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

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 u and 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 lenght 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 $S = \{\mathbf{u}_1, \ldots, \mathbf{u}_p\}$ 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.

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

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

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 writtena s the sum of a vector in 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 $\{\mathbf{u}_1, \ldots, \mathbf{u}_p\}$ is any orthogonal basis of W, then

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

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

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

If $U = \begin{bmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \cdots & \mathbf{u}_p \end{bmatrix}$, 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

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

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

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

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 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 $\mathbf{R}^n$.

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 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 $(x_1, y_1), \ldots, (x_n, y_n)$, find the least-squares solution of $X\beta = \mathbf{y}$, where the design matrix X, the parameter vector β, 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. $\langle \mathbf{u}, \mathbf{u} \rangle \geq 0 \quad \text{and} \quad \langle \mathbf{u}, \mathbf{u} \rangle = 0$ 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-Shwarz 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. $\langle \mathbf{p}, \mathbf{q} \rangle = \mathbf{p}(t_1)\mathbf{q}(t_1) + \cdots + \mathbf{p}(t_n)\mathbf{q}(t_n)$
2. The orthogonal projection of a polynomial in an inner product space is

$$\hat{\mathbf{q}} = \frac{\langle \mathbf{q}, \mathbf{p_1} \rangle}{\langle \mathbf{p_1}, \mathbf{p_1} \rangle}\mathbf{p_1} + \cdots + \frac{\langle \mathbf{q}, \mathbf{p_n} \rangle}{\langle \mathbf{p_n}, \mathbf{p_n} \rangle}\mathbf{p_n}$$

Applications of Inner Product Spaces

Let $C\,[0, 2\pi]$ be a space with the inner product $\langle f, g\rangle = \int_0^{2\pi} f(t)g(t)dt$. The function which approximates as closely as desired for any function in $C\,[0, 2\pi]$ is

$$\frac{a_0}{2} + a_1 \cos t + \cdots a_n \cos nt + b_1 \sin t + \cdots + b_n \sin nt$$

where $\frac{a_0}{2} = \frac{1}{2\pi} \int_0^{2\pi} f(t)\, dt$, $a_k = \frac{1}{\pi} \int_0^{2\pi} f(t) \cos kt\, dt$, and $b_k = \frac{1}{\pi} \int_0^{2\pi} f(t) \sin kt\, dt$