


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

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

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

$$\begin{aligned} \|\mathbf{u}\|^2 &= \mathbf{u} \cdot \mathbf{u} = \left(\frac{1}{3}\right)^2 + \left(-\frac{2}{3}\right)^2 + \left(\frac{2}{3}\right)^2 + (0)^2 \\ &= \frac{1}{9} + \frac{4}{9} + \frac{4}{9} + 0 = 1 \end{aligned}$$



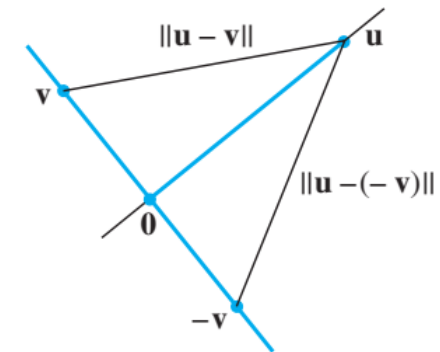
DEFINITION

For \mathbf{u} and \mathbf{v} in \mathbb{R}^n , the **distance between \mathbf{u} and \mathbf{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

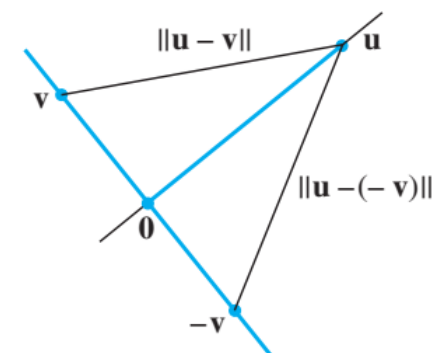


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$$\begin{aligned} [\text{dist}(\mathbf{u}, -\mathbf{v})]^2 &= \|\mathbf{u} - (-\mathbf{v})\|^2 = \|\mathbf{u} + \mathbf{v}\|^2 \\ &= (\mathbf{u} + \mathbf{v}) \cdot (\mathbf{u} + \mathbf{v}) \\ &= \mathbf{u} \cdot (\mathbf{u} + \mathbf{v}) + \mathbf{v}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

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



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



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




$$W^\perp$$

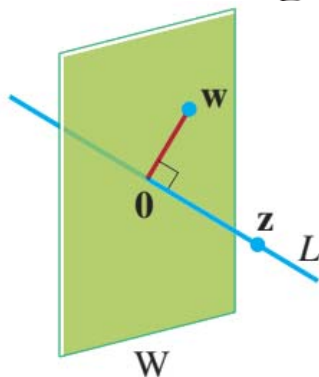
EXAMPLE 6 Let W be a plane through the origin in \mathbb{R}^3 , and let L be the line through the origin and perpendicular to W . If \mathbf{z} and \mathbf{w} are nonzero, \mathbf{z} is on L , and \mathbf{w} is in W , then the line segment from $\mathbf{0}$ to \mathbf{z} is perpendicular to the line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

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

- 
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 $\text{Nul } A$, 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 $\text{Row } A$. Conversely, if \mathbf{x} is orthogonal to $\text{Row } A$, 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 $\text{Row } A^T = \text{Col } A$. ■

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




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3. If $W \neq \{\mathbf{0}\}$, let $\{\mathbf{b}_1, \dots, \mathbf{b}_p\}$ be a basis for W , where $1 \leq p \leq n$. Let A be the $p \times n$ matrix having rows $\mathbf{b}_1^T, \dots, \mathbf{b}_p^T$. 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 $\{\mathbf{u}_1, \dots, \mathbf{u}_p\}$ 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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THEOREM 4

