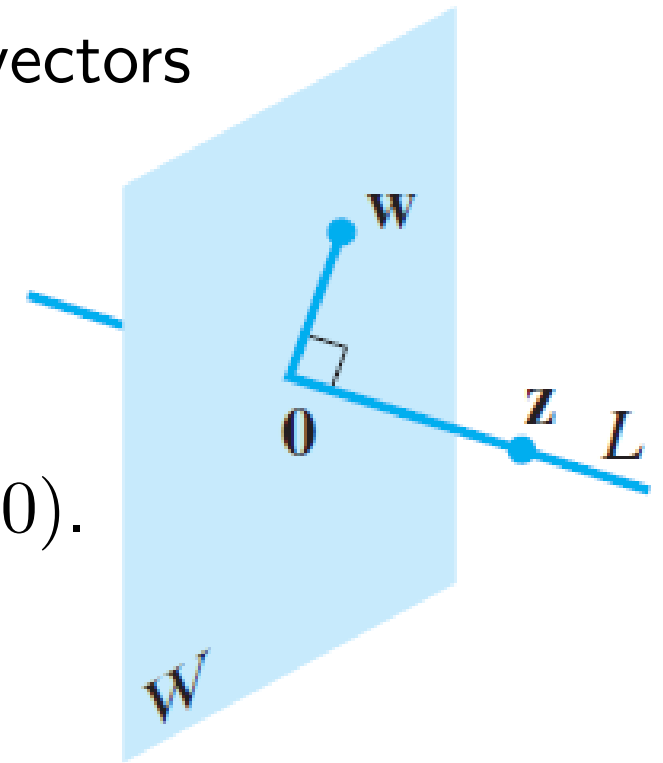
**Definition:** Let  $W$  be a subspace of  $\mathbb{R}^n$  (or more generally a subset). A vector  $\mathbf{z}$  is *orthogonal to  $W$*  if it is orthogonal to every vector in  $W$ . The *orthogonal complement* of  $W$ , written  $W^\perp$ , is the set of all vectors orthogonal to  $W$ . In other words,  $\mathbf{z}$  is in  $W^\perp$  means  $\mathbf{z} \cdot \mathbf{w} = 0$  for all  $\mathbf{w}$  in  $W$ .

**Example:** Let  $W$  be the  $x_1x_3$ -plane in  $\mathbb{R}^3$ , i.e. the set of all vectors

of the form  $\begin{bmatrix} a \\ 0 \\ b \end{bmatrix}$  where  $a, b$  can take any value. Then  $\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$  is

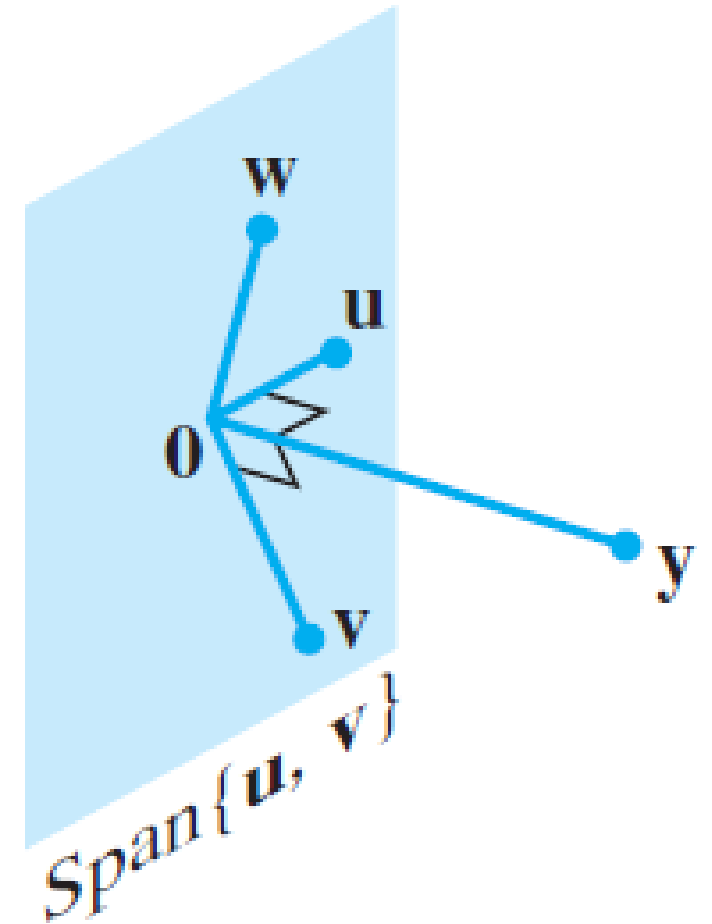
orthogonal to  $W$  (because  $\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \cdot \begin{bmatrix} a \\ 0 \\ b \end{bmatrix} = 0 \cdot a + 1 \cdot 0 + 0 \cdot b = 0$ ).

The orthogonal complement  $W^\perp$  is  $\text{Span} \left\{ \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \right\}$  (see p13).



Key properties of  $W^\perp$ , for a subspace  $W$  of  $\mathbb{R}^n$ :

1. If  $\mathbf{x}$  is in both  $W$  and  $W^\perp$ , then  $\mathbf{x} = \mathbf{0}$  (ex. sheet q2b).
  2. If  $W = \text{Span}\{\mathbf{v}_1, \dots, \mathbf{v}_p\}$ , then  $\mathbf{y}$  is in  $W^\perp$  if and only if  $\mathbf{y}$  is orthogonal to each  $\mathbf{v}_i$  (same idea as ex. sheet q2a, see diagram).
  3.  $W^\perp$  is a subspace of  $\mathbb{R}^n$  (checking the axioms directly is not hard, alternative proof p13).
  4.  $\dim W + \dim W^\perp = n$  (follows from alternative proof of 3, see p13).
  5. If  $W^\perp = U$ , then  $U^\perp = W$ .
  6. For a vector  $\mathbf{y}$  in  $\mathbb{R}^n$ , the closest point in  $W$  to  $\mathbf{y}$  is the unique point  $\hat{\mathbf{y}}$  such that  $\mathbf{y} - \hat{\mathbf{y}}$  is in  $W^\perp$  (see p15-17).
- (1 and 3 are true for any set  $W$ , even when  $W$  is not a subspace.)



