



12.1.1 Orthogonality and Projection

Two vectors are orthogonal if their inner product is zero:

$$\mathbf{u} \perp \mathbf{v} \iff \langle \mathbf{u}, \mathbf{v} \rangle = 0$$
 (if $\mathbf{u}, \mathbf{v} \in \mathbb{R}^n$, then $\mathbf{u}^T \mathbf{v} = 0$.)

And orthogonality among vectors has an important property:

Proposition 12.1

If **nonzero** vectors v_1, \ldots, v_k are mutually orthogonal (mutulally means $v_i \perp v_j$ for any $i \neq j$), then $\{v_1, \ldots, v_k\}$ must be ind.

Proof. We only need to show that

if
$$\alpha_1 v_1 + \cdots + \alpha_k v_k = \mathbf{0}$$
, then $\alpha_i = 0$ for any $i \in \{1, 2, \dots, k\}$.

• We do inner product to show α_1 must be zero:

$$\langle v_1, \alpha_1 v_1 + \dots + \alpha_k v_k \rangle = \langle v_1, \mathbf{0} \rangle = 0$$

$$= \alpha_1 \langle v_1, v_1 \rangle + \alpha_2 \langle v_1, v_2 \rangle + \dots + \alpha_k \langle v_1, v_k \rangle$$

$$= \alpha_1 \langle v_1, v_1 \rangle = \alpha_1 ||v_1||_2^2$$

$$= 0$$

Since $v_1 \neq \mathbf{0}$, we have $\alpha_1 = 0$.

• Similarly, we have $\alpha_i = 0$ for i = 1, ..., k.

Now we can also talk about orthogonality among spaces:

Definition 12.1 — subspace orthogonality. Two subspaces U and V of a vector space are orthogonal if every vector u in U is perpendicular to every vector v in V:

Orthogonal subspaces $u \perp v \quad \forall u \in U, v \in V$.

■ Example 12.1 Two walls look *perpendicular* but they are not orthogonal subspaces! The meeting line is in both U and V-and this line is not perpendicular to itself. Two planes (dimensions 2 and 2 in \mathbb{R}^3) cannot be orthogonal subspaces.

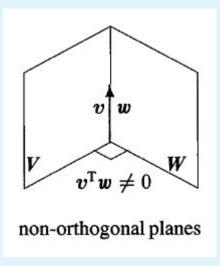


Figure 12.1: Orthogonality is impossible when $\dim U + \dim V > \dim(U \cup V)$

When a vector is in two orthogonal subspaces, it *must* be zero. It is **perpendicular** to itself.

The reason is clear: this vector $\mathbf{u} \in \mathbf{U}$ and $\mathbf{u} \in \mathbf{V}$, so $\langle \mathbf{u}, \mathbf{u} \rangle = 0$. It has to be zero vector.

If two subspaces are perpendicular, their basis must be ind.

Theorem 12.1 Assume $\{u_1, \ldots, u_k\}$ is the basis for U, $\{v_1, \ldots, v_l\}$ is the basis for V. If $U \perp V$ $(u_i \perp v_j)$ for $\forall i, j$, then $u_1, u_2, \ldots, u_k, v_1, v_2, \ldots, v_l$ must be ind.

Proof. Suppose there exists $\{\alpha_1, \dots, \alpha_k\}$ and $\{\beta_1, \dots, \beta_l\}$ such that

$$\alpha_1 u_1 + \cdots + \alpha_k u_k + \beta_1 v_1 + \cdots + \beta_l v_l = \mathbf{0}$$

then equibalently,

$$\alpha_1 u_1 + \cdots + \alpha_k u_k = -(\beta_1 v_1 + \cdots + \beta_l v_l)$$

Then we set $\mathbf{w} = \alpha_1 u_1 + \cdots + \alpha_k u_k$, obviously, $\mathbf{w} \in \mathbf{U}$ and $\mathbf{w} \in \mathbf{V}$. Hence it must be zero (This is due to remark above). Thus we have

$$\alpha_1 u_1 + \cdots + \alpha_k u_k = \mathbf{0}$$

 $\beta_1 v_1 + \cdots + \beta_l v_l = \mathbf{0}$.

