6. ORTHOGONALITY AND LEAST SQUARE

6. INNER PRODUCT, LENGTH AND ORTHOGONALITY

$$\mathbf{u} = \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{bmatrix} \quad \text{and} \quad \mathbf{v} = \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix}$$

The number $\mathbf{u}^T\mathbf{v}$ is called the **inner product** of $\mathbf{u}$ and $\mathbf{v}$, and often it is written as $\mathbf{u}.\mathbf{v}$ (dot product)

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$$\begin{bmatrix} u_1 & u_2 & \cdots & u_n \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix} = u_1 v_1 + u_2 v_2 + \cdots + u_n v_n$$

THEOREM 1

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

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

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

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

d. $\mathbf{u} \cdot \mathbf{u} \geq 0$, and $\mathbf{u} \cdot \mathbf{u} = 0$ if and only if $\mathbf{u} = \mathbf{0}$

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

Length of a vector

DEFINITION The **length** (or **norm**) of $\mathbf{v}$ is the nonnegative scalar $\|\mathbf{v}\|$ defined by

$$\|\mathbf{v}\| = \sqrt{\mathbf{v} \cdot \mathbf{v}} = \sqrt{v_1^2 + v_2^2 + \cdots + v_n^2}, \quad \text{and} \quad \|\mathbf{v}\|^2 = \mathbf{v} \cdot \mathbf{v}$$

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

A vector whose length is 1 is called a **unit vector**. If we *divide* a nonzero vector $\mathbf{v}$ by its length—that is, multiply by $1/\|\mathbf{v}\|$—we obtain a unit vector $\mathbf{u}$ because the length of $\mathbf{u}$ is $(1/\|\mathbf{v}\|)\|\mathbf{v}\|$. The process of creating $\mathbf{u}$ from $\mathbf{v}$ is sometimes called **normalizing** $\mathbf{v}$, and we say that $\mathbf{u}$ is *in the same direction* as $\mathbf{v}$.

EXAMPLE 2 Let $\mathbf{v} = (1, -2, 2, 0)$. Find a unit vector $\mathbf{u}$ in the same direction as $\mathbf{v}$.

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$$\|\mathbf{v}\|^2 = \mathbf{v} \cdot \mathbf{v} = (1)^2 + (-2)^2 + (2)^2 + (0)^2 = 9$$

$$\|\mathbf{v}\| = \sqrt{9} = 3$$

$$\mathbf{u} = \frac{1}{\|\mathbf{v}\|}\mathbf{v} = \frac{1}{3}\mathbf{v} = \frac{1}{3}\begin{bmatrix} 1 \\ -2 \\ 2 \\ 0 \end{bmatrix} = \begin{bmatrix} 1/3 \\ -2/3 \\ 2/3 \\ 0 \end{bmatrix}$$

$$\|\mathbf{u}\|^2 = \mathbf{u} \cdot \mathbf{u} = \left(\tfrac{1}{3}\right)^2 + \left(-\tfrac{2}{3}\right)^2 + \left(\tfrac{2}{3}\right)^2 + (0)^2$$

$$= \tfrac{1}{9} + \tfrac{4}{9} + \tfrac{4}{9} + 0 = 1$$

DEFINITION

For $\mathbf{u}$ and $\mathbf{v}$ in $\mathbb{R}^n$, the **distance between u and v**, written as $\text{dist}(\mathbf{u}, \mathbf{v})$, is the length of the vector $\mathbf{u} - \mathbf{v}$. That is,

$$\text{dist}(\mathbf{u}, \mathbf{v}) = \|\mathbf{u} - \mathbf{v}\|$$

Orthogonal vectors

Consider $\mathbb{R}^2$ or $\mathbb{R}^3$ and two lines through the origin determined by vectors $\mathbf{u}$ and $\mathbf{v}$. The two lines shown in Figure 5 are geometrically perpendicular if and only if the distance from $\mathbf{u}$ to $\mathbf{v}$ is the same as the distance from $\mathbf{u}$ to $-\mathbf{v}$. This is the same as requiring the squares of the distances to be the same. Now
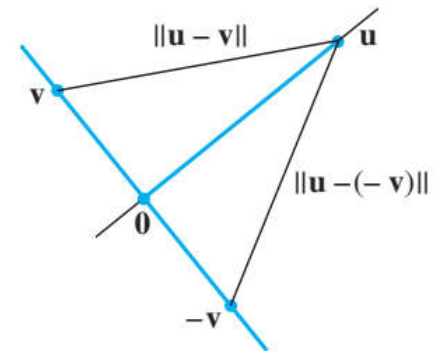
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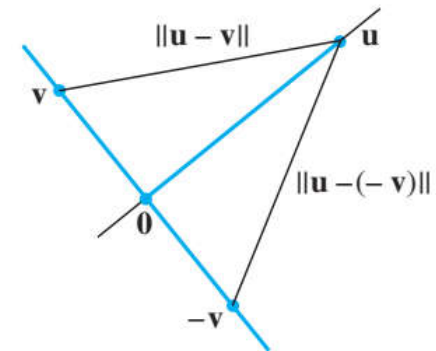
$$\begin{aligned}[\operatorname{dist}(\mathbf{u}, -\mathbf{v})]^2 &= \|\mathbf{u} - (-\mathbf{v})\|^2 = \|\mathbf{u} + \mathbf{v}\|^2 \\ &= (\mathbf{u} + \mathbf{v}) \cdot (\mathbf{u} + \mathbf{v}) \\ &= \mathbf{u} \cdot (\mathbf{u} + \mathbf{v}) + \mathbf{v} \cdot (\mathbf{u} + \mathbf{v}) \\ &= \mathbf{u} \cdot \mathbf{u} + \mathbf{u} \cdot \mathbf{v} + \mathbf{v} \cdot \mathbf{u} + \mathbf{v} \cdot \mathbf{v} \\ &= \|\mathbf{u}\|^2 + \|\mathbf{v}\|^2 + 2\mathbf{u} \cdot \mathbf{v}\end{aligned}$$

$$\begin{aligned}[\operatorname{dist}(\mathbf{u}, \mathbf{v})]^2 &= \|\mathbf{u}\|^2 + \| - \mathbf{v}\|^2 + 2\mathbf{u} \cdot (-\mathbf{v}) \\ &= \|\mathbf{u}\|^2 + \|\mathbf{v}\|^2 - 2\mathbf{u} \cdot \mathbf{v}\end{aligned}$$

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

DEFINITION   Two vectors $\mathbf{u}$ and $\mathbf{v}$ in $\mathbb{R}^n$ are **orthogonal** (to each other) if $\mathbf{u} \cdot \mathbf{v} = 0$.

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

$$\mathbf{u} \cdot \mathbf{v} = \|\mathbf{u}\|\, \|\mathbf{v}\| \cos \vartheta$$

If a vector $\mathbf{z}$ is orthogonal to every vector in a subspace W of $\mathbb{R}^n$, then $\mathbf{z}$ is said to be **orthogonal to** W.

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The set of all vectors $\mathbf{z}$ that are orthogonal to W is called the **orthogonal complement** of W

$$W^{\perp}$$

EXAMPLE 6 Let W be a plane through the origin in $\mathbb{R}^3$, and let L be the line through the origin and perpendicular to W. If $\mathbf{z}$ and $\mathbf{w}$ are nonzero, $\mathbf{z}$ is on L, and $\mathbf{w}$ is in W, then the line segment from $\mathbf{0}$ to $\mathbf{z}$ is perpendicular to the line segment from $\mathbf{0}$ to

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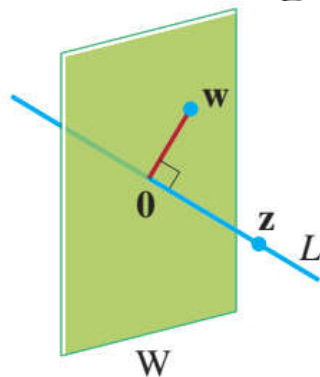
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$$L = W^{\perp} \quad \text{and} \quad W = L^{\perp}$$

1. A vector $\mathbf{x}$ is in $W^{\perp}$ if and only if $\mathbf{x}$ is orthogonal to every vector in a set that spans W.
2. $W^{\perp}$ is a subspace of $\mathbb{R}^n$.

