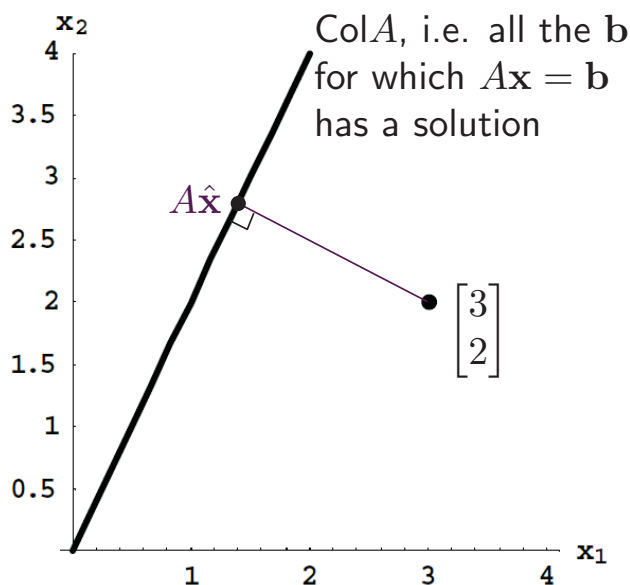


Let $A = \begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix}$. The linear system $A\mathbf{x} = \begin{bmatrix} 3 \\ 2 \end{bmatrix}$ does not have a solution, because

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

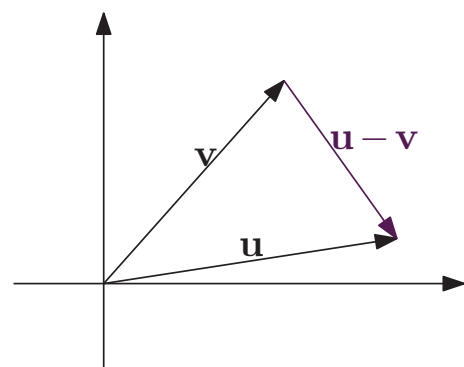


We wish to find a “closest approximate solution”, i.e. a vector $\hat{\mathbf{x}}$ such that $A\hat{\mathbf{x}}$ is the unique point in $\text{Col}A$ that is “closest” to $\begin{bmatrix} 3 \\ 2 \end{bmatrix}$. This is called a **least-squares solution** (p17).

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

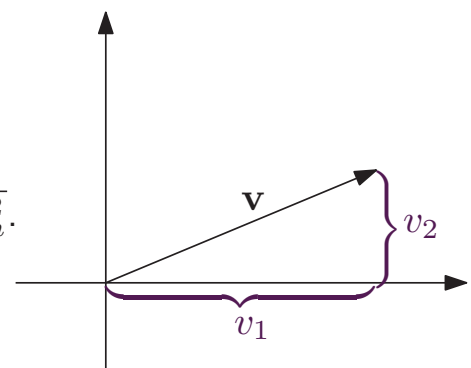
In \mathbb{R}^2 , the distance between \mathbf{u} and \mathbf{v} is the length of their difference $\mathbf{u} - \mathbf{v}$.

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. Do not write \mathbf{u}^2 , which is ambiguous.

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. $(\mathbf{u} + \mathbf{v}) \cdot \mathbf{w} = \mathbf{u} \cdot \mathbf{w} + \mathbf{v} \cdot \mathbf{w}$ } linearity in each input
- c. $(c\mathbf{u}) \cdot \mathbf{v} = c(\mathbf{u} \cdot \mathbf{v}) = \mathbf{u} \cdot (c\mathbf{v})$ } 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: $\mathbf{v} \cdot \mathbf{v} = 8^2 + 5^2 + (-6)^2 = 125$.

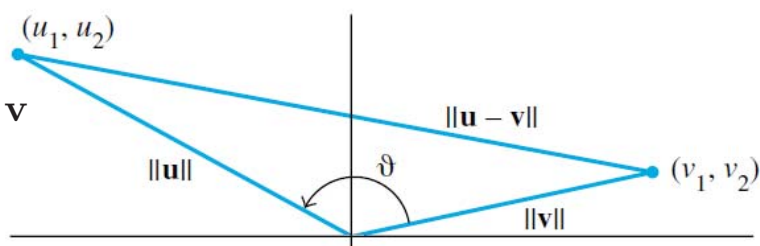
So a unit vector in the same direction as \mathbf{v} is $\frac{\mathbf{v}}{\|\mathbf{v}\|} = \frac{1}{\sqrt{125}} \begin{bmatrix} 8 \\ 5 \\ -6 \end{bmatrix}$.