If $S = \{\mathbf{u}_1, \dots, \mathbf{u}_p\}$ 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 $\mathbf{0} = c_1\mathbf{u}_1 + \dots + c_p\mathbf{u}_p$ for some scalars c_1, \dots, c_p , then

$$\begin{aligned} 0 &= \mathbf{0} \cdot \mathbf{u}_1 = (c_1\mathbf{u}_1 + c_2\mathbf{u}_2 + \dots + c_p\mathbf{u}_p) \cdot \mathbf{u}_1 \\ &= (c_1\mathbf{u}_1) \cdot \mathbf{u}_1 + (c_2\mathbf{u}_2) \cdot \mathbf{u}_1 + \dots + (c_p\mathbf{u}_p) \cdot \mathbf{u}_1 \\ &= c_1(\mathbf{u}_1 \cdot \mathbf{u}_1) + c_2(\mathbf{u}_2 \cdot \mathbf{u}_1) + \dots + c_p(\mathbf{u}_p \cdot \mathbf{u}_1) \\ &= c_1(\mathbf{u}_1 \cdot \mathbf{u}_1) \end{aligned}$$

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



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An **orthogonal basis** for a subspace W of \mathbb{R}^n is a basis for W that is also an orthogonal set.



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THEOREM 5

Let $\{\mathbf{u}_1, \dots, \mathbf{u}_p\}$ 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

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

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PROOF As in the preceding proof, the orthogonality of $\{\mathbf{u}_1, \dots, \mathbf{u}_p\}$ 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 $j = 2, \dots, p$, 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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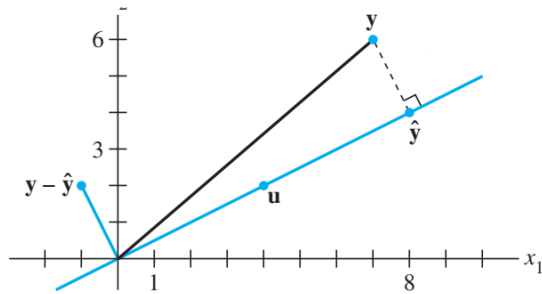
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$$\begin{aligned} \mathbf{y} &= \frac{\mathbf{y} \cdot \mathbf{u}_1}{\mathbf{u}_1 \cdot \mathbf{u}_1} \mathbf{u}_1 + \frac{\mathbf{y} \cdot \mathbf{u}_2}{\mathbf{u}_2 \cdot \mathbf{u}_2} \mathbf{u}_2 + \frac{\mathbf{y} \cdot \mathbf{u}_3}{\mathbf{u}_3 \cdot \mathbf{u}_3} \mathbf{u}_3 \\ &= \frac{11}{11} \mathbf{u}_1 + \frac{-12}{6} \mathbf{u}_2 + \frac{-33}{33/2} \mathbf{u}_3 \\ &= \mathbf{u}_1 - 2\mathbf{u}_2 - 2\mathbf{u}_3 \end{aligned}$$

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

$$\mathbf{y} = \hat{\mathbf{y}} + \mathbf{z} \quad (1)$$

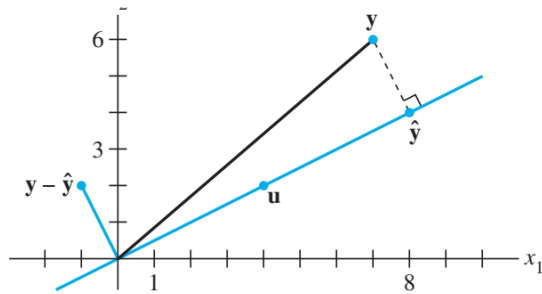


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$$\hat{\mathbf{y}} = \alpha \mathbf{u} \quad \mathbf{z} = \mathbf{y} - \alpha \mathbf{u}$$

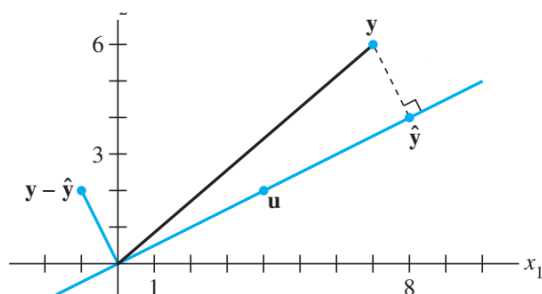


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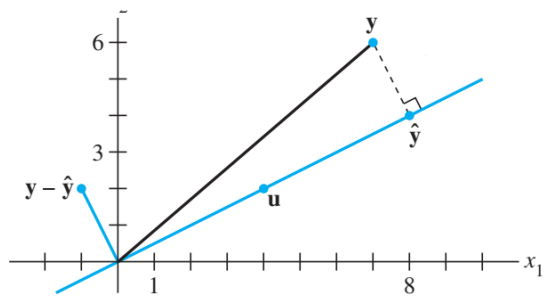


$$0 = (\mathbf{y} - \alpha \mathbf{u}) \cdot \mathbf{u} = \mathbf{y} \cdot \mathbf{u} - (\alpha \mathbf{u}) \cdot \mathbf{u} = \mathbf{y} \cdot \mathbf{u} - \alpha (\mathbf{u} \cdot \mathbf{u})$$