THEOREM 3

Let A be an $m \times n$ matrix. The orthogonal complement of the row space of A is the null space of A, and the orthogonal complement of the column space of A is the null space of A^T:

$$(\text{Row } A)^\perp = \text{Nul } A \quad \text{and} \quad (\text{Col } A)^\perp = \text{Nul } A^T$$

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PROOF   The row–column rule for computing $A\mathbf{x}$ shows that if $\mathbf{x}$ is in Nul A, then $\mathbf{x}$ is orthogonal to each row of A (with the rows treated as vectors in $\mathbb{R}^n$). Since the rows of A span the row space, $\mathbf{x}$ is orthogonal to Row A. Conversely, if $\mathbf{x}$ is orthogonal to Row A, then $\mathbf{x}$ is certainly orthogonal to each row of A, and hence $A\mathbf{x} = \mathbf{0}$. This proves the first statement of the theorem. Since this statement is true for any matrix, it is true for A^T. That is, the orthogonal complement of the row space of A^T is the null space of A^T. This proves the second statement, because Row $A^T = \text{Col } A$. ∎

3. Let W be a subspace of $\mathbf{R}^n$. Exercise 30 establishes that $W^\perp$ is also a subspace of $\mathbf{R}^n$. Prove that $\dim W + \dim W^\perp = n$.

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3. If $W \neq \{\mathbf{0}\}$, let $\{\mathbf{b}_1, \ldots, \mathbf{b}_p\}$ be a basis for W, where $1 \leq p \leq n$. Let A be the $p \times n$ matrix having rows $\mathbf{b}_1^T, \ldots, \mathbf{b}_p^T$. It follows that W is the row space of A. Theorem 3 implies that $W^\perp = (\text{Row } A)^\perp = \text{Nul } A$ and hence $\dim W^\perp = \dim \text{Nul } A$. Thus, $\dim W + \dim W^\perp = \dim \text{Row } A + \dim \text{Nul } A = \text{rank } A + \dim \text{Nul } A = n$, by the Rank Theorem. If $W = \{\mathbf{0}\}$, then $W^\perp = \mathbb{R}^n$, and the result follows.

ORTHOGONAL SETS

A set of vectors $\{\mathbf{u}_1, \ldots, \mathbf{u}_p\}$ in $\mathbb{R}^n$ is said to be an **orthogonal set** if each pair of distinct vectors from the set is orthogonal, that is, if $\mathbf{u}_i \cdot \mathbf{u}_j = 0$ whenever $i \neq j$.

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If $S = \{\mathbf{u}_1, \ldots, \mathbf{u}_p\}$ is an orthogonal set of nonzero vectors in $\mathbb{R}^n$, then S is linearly independent and hence is a basis for the subspace spanned by S.

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PROOF If $\mathbf{0} = c_1\mathbf{u}_1 + \cdots + c_p\mathbf{u}_p$ for some scalars $c_1, \ldots, c_p$, then

$$0 = \mathbf{0} \cdot \mathbf{u}_1 = (c_1\mathbf{u}_1 + c_2\mathbf{u}_2 + \cdots + c_p\mathbf{u}_p) \cdot \mathbf{u}_1$$
$$= (c_1\mathbf{u}_1) \cdot \mathbf{u}_1 + (c_2\mathbf{u}_2) \cdot \mathbf{u}_1 + \cdots + (c_p\mathbf{u}_p) \cdot \mathbf{u}_1$$
$$= c_1(\mathbf{u}_1 \cdot \mathbf{u}_1) + c_2(\mathbf{u}_2 \cdot \mathbf{u}_1) + \cdots + c_p(\mathbf{u}_p \cdot \mathbf{u}_1)$$
$$= c_1(\mathbf{u}_1 \cdot \mathbf{u}_1)$$

because $\mathbf{u}_1$ is orthogonal to $\mathbf{u}_2, \ldots, \mathbf{u}_p$. Since $\mathbf{u}_1$ is nonzero, $\mathbf{u}_1 \cdot \mathbf{u}_1$ is not zero and so $c_1 = 0$. Similarly, $c_2, \ldots, c_p$ must be zero. Thus S is linearly independent. ■

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Let $\{\mathbf{u}_1, \ldots, \mathbf{u}_p\}$ be an orthogonal basis for a subspace W of $\mathbb{R}^n$. For each $\mathbf{y}$ in W, the weights in the linear combination

$$\mathbf{y} = c_1\mathbf{u}_1 + \cdots + c_p\mathbf{u}_p$$

are given by

$$c_j = \frac{\mathbf{y} \cdot \mathbf{u}_j}{\mathbf{u}_j \cdot \mathbf{u}_j} \qquad (j = 1, \ldots, p)$$

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PROOF As in the preceding proof, the orthogonality of $\{\mathbf{u}_1, \ldots, \mathbf{u}_p\}$ shows that

$$\mathbf{y} \cdot \mathbf{u}_1 = (c_1\mathbf{u}_1 + c_2\mathbf{u}_2 + \cdots + c_p\mathbf{u}_p) \cdot \mathbf{u}_1 = c_1(\mathbf{u}_1 \cdot \mathbf{u}_1)$$

Since $\mathbf{u}_1 \cdot \mathbf{u}_1$ is not zero, the equation above can be solved for c_1. To find c_j for $j = 2, \ldots, p$, compute $\mathbf{y} \cdot \mathbf{u}_j$ and solve for c_j. ■

Express the vector $\mathbf{y} = \begin{bmatrix} 6 \\ 1 \\ -8 \end{bmatrix}$ as a linear combination of the vectors in S.

$$\mathbf{u}_1 = \begin{bmatrix} 3 \\ 1 \\ 1 \end{bmatrix}, \quad \mathbf{u}_2 = \begin{bmatrix} -1 \\ 2 \\ 1 \end{bmatrix}, \quad \mathbf{u}_3 = \begin{bmatrix} -1/2 \\ -2 \\ 7/2 \end{bmatrix}$$

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$$\mathbf{y} = \frac{\mathbf{y} \cdot \mathbf{u}_1}{\mathbf{u}_1 \cdot \mathbf{u}_1} \mathbf{u}_1 + \frac{\mathbf{y} \cdot \mathbf{u}_2}{\mathbf{u}_2 \cdot \mathbf{u}_2} \mathbf{u}_2 + \frac{\mathbf{y} \cdot \mathbf{u}_3}{\mathbf{u}_3 \cdot \mathbf{u}_3} \mathbf{u}_3$$

$$= \frac{11}{11} \mathbf{u}_1 + \frac{-12}{6} \mathbf{u}_2 + \frac{-33}{33/2} \mathbf{u}_3$$

$$= \mathbf{u}_1 - 2\mathbf{u}_2 - 2\mathbf{u}_3$$

Orthogonal projection

Given a nonzero vector $\mathbf{u}$ in $\mathbb{R}^n$, consider the problem of decomposing a vector $\mathbf{y}$ in $\mathbb{R}^n$ into the sum of two vectors, one a multiple of $\mathbf{u}$ and the other orthogonal to $\mathbf{u}$. We wish to write
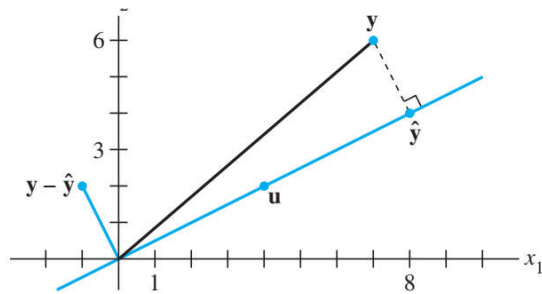
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$$\mathbf{y} = \hat{\mathbf{y}} + \mathbf{z} \tag{1}$$

$$\hat{\mathbf{y}} = \alpha\mathbf{u} \qquad \mathbf{z} = \mathbf{y} - \alpha\mathbf{u}$$
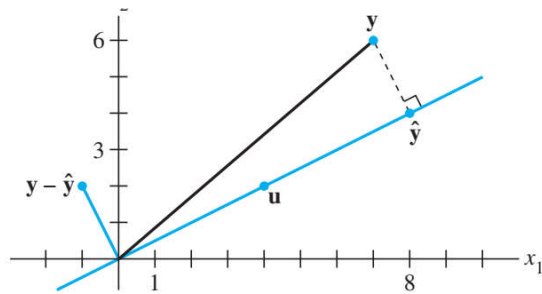
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$$\mathbf{y} = \hat{\mathbf{y}} + \mathbf{z} \tag{1}$$

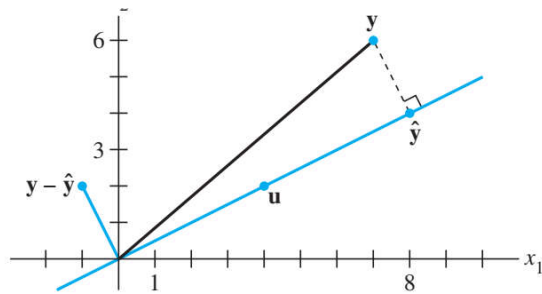$$\hat{\mathbf{y}} = \alpha\mathbf{u} \qquad \mathbf{z} = \mathbf{y} - \alpha\mathbf{u}$$

$$0 = (\mathbf{y} - \alpha\mathbf{u})\cdot\mathbf{u} = \mathbf{y}\cdot\mathbf{u} - (\alpha\mathbf{u})\cdot\mathbf{u} = \mathbf{y}\cdot\mathbf{u} - \alpha(\mathbf{u}\cdot\mathbf{u})$$

$$\alpha = \frac{\mathbf{y}\cdot\mathbf{u}}{\mathbf{u}\cdot\mathbf{u}} \text{ and } \hat{\mathbf{y}} = \frac{\mathbf{y}\cdot\mathbf{u}}{\mathbf{u}\cdot\mathbf{u}}\mathbf{u}.$$

