

# Chapter 6 Orthogonality and Least Squares

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## Inner Product, Length, and Orthogonality

### Theorem 1

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

1.  $\mathbf{u} \cdot \mathbf{v} = \mathbf{v} \cdot \mathbf{u}$
2.  $(\mathbf{u} + \mathbf{v}) \cdot \mathbf{w} = \mathbf{u} \cdot \mathbf{w} + \mathbf{v} \cdot \mathbf{w}$
3.  $(c\mathbf{u}) \cdot \mathbf{v} = c(\mathbf{u} \cdot \mathbf{v}) = \mathbf{u} \cdot (c\mathbf{v})$
4.  $\mathbf{u} \cdot \mathbf{u} \geq 0$ , and  $\mathbf{u} \cdot \mathbf{u} = 0$  if and only if  $\mathbf{u} = \mathbf{0}$

### The Length of a Vector

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

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

### Distance in $\mathbb{R}^n$

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  $\mathbf{u} - \mathbf{v}$ .

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

### Orthogonal Vectors

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

### Theorem 2 — The Pythagorean Theorem

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

### 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  $A^T$

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

## Key Points

1.  $\mathbf{u} \cdot \mathbf{v} = \mathbf{u}^T \times \mathbf{v}$
2. A unit vector in the direction of a vector can be determined by dividing that vector by its length.
3.  $\|c\mathbf{v}\|$  is not always equal to  $c\|\mathbf{v}\|$ . Since length is always positive, the value of  $\|c\mathbf{v}\|$  is positive for all values of  $c$ . However,  $c\|\mathbf{v}\|$  is negative if  $c$  is negative.

## Orthogonal Sets

### 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  $S$ .

### Orthogonal Basis

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

### 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 are

$$\mathbf{y} = c_1\mathbf{u}_1 + \dots + c_p\mathbf{u}_p \quad \text{given by} \quad c_j = \frac{\mathbf{y} \cdot \mathbf{u}_j}{\mathbf{u}_j \cdot \mathbf{u}_j} \quad (j = 1, \dots, p)$$

### Theorem 6

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

### 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

1.  $\|U\mathbf{x}\| = \|\mathbf{x}\|$
2.  $(U\mathbf{x}) \cdot (U\mathbf{y}) = \mathbf{x} \cdot \mathbf{y}$
3.  $(U\mathbf{x}) \cdot (U\mathbf{y}) = 0$  if and only if  $\mathbf{x} \cdot \mathbf{y} = 0$

## Key Points

1. A set of vectors is orthogonal if each pair of distinct vectors from the set is orthogonal.
2. The vector  $\hat{\mathbf{y}}$  is the orthogonal projection of  $\mathbf{y}$  onto  $\mathbf{u}$ .

$$\hat{\mathbf{y}} = \left( \frac{\mathbf{y} \cdot \mathbf{u}}{\mathbf{u} \cdot \mathbf{u}} \right) \mathbf{u}$$

3.  $\mathbf{y}$  can be written as the sum of a vector in  $\text{Span}\{\mathbf{u}\}$  and a vector orthogonal to  $\mathbf{u}$ .

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

4. An orthonormal set is an orthogonal set where all of the vectors are unit vectors.
5. If  $A$  is a matrix with orthonormal columns, then  $\|A\mathbf{x}\| = \|\mathbf{x}\|$ .
6. If  $U$  is an orthogonal matrix,  $U^T = U^{-1}$ .
7. A matrix with orthogonal columns is an orthonormal matrix if the matrix is also square.
8. If  $U$  is a  $m \times n$  matrix with orthonormal columns,  $\mathbf{x}$  is in  $\mathbb{R}^n$ ,  $\|U\mathbf{x}\| = (U\mathbf{x})^T(U\mathbf{x})$

## Orthogonal Projections

### 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

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

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

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

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

### 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

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

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

**Theorem 10**

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

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

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

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

**Key Points**

1. If  $\mathbf{u}_1$  and  $\mathbf{u}_2$  are orthogonal but  $\mathbf{u}_3$  is not orthogonal to  $\mathbf{u}_1$  or  $\mathbf{u}_2$ , a nonzero vector  $\mathbf{v}$  in  $\mathbb{R}^3$  that is orthogonal to  $\mathbf{u}_1$  and  $\mathbf{u}_2$  can be constructed through  $\mathbf{v} = \mathbf{u}_3 - \hat{\mathbf{u}}_3$ .