## Dot product and matrix multiplication:

Remember from Week 2 (§1.4) the row-column method of matrix-vector multiplication:

**Example:** 
$$\begin{bmatrix} 4 & 3 \\ 2 & 6 \\ 14 & 10 \end{bmatrix} \begin{bmatrix} -2 \\ 2 \end{bmatrix} = \begin{bmatrix} 4(-2) + 3(2) \\ 2(-2) + 6(2) \\ 14(-2) + 10(2) \end{bmatrix} = \begin{bmatrix} -2 \\ 8 \\ -8 \end{bmatrix}.$$

↖ This last entry is  $\begin{bmatrix} 14 \\ 10 \end{bmatrix} \cdot \begin{bmatrix} -2 \\ 2 \end{bmatrix}.$

In general,

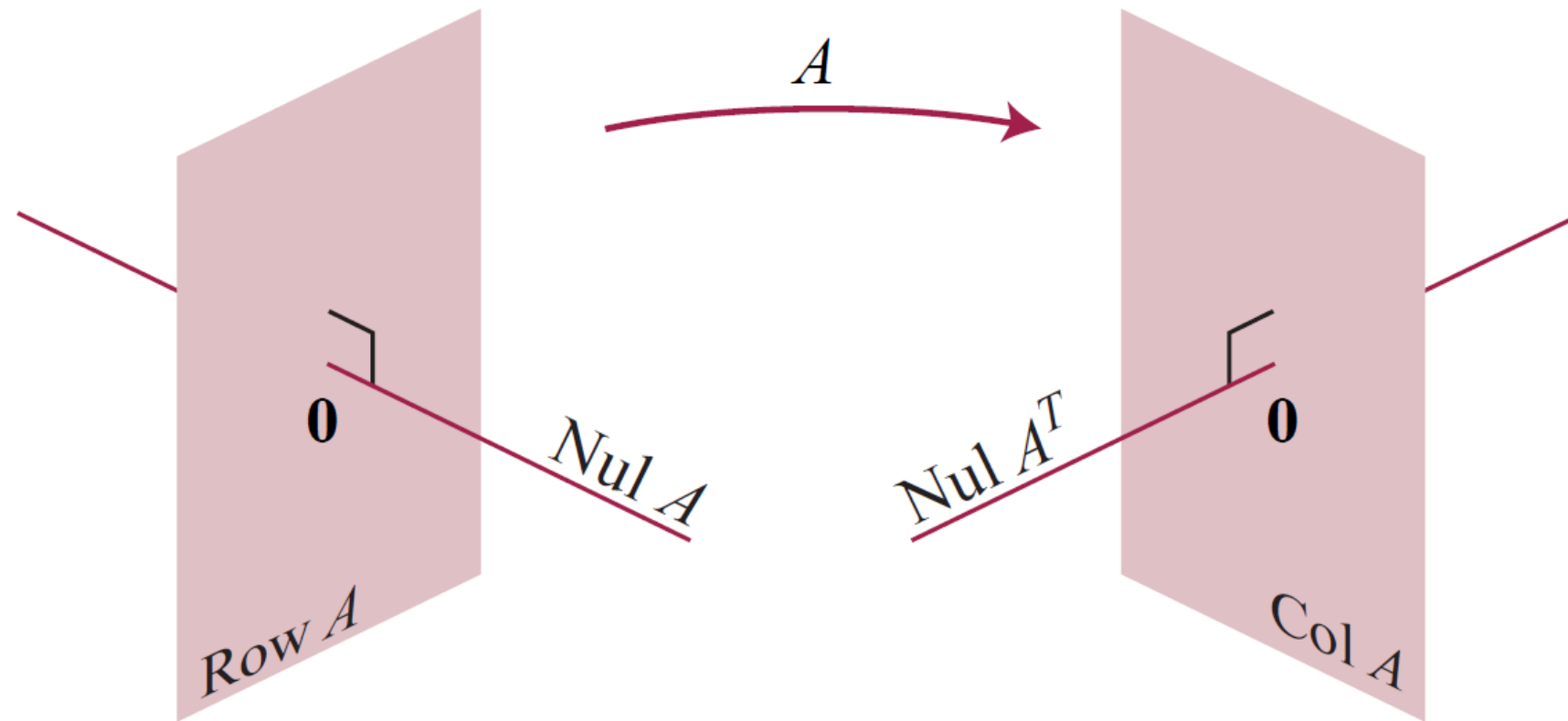
$$\begin{bmatrix} \text{---} & \mathbf{r}_1 & \text{---} \\ \text{---} & \vdots & \text{---} \\ \text{---} & \mathbf{r}_m & \text{---} \end{bmatrix} \mathbf{x} = \begin{bmatrix} \mathbf{r}_1 \cdot \mathbf{x} \\ \vdots \\ \mathbf{r}_m \cdot \mathbf{x} \end{bmatrix}.$$

So  $\mathbf{x}$  is in the null space of  $A$  if and only if  $\mathbf{r}_i \cdot \mathbf{x} = 0$  for every row  $\mathbf{r}_i$  of  $A$ . By property 2 on the previous page, this precisely means  $\mathbf{x}$  is in  $(\text{Span}\{\mathbf{r}_1, \dots, \mathbf{r}_m\})^\perp$ . So

**Theorem 3: Orthogonality of Subspaces associated to Matrices:**

$(\text{Row } A)^\perp = \text{Nul } A$ , and ...

**Theorem 3: Orthogonality of Subspaces associated to Matrices:** For a matrix  $A$ ,  $(\text{Row } A)^\perp = \text{Nul } A$  and  $(\text{Col } A)^\perp = \text{Nul } A^T$ .  
 The second assertion comes from applying the first statement to  $A^T$  instead of  $A$ , remembering that  $\text{Row } A^T = \text{Col } A$ .



**Theorem 3: Orthogonality of Subspaces associated to Matrices:** For a matrix  $A$ ,  $(\text{Row}A)^\perp = \text{Nul}A$  and  $(\text{Col}A)^\perp = \text{Nul}A^T$ .

We can use this theorem to prove that  $W^\perp$  is a subspace: given a subspace  $W$  of  $\mathbb{R}^n$ , let  $A$  be the matrix whose rows is a basis for  $W$ , so  $\text{Row}A = W$ . Then  $W^\perp = \text{Nul}A$ , and null spaces are subspaces, so  $W^\perp$  is a subspace.

Futhermore, the Rank Nullity Theorem says  $\dim \text{Row}A + \dim \text{Nul}A = n$ , so  $\dim W + \dim W^\perp = n$ .

The argument above also gives us a way to compute orthogonal complements:

**Example:** Let  $W$  be the set of vectors of the form  $\begin{bmatrix} a \\ 0 \\ b \end{bmatrix}$  where  $a, b$  can take any value. A basis for  $W$  is  $\left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \right\}$ , so  $W^\perp$  is the solutions to  $\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \mathbf{x} = \mathbf{0}$ , which is  $s \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$  where  $s$  can take any value. Notice  $\dim W + \dim W^\perp = 2 + 1 = 3$ .