The vector $\hat{\mathbf{y}}$ is called the **orthogonal projection of y onto u**, and the vector $\mathbf{z}$ is called the **component of y orthogonal to u**.

subspace L spanned by **u**
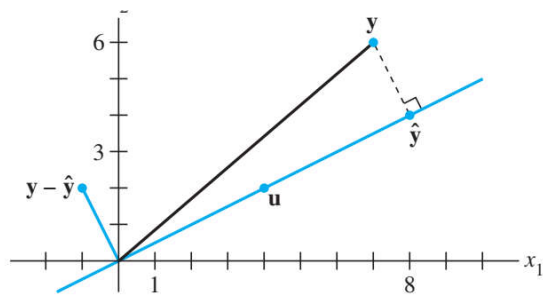
subspace L spanned by **u**

Sometimes **y**O is denoted by proj$_L$ **y** and is called the **orthogonal projection of y onto** L. That is,
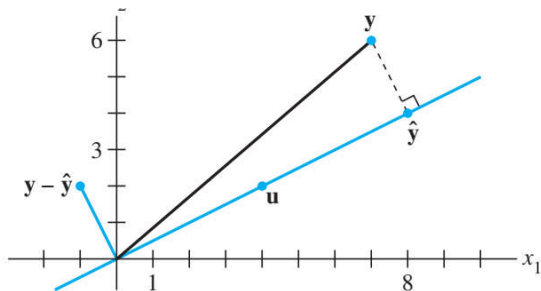
$$\hat{\mathbf{y}} = \text{proj}_L \mathbf{y} = \frac{\mathbf{y} \cdot \mathbf{u}}{\mathbf{u} \cdot \mathbf{u}} \mathbf{u}$$

EXAMPLE 3 Let $\mathbf{y} = \begin{bmatrix} 7 \\ 6 \end{bmatrix}$ and $\mathbf{u} = \begin{bmatrix} 4 \\ 2 \end{bmatrix}$. Find the orthogonal projection of $\mathbf{y}$ onto $\mathbf{u}$. Then write $\mathbf{y}$ as the sum of two orthogonal vectors, one in Span $\{\mathbf{u}\}$ and one orthogonal to $\mathbf{u}$.

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$$\hat{\mathbf{y}} = \frac{\mathbf{y} \cdot \mathbf{u}}{\mathbf{u} \cdot \mathbf{u}} \mathbf{u} = \frac{40}{20} \mathbf{u} = 2 \begin{bmatrix} 4 \\ 2 \end{bmatrix} = \begin{bmatrix} 8 \\ 4 \end{bmatrix} \qquad \mathbf{y} - \hat{\mathbf{y}} = \begin{bmatrix} 7 \\ 6 \end{bmatrix} - \begin{bmatrix} 8 \\ 4 \end{bmatrix} = \begin{bmatrix} -1 \\ 2 \end{bmatrix}$$

$$\begin{bmatrix} 7 \\ 6 \end{bmatrix} = \begin{bmatrix} 8 \\ 4 \end{bmatrix} + \begin{bmatrix} -1 \\ 2 \end{bmatrix}$$

$$\uparrow \qquad \uparrow \qquad \uparrow$$

$$\mathbf{y} \qquad \hat{\mathbf{y}} \qquad (\mathbf{y} - \hat{\mathbf{y}})$$

Orthonormal Sets

A set $\{\mathbf{u}_1, \ldots, \mathbf{u}_p\}$ is an **orthonormal set** if it is an orthogonal set of unit vectors. If W is the subspace spanned by such a set, then $\{\mathbf{u}_1, \ldots, \mathbf{u}_p\}$ is an **orthonormal basis**

$$\{\mathbf{e}_1, \ldots, \mathbf{e}_n\}$$

$$\mathbf{v}_1 = \begin{bmatrix} 3/\sqrt{11} \\ 1/\sqrt{11} \\ 1/\sqrt{11} \end{bmatrix}, \quad \mathbf{v}_2 = \begin{bmatrix} -1/\sqrt{6} \\ 2/\sqrt{6} \\ 1/\sqrt{6} \end{bmatrix}, \quad \mathbf{v}_3 = \begin{bmatrix} -1/\sqrt{66} \\ -4/\sqrt{66} \\ 7/\sqrt{66} \end{bmatrix}$$

THEOREM 6   An $m \times n$ matrix U has orthonormal columns if and only if $U^T U = I$.

THEOREM 6 An $m \times n$ matrix U has orthonormal columns if and only if $U^T U = I$.

$$U = \begin{bmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \mathbf{u}_3 \end{bmatrix}$$

$$U^T U = \begin{bmatrix} \mathbf{u}_1^T \\ \mathbf{u}_2^T \\ \mathbf{u}_3^T \end{bmatrix} \begin{bmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \mathbf{u}_3 \end{bmatrix} = \begin{bmatrix} \mathbf{u}_1^T \mathbf{u}_1 & \mathbf{u}_1^T \mathbf{u}_2 & \mathbf{u}_1^T \mathbf{u}_3 \\ \mathbf{u}_2^T \mathbf{u}_1 & \mathbf{u}_2^T \mathbf{u}_2 & \mathbf{u}_2^T \mathbf{u}_3 \\ \mathbf{u}_3^T \mathbf{u}_1 & \mathbf{u}_3^T \mathbf{u}_2 & \mathbf{u}_3^T \mathbf{u}_3 \end{bmatrix}$$

THEOREM 7   Let U be an $m \times n$ matrix with orthonormal columns, and let $\mathbf{x}$ and $\mathbf{y}$ be in $\mathbb{R}^n$. Then

a. $\|U\mathbf{x}\| = \|\mathbf{x}\|$

b. $(U\mathbf{x}) \cdot (U\mathbf{y}) = \mathbf{x} \cdot \mathbf{y}$

c. $(U\mathbf{x}) \cdot (U\mathbf{y}) = 0$ if and only if $\mathbf{x} \cdot \mathbf{y} = 0$

orthogonal matrix is a square invertible matrix U such that $U^{-1} = U^T$.

It is easy to see that any *square* matrix with orthonormal columns is an orthogonal matrix.

6.3. ORTHOGONAL PROJECTIONS

The orthogonal projection of a point in R_2 onto a line through the origin has an important analogue in R_n

$$\mathbf{y} = \hat{\mathbf{y}} + \mathbf{z}$$
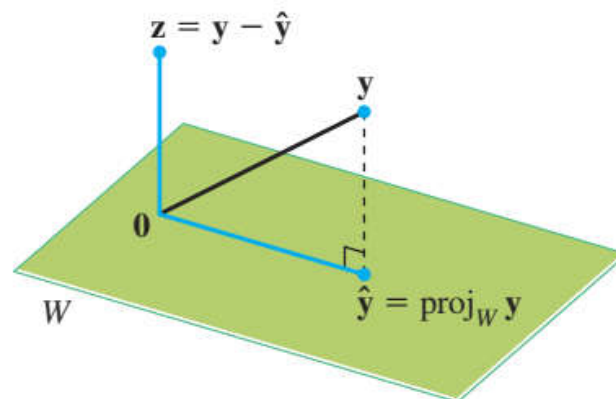
FIGURE 2 The orthogonal projection of **y** onto W.

THEOREM 8

The Orthogonal Decomposition Theorem

Let W be a subspace of $\mathbb{R}^n$. Then each $\mathbf{y}$ in $\mathbb{R}^n$ can be written uniquely in the form

$$\mathbf{y} = \hat{\mathbf{y}} + \mathbf{z} \tag{1}$$

where $\hat{\mathbf{y}}$ is in W and $\mathbf{z}$ is in $W^{\perp}$. In fact, if $\{\mathbf{u}_1, \ldots, \mathbf{u}_p\}$ is any orthogonal basis of W, then

$$\hat{\mathbf{y}} = \frac{\mathbf{y} \cdot \mathbf{u}_1}{\mathbf{u}_1 \cdot \mathbf{u}_1} \mathbf{u}_1 + \cdots + \frac{\mathbf{y} \cdot \mathbf{u}_p}{\mathbf{u}_p \cdot \mathbf{u}_p} \mathbf{u}_p \tag{2}$$

and $\mathbf{z} = \mathbf{y} - \hat{\mathbf{y}}$.