**The Gram-Schmidt Process****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

$$\begin{aligned} \mathbf{v}_1 &= \mathbf{x}_1 \\ \mathbf{v}_2 &= \mathbf{x}_2 - \frac{\mathbf{x}_2 \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v}_1} \mathbf{v}_1 \\ \mathbf{v}_3 &= \mathbf{x}_3 - \frac{\mathbf{x}_3 \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v}_1} \mathbf{v}_1 - \frac{\mathbf{x}_3 \cdot \mathbf{v}_2}{\mathbf{v}_2 \cdot \mathbf{v}_2} \mathbf{v}_2 \\ &\vdots \\ \mathbf{v}_p &= \mathbf{x}_p - \frac{\mathbf{x}_p \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v}_1} \mathbf{v}_1 - \frac{\mathbf{x}_p \cdot \mathbf{v}_2}{\mathbf{v}_2 \cdot \mathbf{v}_2} \mathbf{v}_2 - \dots - \frac{\mathbf{x}_p \cdot \mathbf{v}_{p-1}}{\mathbf{v}_{p-1} \cdot \mathbf{v}_{p-1}} \mathbf{v}_{p-1} \end{aligned}$$

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

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

**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.

## Least-Squares Problems

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  $\mathbb{R}^n$ .

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

### Theorem 14

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

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

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

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

### Theorem 15

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

$$\hat{\mathbf{x}} = R^{-1} Q^T \mathbf{b}$$

## Key Points

1. The least-squares error is the distance from  $\mathbf{b}$  to  $A\hat{\mathbf{x}}$ ,  $\|\mathbf{b} - A\hat{\mathbf{x}}\|$ .
2. If  $A$  is an orthogonal set, the weights that form the orthogonal projection of  $\mathbf{b}$  onto  $\text{Col } A$ ,  $\frac{\mathbf{y} \cdot \mathbf{u}_j}{\mathbf{u}_j \cdot \mathbf{u}_j}$ , form the least-squares solution of  $A\mathbf{x} = \mathbf{b}$ .

## Machine Learning and Linear Models

To find the equation  $y = \beta_0 + \beta_1 X$  of the least-squares line that best fits data points  $(x_1, y_1), \dots, (x_n, y_n)$ , find the least-squares solution of  $X\beta = \mathbf{y}$ , where the design matrix  $X$ , the parameter vector  $\beta$ , and observation vector  $\mathbf{y}$  are

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

$$\beta = (X^T X)^{-1} X^T \mathbf{y}$$

## Inner Product Spaces

An **inner product** on a vector space  $V$  is a function that, to each pair of vectors  $\mathbf{u}$  and  $\mathbf{v}$  in  $V$ , associates a real number  $\langle \mathbf{u}, \mathbf{v} \rangle$  and satisfies the following axioms, for all  $\mathbf{u}, \mathbf{v}$ , and  $\mathbf{w}$  in  $V$  and all scalars  $c$ :

1.  $\langle \mathbf{u}, \mathbf{v} \rangle = \langle \mathbf{v}, \mathbf{u} \rangle$
2.  $\langle \mathbf{u} + \mathbf{v}, \mathbf{w} \rangle = \langle \mathbf{u}, \mathbf{w} \rangle + \langle \mathbf{v}, \mathbf{w} \rangle$
3.  $\langle c\mathbf{u}, \mathbf{v} \rangle = c\langle \mathbf{u}, \mathbf{v} \rangle$
4.  $\langle \mathbf{u}, \mathbf{u} \rangle \geq 0$  and  $\langle \mathbf{u}, \mathbf{u} \rangle = 0$  if and only if  $\mathbf{u} = \mathbf{0}$

A vector space with an inner product is called an **inner product space**.

### Theorem 16 — The Cauchy-Schwarz Inequality

For all  $\mathbf{u}, \mathbf{v}$  in  $V$ ,

$$|\langle \mathbf{u}, \mathbf{v} \rangle| \leq \|\mathbf{u}\| \|\mathbf{v}\|$$

### Theorem 17 — The Triangle Inequality

For all  $\mathbf{u}, \mathbf{v}$  in  $V$ ,

$$\|\mathbf{u} + \mathbf{v}\| \leq \|\mathbf{u}\| + \|\mathbf{v}\|$$

## Key Points

1.  $\langle \mathbf{p}, \mathbf{q} \rangle = \mathbf{p}(t_1)\mathbf{q}(t_1) + \dots + \mathbf{p}(t_n)\mathbf{q}(t_n)$
2. The orthogonal projection of a polynomial in an inner product space is

$$\hat{\mathbf{q}} = \frac{\langle \mathbf{q}, \mathbf{p}_1 \rangle}{\langle \mathbf{p}_1, \mathbf{p}_1 \rangle} \mathbf{p}_1 + \dots + \frac{\langle \mathbf{q}, \mathbf{p}_n \rangle}{\langle \mathbf{p}_n, \mathbf{p}_n \rangle} \mathbf{p}_n$$