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:

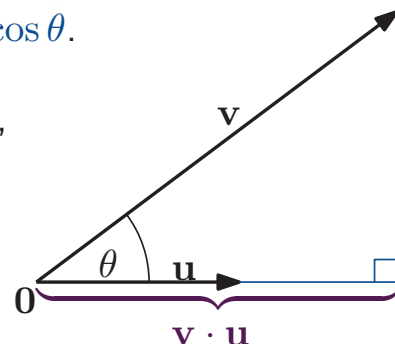
$$\begin{aligned}\|\mathbf{u} - \mathbf{v}\|^2 &= (\mathbf{u} - \mathbf{v}) \cdot (\mathbf{u} - \mathbf{v}) \\ &= \mathbf{u} \cdot \mathbf{u} - \mathbf{u} \cdot \mathbf{v} - \mathbf{v} \cdot \mathbf{u} + \mathbf{v} \cdot \mathbf{v} \\ &= \|\mathbf{u}\|^2 - 2\mathbf{u} \cdot \mathbf{v} + \|\mathbf{v}\|^2.\end{aligned}$$



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} .

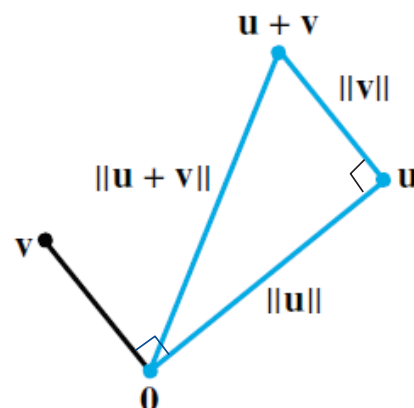
Another way to see that orthogonality generalises perpendicularity:

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 $\mathbf{u} \cdot \mathbf{v} = 0$.



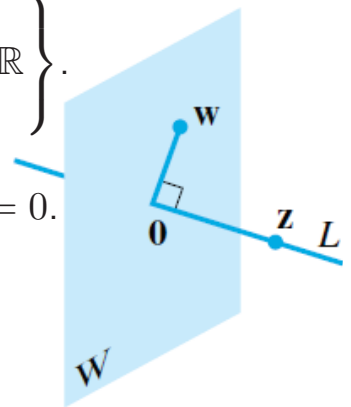
Instead of \mathbf{v} being orthogonal to just a single vector \mathbf{u} , we can consider orthogonality to a set of vectors:

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. $W = \left\{ \begin{bmatrix} a \\ 0 \\ b \end{bmatrix} \mid a, b \in \mathbb{R} \right\}$.

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

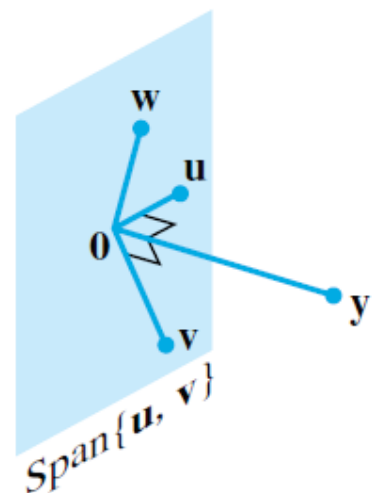
We show on p13 that W^\perp is $\text{Span} \left\{ \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \right\}$.