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where $\hat{\mathbf{y}}$ is in W and $\mathbf{z}$ is in $W^{\perp}$. In fact, if $\{\mathbf{u}_1, \ldots, \mathbf{u}_p\}$ is any orthogonal basis of W, then

$$\hat{\mathbf{y}} = \frac{\mathbf{y} \cdot \mathbf{u}_1}{\mathbf{u}_1 \cdot \mathbf{u}_1} \mathbf{u}_1 + \cdots + \frac{\mathbf{y} \cdot \mathbf{u}_p}{\mathbf{u}_p \cdot \mathbf{u}_p} \mathbf{u}_p \tag{2}$$

and $\mathbf{z} = \mathbf{y} - \hat{\mathbf{y}}$.

$$\mathbf{z} = \mathbf{y} - \hat{\mathbf{y}} \qquad \mathbf{z} \cdot \mathbf{u}_1 = (\mathbf{y} - \hat{\mathbf{y}}) \cdot \mathbf{u}_1 = \mathbf{y} \cdot \mathbf{u}_1 - \left(\frac{\mathbf{y} \cdot \mathbf{u}_1}{\mathbf{u}_1 \cdot \mathbf{u}_1} \right) \mathbf{u}_1 \cdot \mathbf{u}_1 - 0 - \cdots - 0$$

$$= \mathbf{y} \cdot \mathbf{u}_1 - \mathbf{y} \cdot \mathbf{u}_1 = 0$$

THEOREM 8

The Orthogonal Decomposition Theorem

Let W be a subspace of $\mathbb{R}^n$. Then each $\mathbf{y}$ in $\mathbb{R}^n$ can be written uniquely in the form

$$\mathbf{y} = \hat{\mathbf{y}} + \mathbf{z} \tag{1}$$

where $\hat{\mathbf{y}}$ is in W and $\mathbf{z}$ is in $W^{\perp}$. In fact, if $\{\mathbf{u}_1, \ldots, \mathbf{u}_p\}$ is any orthogonal basis of W, then

$$\hat{\mathbf{y}} = \frac{\mathbf{y} \cdot \mathbf{u}_1}{\mathbf{u}_1 \cdot \mathbf{u}_1} \mathbf{u}_1 + \cdots + \frac{\mathbf{y} \cdot \mathbf{u}_p}{\mathbf{u}_p \cdot \mathbf{u}_p} \mathbf{u}_p \tag{2}$$

and $\mathbf{z} = \mathbf{y} - \hat{\mathbf{y}}$.

$$\mathbf{z} = \mathbf{y} - \hat{\mathbf{y}} \qquad \mathbf{z} \cdot \mathbf{u}_1 = (\mathbf{y} - \hat{\mathbf{y}}) \cdot \mathbf{u}_1 = \mathbf{y} \cdot \mathbf{u}_1 - \left(\frac{\mathbf{y} \cdot \mathbf{u}_1}{\mathbf{u}_1 \cdot \mathbf{u}_1} \right) \mathbf{u}_1 \cdot \mathbf{u}_1 - 0 - \cdots - 0$$

$$= \mathbf{y} \cdot \mathbf{u}_1 - \mathbf{y} \cdot \mathbf{u}_1 = 0$$

$$\mathbf{y} = \hat{\mathbf{y}}_1 + \mathbf{z}_1 \qquad \hat{\mathbf{y}} + \mathbf{z} = \hat{\mathbf{y}}_1 + \mathbf{z}_1 \qquad \hat{\mathbf{y}} - \hat{\mathbf{y}}_1 = \mathbf{z}_1 - \mathbf{z}$$

EXAMPLE 2 Let $\mathbf{u}_1 = \begin{bmatrix} 2 \\ 5 \\ -1 \end{bmatrix}, \mathbf{u}_2 = \begin{bmatrix} -2 \\ 1 \\ 1 \end{bmatrix}$, and $\mathbf{y} = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$. Observe that $\{\mathbf{u}_1, \mathbf{u}_2\}$ is an orthogonal basis for $W = \text{Span}\{\mathbf{u}_1, \mathbf{u}_2\}$. Write $\mathbf{y}$ as the sum of a vector in W and a vector orthogonal to W.

EXAMPLE 2 Let $\mathbf{u}_1 = \begin{bmatrix} 2 \\ 5 \\ -1 \end{bmatrix}, \mathbf{u}_2 = \begin{bmatrix} -2 \\ 1 \\ 1 \end{bmatrix}$, and $\mathbf{y} = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$. Observe that $\{\mathbf{u}_1, \mathbf{u}_2\}$

is an orthogonal basis for $W = \text{Span}\,\{\mathbf{u}_1, \mathbf{u}_2\}$. Write $\mathbf{y}$ as the sum of a vector in W and a vector orthogonal to W.

$$\hat{\mathbf{y}} = \frac{\mathbf{y} \cdot \mathbf{u}_1}{\mathbf{u}_1 \cdot \mathbf{u}_1}\mathbf{u}_1 + \frac{\mathbf{y} \cdot \mathbf{u}_2}{\mathbf{u}_2 \cdot \mathbf{u}_2}\mathbf{u}_2$$

$$= \frac{9}{30}\begin{bmatrix} 2 \\ 5 \\ -1 \end{bmatrix} + \frac{3}{6}\begin{bmatrix} -2 \\ 1 \\ 1 \end{bmatrix} = \frac{9}{30}\begin{bmatrix} 2 \\ 5 \\ -1 \end{bmatrix} + \frac{15}{30}\begin{bmatrix} -2 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} -2/5 \\ 2 \\ 1/5 \end{bmatrix}$$

$$\mathbf{y} - \hat{\mathbf{y}} = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} - \begin{bmatrix} -2/5 \\ 2 \\ 1/5 \end{bmatrix} = \begin{bmatrix} 7/5 \\ 0 \\ 14/5 \end{bmatrix}$$

$$\mathbf{y} = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} = \begin{bmatrix} -2/5 \\ 2 \\ 1/5 \end{bmatrix} + \begin{bmatrix} 7/5 \\ 0 \\ 14/5 \end{bmatrix}$$

If $\{\mathbf{u}_1, \ldots, \mathbf{u}_p\}$ is an orthogonal basis for W and if $\mathbf{y}$ happens to be in W, then the formula for $\text{proj}_W \mathbf{y}$ is exactly the same as the representation of $\mathbf{y}$ given in Theorem 5 in Section 6.2. In this case, $\text{proj}_W \mathbf{y} = \mathbf{y}$.

If $\mathbf{y}$ is in $W = \text{Span}\{\mathbf{u}_1, \ldots, \mathbf{u}_p\}$, then $\text{proj}_W \mathbf{y} = \mathbf{y}$.

THEOREM 9

The Best Approximation Theorem

Let W be a subspace of $\mathbb{R}^n$, let $\mathbf{y}$ be any vector in $\mathbb{R}^n$, and let $\hat{\mathbf{y}}$ be the orthogonal projection of $\mathbf{y}$ onto W. Then $\hat{\mathbf{y}}$ is the closest point in W to $\mathbf{y}$, in the sense that

$$\|\mathbf{y} - \hat{\mathbf{y}}\| < \|\mathbf{y} - \mathbf{v}\| \tag{3}$$

for all $\mathbf{v}$ in W distinct from $\hat{\mathbf{y}}$.

the best approximation to y by elements of W

Min error

THEOREM 9

The Best Approximation Theorem

Let W be a subspace of $\mathbb{R}^n$, let $\mathbf{y}$ be any vector in $\mathbb{R}^n$, and let $\hat{\mathbf{y}}$ be the orthogonal projection of $\mathbf{y}$ onto W. Then $\hat{\mathbf{y}}$ is the closest point in W to $\mathbf{y}$, in the sense that

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$$\mathbf{y} - \mathbf{v} = (\mathbf{y} - \hat{\mathbf{y}}) + (\hat{\mathbf{y}} - \mathbf{v})$$
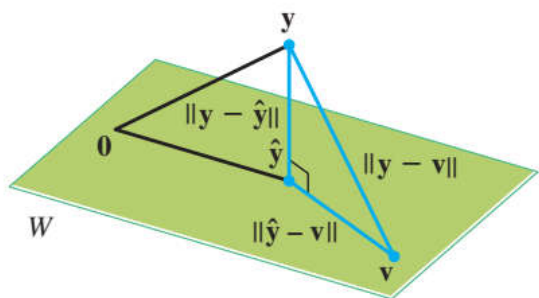
THEOREM 9

The Best Approximation Theorem

Let W be a subspace of $\mathbb{R}^n$, let $\mathbf{y}$ be any vector in $\mathbb{R}^n$, and let $\hat{\mathbf{y}}$ be the orthogonal projection of $\mathbf{y}$ onto W. Then $\hat{\mathbf{y}}$ is the closest point in W to $\mathbf{y}$, in the sense that

$$\|\mathbf{y} - \hat{\mathbf{y}}\| < \|\mathbf{y} - \mathbf{v}\| \tag{3}$$

for all $\mathbf{v}$ in W distinct from $\hat{\mathbf{y}}$.