On p11, we related the matrix-vector product to the dot product:

$$\begin{bmatrix} \text{---} & \mathbf{r}_1 & \text{---} \\ \text{---} & \vdots & \text{---} \\ \text{---} & \mathbf{r}_m & \text{---} \end{bmatrix} \mathbf{x} = \begin{bmatrix} \mathbf{r}_1 \cdot \mathbf{x} \\ \vdots \\ \mathbf{r}_m \cdot \mathbf{x} \end{bmatrix}.$$

Because each column of a matrix-matrix product is a matrix-vector product,

$$AB = A \begin{bmatrix} | & & | \\ \mathbf{b}_1 & \dots & \mathbf{b}_p \\ | & & | \end{bmatrix} = \begin{bmatrix} | & & | \\ A\mathbf{b}_1 & \dots & A\mathbf{b}_p \\ | & & | \end{bmatrix},$$

we can also express matrix-matrix products in terms of the dot product:

the  $(i, j)$ -entry of the product  $AB$  is  $(i\text{th row of } A) \cdot (j\text{th column of } B)$

$$\begin{bmatrix} \text{---} & \mathbf{r}_1 & \text{---} \\ \text{---} & \vdots & \text{---} \\ \text{---} & \mathbf{r}_m & \text{---} \end{bmatrix} \begin{bmatrix} | & & | \\ \mathbf{b}_1 & \dots & \mathbf{b}_p \\ | & & | \end{bmatrix} = \begin{bmatrix} \mathbf{r}_1 \cdot \mathbf{b}_1 & \dots & \mathbf{r}_1 \cdot \mathbf{b}_p \\ \vdots & & \vdots \\ \mathbf{r}_m \cdot \mathbf{b}_1 & \dots & \mathbf{r}_m \cdot \mathbf{b}_p \end{bmatrix}.$$

Closest point to a subspace:

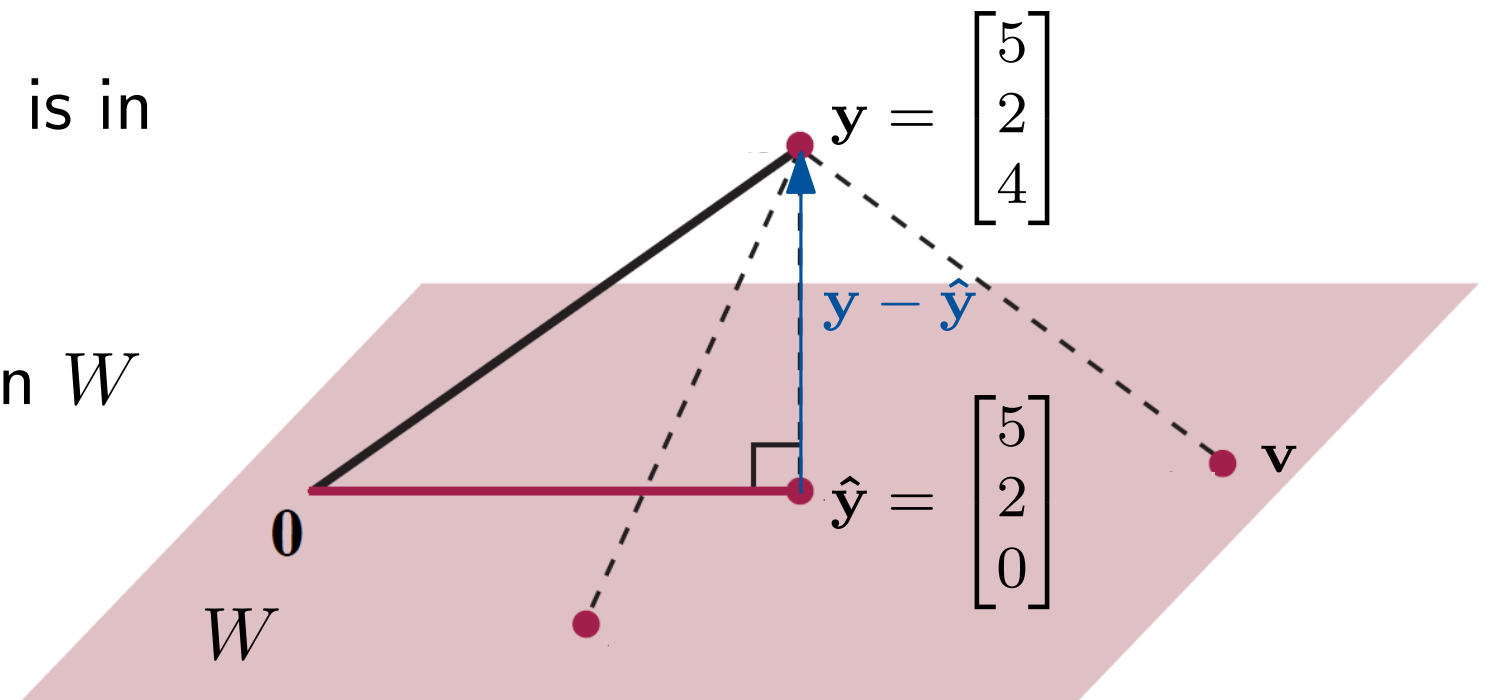
**Theorem 9: Best Approximation Theorem:** Let  $W$  be a subspace of  $\mathbb{R}^n$ , and  $\mathbf{y}$  a vector in  $\mathbb{R}^n$ . Then the **closest point in  $W$  to  $\mathbf{y}$**  is the **unique** point  $\hat{\mathbf{y}}$  in  $W$  such that  $\mathbf{y} - \hat{\mathbf{y}}$  is in  $W^\perp$ . In other words,  $\|\mathbf{y} - \hat{\mathbf{y}}\| < \|\mathbf{y} - \mathbf{v}\|$  for all  $\mathbf{v}$  in  $W$  with  $\mathbf{v} \neq \hat{\mathbf{y}}$ .

**Example:** Let  $W = \text{Span} \left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \right\}$ , so  $W^\perp = \text{Span} \left\{ \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \right\}$ . Let  $\mathbf{y} = \begin{bmatrix} 5 \\ 2 \\ 4 \end{bmatrix}$ .

Take  $\hat{\mathbf{y}} = \begin{bmatrix} 5 \\ 2 \\ 0 \end{bmatrix}$ , then  $\mathbf{y} - \hat{\mathbf{y}} = \begin{bmatrix} 0 \\ 0 \\ 4 \end{bmatrix}$  is in

$W^\perp$ , so  $\hat{\mathbf{y}} = \begin{bmatrix} 5 \\ 2 \\ 0 \end{bmatrix}$  is unique point in  $W$

that is closest to  $\begin{bmatrix} 5 \\ 2 \\ 4 \end{bmatrix}$ .



**Theorem 9: Best Approximation Theorem:** Let  $W$  be a subspace of  $\mathbb{R}^n$ , and  $\mathbf{y}$  a vector in  $\mathbb{R}^n$ . Then the **closest point in  $W$  to  $\mathbf{y}$**  is the **unique** point  $\hat{\mathbf{y}}$  in  $W$  such that  $\mathbf{y} - \hat{\mathbf{y}}$  is in  $W^\perp$ . In other words,  $\|\mathbf{y} - \hat{\mathbf{y}}\| < \|\mathbf{y} - \mathbf{v}\|$  for all  $\mathbf{v}$  in  $W$  with  $\mathbf{v} \neq \hat{\mathbf{y}}$ .