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 #21 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 (week 2 p16, §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,

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

Now consider

$$\mathbf{x} \in \text{Nul } A$$

By (*), this is equivalent to

$$\mathbf{r}_i \cdot \mathbf{x} = 0 \text{ for all } i.$$

By property 2 on the previous page,
this is equivalent to

$$\mathbf{r} \cdot \mathbf{x} = 0 \text{ for all } \mathbf{r} \in \text{Span}\{\mathbf{r}_1, \dots, \mathbf{r}_m\} = \text{Row } A.$$

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By definition of orthogonal

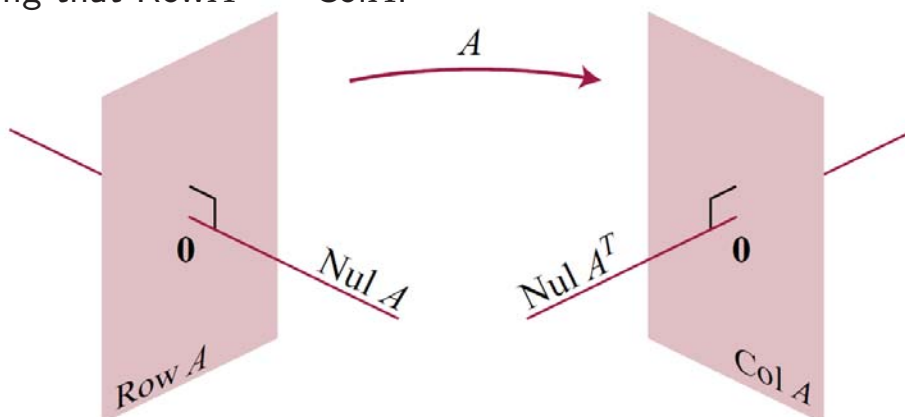
$$\mathbf{x} \in (\text{Row } A)^\perp$$

complement, this is equivalent to

So $\mathbf{x} \in \text{Nul } A$ if and only if $\mathbf{x} \in (\text{Row } A)^\perp$. We have proved

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 $W = \left\{ \begin{bmatrix} a \\ 0 \\ b \end{bmatrix} \mid a, b \in \mathbb{R} \right\}$. 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 $\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \mathbf{x} = \mathbf{0}$, i.e. $W^\perp = \left\{ s \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \mid s \in \mathbb{R} \right\}$.

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:

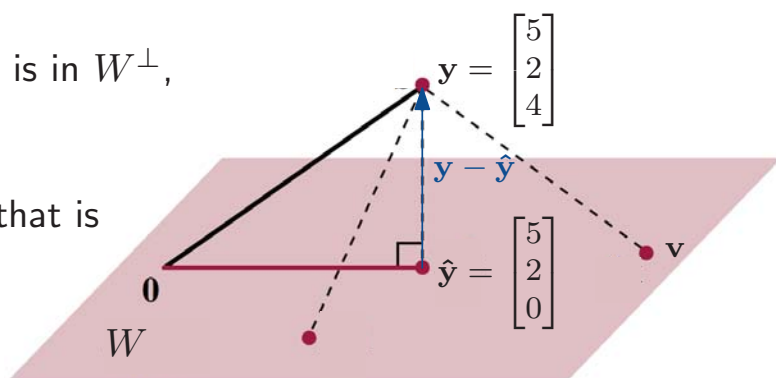
Theorem 9: Best Approximation Theorem: Let W be a subspace of \mathbb{R}^n , and \mathbf{y} a vector in \mathbb{R}^n . Then there is a **unique** point $\hat{\mathbf{y}}$ in W such that $\mathbf{y} - \hat{\mathbf{y}}$ is in W^\perp , and this $\hat{\mathbf{y}}$ is the **closest point in W to \mathbf{y}** in the sense that $\|\mathbf{y} - \hat{\mathbf{y}}\| < \|\mathbf{y} - \mathbf{v}\|$ 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 there is a **unique** point $\hat{\mathbf{y}}$ in W such that $\mathbf{y} - \hat{\mathbf{y}}$ is in W^\perp , and this $\hat{\mathbf{y}}$ is the **closest point in W to \mathbf{y}** in the sense that $\|\mathbf{y} - \hat{\mathbf{y}}\| < \|\mathbf{y} - \mathbf{v}\|$ 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 inequality). 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 12 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)

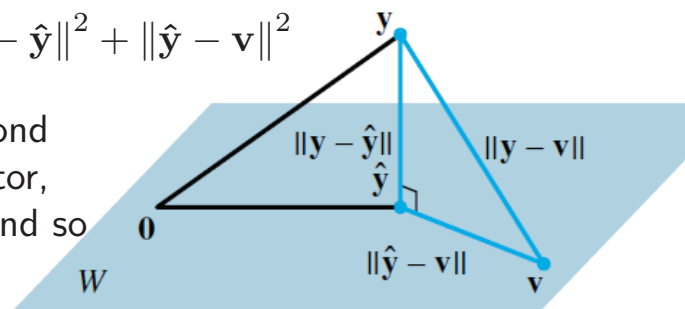
So $\mathbf{y} - \hat{\mathbf{y}}$ and $\hat{\mathbf{y}} - \mathbf{v}$ are orthogonal. Apply the Pythagorean Theorem (blue triangle):

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

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 .