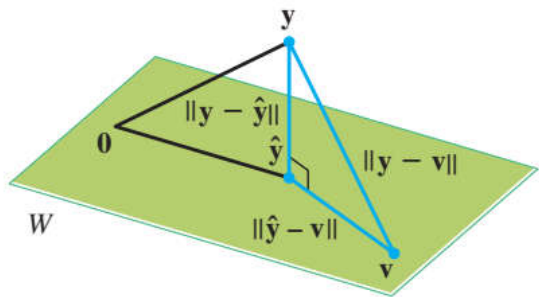$$\mathbf{y} - \mathbf{v} = (\mathbf{y} - \hat{\mathbf{y}}) + (\hat{\mathbf{y}} - \mathbf{v})$$

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

$$\|\hat{\mathbf{y}} - \mathbf{v}\|^2 > 0$$

EXAMPLE 3 If $\mathbf{u}_1 = \begin{bmatrix} 2 \\ 5 \\ -1 \end{bmatrix}$, $\mathbf{u}_2 = \begin{bmatrix} -2 \\ 1 \\ 1 \end{bmatrix}$, $\mathbf{y} = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$, and $W = \mathrm{Span}\,\{\mathbf{u}_1, \mathbf{u}_2\}$,

as in Example 2, then the closest point in W to $\mathbf{y}$ is

$$\hat{\mathbf{y}} = \frac{\mathbf{y} \cdot \mathbf{u}_1}{\mathbf{u}_1 \cdot \mathbf{u}_1} \mathbf{u}_1 + \frac{\mathbf{y} \cdot \mathbf{u}_2}{\mathbf{u}_2 \cdot \mathbf{u}_2} \mathbf{u}_2 = \begin{bmatrix} -2/5 \\ 2 \\ 1/5 \end{bmatrix}$$ ∎

EXAMPLE 4 The distance from a point $\mathbf{y}$ in $\mathbb{R}^n$ to a subspace W is defined as the distance from $\mathbf{y}$ to the nearest point in W. Find the distance from $\mathbf{y}$ to $W = \text{Span}\{\mathbf{u}_1, \mathbf{u}_2\}$, where

$$\mathbf{y} = \begin{bmatrix} -1 \\ -5 \\ 10 \end{bmatrix}, \quad \mathbf{u}_1 = \begin{bmatrix} 5 \\ -2 \\ 1 \end{bmatrix}, \quad \mathbf{u}_2 = \begin{bmatrix} 1 \\ 2 \\ -1 \end{bmatrix}$$

EXAMPLE 4 The distance from a point $\mathbf{y}$ in $\mathbb{R}^n$ to a subspace W is defined as the distance from $\mathbf{y}$ to the nearest point in W. Find the distance from $\mathbf{y}$ to $W = \text{Span}\{\mathbf{u}_1, \mathbf{u}_2\}$, where

$$\mathbf{y} = \begin{bmatrix} -1 \\ -5 \\ 10 \end{bmatrix}, \quad \mathbf{u}_1 = \begin{bmatrix} 5 \\ -2 \\ 1 \end{bmatrix}, \quad \mathbf{u}_2 = \begin{bmatrix} 1 \\ 2 \\ -1 \end{bmatrix}$$

$$\hat{\mathbf{y}} = \frac{15}{30}\mathbf{u}_1 + \frac{-21}{6}\mathbf{u}_2 = \frac{1}{2}\begin{bmatrix} 5 \\ -2 \\ 1 \end{bmatrix} - \frac{7}{2}\begin{bmatrix} 1 \\ 2 \\ -1 \end{bmatrix} = \begin{bmatrix} -1 \\ -8 \\ 4 \end{bmatrix}$$

$$\mathbf{y} - \hat{\mathbf{y}} = \begin{bmatrix} -1 \\ -5 \\ 10 \end{bmatrix} - \begin{bmatrix} -1 \\ -8 \\ 4 \end{bmatrix} = \begin{bmatrix} 0 \\ 3 \\ 6 \end{bmatrix}$$

$$\|\mathbf{y} - \hat{\mathbf{y}}\|^2 = 3^2 + 6^2 = 45$$

THEOREM 10   If $\{\mathbf{u}_1, \ldots, \mathbf{u}_p\}$ is an orthonormal basis for a subspace W of $\mathbb{R}^n$, then

$$\text{proj}_W \mathbf{y} = (\mathbf{y}\cdot\mathbf{u}_1)\mathbf{u}_1 + (\mathbf{y}\cdot\mathbf{u}_2)\mathbf{u}_2 + \cdots + (\mathbf{y}\cdot\mathbf{u}_p)\mathbf{u}_p \tag{4}$$

If $U = [\,\mathbf{u}_1 \quad \mathbf{u}_2 \quad \cdots \quad \mathbf{u}_p\,]$, then

$$\text{proj}_W \mathbf{y} = UU^T\mathbf{y} \quad \text{for all } \mathbf{y} \text{ in } \mathbb{R}^n \tag{5}$$

THEOREM 10

If $\{\mathbf{u}_1, \ldots, \mathbf{u}_p\}$ is an orthonormal basis for a subspace W of $\mathbb{R}^n$, then

$$\text{proj}_W \mathbf{y} = (\mathbf{y} \cdot \mathbf{u}_1)\mathbf{u}_1 + (\mathbf{y} \cdot \mathbf{u}_2)\mathbf{u}_2 + \cdots + (\mathbf{y} \cdot \mathbf{u}_p)\mathbf{u}_p \qquad (4)$$

If $U = [\,\mathbf{u}_1 \quad \mathbf{u}_2 \quad \cdots \quad \mathbf{u}_p\,]$, then

$$\text{proj}_W \mathbf{y} = UU^T\mathbf{y} \quad \text{for all } \mathbf{y} \text{ in } \mathbb{R}^n \qquad (5)$$

PROOF Formula (4) follows immediately from (2) in Theorem 8. Also, (4) shows that $\text{proj}_W \mathbf{y}$ is a linear combination of the columns of U using the weights $\mathbf{y} \cdot \mathbf{u}_1$, $\mathbf{y} \cdot \mathbf{u}_2, \ldots, \mathbf{y} \cdot \mathbf{u}_p$. The weights can be written as $\mathbf{u}_1^T\mathbf{y}, \mathbf{u}_2^T\mathbf{y}, \ldots, \mathbf{u}_p^T\mathbf{y}$, showing that they are the entries in $U^T\mathbf{y}$ and justifying (5). ∎

Suppose U is an $n \times p$ matrix with orthonormal columns, and let W be the column space of U. Then

$$U^T U \mathbf{x} = I_p \mathbf{x} = \mathbf{x} \quad \text{for all } \mathbf{x} \text{ in } \mathbb{R}^p \qquad \text{Theorem 6}$$

$$U U^T \mathbf{y} = \text{proj}_W \mathbf{y} \quad \text{for all } \mathbf{y} \text{ in } \mathbb{R}^n \qquad \text{Theorem 10}$$

How find orthonormal basis for subspaces

GRAM-SCHMIDT PROCESS

The Gram–Schmidt process is a simple algorithm for producing an orthogonal or orthonormal basis for any nonzero subspace of R_n

EXAMPLE 1 Let $W = \text{Span}\{\mathbf{x}_1, \mathbf{x}_2\}$, where $\mathbf{x}_1 = \begin{bmatrix} 3 \\ 6 \\ 0 \end{bmatrix}$ and $\mathbf{x}_2 = \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix}$. Construct an orthogonal basis $\{\mathbf{v}_1, \mathbf{v}_2\}$ for W.

The Gram–Schmidt process is a simple algorithm for producing an orthogonal or orthonormal basis for any nonzero subspace of R_n

EXAMPLE 1 Let $W = \text{Span}\{\mathbf{x}_1, \mathbf{x}_2\}$, where $\mathbf{x}_1 = \begin{bmatrix} 3 \\ 6 \\ 0 \end{bmatrix}$ and $\mathbf{x}_2 = \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix}$. Construct an orthogonal basis $\{\mathbf{v}_1, \mathbf{v}_2\}$ for W.

$$\mathbf{v}_1 = \mathbf{x}_1 \qquad \mathbf{v}_2 = \mathbf{x}_2 - \mathbf{p} = \mathbf{x}_2 - \frac{\mathbf{x}_2 \cdot \mathbf{x}_1}{\mathbf{x}_1 \cdot \mathbf{x}_1}\mathbf{x}_1 = \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix} - \frac{15}{45}\begin{bmatrix} 3 \\ 6 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 2 \end{bmatrix}$$

Then $\{\mathbf{v}_1, \mathbf{v}_2\}$ is an orthogonal set of nonzero vectors in W. Since $\dim W = 2$, the set $\{\mathbf{v}_1, \mathbf{v}_2\}$ is a basis for W. ■

EXAMPLE 2 Let $\mathbf{x}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$, $\mathbf{x}_2 = \begin{bmatrix} 0 \\ 1 \\ 1 \\ 1 \end{bmatrix}$, and $\mathbf{x}_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}$. Then $\{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3\}$ is

clearly linearly independent and thus is a basis for a subspace W of $\mathbb{R}^4$. Construct an orthogonal basis for W.