**Partial Proof:** We show here that, if  $\mathbf{y} - \hat{\mathbf{y}}$  is in  $W^\perp$ , then  $\hat{\mathbf{y}}$  is the unique closest point (i.e. it satisfies the last sentence of the theorem). We will not show here that there is always a  $\hat{\mathbf{y}}$  such that  $\mathbf{y} - \hat{\mathbf{y}}$  is in  $W^\perp$ . (See §6.3 on orthogonal projections, in Week 13 notes.)

We are assuming that  $\mathbf{y} - \hat{\mathbf{y}}$  is in  $W^\perp$ . (vertical blue edge)

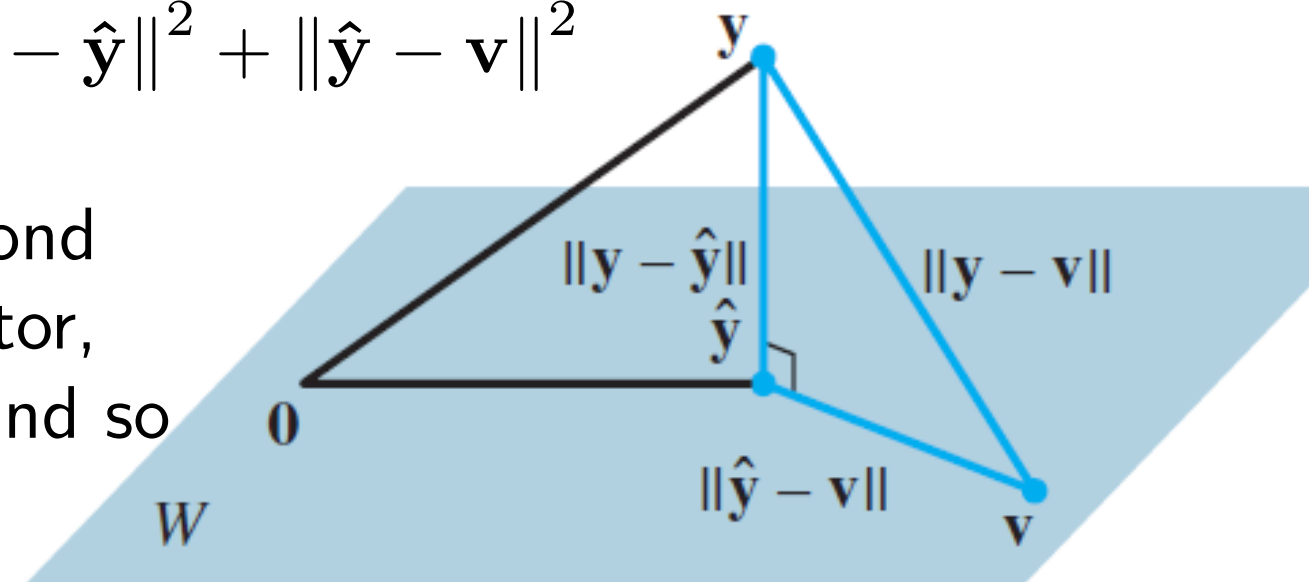
$\hat{\mathbf{y}} - \mathbf{v}$  is a difference of vectors in  $W$ , so it is in  $W$ . (horizontal blue edge)

So  $\mathbf{y} - \hat{\mathbf{y}}$  and  $\hat{\mathbf{y}} - \mathbf{v}$  are orthogonal. Apply the Pythagorean Theorem (blue triangle):

$$\|(\mathbf{y} - \hat{\mathbf{y}}) + (\hat{\mathbf{y}} - \mathbf{v})\|^2 = \|\mathbf{y} - \hat{\mathbf{y}}\|^2 + \|\hat{\mathbf{y}} - \mathbf{v}\|^2$$

The left hand side is  $\|\mathbf{y} - \mathbf{v}\|^2$ .

The right hand side: if  $\mathbf{v} \neq \hat{\mathbf{y}}$ , then the second term is the squared-length of a nonzero vector, so it is positive. So  $\|\mathbf{y} - \mathbf{v}\|^2 > \|\mathbf{y} - \hat{\mathbf{y}}\|^2$  and so  $\|\mathbf{y} - \mathbf{v}\| > \|\mathbf{y} - \hat{\mathbf{y}}\|$ .





## §6.5-6.6: Least Squares, Application to Regression

Remember our motivation: we have an inconsistent equation  $A\mathbf{x} = \mathbf{b}$ , and we want to find a “closest approximate solution”  $\hat{\mathbf{x}}$  such that  $A\hat{\mathbf{x}}$  is the point in  $\text{Col}A$  that is closest to  $\mathbf{b}$ .

**Definition:** If  $A$  is an  $m \times n$  matrix and  $\mathbf{b}$  is in  $\mathbb{R}^m$ , then a *least-squares solution* of  $A\mathbf{x} = \mathbf{b}$  is a vector  $\hat{\mathbf{x}}$  in  $\mathbb{R}^n$  such that  $\|\mathbf{b} - A\hat{\mathbf{x}}\| \leq \|\mathbf{b} - A\mathbf{x}\|$  for all  $\mathbf{x}$  in  $\mathbb{R}^n$ .

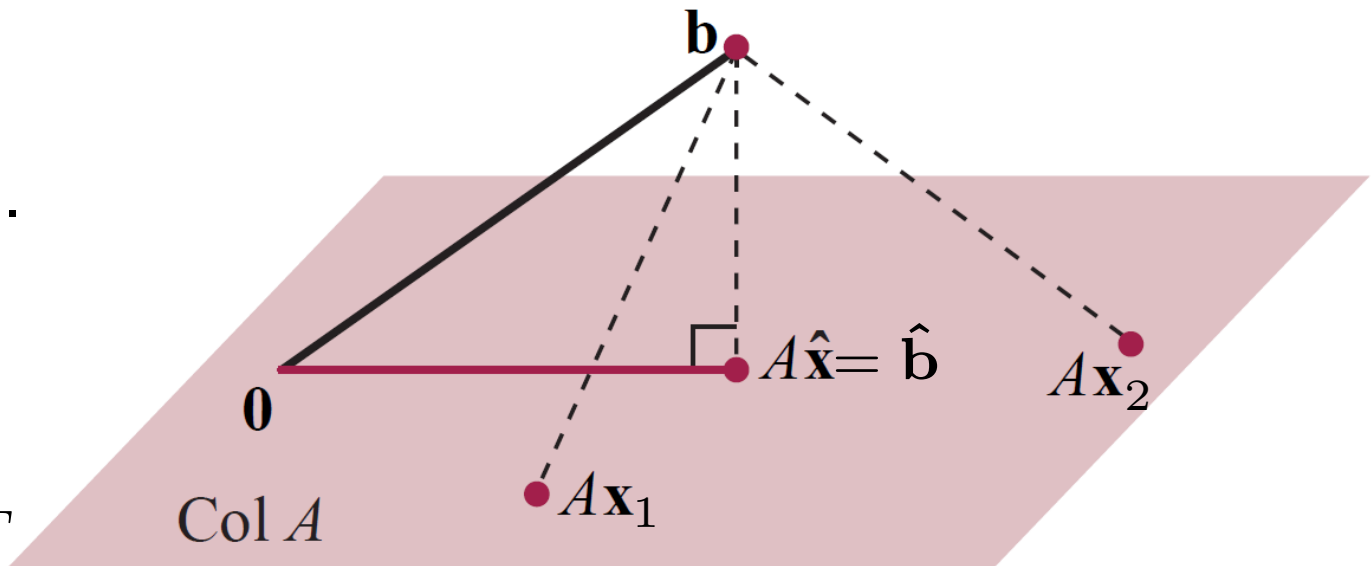
Equivalently: we want to find a vector  $\hat{\mathbf{b}}$  in  $\text{Col}A$  that is closest to  $\mathbf{b}$ , and then solve  $A\hat{\mathbf{x}} = \hat{\mathbf{b}}$ .