Due to the independence, we have $\alpha_i = 0$ and $\beta_j = 0$ for $\forall i, j$.

Corollary 12.1 If $\{u_1, u_2, \dots, u_k, v_1, v_2, \dots, v_l\} \in \mathbf{W}$, then $\dim(\mathbf{W}) \ge \dim(\mathbf{U}) + \dim(\mathbf{V})$. Note that $\mathbf{U} \cup \mathbf{V} \subset \mathbf{W}$.

For subspaces U and $V \in \mathbb{R}^n$, if $\mathbb{R}^n = U \cup V$, and moreover, $n = \dim(U) + \dim(V)$, then we say V is the **orthogonal complement** of U.

Definition 12.2 — **orthogonal complement.** For subspaces \boldsymbol{U} and $\boldsymbol{V} \in \mathbb{R}^n$, if $\dim(\boldsymbol{U}) + \dim(\boldsymbol{V}) = n$ and $\boldsymbol{U} \perp \boldsymbol{V}$, then we say \boldsymbol{V} is the **orthogonal complement** of \boldsymbol{U} . And we denote \boldsymbol{V} as \boldsymbol{U}^{\perp} .

Moreover,
$$V = U^{\perp} \Longleftrightarrow V^{\perp} = U$$
.

■ Example 12.2 Suppose $U \cup V = \mathbb{R}^3$, $U = \text{span}\{e_1, e_2\}$. If V is the orthogonal complement of U, then $V = \text{span}\{e_3\}$.

Moreover,
$$U$$
 could also be expressed as span $\left\{ \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \right\}$.

Example:

Next let's show the nullspace is the orthogonal complement of the row space. (In \mathbb{R}^n). Suppose \mathbf{A} is a $m \times n$ matrix.

- Firstly, we show $\dim(N(\mathbf{A})) + \dim(C(\mathbf{A}^T)) = \dim(N(\mathbf{A}) \cup C(\mathbf{A}^T)) = \dim(\mathbb{R}^n) = n$: We know $\dim(N(\mathbf{A})) = n r$, where $r = \operatorname{rank}(\mathbf{A})$. And $r = C(\mathbf{A}^T)$. Hence $\dim(N(\mathbf{A})) + \dim(C(\mathbf{A}^T)) = n$.
- Then we show $N(\mathbf{A}) \perp C(\mathbf{A}^{\mathrm{T}})$:

For any $x \in N(\mathbf{A})$, if we set $\mathbf{A} = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_m \end{bmatrix}$, then we obtain:

$$\mathbf{A}\mathbf{x} = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_m \end{bmatrix} \begin{bmatrix} \mathbf{x} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

Hence every row has a zero product with x. In other words, $\langle a_i, x \rangle = 0$ for $\forall i \in \{1, 2, ..., m\}$. Hence for any $y = \sum_{i=1}^m \alpha_i a_i \in C(\mathbf{A}^T)$, we obtain:

$$\langle x, y \rangle = \langle y, x \rangle = \langle \sum_{i=1}^{m} \alpha_i a_i, x \rangle$$

= $\sum_{i=1}^{m} \alpha_i \langle a_i, x \rangle = 0.$

Hence $x \perp y$ for $\forall x \in N(\mathbf{A})$ and $y \in C(\mathbf{A}^{\mathrm{T}})$.

Hence $N(\mathbf{A})^{\perp} = C(\mathbf{A}^{\mathrm{T}})$.

If we applying this equation to \mathbf{A}^{T} , then we have $N(\mathbf{A}^{T})^{\perp} = C(\mathbf{A})$.

Theorem 12.2 — Fundamental theorem for linear alegbra, part 2. $N(\mathbf{A})$ is the orthogonal complement of the row space $C(\mathbf{A}^T)$ (in \mathbb{R}^n). $N(\mathbf{A}^T)$ is the orthogonal complement of the row space $C(\mathbf{A})$ (in \mathbb{R}^m).