EXAMPLE 2 Let $\mathbf{x}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$, $\mathbf{x}_2 = \begin{bmatrix} 0 \\ 1 \\ 1 \\ 1 \end{bmatrix}$, and $\mathbf{x}_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}$. Then $\{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3\}$ is

clearly linearly independent and thus is a basis for a subspace W of $\mathbb{R}^4$. Construct an orthogonal basis for W.

Step 1. Let $\mathbf{v}_1 = \mathbf{x}_1$ and $W_1 = \mathrm{Span}\,\{\mathbf{x}_1\} = \mathrm{Span}\,\{\mathbf{v}_1\}$.

Step 2. Let $\mathbf{v}_2$ be the vector produced by subtracting from $\mathbf{x}_2$ its projection onto the subspace W_1. That is, let

$$\mathbf{v}_2 = \mathbf{x}_2 - \mathrm{proj}_{W_1} \mathbf{x}_2$$

$$= \mathbf{x}_2 - \frac{\mathbf{x}_2 \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v}_1} \mathbf{v}_1 \qquad \text{\color{blue}{Since } } \mathbf{v}_1 = \mathbf{x}_1$$

$$= \begin{bmatrix} 0 \\ 1 \\ 1 \\ 1 \end{bmatrix} - \frac{3}{4} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} -3/4 \\ 1/4 \\ 1/4 \\ 1/4 \end{bmatrix}$$

As in Example 1, $\mathbf{v}_2$ is the component of $\mathbf{x}_2$ orthogonal to $\mathbf{x}_1$, and $\{\mathbf{v}_1, \mathbf{v}_2\}$ is an orthogonal basis for the subspace W_2 spanned by $\mathbf{x}_1$ and $\mathbf{x}_2$.

$$\mathbf{v}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}, \quad \mathbf{v}_2' = \begin{bmatrix} -3 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

Step 3. Let $\mathbf{v}_3$ be the vector produced by subtracting from $\mathbf{x}_3$ its projection onto the subspace W_2. Use the orthogonal basis $\{\mathbf{v}_1, \mathbf{v}_2'\}$ to compute this projection onto W_2:

$$\text{proj}_{W_2}\, \mathbf{x}_3 = \underbrace{\frac{\mathbf{x}_3 \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v}_1} \mathbf{v}_1}_{\substack{\text{Projection of} \\ \mathbf{x}_3 \text{ onto } \mathbf{v}_1}} + \underbrace{\frac{\mathbf{x}_3 \cdot \mathbf{v}_2'}{\mathbf{v}_2' \cdot \mathbf{v}_2'} \mathbf{v}_2'}_{\substack{\text{Projection of} \\ \mathbf{x}_3 \text{ onto } \mathbf{v}_2'}} = \frac{2}{4}\begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} + \frac{2}{12}\begin{bmatrix} -3 \\ 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 2/3 \\ 2/3 \\ 2/3 \end{bmatrix}$$

Then $\mathbf{v}_3$ is the component of $\mathbf{x}_3$ orthogonal to W_2, namely,

$$\mathbf{v}_3 = \mathbf{x}_3 - \text{proj}_{W_2}\, \mathbf{x}_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix} - \begin{bmatrix} 0 \\ 2/3 \\ 2/3 \\ 2/3 \end{bmatrix} = \begin{bmatrix} 0 \\ -2/3 \\ 1/3 \\ 1/3 \end{bmatrix}$$

THEOREM 11

The Gram–Schmidt Process

Given a basis $\{\mathbf{x}_1, \ldots, \mathbf{x}_p\}$ for a nonzero subspace W of $\mathbb{R}^n$, define

$$\mathbf{v}_1 = \mathbf{x}_1$$

$$\mathbf{v}_2 = \mathbf{x}_2 - \frac{\mathbf{x}_2 \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v}_1} \mathbf{v}_1$$

$$\mathbf{v}_3 = \mathbf{x}_3 - \frac{\mathbf{x}_3 \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v}_1} \mathbf{v}_1 - \frac{\mathbf{x}_3 \cdot \mathbf{v}_2}{\mathbf{v}_2 \cdot \mathbf{v}_2} \mathbf{v}_2$$

$$\vdots$$

$$\mathbf{v}_p = \mathbf{x}_p - \frac{\mathbf{x}_p \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v}_1} \mathbf{v}_1 - \frac{\mathbf{x}_p \cdot \mathbf{v}_2}{\mathbf{v}_2 \cdot \mathbf{v}_2} \mathbf{v}_2 - \cdots - \frac{\mathbf{x}_p \cdot \mathbf{v}_{p-1}}{\mathbf{v}_{p-1} \cdot \mathbf{v}_{p-1}} \mathbf{v}_{p-1}$$

Then $\{\mathbf{v}_1, \ldots, \mathbf{v}_p\}$ is an orthogonal basis for W. In addition

$$\text{Span}\,\{\mathbf{v}_1, \ldots, \mathbf{v}_k\} = \text{Span}\,\{\mathbf{x}_1, \ldots, \mathbf{x}_k\} \qquad \text{for } 1 \le k \le p \qquad (1)$$

PROOF For $1 \le k \le p$, let $W_k = \text{Span}\{x_1, \ldots, x_k\}$. Set $v_1 = x_1$, so that $\text{Span}\{v_1\} = \text{Span}\{x_1\}$. Suppose, for some $k < p$, we have constructed $v_1, \ldots, v_k$ so that $\{v_1, \ldots, v_k\}$ is an orthogonal basis for W_k. Define

$$v_{k+1} = x_{k+1} - \text{proj}_{W_k} x_{k+1} \tag{2}$$

By the Orthogonal Decomposition Theorem, v_{k+1} is orthogonal to W_k. Note that $\text{proj}_{W_k} x_{k+1}$ is in W_k and hence also in W_{k+1}. Since x_{k+1} is in W_{k+1}, so is v_{k+1} (because W_{k+1} is a subspace and is closed under subtraction). Furthermore, $v_{k+1} \ne 0$ because x_{k+1} is not in $W_k = \text{Span}\{x_1, \ldots, x_k\}$. Hence $\{v_1, \ldots, v_{k+1}\}$ is an orthogonal set of nonzero vectors in the $(k+1)$-dimensional space W_{k+1}. By the Basis Theorem in Section 4.5, this set is an orthogonal basis for W_{k+1}. Hence $W_{k+1} = \text{Span}\{v_1, \ldots, v_{k+1}\}$. When $k + 1 = p$, the process stops. ∎

Orthonormal Bases

THEOREM 12

The QR Factorization

If A is an $m \times n$ matrix with linearly independent columns, then A can be factored as $A = QR$, where Q is an $m \times n$ matrix whose columns form an orthonormal basis for Col A and R is an $n \times n$ upper triangular invertible matrix with positive entries on its diagonal.

THEOREM 12 **The QR Factorization**

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The columns of A form a basis $\{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ for Col A.

$Q = [\, \mathbf{u}_1 \quad \mathbf{u}_2 \quad \cdots \quad \mathbf{u}_n \,]$

$\mathbf{x}_k = r_{1k}\mathbf{u}_1 + \cdots + r_{kk}\mathbf{u}_k + 0 \cdot \mathbf{u}_{k+1} + \cdots + 0 \cdot \mathbf{u}_n$

$\{\mathbf{u}_1, \ldots, \mathbf{u}_n\}$

$$\mathbf{r}_k = \begin{bmatrix} r_{1k} \\ \vdots \\ r_{kk} \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

THEOREM 12 The QR Factorization

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The columns of A form a basis $\{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ for Col A.

$$Q = \begin{bmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \cdots & \mathbf{u}_n \end{bmatrix}$$

$$\mathbf{x}_k = r_{1k}\mathbf{u}_1 + \cdots + r_{kk}\mathbf{u}_k + 0 \cdot \mathbf{u}_{k+1} + \cdots + 0 \cdot \mathbf{u}_n$$

$\{\mathbf{u}_1, \ldots, \mathbf{u}_n\}$

$$\mathbf{r}_k = \begin{bmatrix} r_{1k} \\ \vdots \\ r_{kk} \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

$\mathbf{x}_k = Q\mathbf{r}_k$ for $k = 1, \ldots, n$. Let $R = \begin{bmatrix} \mathbf{r}_1 & \cdots & \mathbf{r}_n \end{bmatrix}$. Then

$$A = \begin{bmatrix} \mathbf{x}_1 & \cdots & \mathbf{x}_n \end{bmatrix} = \begin{bmatrix} Q\mathbf{r}_1 & \cdots & Q\mathbf{r}_n \end{bmatrix} = QR$$

EXAMPLE 4   Find a QR factorization of $A = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}$.