Because of the Best Approximation Theorem (p15-16):  $\mathbf{b} - \hat{\mathbf{b}}$  is in  $(\text{Col}A)^\perp$ .

Because of Orthogonality of Subspaces associated to Matrices (p11-13):

$$(\text{Col}A)^\perp = \text{Nul}A^T.$$

So we need  $\hat{\mathbf{b}}$  so that  $\mathbf{b} - \hat{\mathbf{b}}$  is in  $\text{Nul}A^T$ .



The least-squares solutions to  $A\mathbf{x} = \mathbf{b}$  are the solutions to  $A\hat{\mathbf{x}} = \hat{\mathbf{b}}$  where  $\hat{\mathbf{b}}$  is the unique vector such that  $\mathbf{b} - \hat{\mathbf{b}}$  is in  $\text{Nul}A^T$ .

Equivalently,

$$A^T(\mathbf{b} - \hat{\mathbf{b}}) = \mathbf{0}$$

$$A^T\mathbf{b} - A^T\hat{\mathbf{b}} = \mathbf{0}$$

$$A^T\mathbf{b} = A^T\hat{\mathbf{b}}$$

$$A^T\mathbf{b} = A^T A\hat{\mathbf{x}}$$

So we have proved:

**Theorem 13: Least-Squares Theorem:** The set of least-squares solutions of  $A\mathbf{x} = \mathbf{b}$  is the set of solutions of the **normal equations**  $A^T A\hat{\mathbf{x}} = A^T\mathbf{b}$ .

Because of the existence part of the Best Approximation Theorem (that we will prove later),  $A^T A\hat{\mathbf{x}} = A^T\mathbf{b}$  is always consistent.

**Warning:** The terminology is confusing: a least-squares solution  $\hat{\mathbf{x}}$ , satisfying  $A^T A\hat{\mathbf{x}} = A^T\mathbf{b}$ , is in general **not** a solution to  $A\mathbf{x} = \mathbf{b}$ . That is, usually  $A\hat{\mathbf{x}} \neq \mathbf{b}$ .

**Theorem 13: Least-Squares Theorem:** The set of least-squares solutions of  $A\mathbf{x} = \mathbf{b}$  is the set of solutions of the **normal equations**  $A^T A\hat{\mathbf{x}} = A^T \mathbf{b}$ .

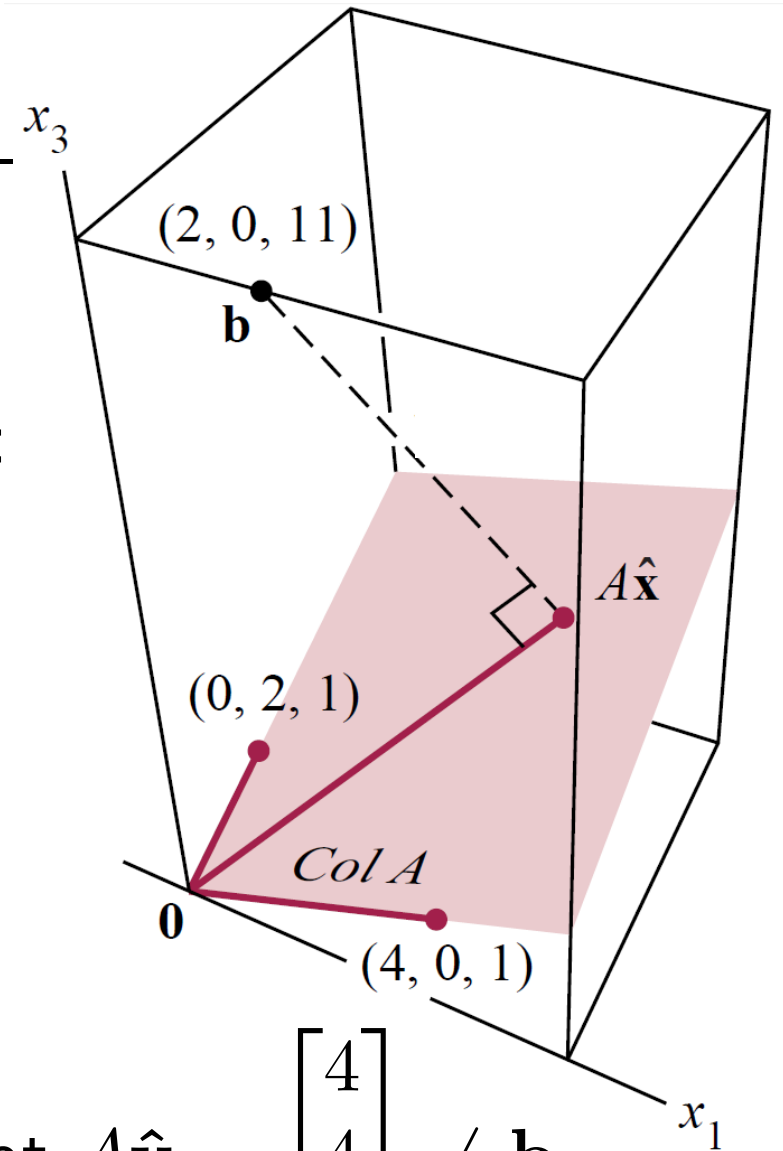
**Example:** Let  $A = \begin{bmatrix} 4 & 0 \\ 0 & 2 \\ 1 & 1 \end{bmatrix}$  and  $\mathbf{b} = \begin{bmatrix} 2 \\ 0 \\ 11 \end{bmatrix}$ . Find a least-squares solution of the inconsistent equation  $A\mathbf{x} = \mathbf{b}$ .