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

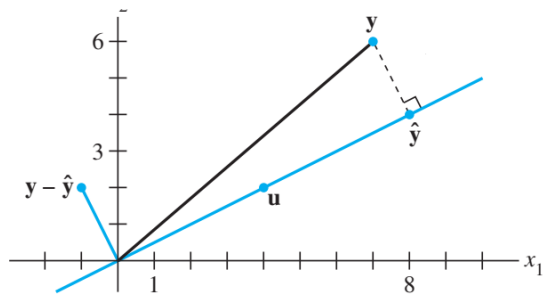
The vector $\hat{\mathbf{y}}$ is called the **orthogonal projection of \mathbf{y} onto \mathbf{u}** , and the vector \mathbf{z} is called the **component of \mathbf{y} orthogonal to \mathbf{u}** .

subspace L spanned by \mathbf{u}




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Sometimes \mathbf{y}_O is denoted by $\text{proj}_L \mathbf{y}$ and is called the **orthogonal projection of \mathbf{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 $\text{Span}\{\mathbf{u}\}$ and one orthogonal to \mathbf{u} .

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

$$\begin{array}{ccc} \begin{bmatrix} 7 \\ 6 \end{bmatrix} & = & \begin{bmatrix} 8 \\ 4 \end{bmatrix} + \begin{bmatrix} -1 \\ 2 \end{bmatrix} \\ \uparrow & & \uparrow \quad \uparrow \\ \mathbf{y} & & \hat{\mathbf{y}} \quad (\mathbf{y} - \hat{\mathbf{y}}) \end{array}$$

Orthonormal Sets

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

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

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



THEOREM 6

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

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$$U = [\mathbf{u}_1 \quad \mathbf{u}_2 \quad \mathbf{u}_3]$$

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

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 \mathbb{R}_2 onto a line through the origin has an important analogue in \mathbb{R}_n

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

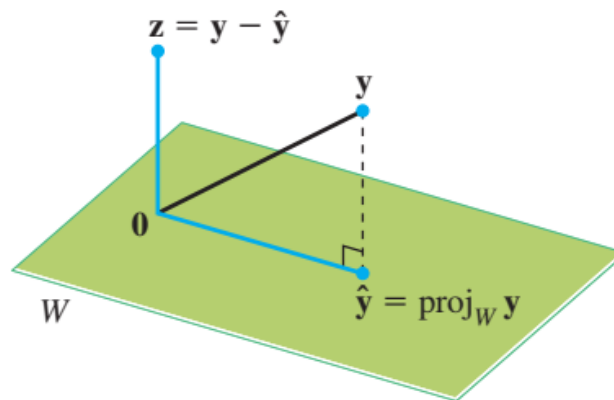


FIGURE 2 The orthogonal projection of \mathbf{y} onto W .

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

$$\mathbf{y} = \hat{\mathbf{y}} + \mathbf{z} \quad (1)$$

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

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

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

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$$\mathbf{y} = \hat{\mathbf{y}} + \mathbf{z} \quad (1)$$

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

$$\hat{\mathbf{y}} = \frac{\mathbf{y} \cdot \mathbf{u}_1}{\mathbf{u}_1 \cdot \mathbf{u}_1} \mathbf{u}_1 + \dots + \frac{\mathbf{y} \cdot \mathbf{u}_p}{\mathbf{u}_p \cdot \mathbf{u}_p} \mathbf{u}_p \quad (2)$$