Corollary 12.2 Ax = b is solvable if and only if $y^TA = 0$ implies $y^Tb = 0$.

Proof.

$$Ax = b$$
 is solvable. $\iff b \in C(A)$. $\iff b \in N(A^T)^{\perp}$
 $\iff y^Tb = 0$ for $\forall y \in N(A^T) \iff y^TA = 0$ implies $y^Tb = 0$.

The Inverse Negative Propositions is more important:

Corollary 12.3 Ax = b has no solution if and and only if $\exists y$ s.t. $y^TA = 0$ and $y^Tb \neq 0$.



Theorem 12.3 $Ax \ge b$ has no solution if and only if $\exists y \ge 0$ such that $y^TA = 0$ and $y^Tb \ge 0$.

 $\mathbf{y}^{\mathrm{T}}\mathbf{A} = 0$ requires exists one linear combination of the row space to be zero.

Necessity case. Suppose $\exists y \ge 0$ such that $y^T A = 0$ and $y^T b \ge 0$. And we assume there exists x^* such that $Ax^* \ge b$. By postmultiplying y^T we have

$$\mathbf{y}^{\mathrm{T}}\mathbf{A}\mathbf{x}^{*} > \mathbf{y}^{\mathrm{T}}\mathbf{b} > \mathbf{0} \implies \mathbf{0} > \mathbf{0}.$$

which is a contradiction!

The complete proof for this theorem is not required in this course.

■ Example 12.3 Given the system

$$x_1 + x_2 \ge 1$$

 $-x_1 \ge -1$
 $-x_2 \ge 2$ (12.1)

 $Eq(1)\times 1+Eq(2)\times 1+Eq(3)\times 1$ gives

$$0 \ge 2$$

which is a contradiction!

So the key idea of theorem (12.3) is to construct a linear combination of row space to let it become zero. Then if the right hand is larger than zero, then this system has no solution.



Corollary 12.4 If
$$\mathbf{A} = \mathbf{A}^{\mathrm{T}}$$
, then $N(\mathbf{A}^{\mathrm{T}})^{\perp} = C(A) = C(\mathbf{A}^{\mathrm{T}}) = N(\mathbf{A})$.

Corollary 12.5 The system Ax = b may not have a solution, but $A^{T}Ax = A^{T}b$ always have at least one solution for $\forall b$.

Proof. Since $\mathbf{A}^{\mathrm{T}}\mathbf{A}$ is symmetric, we have $C(\mathbf{A}^{\mathrm{T}}\mathbf{A}) = C(\mathbf{A}\mathbf{A}^{\mathrm{T}})$. You can check by yourself that $C(\mathbf{A}\mathbf{A}^{\mathrm{T}}) = C(\mathbf{A}^{\mathrm{T}})$. Hence $C(\mathbf{A}^{\mathrm{T}}\mathbf{A}) = C(\mathbf{A}^{\mathrm{T}})$.

For any vector \boldsymbol{b} we have $\boldsymbol{A}^T\boldsymbol{b} \in C(\boldsymbol{A}^T) \implies \boldsymbol{A}^T\boldsymbol{b} \in C(\boldsymbol{A}^T\boldsymbol{A})$, which means there exists a linear combination of the columns of $A^{T}A$ that equals to b. Equivalently, there exists a solution to $\mathbf{A}^{\mathrm{T}} \mathbf{A} \mathbf{x} = \mathbf{A}^{\mathrm{T}} \mathbf{b}$.

Corollary 12.6 $A^{T}A$ is invertible if and only if columns of A are ind.

Proof. We have shown that $C(\mathbf{A}^{T}\mathbf{A}) = C(\mathbf{A}^{T})$. Hence $C(\mathbf{A}^{\mathrm{T}}\mathbf{A})^{\perp} = C(\mathbf{A}^{\mathrm{T}})^{\perp} \implies N(\mathbf{A}^{\mathrm{T}}\mathbf{A}) = N(\mathbf{A}).$ **A** has ind. columns \iff $N(\mathbf{A}) = \{\mathbf{0}\} \iff N(\mathbf{A}^T\mathbf{A}) = \{\mathbf{0}\} \iff \mathbf{A}^T\mathbf{A}$ is invertible.