**Answer:** We solve the normal equations  $A^T A\hat{\mathbf{x}} = A^T \mathbf{b}$ :

$$\begin{bmatrix} 4 & 0 & 1 \\ 0 & 2 & 1 \end{bmatrix} \begin{bmatrix} 4 & 0 \\ 0 & 2 \\ 1 & 1 \end{bmatrix} \hat{\mathbf{x}} = \begin{bmatrix} 4 & 0 & 1 \\ 0 & 2 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 0 \\ 11 \end{bmatrix}$$

$$\begin{bmatrix} 17 & 1 \\ 1 & 5 \end{bmatrix} \hat{\mathbf{x}} = \begin{bmatrix} 19 \\ 11 \end{bmatrix}$$

By row-reducing  $\begin{bmatrix} 17 & 1 & | & 19 \\ 1 & 5 & | & 11 \end{bmatrix}$ , we find  $\hat{\mathbf{x}} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$ . Note that  $A\hat{\mathbf{x}} = \begin{bmatrix} 4 \\ 4 \\ 3 \end{bmatrix} \neq \mathbf{b}$ .



**Example:** (from p1) Let  $A = \begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix}$  and  $\mathbf{b} = \begin{bmatrix} 3 \\ 2 \end{bmatrix}$ . Find the set of least-squares solutions of the inconsistent equation  $A\mathbf{x} = \mathbf{b}$ .

**Answer:** We solve  $A^T A \hat{\mathbf{x}} = A^T \mathbf{b}$ :

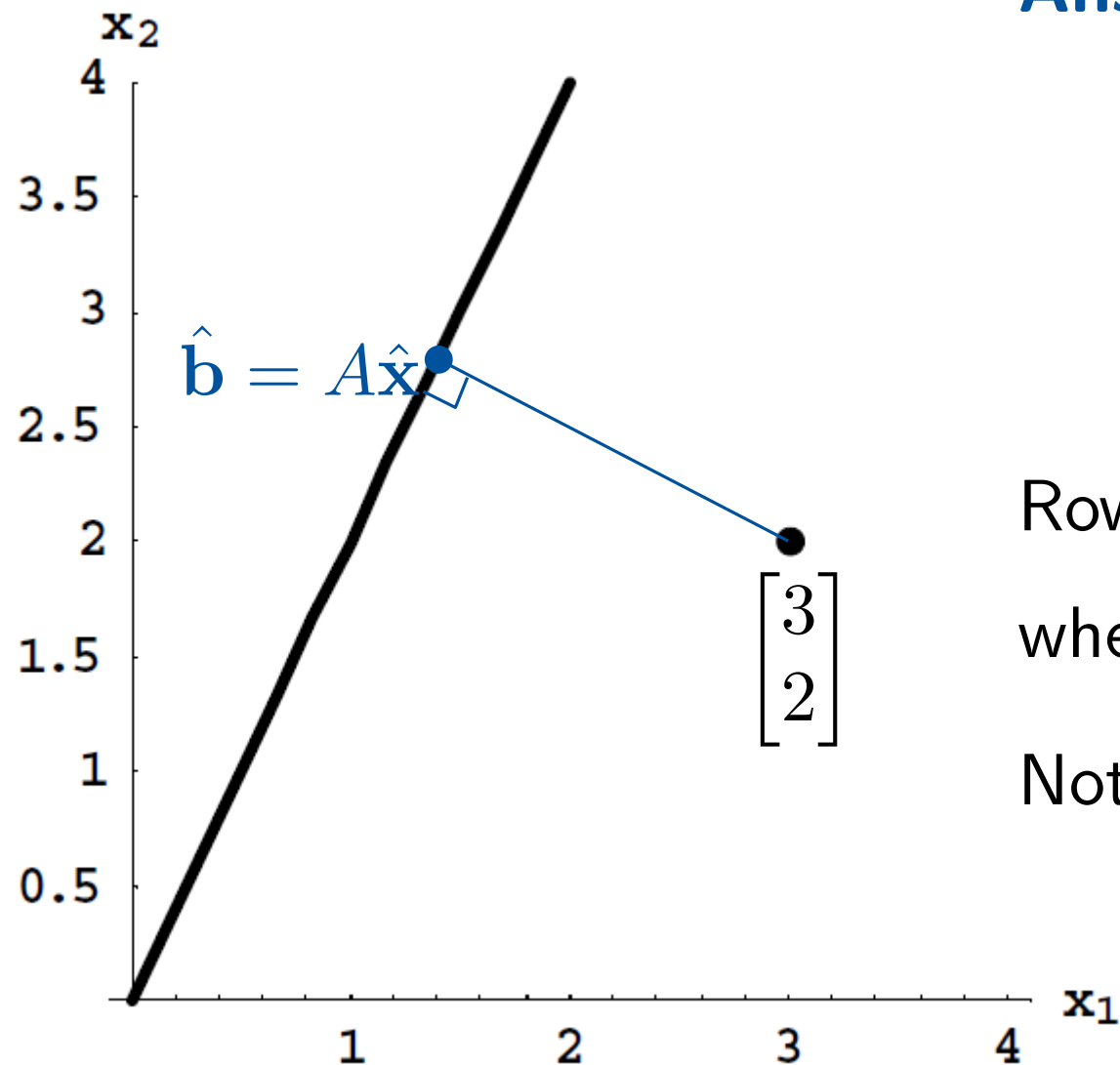
$$\begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix} \hat{\mathbf{x}} = \begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix} \begin{bmatrix} 3 \\ 2 \end{bmatrix}$$

$$\begin{bmatrix} 5 & 10 \\ 10 & 20 \end{bmatrix} \hat{\mathbf{x}} = \begin{bmatrix} 7 \\ 14 \end{bmatrix}$$

Row-reducing  $\begin{bmatrix} 5 & 10 & | & 7 \\ 10 & 20 & | & 14 \end{bmatrix}$  gives  $\hat{\mathbf{x}} = \begin{bmatrix} 7/5 \\ 0 \end{bmatrix} + s \begin{bmatrix} -2 \\ 1 \end{bmatrix}$  where  $s$  can take any value.

Note that  $A\hat{\mathbf{x}} = A \left( \begin{bmatrix} 7/5 \\ 0 \end{bmatrix} + s \begin{bmatrix} -2 \\ 1 \end{bmatrix} \right) = \begin{bmatrix} 7/5 \\ 14/5 \end{bmatrix}$ ,

independent of  $s$ :  $A\hat{\mathbf{x}}$  is the closest point in  $\text{Col}A$  to  $\mathbf{b}$ , which by the Best Approximation Theorem is unique.



Observations from the previous examples:

- $A^T A$  is a square matrix and is symmetric. (Exercise: prove it!)
- The normal equations sometimes have a unique solution and sometimes have infinitely many solutions, but  $A\hat{\mathbf{x}}$  is unique.

When is the least-squares solution unique?

**Theorem 14: Uniqueness of Least-Squares Solutions:** The equation  $A\mathbf{x} = \mathbf{b}$  has a **unique least-squares solution** if and only if the **columns of  $A$  are linearly independent**.