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$$\mathbf{v}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}, \quad \mathbf{v}_2' = \begin{bmatrix} -3 \\ 1 \\ 1 \\ 1 \end{bmatrix}, \quad \mathbf{v}_3 = \begin{bmatrix} 0 \\ -2/3 \\ 1/3 \\ 1/3 \end{bmatrix} \qquad Q = \begin{bmatrix} 1/2 & -3/\sqrt{12} & 0 \\ 1/2 & 1/\sqrt{12} & -2/\sqrt{6} \\ 1/2 & 1/\sqrt{12} & 1/\sqrt{6} \\ 1/2 & 1/\sqrt{12} & 1/\sqrt{6} \end{bmatrix}$$

EXAMPLE 4 Find a QR factorization of $A = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}$.

$$\mathbf{v}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}, \quad \mathbf{v}_2' = \begin{bmatrix} -3 \\ 1 \\ 1 \\ 1 \end{bmatrix}, \quad \mathbf{v}_3 = \begin{bmatrix} 0 \\ -2/3 \\ 1/3 \\ 1/3 \end{bmatrix} \qquad Q = \begin{bmatrix} 1/2 & -3/\sqrt{12} & 0 \\ 1/2 & 1/\sqrt{12} & -2/\sqrt{6} \\ 1/2 & 1/\sqrt{12} & 1/\sqrt{6} \\ 1/2 & 1/\sqrt{12} & 1/\sqrt{6} \end{bmatrix}$$

$A = QR$ for some R. To find R, observe that $Q^T Q = I$ $\qquad Q^T A = Q^T (QR) = IR = R$

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$A = QR$ for some R. To find R, observe that $Q^T Q = I$ $\qquad\qquad$ $Q^T A = Q^T(QR) = IR = R$

$$R = \begin{bmatrix} 1/2 & 1/2 & 1/2 & 1/2 \\ -3/\sqrt{12} & 1/\sqrt{12} & 1/\sqrt{12} & 1/\sqrt{12} \\ 0 & -2/\sqrt{6} & 1/\sqrt{6} & 1/\sqrt{6} \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}$$

$$= \begin{bmatrix} 2 & 3/2 & 1 \\ 0 & 3/\sqrt{12} & 2/\sqrt{12} \\ 0 & 0 & 2/\sqrt{6} \end{bmatrix}$$

LEAST SQUARE PROBLEMS

$$Ax = b$$

When a solution is demanded and none exists, the best one can do is to find an **x** that makes A**x** as close as possible to **b**.

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

When a solution is demanded and none exists, the best one can do is to find an **x** that makes A**x** as close as possible to **b**.

Think of $A\mathbf{x}$ as an *approximation* to $\mathbf{b}$. The smaller the distance between $\mathbf{b}$ and $A\mathbf{x}$, given by $\|\mathbf{b} - A\mathbf{x}\|$, the better the approximation. The **general least-squares problem** is to find an **x** that makes $\|\mathbf{b} - A\mathbf{x}\|$ as small as possible. The adjective "least-squares" arises from the fact that $\|\mathbf{b} - A\mathbf{x}\|$ is the square root of a sum of squares.

DEFINITION

If A is $m \times n$ and $\mathbf{b}$ is in $\mathbb{R}^m$, a **least-squares solution** of $A\mathbf{x} = \mathbf{b}$ is an $\hat{\mathbf{x}}$ in $\mathbb{R}^n$ such that

$$\|\mathbf{b} - A\hat{\mathbf{x}}\| \leq \|\mathbf{b} - A\mathbf{x}\|$$

for all $\mathbf{x}$ in $\mathbb{R}^n$.

we seek an **x** that makes A**x** the closest point in Col A to **b**

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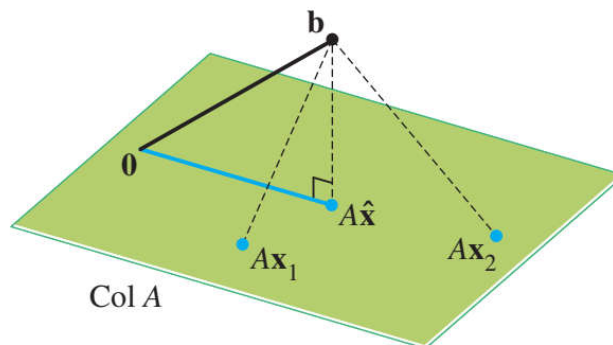
for all $\mathbf{x}$ in $\mathbb{R}^n$.

FIGURE 1 The vector $\mathbf{b}$ is closer to $A\hat{\mathbf{x}}$ than to $A\mathbf{x}$ for other $\mathbf{x}$.

Solution of the General Least-Squares Problem

apply the Best Approximation Theorem

$$\hat{\mathbf{b}} = \text{proj}_{\text{Col } A} \mathbf{b}$$

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Solution of the General Least-Squares Problem

apply the Best Approximation Theorem

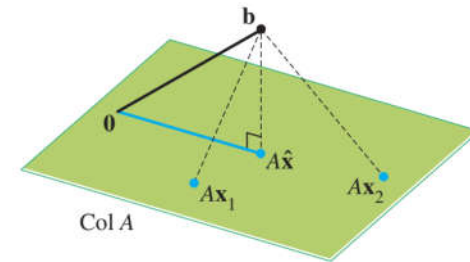$$\hat{\mathbf{b}} = \text{proj}_{\text{Col } A}\, \mathbf{b}$$

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

$\mathbf{b} - A\hat{\mathbf{x}}$ is orthogonal to each column of A

If $\mathbf{a}_j$ is any column of A

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

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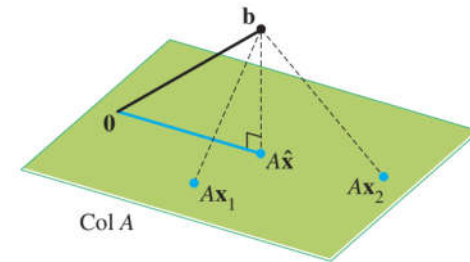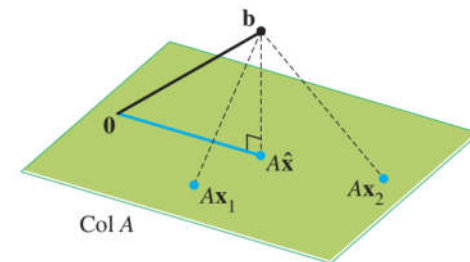
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$$A^T A\hat{\mathbf{x}} = A^T \mathbf{b} \qquad\qquad \text{\textbf{normal equations} for A\textbf{x}=b}$$
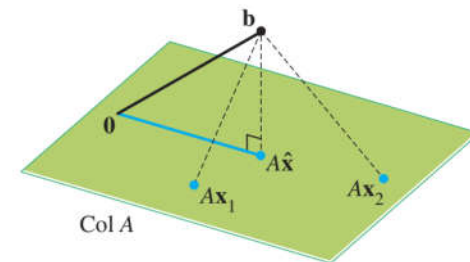
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THEOREM 13 The set of least-squares solutions of $A\mathbf{x} = \mathbf{b}$ coincides with the nonempty set of solutions of the normal equations $A^TA\mathbf{x} = A^T\mathbf{b}$.

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$$\mathbf{b} = A\hat{\mathbf{x}} + (\mathbf{b} - A\hat{\mathbf{x}})$$

By the uniqueness of the orthogonal decomposition, $A\hat{\mathbf{x}}$ must be the orthogonal projection of $\mathbf{b}$ onto Col A. That is, $A\hat{\mathbf{x}} = \hat{\mathbf{b}}$, and $\hat{\mathbf{x}}$ is a least-squares solution. ■

EXAMPLE 1 Find a least-squares solution of the inconsistent system $A\mathbf{x} = \mathbf{b}$ for

$$A = \begin{bmatrix} 4 & 0 \\ 0 & 2 \\ 1 & 1 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} 2 \\ 0 \\ 11 \end{bmatrix}$$

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$$A^{T}A = \begin{bmatrix} 4 & 0 & 1 \\ 0 & 2 & 1 \end{bmatrix} \begin{bmatrix} 4 & 0 \\ 0 & 2 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 17 & 1 \\ 1 & 5 \end{bmatrix}$$

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$$\begin{bmatrix} 17 & 1 \\ 1 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 19 \\ 11 \end{bmatrix}$$

EXAMPLE 2 Find a least-squares solution of $A\mathbf{x} = \mathbf{b}$ for

$$A = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} -3 \\ -1 \\ 0 \\ 2 \\ 5 \\ 1 \end{bmatrix}$$

$$A^T A = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 6 & 2 & 2 & 2 \\ 2 & 2 & 0 & 0 \\ 2 & 0 & 2 & 0 \\ 2 & 0 & 0 & 2 \end{bmatrix}$$

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$$\hat{\mathbf{x}} = \begin{bmatrix} 3 \\ -5 \\ -2 \\ 0 \end{bmatrix} + x_4 \begin{bmatrix} -1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

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$$\begin{bmatrix} 6 & 2 & 2 & 2 & 4 \\ 2 & 2 & 0 & 0 & -4 \\ 2 & 0 & 2 & 0 & 2 \\ 2 & 0 & 0 & 2 & 6 \end{bmatrix} \sim \begin{bmatrix} 1 & 0 & 0 & 1 & 3 \\ 0 & 1 & 0 & -1 & -5 \\ 0 & 0 & 1 & -1 & -2 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

THEOREM 14   Let A be an $m \times n$ matrix. The following statements are logically equivalent:

a. The equation $A\mathbf{x} = \mathbf{b}$ has a unique least-squares solution for each $\mathbf{b}$ in $\mathbb{R}^m$.
b. The columns of A are linearly independent.
c. The matrix A^TA is invertible.