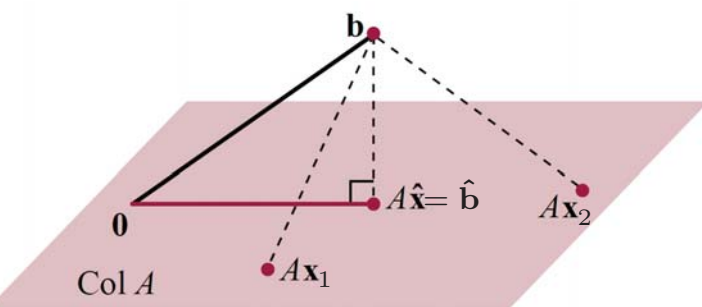
Equivalently: we want to find a vector $\hat{\mathbf{b}}$ in $\text{Col}A$ that is closest to \mathbf{b} , and then solve $A\hat{\mathbf{x}} = \hat{\mathbf{b}}$.

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

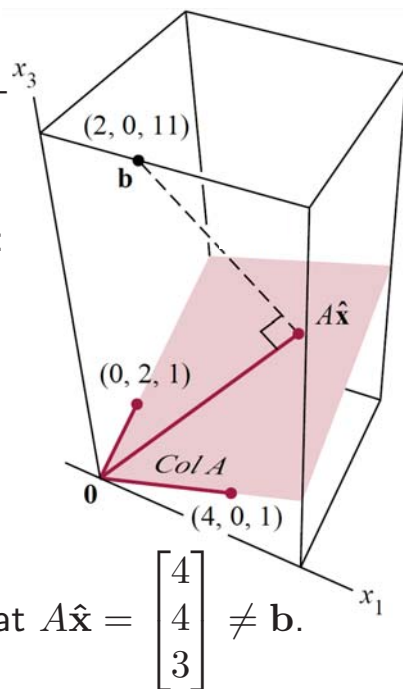
Example: Let $A = \begin{bmatrix} 4 & 0 \\ 0 & 2 \\ 1 & 1 \end{bmatrix}$ and $\mathbf{b} = \begin{bmatrix} 2 \\ 0 \\ 11 \end{bmatrix}$. Find a least-squares solution of the inconsistent equation $A\mathbf{x} = \mathbf{b}$.

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 $A\mathbf{x} = \mathbf{b}$.

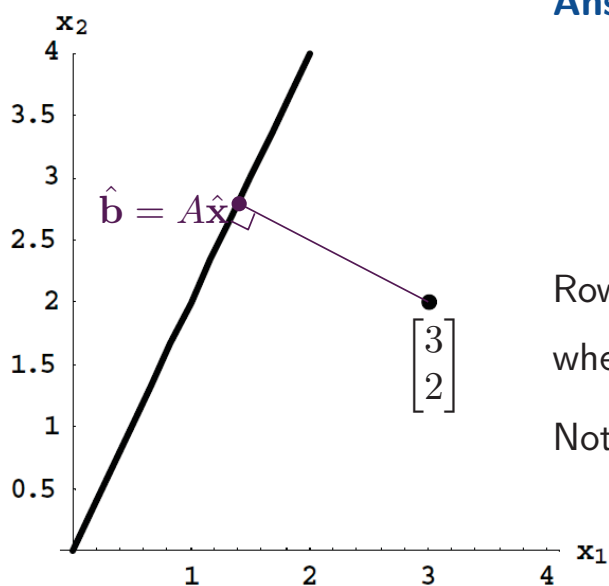
Answer: We solve $A^T A \hat{\mathbf{x}} = A^T \mathbf{b}$:

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

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

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 β_0, β_1 .