Consequences:

- The number of least-squares solutions to  $A\mathbf{x} = \mathbf{b}$  does not depend on  $\mathbf{b}$ , only on  $A$ .
- Because  $A^T A$  is a square matrix, if the least-squares solution is unique, then it is  $\hat{\mathbf{x}} = (A^T A)^{-1} A^T \mathbf{b}$ . This formula is useful theoretically (e.g. for deriving general expressions for regression coefficients, see Homework 6 q5).

**Theorem 14: Uniqueness of Least-Squares Solutions:** The equation  $A\mathbf{x} = \mathbf{b}$  has a unique least-squares solution if and only if the columns of  $A$  are linearly independent.

**Proof 1:** The least-squares solutions are the solutions to the normal equations  $A^T A\hat{\mathbf{x}} = A^T \mathbf{b}$ . So

- “unique least-squares solution” is equivalent to  $\text{Nul}(A^T A) = \{\mathbf{0}\}$ .
- “columns of  $A$  are linearly independent” is equivalent to  $\text{Nul}A = \{\mathbf{0}\}$ .

So the theorem will follow if we prove the stronger fact  $\text{Nul}(A^T A) = \text{Nul}A$ ; in other words,  $A^T A\mathbf{x} = \mathbf{0}$  if and only if  $A\mathbf{x} = \mathbf{0}$ .

- If  $A\mathbf{x} = \mathbf{0}$ , then  $A^T A\mathbf{x} = A^T (A\mathbf{x}) = A^T \mathbf{0} = \mathbf{0}$ .
- If  $A^T A\mathbf{x} = \mathbf{0}$ , then  $\|A\mathbf{x}\|^2 = (A\mathbf{x}) \cdot (A\mathbf{x}) = (A\mathbf{x})^T (A\mathbf{x}) = \mathbf{x}^T A^T A\mathbf{x} = \mathbf{x}^T (A^T A\mathbf{x}) = \mathbf{x}^T \mathbf{0} = 0$ . So the length of  $A\mathbf{x}$  is 0, which means it must be the zero vector.

**Proof 2:** The least-squares solutions are the solutions to  $A\hat{\mathbf{x}} = \hat{\mathbf{b}}$  where  $\hat{\mathbf{b}}$  is unique (the closest point in  $\text{Col}A$  to  $\mathbf{b}$ ). The equation  $A\hat{\mathbf{x}} = \hat{\mathbf{b}}$  has a unique solution precisely when the columns of  $A$  are linearly independent.

## Application: least-squares line

Suppose we have a model that relates two quantities  $x$  and  $y$  linearly, i.e. we expect  $y = \beta_0 + \beta_1 x$ , for some unknown numbers  $\beta_0, \beta_1$ .

To estimate  $\beta_0$  and  $\beta_1$ , we do an experiment, whose results are  $(x_1, y_1), \dots, (x_n, y_n)$ .

Now we wish to solve (for  $\beta_0, \beta_1$ ):

$$\beta_0 + \beta_1 x_1 = y_1$$

$$\beta_0 + \beta_1 x_2 = y_2$$

$$\vdots \quad \vdots$$

$$\beta_0 + \beta_1 x_n = y_n$$

$$\text{i.e.} \quad \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

$A\mathbf{x} = \mathbf{b}$  with  
different notation

$X$   
//  
design  
matrix

$\beta$   
//  
parameter  
vector

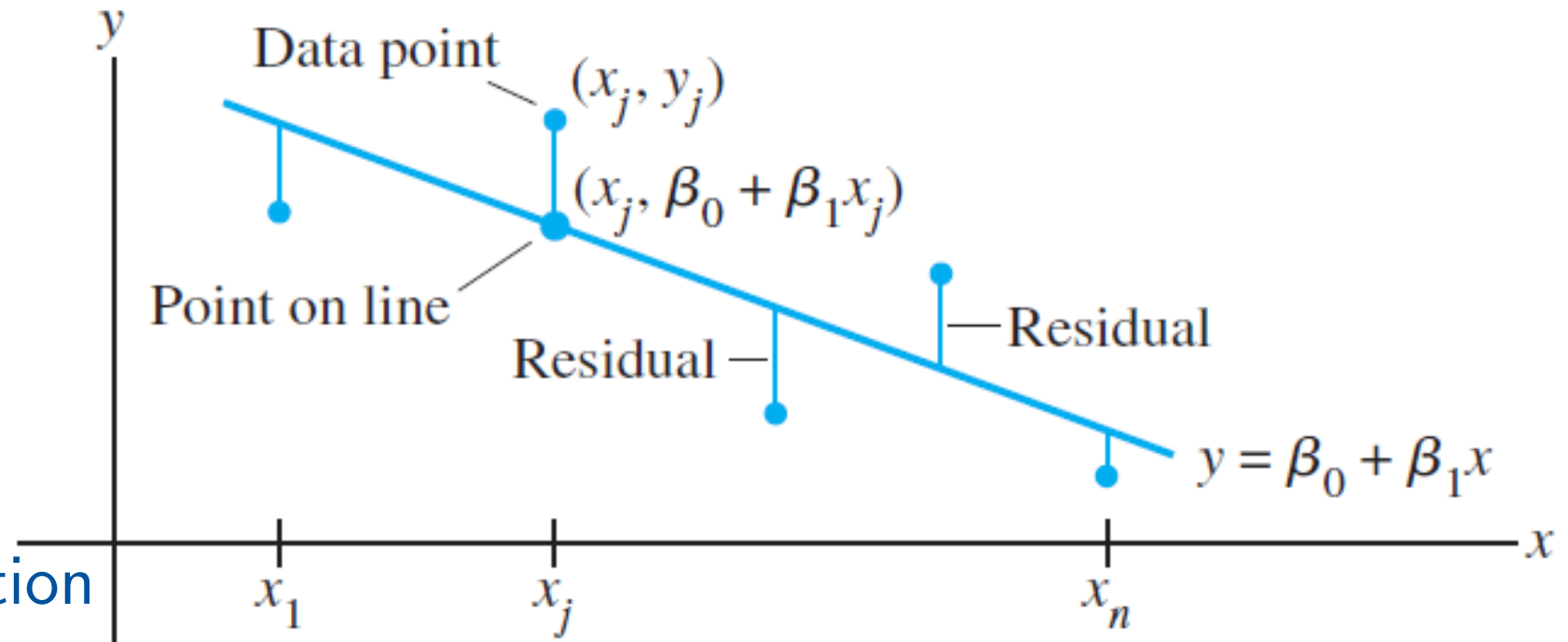
$=$

$y$   
//  
observation  
vector

We wish to solve (for  $\beta_0, \beta_1$ ):

$$\begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

$\begin{matrix} \text{design} \\ \text{matrix} \end{matrix}$ 
 $\begin{matrix} \beta \\ \text{parameter} \\ \text{vector} \end{matrix}$ 
 $=$ 
 $\begin{matrix} \mathbf{y} \\ \text{observation} \\ \text{vector} \end{matrix}$



Because experiments are rarely perfect, our data points  $(x_i, y_i)$  probably don't all lie exactly on any line, i.e. this system probably doesn't have a solution. So we ask for a least-squares solution.