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

$$\begin{aligned} \mathbf{z} = \mathbf{y} - \hat{\mathbf{y}} \quad \mathbf{z} \cdot \mathbf{u}_1 &= (\mathbf{y} - \hat{\mathbf{y}}) \cdot \mathbf{u}_1 = \mathbf{y} \cdot \mathbf{u}_1 - \left(\frac{\mathbf{y} \cdot \mathbf{u}_1}{\mathbf{u}_1 \cdot \mathbf{u}_1} \right) \mathbf{u}_1 \cdot \mathbf{u}_1 - 0 - \dots - 0 \\ &= \mathbf{y} \cdot \mathbf{u}_1 - \mathbf{y} \cdot \mathbf{u}_1 = 0 \end{aligned}$$

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

$$\mathbf{y} = \hat{\mathbf{y}} + \mathbf{z} \quad (1)$$


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

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

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

$$\begin{aligned} \mathbf{z} = \mathbf{y} - \hat{\mathbf{y}} \quad \mathbf{z} \cdot \mathbf{u}_1 &= (\mathbf{y} - \hat{\mathbf{y}}) \cdot \mathbf{u}_1 = \mathbf{y} \cdot \mathbf{u}_1 - \left(\frac{\mathbf{y} \cdot \mathbf{u}_1}{\mathbf{u}_1 \cdot \mathbf{u}_1} \right) \mathbf{u}_1 \cdot \mathbf{u}_1 - 0 - \cdots - 0 \\ &= \mathbf{y} \cdot \mathbf{u}_1 - \mathbf{y} \cdot \mathbf{u}_1 = 0 \end{aligned}$$

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




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 .

$$\begin{aligned}\hat{\mathbf{y}} &= \frac{\mathbf{y} \cdot \mathbf{u}_1}{\mathbf{u}_1 \cdot \mathbf{u}_1} \mathbf{u}_1 + \frac{\mathbf{y} \cdot \mathbf{u}_2}{\mathbf{u}_2 \cdot \mathbf{u}_2} \mathbf{u}_2 \\ &= \frac{9}{30} \begin{bmatrix} 2 \\ 5 \\ -1 \end{bmatrix} + \frac{3}{6} \begin{bmatrix} -2 \\ 1 \\ 1 \end{bmatrix} = \frac{9}{30} \begin{bmatrix} 2 \\ 5 \\ -1 \end{bmatrix} + \frac{15}{30} \begin{bmatrix} -2 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} -2/5 \\ 2 \\ 1/5 \end{bmatrix}\end{aligned}$$

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

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



If $\{\mathbf{u}_1, \dots, \mathbf{u}_p\}$ 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 $W = \text{Span}\{\mathbf{u}_1, \dots, \mathbf{u}_p\}$, 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

$$\|\mathbf{y} - \hat{\mathbf{y}}\| < \|\mathbf{y} - \mathbf{v}\| \quad (3)$$

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



the best approximation to \mathbf{y} by elements of W

Min error

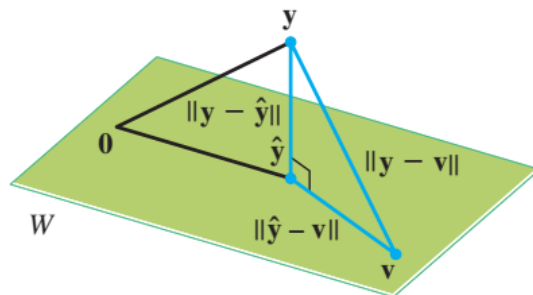
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$$\mathbf{y} - \mathbf{v} = (\mathbf{y} - \hat{\mathbf{y}}) + (\hat{\mathbf{y}} - \mathbf{v})$$

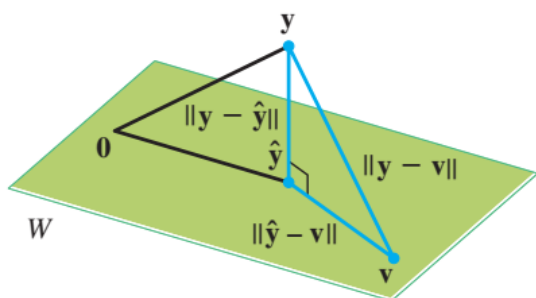
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for all \mathbf{v} in W distinct from $\hat{\mathbf{y}}$.