Least Squares Approximations *12.1.2*

Ax = b often has no solution, if so, what should we do?

We cannot always get the error e = b - Ax down to zero, so we want to use least square method to minimize the error. In other words, our goal is to

$$\min_{\mathbf{x}} \mathbf{e}^2 = \min_{\mathbf{x}} ||\mathbf{A}\mathbf{x} - \mathbf{b}||^2 = \sum_{i=1}^{m} (a_i^{\mathsf{T}}\mathbf{x} - b_i)^2$$

where
$$\mathbf{A} = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_m \end{bmatrix}$$
 and $\mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix}$.

The minimizer \bar{x} is called linear least squares solution.

Matrix Calculus

Firstly, you should know some basic calculus knowledge for matrix:

•
$$\frac{\partial (f^{\mathrm{T}}g)}{\partial x} = \frac{\partial f(x)}{\partial x}g(x) + \frac{\partial g(x)}{\partial x}f(x)$$

Example:

$$\bullet \ \frac{\partial (a^{\mathrm{T}} \mathbf{x})}{\partial \mathbf{x}} = a$$

ample.

•
$$\frac{\partial (a^{T}x)}{\partial x} = a$$

• $\frac{\partial (a^{T}Ax)}{\partial x} = \frac{\partial ((A^{T}a)^{T}x)}{\partial x} = A^{T}a$

• $\frac{\partial (Ax)}{\partial x} = A^{T}$

• $\frac{\partial (x^{T}Ax)}{\partial x} = Ax + A^{T}x$

$$\bullet \ \frac{\partial (\mathbf{A}\mathbf{x})}{\partial \mathbf{r}} = \mathbf{A}^{\mathrm{T}}$$

$$\frac{\partial (\mathbf{x}^{\mathrm{T}} \mathbf{A} \mathbf{x})}{\partial \mathbf{x}} = \mathbf{A} \mathbf{x} + \mathbf{A}^{\mathrm{T}} \mathbf{x}$$

Thus, in order to minimize $\|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2 = (\mathbf{A}\mathbf{x} - \mathbf{b})^{\mathrm{T}}(\mathbf{A}\mathbf{x} - \mathbf{b})$, we only need to let its partial **derivative** with respect to x to be **zero.** (Since its second derivative is non-negative, we will talk about it in detail in other courses.) Hence we have

$$\frac{\partial (\mathbf{A}\mathbf{x} - \mathbf{b})^{\mathrm{T}} (\mathbf{A}\mathbf{x} - \mathbf{b})}{\partial \mathbf{x}} = \frac{\partial (\mathbf{A}\mathbf{x} - \mathbf{b})}{\partial \mathbf{x}} (\mathbf{A}\mathbf{x} - \mathbf{b}) + \frac{\partial (\mathbf{A}\mathbf{x} - \mathbf{b})}{\partial \mathbf{x}} (\mathbf{A}\mathbf{x} - \mathbf{b}) = 2\frac{\partial (\mathbf{A}\mathbf{x} - \mathbf{b})}{\partial \mathbf{x}} (\mathbf{A}\mathbf{x} - \mathbf{b})$$

$$= 2(\frac{\partial (\mathbf{A}\mathbf{x})}{\partial \mathbf{x}} - \frac{\partial (\mathbf{b})}{\partial \mathbf{x}})(\mathbf{A}\mathbf{x} - \mathbf{b})$$

$$= 2\mathbf{A}^{\mathrm{T}} (\mathbf{A}\mathbf{x} - \mathbf{b}) = \mathbf{0}.$$

Or equivalently,

$$\mathbf{A}^{\mathrm{T}}\mathbf{A}\mathbf{r} = \mathbf{A}^{\mathrm{T}}\mathbf{b}$$

According to corollary (12.5), this equation always exists a solution. And this equation is called normal equation.

