Math 304–504

Linear Algebra

Lecture 25:
Least squares problems.

Orthogonality

Definition 1. Vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ are said to be **orthogonal** (denoted $\mathbf{x} \perp \mathbf{y}$) if $\boxed{\mathbf{x} \cdot \mathbf{y} = 0.}$

Definition 2. A vector $\mathbf{x} \in \mathbb{R}^n$ is said to be **orthogonal** to a nonempty set $Y \subset \mathbb{R}^n$ (denoted $\mathbf{x} \perp Y$) if $\mathbf{x} \cdot \mathbf{y} = 0$ for any $\mathbf{y} \in Y$.

Definition 3. Nonempty sets $X, Y \subset \mathbb{R}^n$ are said to be **orthogonal** (denoted $X \perp Y$) if $\mathbf{x} \cdot \mathbf{y} = 0$ for any $\mathbf{x} \in X$ and $\mathbf{y} \in Y$.

Orthogonal complement

Definition. Let S be a subset of $\mathbb{R}^n$. The **orthogonal complement** of S, denoted $S^\perp$, is the set of all vectors $\mathbf{x} \in \mathbb{R}^n$ that are orthogonal to S.

Theorem Let V be a subspace of $\mathbb{R}^n$. Then

(i) $V^\perp$ is also a subspace of $\mathbb{R}^n$;

(ii) $V \cap V^\perp = \{\mathbf{0}\}$;

(iii) $\dim V + \dim V^\perp = n$;

(iv) $\mathbb{R}^n = V \oplus V^\perp$, that is, any vector $\mathbf{x} \in \mathbb{R}^n$ is uniquely represented as $\mathbf{x} = \mathbf{p} + \mathbf{o}$, where $\mathbf{p} \in V$ and $\mathbf{o} \in V^\perp$.

In the above expansion, $\mathbf{p}$ is called the **orthogonal projection** of the vector $\mathbf{x}$ onto the subspace V.

Let V be a subspace of $\mathbb{R}^n$. Let $\mathbf{p}$ be the orthogonal projection of a vector $\mathbf{x} \in \mathbb{R}^n$ onto V.

Theorem $\|\mathbf{x}-\mathbf{v}\| > \|\mathbf{x}-\mathbf{p}\|$ for any $\mathbf{v} \neq \mathbf{p}$ in V.

Proof: Let $\mathbf{o} = \mathbf{x} - \mathbf{p}$, $\mathbf{o}_1 = \mathbf{x} - \mathbf{v}$, and $\mathbf{v}_1 = \mathbf{p} - \mathbf{v}$. Then $\mathbf{o}_1 = \mathbf{o} + \mathbf{v}_1$, $\mathbf{v}_1 \in V$, and $\mathbf{v}_1 \neq \mathbf{0}$. Since $\mathbf{o} \perp V$, it follows that $\mathbf{o} \cdot \mathbf{v}_1 = 0$.

$$\begin{aligned}
\|\mathbf{o}_1\|^2 &= \mathbf{o}_1 \cdot \mathbf{o}_1 = (\mathbf{o} + \mathbf{v}_1) \cdot (\mathbf{o} + \mathbf{v}_1) \\
&= \mathbf{o} \cdot \mathbf{o} + \mathbf{v}_1 \cdot \mathbf{o} + \mathbf{o} \cdot \mathbf{v}_1 + \mathbf{v}_1 \cdot \mathbf{v}_1 \\
&= \mathbf{o} \cdot \mathbf{o} + \mathbf{v}_1 \cdot \mathbf{v}_1 = \|\mathbf{o}\|^2 + \|\mathbf{v}_1\|^2 > \|\mathbf{o}\|^2.
\end{aligned}$$

Thus $\|\mathbf{x}-\mathbf{p}\| = \min_{\mathbf{v} \in V} \|\mathbf{x}-\mathbf{v}\|$ is the **distance** from the vector $\mathbf{x}$ to the subspace V.

Problem. Let Π be the plane spanned by vectors $\mathbf{v}_1 = (1,1,0)$ and $\mathbf{v}_2 = (0,1,1)$.

(i) Find the orthogonal projection of the vector $\mathbf{x} = (2,0,1)$ onto the plane Π.