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

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

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

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 $W = \text{Span}\{\mathbf{u}_1, \mathbf{u}_2\}$, 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 $\{\mathbf{u}_1, \dots, \mathbf{u}_p\}$ is an orthonormal basis for a subspace W of \mathbb{R}^n , then

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

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

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

THEOREM 10

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

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

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

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

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 $\mathbf{y} \cdot \mathbf{u}_1, \mathbf{y} \cdot \mathbf{u}_2, \dots, \mathbf{y} \cdot \mathbf{u}_p$. The weights can be written as $\mathbf{u}_1^T \mathbf{y}, \mathbf{u}_2^T \mathbf{y}, \dots, \mathbf{u}_p^T \mathbf{y}$, 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

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

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

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 \mathbb{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 \mathbb{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 $W_1 = \text{Span}\{\mathbf{x}_1\} = \text{Span}\{\mathbf{v}_1\}$.

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

$$\begin{aligned}\mathbf{v}_2 &= \mathbf{x}_2 - \text{proj}_{W_1} \mathbf{x}_2 \\ &= \mathbf{x}_2 - \frac{\mathbf{x}_2 \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v}_1} \mathbf{v}_1 \quad \text{Since } \mathbf{v}_1 = \mathbf{x}_1 \\ &= \begin{bmatrix} 0 \\ 1 \\ 1 \\ 1 \end{bmatrix} - \frac{3}{4} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} -3/4 \\ 1/4 \\ 1/4 \\ 1/4 \end{bmatrix}\end{aligned}$$

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 :

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

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

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

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

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

$$\vdots$$

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

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

$$\text{Span}\{\mathbf{v}_1, \dots, \mathbf{v}_k\} = \text{Span}\{\mathbf{x}_1, \dots, \mathbf{x}_k\} \quad \text{for } 1 \leq k \leq p \quad (1)$$

PROOF For $1 \leq k \leq p$, let $W_k = \text{Span}\{\mathbf{x}_1, \dots, \mathbf{x}_k\}$. Set $\mathbf{v}_1 = \mathbf{x}_1$, so that $\text{Span}\{\mathbf{v}_1\} = \text{Span}\{\mathbf{x}_1\}$. Suppose, for some $k < p$, we have constructed $\mathbf{v}_1, \dots, \mathbf{v}_k$ so that $\{\mathbf{v}_1, \dots, \mathbf{v}_k\}$ is an orthogonal basis for W_k . Define

$$\mathbf{v}_{k+1} = \mathbf{x}_{k+1} - \text{proj}_{W_k} \mathbf{x}_{k+1} \quad (2)$$

By the Orthogonal Decomposition Theorem, \mathbf{v}_{k+1} is orthogonal to W_k . Note that $\text{proj}_{W_k} \mathbf{x}_{k+1}$ is in W_k and hence also in W_{k+1} . Since \mathbf{x}_{k+1} is in W_{k+1} , so is \mathbf{v}_{k+1} (because W_{k+1} is a subspace and is closed under subtraction). Furthermore, $\mathbf{v}_{k+1} \neq \mathbf{0}$ because \mathbf{x}_{k+1} is not in $W_k = \text{Span}\{\mathbf{x}_1, \dots, \mathbf{x}_k\}$. Hence $\{\mathbf{v}_1, \dots, \mathbf{v}_{k+1}\}$ 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 $W_{k+1} = \text{Span}\{\mathbf{v}_1, \dots, \mathbf{v}_{k+1}\}$. 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 $\text{Col } A$ and R is an $n \times n$ upper triangular invertible matrix with positive entries on its diagonal.