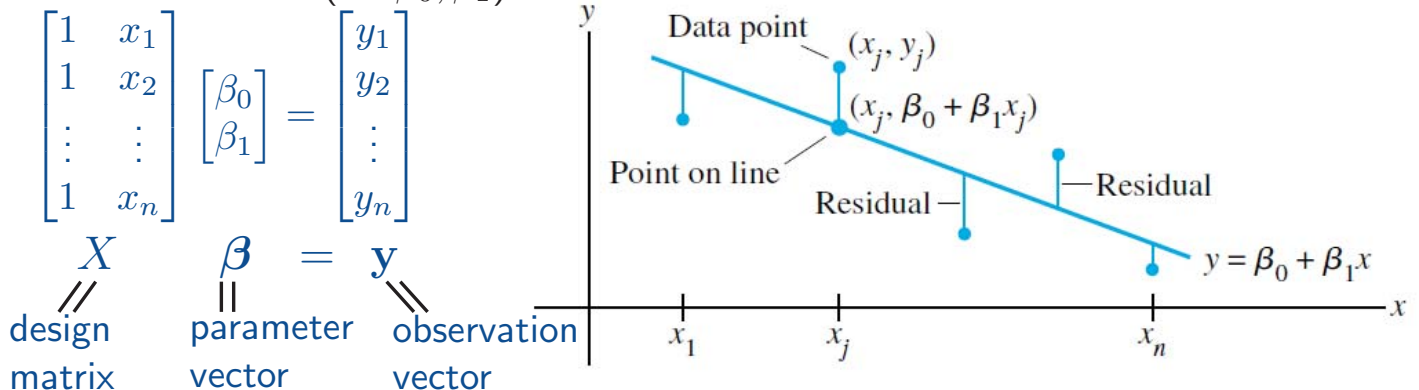
To estimate β_0 and β_1 , we do an experiment, whose results are $(x_1, y_1), \dots, (x_n, y_n)$.

Now we wish to solve (for β_0, β_1):

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

$$A\mathbf{x} = \mathbf{b} \text{ with different notation} \quad \begin{matrix} \nearrow \\ X \\ // \\ \text{design} \\ \text{matrix} \end{matrix} \quad \begin{matrix} \beta \\ // \\ \text{parameter} \\ \text{vector} \end{matrix} = \begin{matrix} \mathbf{y} \\ // \\ \text{observation} \\ \text{vector} \end{matrix}$$

We wish to solve (for β_0, β_1):



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 $\|\mathbf{y} - X\boldsymbol{\beta}\|^2 = (y_1 - (\beta_0 + \beta_1 x_1))^2 + \dots + (y_n - (\beta_0 + \beta_1 x_n))^2$, 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 $X\beta = \mathbf{y}$ is

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

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

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

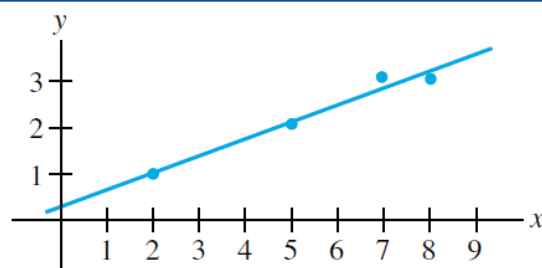
$$\begin{bmatrix} 4 & 22 \\ 22 & 142 \end{bmatrix} \hat{\beta} = \begin{bmatrix} 9 \\ 57 \end{bmatrix}.$$

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

We wish to solve (for β_0, β_1):

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

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



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 β_0, \dots, β_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 β_0, \dots, β_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 β_0, \dots, β_k in a linear model

$y = \beta_0 f_0(x) + \beta_1 f_1(x) + \cdots + \beta_k f_k(x)$, we find the least-squares solution to

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

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

more general design matrix \rightarrow i.e.
$$\begin{bmatrix} f_0(x_1) & f_1(x_1) & \cdots & f_k(x_1) \\ f_0(x_2) & f_1(x_2) & \cdots & f_k(x_2) \\ \vdots & \vdots & & \vdots \\ f_0(x_n) & f_1(x_n) & \cdots & f_k(x_n) \end{bmatrix} \begin{bmatrix} \beta_0 \\ \vdots \\ \beta_k \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

parameter vector with more rows \rightarrow $\begin{bmatrix} \beta_0 \\ \vdots \\ \beta_k \end{bmatrix}$

same observation vector \rightarrow $\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$

(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.