(ii) Find the distance from $\mathbf{x}$ to Π.

We have $\mathbf{x} = \mathbf{p} + \mathbf{o}$, where $\mathbf{p} \in \Pi$ and $\mathbf{o} \perp \Pi$. Then the orthogonal projection of $\mathbf{x}$ onto Π is $\mathbf{p}$ and the distance from $\mathbf{x}$ to Π is $\|\mathbf{o}\|$.

We have $\mathbf{p} = \alpha\mathbf{v}_1 + \beta\mathbf{v}_2$ for some $\alpha, \beta \in \mathbb{R}$. Then $\mathbf{o} = \mathbf{x} - \mathbf{p} = \mathbf{x} - \alpha\mathbf{v}_1 - \beta\mathbf{v}_2$.

$$\begin{cases} \mathbf{o} \cdot \mathbf{v}_1 = 0 \\ \mathbf{o} \cdot \mathbf{v}_2 = 0 \end{cases} \iff \begin{cases} \alpha(\mathbf{v}_1 \cdot \mathbf{v}_1) + \beta(\mathbf{v}_2 \cdot \mathbf{v}_1) = \mathbf{x} \cdot \mathbf{v}_1 \\ \alpha(\mathbf{v}_1 \cdot \mathbf{v}_2) + \beta(\mathbf{v}_2 \cdot \mathbf{v}_2) = \mathbf{x} \cdot \mathbf{v}_2 \end{cases}$$

$$\mathbf{x} = (4, 0, -1), \;\; \mathbf{v}_1 = (1, 1, 0), \;\; \mathbf{v}_2 = (0, 1, 1)$$

$$\begin{cases} \alpha(\mathbf{v}_1 \cdot \mathbf{v}_1) + \beta(\mathbf{v}_2 \cdot \mathbf{v}_1) = \mathbf{x} \cdot \mathbf{v}_1 \\ \alpha(\mathbf{v}_1 \cdot \mathbf{v}_2) + \beta(\mathbf{v}_2 \cdot \mathbf{v}_2) = \mathbf{x} \cdot \mathbf{v}_2 \end{cases}$$

$$\Longleftrightarrow \begin{cases} 2\alpha + \beta = 4 \\ \alpha + 2\beta = -1 \end{cases} \Longleftrightarrow \begin{cases} \alpha = 3 \\ \beta = -2 \end{cases}$$

$$\mathbf{p} = 3\mathbf{v}_1 - 2\mathbf{v}_2 = (3, 1, -2)$$

$$\mathbf{o} = \mathbf{x} - \mathbf{p} = (1, -1, 1)$$

$$\|\mathbf{o}\| = \sqrt{3}$$

Overdetermined system of linear equations:

$$\begin{cases} x + 2y = 3 \\ 3x + 2y = 5 \\ x + y = 2.09 \end{cases} \iff \begin{cases} x + 2y = 3 \\ -4y = -4 \\ -y = -0.91 \end{cases}$$

No solution: inconsistent system

Assume that a solution (x_0, y_0) does exist but the system is not quite accurate, namely, there may be some errors in the right-hand sides.

Problem. Find a good approximation of (x_0, y_0).

One approach is the **least squares fit**. Namely, we look for a pair (x, y) that minimizes the sum $(x + 2y - 3)^2 + (3x + 2y - 5)^2 + (x + y - 2.09)^2$.

Least squares solution

System of linear equations:

$$\left\{\begin{array}{c} a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n = b_1 \\ a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n = b_2 \\ \cdots\cdots\cdots \\ a_{m1}x_1 + a_{m2}x_2 + \cdots + a_{mn}x_n = b_m \end{array}\right. \iff A\mathbf{x} = \mathbf{b}$$

For any $\mathbf{x} \in \mathbb{R}^n$ define a **residual** $r(\mathbf{x}) = \mathbf{b} - A\mathbf{x}$.

The **least squares solution x** to the system is the one that minimizes $\|r(\mathbf{x})\|$ (or, equivalently, $\|r(\mathbf{x})\|^2$).

$$\|r(\mathbf{x})\|^2 = \sum_{i=1}^{m} (a_{i1}x_1 + a_{i2}x_2 + \cdots + a_{in}x_n - b_i)^2$$

Let A be an $m \times n$ matrix and let $\mathbf{b} \in \mathbb{R}^m$.