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

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

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

$$\{\mathbf{u}_1, \dots, \mathbf{u}_n\} \quad \mathbf{r}_k = \begin{bmatrix} r_{1k} \\ \vdots \\ r_{kk} \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

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

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

$$\{\mathbf{u}_1, \dots, \mathbf{u}_n\} \quad \mathbf{r}_k = \begin{bmatrix} r_{1k} \\ \vdots \\ r_{kk} \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

$\mathbf{x}_k = Q\mathbf{r}_k$ for $k = 1, \dots, n$. Let $R = [\mathbf{r}_1 \quad \cdots \quad \mathbf{r}_n]$. Then

$$A = [\mathbf{x}_1 \quad \cdots \quad \mathbf{x}_n] = [Q\mathbf{r}_1 \quad \cdots \quad Q\mathbf{r}_n] = QR$$



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

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

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

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


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

LEAST SQUARE PROBLEMS




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

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


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

When a solution is demanded and none exists, the best one can do is to find an \mathbf{x} that makes $A\mathbf{x}$ as close as possible to \mathbf{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 \mathbf{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 \mathbf{x} that makes $A\mathbf{x}$ the closest point in Col A to \mathbf{b}

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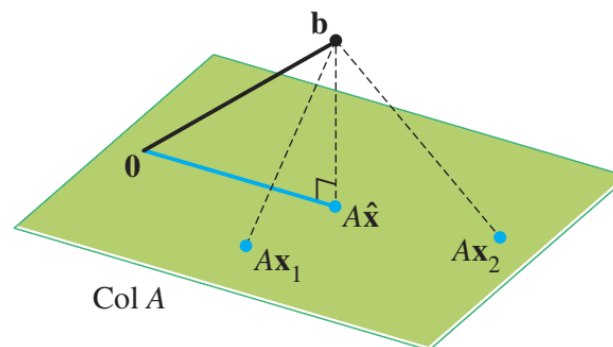


FIGURE 1 The vector \mathbf{b} is closer to $A\hat{\mathbf{x}}$ than to $A\mathbf{x}$ for other \mathbf{x} .

Solution of the General Least-Squares Problem

apply the Best Approximation Theorem

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

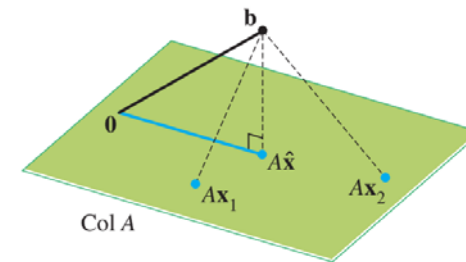


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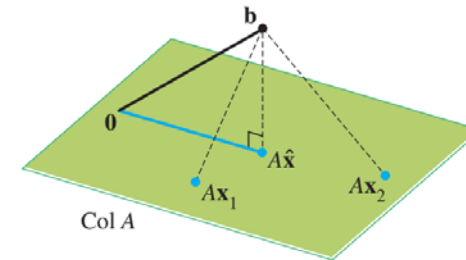


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$$A\hat{\mathbf{x}} = \hat{\mathbf{b}}$$

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

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

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

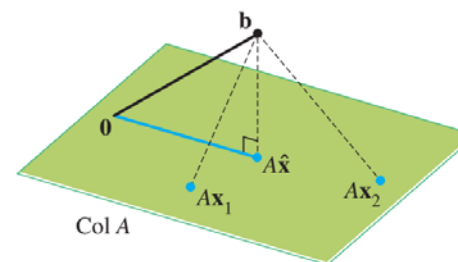


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$$A^T (\mathbf{b} - A\hat{\mathbf{x}}) = \mathbf{0}$$

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

normal equations for $A\mathbf{x}=\mathbf{b}$

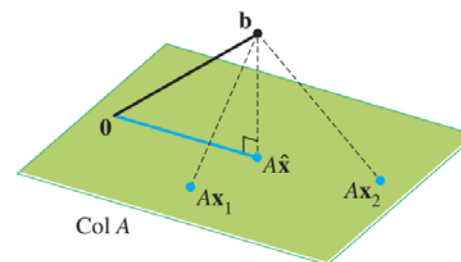


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THEOREM 13

The set of least-squares solutions of $A\mathbf{x} = \mathbf{b}$ coincides with the nonempty set of solutions of the normal equations $A^T A\mathbf{x} = A^T \mathbf{b}$.