Theorem 12.4 The partial derivatives of $\|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2$ are zero when $\mathbf{A}^T \mathbf{A}\mathbf{x} = \mathbf{A}^T \mathbf{b}$.

Fit a stright line

Given a collection of data (x_i, y_i) for i = 1, ..., m, we can fit the model parameters:

$$\begin{cases} y_1 = a_0 + a_1 x_{1,1} + a_2 x_{1,2} + \dots + a_n x_{1,n} + \varepsilon_1 \\ y_2 = a_0 + a_1 x_{2,1} + a_2 x_{2,2} + \dots + a_n x_{2,n} + \varepsilon_2 \\ \vdots \\ y_m = a_0 + a_1 x_{m,1} + a_2 x_{m,2} + \dots + a_n x_{m,n} + \varepsilon_m \end{cases}$$

Our fit line is

$$\hat{y} = a_0 + a_1 x_1 + a_2 x_2 + \dots + a_n x_n$$

In compact matrix form, we have

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 & x_{1,1} & x_{1,2} & \dots & x_{1,n} \\ 1 & x_{2,1} & x_{2,2} & \dots & x_{2,n} \\ \vdots & \vdots & & & \\ 1 & x_{m,1} & x_{m,2} & \dots & x_{m,n} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_m \end{bmatrix}$$

Or equivalently, we have

$$\mathbf{v} = \mathbf{A}\mathbf{x} + \boldsymbol{\varepsilon}$$

where
$$\mathbf{A} = \begin{bmatrix} 1 & x_{1,1} & x_{1,2} & \dots & x_{1,n} \\ 1 & x_{2,1} & x_{2,2} & \dots & x_{2,n} \\ \vdots & \vdots & & & & \\ 1 & x_{m,1} & x_{m,2} & \dots & x_{m,n} \end{bmatrix}_{m \times (n+1)}, \mathbf{x} = \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix}, \mathbf{\varepsilon} = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_m \end{bmatrix}_{m \times 1}.$$

Our goal is to minimize $\|\hat{\mathbf{y}} - \mathbf{y}\|^2 = \|\mathbf{A}\mathbf{x} - \mathbf{y}\|^2$. Then by theorem (12.4), we only need to sovle $\mathbf{A}^T \mathbf{A}\mathbf{x} = \mathbf{A}^T \mathbf{y}$.

12.1.3 Projections

In corollary (12.6), we know that if \mathbf{A} has ind. columns, then $\mathbf{A}^T \mathbf{A}$ is invertible. On this condition, the normal equation $\mathbf{A}^T \mathbf{A} \mathbf{x} = \mathbf{A}^T \mathbf{b}$ has unique solution $\mathbf{x}^* = (\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T \mathbf{b}$. Thus the error $\mathbf{b} - \mathbf{A} \mathbf{x}^*$ is minimum. And $\mathbf{A} \mathbf{x}^* = \mathbf{A} (\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T \mathbf{b}$ approximately equals to \mathbf{b} .

- If **b** and Ax^* are exactly in the same space, then $Ax^* = b$.
- Otherwise, just as the Figure (12.2) shown, Ax^* is the projection of b to subspace C(A).

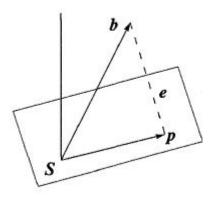


Figure 12.2: The projection of \boldsymbol{b} onto a subspace $C(\boldsymbol{A})$.

Definition 12.3 — **Projection**. The projection of \boldsymbol{b} onto the subspace $C(\boldsymbol{A})$ is denoted as $\text{Proj}_{C(\boldsymbol{A})}(\boldsymbol{b})$.

Definition 12.4 — Projection matrix. Given $Ax^* = A(A^TA)^{-1}A^Tb = \operatorname{Proj}_{C(A)}(b)$. Since $[A(A^TA)^{-1}A^T]b$ is the projection of b, we call $P = A(A^TA)^{-1}A^T$ as projection matrix.