Theorem A vector $\hat{\mathbf{x}}$ is a least squares solution of the system $A\mathbf{x} = \mathbf{b}$ if and only if it is a solution of the associated **normal system** $\boxed{A^T A\mathbf{x} = A^T\mathbf{b}.}$

Proof: $A\mathbf{x}$ is an arbitrary vector in $R(A)$, the column space of A. Hence the length of $r(\mathbf{x}) = \mathbf{b} - A\mathbf{x}$ is minimal if $A\mathbf{x}$ is the orthogonal projection of $\mathbf{b}$ onto $R(A)$. That is, if $r(\mathbf{x})$ is orthogonal to $R(A)$.

We know that $R(A)^{\perp} = N(A^T)$, the nullspace of the transpose matrix. Thus $\hat{\mathbf{x}}$ is a least squares solution if and only if

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

Problem. Find the least squares solution to

$$\begin{cases} x + 2y = 3 \\ 3x + 2y = 5 \\ x + y = 2.09 \end{cases}$$

$$\begin{pmatrix} 1 & 2 \\ 3 & 2 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 3 \\ 5 \\ 2.09 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 3 & 1 \\ 2 & 2 & 1 \end{pmatrix} \begin{pmatrix} 1 & 2 \\ 3 & 2 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 1 & 3 & 1 \\ 2 & 2 & 1 \end{pmatrix} \begin{pmatrix} 3 \\ 5 \\ 2.09 \end{pmatrix}$$

$$\begin{pmatrix} 11 & 9 \\ 9 & 9 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 20.09 \\ 18.09 \end{pmatrix} \iff \begin{cases} x = 1 \\ y = 1.01 \end{cases}$$

Consider a system of linear equations $A\mathbf{x} = \mathbf{b}$ and the associated normal system $A^T A\mathbf{x} = A^T\mathbf{b}$.

Theorem The normal system $A^T A\mathbf{x} = A^T\mathbf{b}$ is always consistent. Also, the following conditions are equivalent:

(i) the least squares problem has a unique solution,
(ii) the system $A\mathbf{x} = \mathbf{0}$ has only zero solution,
(iii) columns of A are linearly independent.

Proof: $\mathbf{x}$ is a solution of the least squares problem if and only if $A\mathbf{x}$ is the orthogonal projection of $\mathbf{b}$ onto $R(A)$. Clearly, such $\mathbf{x}$ exists. If $\mathbf{x}_1$ and $\mathbf{x}_2$ are two solutions then $A\mathbf{x}_1 = A\mathbf{x}_2$ $\iff A(\mathbf{x}_1 - \mathbf{x}_2) = \mathbf{0}$.

Problem. Find the constant function that is the least squares fit to the following data:

x	0	1	2	3
$f(x)$	1	0	1	2

$$f(x) = c \implies \begin{cases} c = 1 \\ c = 0 \\ c = 1 \\ c = 2 \end{cases} \implies \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} (c) = \begin{pmatrix} 1 \\ 0 \\ 1 \\ 2 \end{pmatrix}$$

$$(1, 1, 1, 1) \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} (c) = (1, 1, 1, 1) \begin{pmatrix} 1 \\ 0 \\ 1 \\ 2 \end{pmatrix}$$

$c = \frac{1}{4}(1 + 0 + 1 + 2) = 1$ (mean arithmetic value)

Problem. Find the linear polynomial that is the least squares fit to the following data:

x	0	1	2	3
$f(x)$	1	0	1	2

$$f(x) = c_1 + c_2 x \implies \begin{cases} c_1 = 1 \\ c_1 + c_2 = 0 \\ c_1 + 2c_2 = 1 \\ c_1 + 3c_2 = 2 \end{cases} \implies \begin{pmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 1 \\ 2 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 1 \\ 2 \end{pmatrix}$$

$$\begin{pmatrix} 4 & 6 \\ 6 & 14 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 4 \\ 8 \end{pmatrix} \iff \begin{cases} c_1 = 2/5 \\ c_2 = 2/5 \end{cases}$$