When these statements are true, the least-squares solution $\hat{\mathbf{x}}$ is given by

$$\hat{\mathbf{x}} = (A^TA)^{-1}A^T\mathbf{b} \tag{4}$$

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When a least-squares solution $\hat{\mathbf{x}}$ is used to produce $A\hat{\mathbf{x}}$ as an approximation to $\mathbf{b}$, the distance from $\mathbf{b}$ to $A\hat{\mathbf{x}}$ is called the **least-squares error** of this approximation.

EXAMPLE 4 Find a least-squares solution of $A\mathbf{x} = \mathbf{b}$ for

$$A = \begin{bmatrix} 1 & -6 \\ 1 & -2 \\ 1 & 1 \\ 1 & 7 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} -1 \\ 2 \\ 1 \\ 6 \end{bmatrix}$$

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$$\hat{\mathbf{b}} = \frac{\mathbf{b} \cdot \mathbf{a}_1}{\mathbf{a}_1 \cdot \mathbf{a}_1} \mathbf{a}_1 + \frac{\mathbf{b} \cdot \mathbf{a}_2}{\mathbf{a}_2 \cdot \mathbf{a}_2} \mathbf{a}_2 = \frac{8}{4} \mathbf{a}_1 + \frac{45}{90} \mathbf{a}_2 = \begin{bmatrix} -1 \\ 1 \\ 5/2 \\ 11/2 \end{bmatrix} \qquad A\hat{\mathbf{x}} = \hat{\mathbf{b}}$$

$$\hat{\mathbf{x}} = \begin{bmatrix} 8/4 \\ 45/90 \end{bmatrix} = \begin{bmatrix} 2 \\ 1/2 \end{bmatrix}$$

THEOREM 15   Given an $m \times n$ matrix A with linearly independent columns, let $A = QR$ be a QR factorization of A as in Theorem 12. Then, for each $\mathbf{b}$ in $\mathbb{R}^m$, the equation $A\mathbf{x} = \mathbf{b}$ has a unique least-squares solution, given by

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PROOF Let $\hat{\mathbf{x}} = R^{-1}Q^T\mathbf{b}$. Then

$$A\hat{\mathbf{x}} = QR\hat{\mathbf{x}} = QRR^{-1}Q^T\mathbf{b} = QQ^T\mathbf{b}$$

By Theorem 12, the columns of Q form an orthonormal basis for Col A. Hence, by Theorem 10, $QQ^T\mathbf{b}$ is the orthogonal projection $\hat{\mathbf{b}}$ of $\mathbf{b}$ onto Col A. Then $A\hat{\mathbf{x}} = \hat{\mathbf{b}}$, which shows that $\hat{\mathbf{x}}$ is a least-squares solution of $A\mathbf{x} = \mathbf{b}$. The uniqueness of $\hat{\mathbf{x}}$ follows from Theorem 14. ∎

APPLICATIONS TO LINEAR MODELS

Least Square line

❖A common task in science and engineering is to analyze and understand relationships among several quantities that vary

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Least-Squares Lines

$$y = \beta_0 + \beta_1 x$$

$$(x_1, y_1), \ldots, (x_n, y_n)$$

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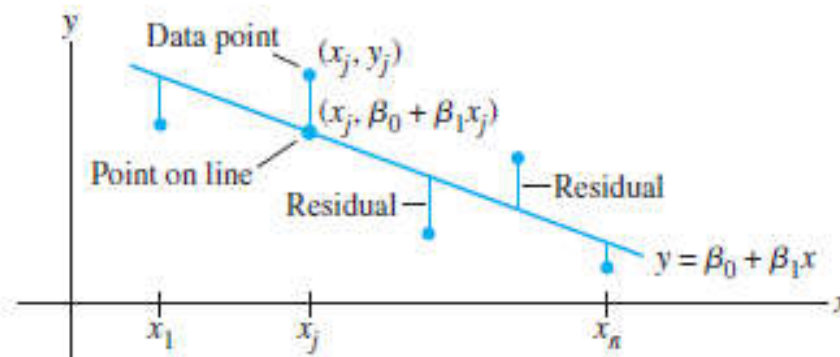$$y = \beta_0 + \beta_1 x$$

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FIGURE 1 Fitting a line to experimental data.

Goal: determine the parameters B0 and B1 that make the line as "close" to the points as possible

Least Square line

There are several ways to measure how "close" the line is to the data.
Usual choice is to add the squares of the residuals

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line of regression of y on x   **Linear regression coefficients**

$$(x_1, y_1), \ldots, (x_n, y_n)$$

Predicted y-value		Observed y-value
$\beta_0 + \beta_1 x_1$	$=$	y_1
$\beta_0 + \beta_1 x_2$	$=$	y_2
$\vdots$		$\vdots$
$\beta_0 + \beta_1 x_n$	$=$	y_n

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$$\beta = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \quad X = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \qquad X\beta = \mathbf{y}$$

Predicted y-value		Observed y-value
$\beta_0 + \beta_1 x_1$	=	y_1
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$\vdots$		$\vdots$
$\beta_0 + \beta_1 x_n$	=	y_n

Least Square line

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

*Computing the least-squares solution of XB=y **is equivalent to** finding the B   that determines the least-squares line in Figure 1*

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

Least Square line

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*Computing the least-squares solution of XB=y **is equivalent to** finding the B that determines the least-squares line in Figure 1*

$$X^T X \beta = X^T y$$

$$y = X\beta + \epsilon$$

goal is to minimize the length of residual (error), which amounts to finding a least-squares solution

example

$$y = \beta_0 + \beta_1 x + \beta_2 x^2$$

$(x_1, y_1), \ldots, (x_n, y_n)$

$$y_1 = \beta_0 + \beta_1 x_1 + \beta_2 x_1^2 + \epsilon_1$$
$$y_2 = \beta_0 + \beta_1 x_2 + \beta_2 x_2^2 + \epsilon_2$$
$$\vdots \qquad \vdots$$
$$y_n = \beta_0 + \beta_1 x_n + \beta_2 x_n^2 + \epsilon_n$$

$$
\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}
=
\begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ \vdots & \vdots & \vdots \\ 1 & x_n & x_n^2 \end{bmatrix}
\begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}
+
\begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}
$$

$$\mathbf{y} \qquad = \qquad X \qquad\qquad \beta \quad + \quad \epsilon$$

$$y = \beta_0 f_0(x) + \beta_1 f_1(x) + \cdots + \beta_k f_k(x)$$

Multiple Regression

$$y = \beta_0 + \beta_1 u + \beta_2 v$$

$$y = \beta_0 + \beta_1 u + \beta_2 v + \beta_3 u^2 + \beta_4 uv + \beta_5 v^2$$

$$y = \beta_0 f_0(u, v) + \beta_1 f_1(u, v) + \cdots + \beta_k f_k(u, v)$$

$$
\begin{aligned}
y_1 &= \beta_0 + \beta_1 u_1 + \beta_2 v_1 + \epsilon_1 \\
y_2 &= \beta_0 + \beta_1 u_2 + \beta_2 v_2 + \epsilon_2 \\
&\;\;\vdots \\
y_n &= \beta_0 + \beta_1 u_n + \beta_2 v_n + \epsilon_n
\end{aligned}
$$

Observation vector

Design matrix

Parameter vector

Residual vector

$$
\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, \quad
X = \begin{bmatrix} 1 & u_1 & v_1 \\ 1 & u_2 & v_2 \\ \vdots & \vdots & \vdots \\ 1 & u_n & v_n \end{bmatrix}, \quad
\beta = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}, \quad
\epsilon = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}
$$