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

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

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

By the uniqueness of the orthogonal decomposition, $A\hat{\mathbf{x}}$ must be the orthogonal projection of \mathbf{b} onto $\text{Col } A$. 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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$$A^T A = \begin{bmatrix} 4 & 0 & 1 \\ 0 & 2 & 1 \end{bmatrix} \begin{bmatrix} 4 & 0 \\ 0 & 2 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 17 & 1 \\ 1 & 5 \end{bmatrix}$$

$$A^T \mathbf{b} = \begin{bmatrix} 4 & 0 & 1 \\ 0 & 2 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 0 \\ 11 \end{bmatrix} = \begin{bmatrix} 19 \\ 11 \end{bmatrix}$$

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

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

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

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$$A^T \mathbf{b} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} -3 \\ -1 \\ 0 \\ 2 \\ 5 \\ 1 \end{bmatrix} = \begin{bmatrix} 4 \\ -4 \\ 2 \\ 6 \end{bmatrix}$$

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

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

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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 $A^T A$ is invertible.

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

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

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

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



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

$$\hat{\mathbf{x}} = R^{-1}Q^T\mathbf{b} \quad (6)$$

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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 $\text{Col } A$. Hence, by Theorem 10, $QQ^T\mathbf{b}$ is the orthogonal projection $\hat{\mathbf{b}}$ of \mathbf{b} onto $\text{Col } A$. 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
- ❖ data are used to build or verify a formula that predicts the value of one variable as a function of other variables

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Least-Squares Lines

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

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

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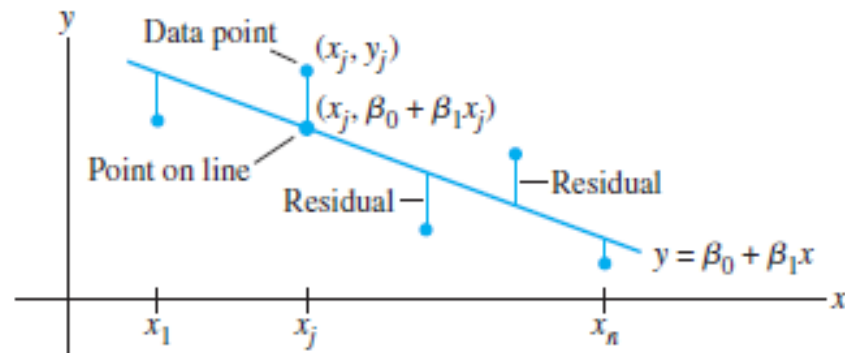


FIGURE 1 Fitting a line to experimental data.

Goal: determine the parameters β_0 and β_1 that make the line as “close” to the points as possible

Least Square line

line of regression of y on x

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

Linear regression coefficients

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

Least Square line

line of regression of y on x

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

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

Linear regression coefficients

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

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

least-squares line is the line that minimizes the sum of the squares of the residuals

line of regression of y on x

Linear regression coefficients

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

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

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Least Square line



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

*Computing the least-squares solution of $X\beta = \mathbf{y}$ is **equivalent** to finding the β 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 $X\beta = \mathbf{y}$ is **equivalent** to finding the β that determines the least-squares line in Figure 1

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

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

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

example



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

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

example

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

$$(x_1, y_1), \dots, (x_n, y_n)$$
$$\begin{aligned} y_1 &= \beta_0 + \beta_1 x_1 + \beta_2 x_1^2 + \epsilon_1 \\ y_2 &= \beta_0 + \beta_1 x_2 + \beta_2 x_2^2 + \epsilon_2 \\ &\vdots \\ y_n &= \beta_0 + \beta_1 x_n + \beta_2 x_n^2 + \epsilon_n \end{aligned}$$

example

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

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

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

Multiple Regression



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

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

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

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$$\vdots \quad \quad \quad \vdots$$

$$y_n = \beta_0 + \beta_1 u_n + \beta_2 v_n + \epsilon_n$$

Observation
vector

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix},$$

Design
matrix

$$X = \begin{bmatrix} 1 & u_1 & v_1 \\ 1 & u_2 & v_2 \\ \vdots & \vdots & \vdots \\ 1 & u_n & v_n \end{bmatrix},$$

Parameter
vector

$$\boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix},$$

Residual
vector

$$\boldsymbol{\epsilon} = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$