A least-squares solution minimises  $\|\mathbf{y} - X\boldsymbol{\beta}\|$ , which is equivalent to minimising  $\|\mathbf{y} - X\boldsymbol{\beta}\|^2 = (y_1 - (\beta_0 + \beta_1 x_1))^2 + \cdots + (y_n - (\beta_0 + \beta_1 x_n))^2$ , the sums of the squares of the residuals. (The residuals are the vertical distances between each data point and the line, as in the diagram above).



**Example:** Find the equation  $y = \hat{\beta}_0 + \hat{\beta}_1 x$  for the least-squares line for the following data points:

$x_i$	2	5	7	8
$y_i$	1	2	3	3

**Answer:** The model  $X\boldsymbol{\beta} = \mathbf{y}$  is

$$\begin{bmatrix} 1 & 2 \\ 1 & 5 \\ 1 & 7 \\ 1 & 8 \end{bmatrix} \boldsymbol{\beta} = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 3 \end{bmatrix}$$

The normal equations  $X^T X \hat{\boldsymbol{\beta}} = X^T \mathbf{y}$  are

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 2 & 5 & 7 & 8 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 1 & 5 \\ 1 & 7 \\ 1 & 8 \end{bmatrix} \hat{\boldsymbol{\beta}} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 2 & 5 & 7 & 8 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ 3 \\ 3 \end{bmatrix}$$

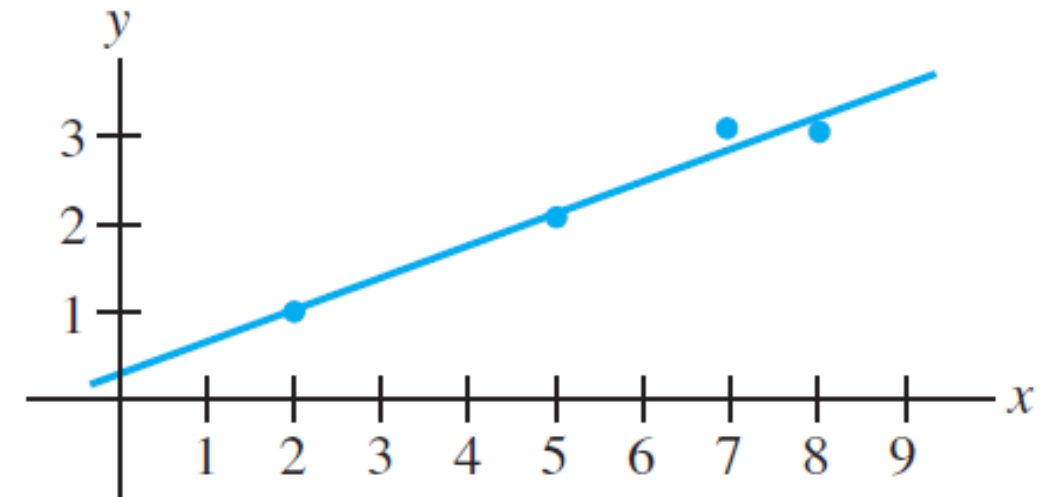
$$\begin{bmatrix} 4 & 22 \\ 22 & 142 \end{bmatrix} \hat{\boldsymbol{\beta}} = \begin{bmatrix} 9 \\ 57 \end{bmatrix}.$$

Row-reducing gives  $\hat{\boldsymbol{\beta}} = \begin{bmatrix} 2/7 \\ 5/14 \end{bmatrix}$ , so the equation of the least-squares line is  $y = 2/7 + 5/14x$ .

We wish to solve (for  $\beta_0, \beta_1$ ):

$$\begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

$X \quad \boldsymbol{\beta} \quad = \quad \mathbf{y}$



## Application: least-squares fitting of other curves

Suppose we model  $y$  as a more complicated function of  $x$ , i.e.

$y = \beta_0 f_0(x) + \beta_1 f_1(x) + \cdots + \beta_k f_k(x)$ , where  $f_0, \dots, f_k$  are known functions, and  $\beta_0, \dots, \beta_k$  are unknown parameters that we will estimate from experimental data. Such a model is still called a “linear model”, because it is linear in the parameters  $\beta_0, \dots, \beta_k$ .

**Example:** Estimate the parameters  $\beta_1, \beta_2, \beta_3$  in the model  $y = \beta_1 x + \beta_2 x^2 + \beta_3 x^3$ , given the data

$x_i$	2	3	4	6	7
$y_i$	1.6	2.0	2.5	3.1	3.4

**Answer:** The model equations are  $\beta_1 2 + \beta_2 2^2 + \beta_3 2^3 = 1.6$   
 $\beta_1 3 + \beta_2 3^2 + \beta_3 3^3 = 2.0$ , and so on.

In matrix form:  $\begin{bmatrix} 2 & 4 & 8 \\ 3 & 9 & 27 \\ 4 & 16 & 64 \\ 6 & 36 & 216 \\ 7 & 49 & 343 \end{bmatrix} \beta = \begin{bmatrix} 1.6 \\ 2.0 \\ 2.5 \\ 3.1 \\ 3.4 \end{bmatrix}$ . Then we solve the normal equations etc...

So in general, to estimate the parameters  $\beta_0, \dots, \beta_k$  in a linear model  $y = \beta_0 f_0(x) + \beta_1 f_1(x) + \dots + \beta_k f_k(x)$ , we find the least-squares solution to

$$\beta_0 f_0(x_1) + \beta_1 f_1(x_1) + \dots + \beta_k f_k(x_1) = y_1$$

$$\beta_0 f_0(x_2) + \beta_1 f_1(x_2) + \dots + \beta_k f_k(x_2) = y_2$$

more general  
design matrix

i.e.

$$\begin{bmatrix} \vdots & & & \\ f_0(x_1) & f_1(x_1) & \dots & f_k(x_1) \\ f_0(x_2) & f_1(x_2) & \dots & f_k(x_2) \\ \vdots & \vdots & & \vdots \\ f_0(x_n) & f_1(x_n) & \dots & f_k(x_n) \end{bmatrix} \begin{bmatrix} \beta_0 \\ \vdots \\ \beta_k \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

parameter  
vector with  
more rows

same  
observation  
vector

(Least-squares lines correspond to the case  $f_0(x) = 1, f_1(x) = x$ .)

Least-squares techniques can also be used to fit a surface to experimental data, for linear models with more than one input variable (e.g.  $y = \beta_0 + \beta_1 x + \beta_2 xw$ , for input variables  $x$  and  $w$ ) - this is called multiple regression.