Definition 12.5 — **Idempotent.** Let A be a **square** matrix that satisfies A = AA, then A is called a **idempotent** matrix.

Let's show the projection matrix is *idempotent*:

$$P^{2} = A(A^{T}A)^{-1}A^{T}A(A^{T}A)^{-1}A^{T}$$

$$= A(A^{T}A)^{-1}(A^{T}A)(A^{T}A)^{-1}A^{T}$$

$$= A(A^{T}A)^{-1}A^{T} = P.$$

Observations

• If $b \in C(A)$, then $\exists x$ s.t. Ax = b. Moreover, the projection of b is exactly b:

$$Pb = A(A^{T}A)^{-1}A^{T}(b)$$

$$= A(A^{T}A)^{-1}A^{T}(Ax)$$

$$= A(A^{T}A)^{-1}(A^{T}A)x$$

$$= Ax = b.$$

• Assume **A** has only one column, say, **a**. Then we have

$$\mathbf{x}^* = (\mathbf{A}^{\mathrm{T}}\mathbf{A})^{-1}\mathbf{A}^{\mathrm{T}}\mathbf{b} = \frac{\mathbf{a}^{\mathrm{T}}\mathbf{b}}{\mathbf{a}^{\mathrm{T}}\mathbf{a}}$$
$$\mathbf{A}\mathbf{x}^* = \mathbf{P}\mathbf{b} = \mathbf{A}(\mathbf{A}^{\mathrm{T}}\mathbf{A})^{-1}\mathbf{A}^{\mathrm{T}}(\mathbf{b}) = \frac{\mathbf{a}^{\mathrm{T}}\mathbf{b}}{\mathbf{a}^{\mathrm{T}}\mathbf{a}} \times \mathbf{a} = \frac{\mathbf{a}^{\mathrm{T}}\mathbf{b}}{\|\mathbf{a}\|^2} \times \mathbf{a}$$

More interestingly,

$$\frac{\boldsymbol{a}^{\mathrm{T}}\boldsymbol{b}}{\|\boldsymbol{a}\|^{2}} \times \boldsymbol{a} = \frac{\|\boldsymbol{a}\|\|\boldsymbol{b}\|\cos\theta}{\|\boldsymbol{a}\|^{2}} \times \boldsymbol{a} = \|\boldsymbol{b}\|\cos\theta \times \frac{\boldsymbol{a}}{\|\boldsymbol{a}\|}$$

which is the projection of \boldsymbol{b} onto a line \boldsymbol{a} . (Shown in figure below.)

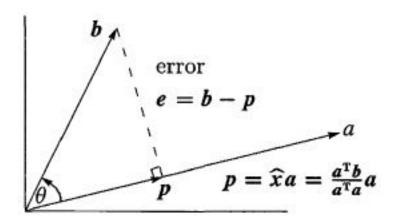


Figure 12.3: The projection of **b** onto a line **a**.

More generally, we can write the projection of \boldsymbol{b} as:

$$\operatorname{Proj}_{\boldsymbol{a}}(\boldsymbol{b}) = \frac{\langle \boldsymbol{a}, \boldsymbol{b} \rangle}{\langle \boldsymbol{a}, \boldsymbol{a} \rangle} \boldsymbol{a}$$

Look at the figure above! The error is $\boldsymbol{b} - \operatorname{Proj}_{\boldsymbol{a}}(\boldsymbol{b})$, which is obviously perpendicular to \boldsymbol{a} . And $\boldsymbol{b} - \operatorname{Proj}_{\boldsymbol{a}}(\boldsymbol{b}) \in \operatorname{span}\{\boldsymbol{a}, \boldsymbol{b}\}$.

If we define $b' = b - \operatorname{Proj}_{a}(b)$, then it's easy to check $\operatorname{span}\{a,b'\} = \operatorname{span}\{a,b\}$ and $a \perp b'$. Hence we convert a basis to another basis such that the elements are orthogonal to each other. We will discuss it in detail in next lecture.