

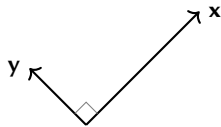
Applied Linear Algebra in Data Analysis

Orthogonality

Sivakumar Balasubramanian

Department of Bioengineering
Christian Medical College, Bagayam
Vellore 632002

- ▶ Two vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ are orthogonal if $\mathbf{x}^\top \mathbf{y} = 0$.



- ▶ The set of non-zero vectors, $V = \{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3, \dots, \mathbf{v}_r\}$ is a set of mutually orthogonal vectors, if and only if,

$$\mathbf{v}_i^\top \mathbf{v}_j = 0, \quad 1 \leq i, j \leq r \text{ and } i \neq j$$

- ▶ V is also a linearly independent set of vectors. Why?

- ▶ If $\|\mathbf{v}_i\| = 1$, then V is an **orthonormal** set of vectors.
- ▶ A set of orthonormal vectors V also form an **orthonormal basis** of the subspace $\text{span}(V)$.

Orthogonal Subspaces

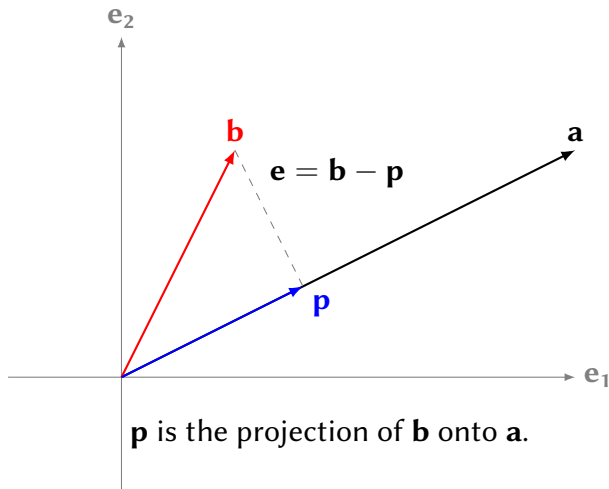
- ▶ Two subspaces $\mathcal{V}, \mathcal{W} \subset \mathbb{R}^n$ are orthogonal if every vector in one subspace is orthogonal to every vector in the other subspace.

$$\mathbf{v}^\top \mathbf{w} = 0, \quad \forall \mathbf{v} \in \mathcal{V} \text{ and } \forall \mathbf{w} \in \mathcal{W} \implies \mathcal{V} \perp \mathcal{W}$$

- ▶ If $\mathcal{V} + \mathcal{W} = \mathbb{R}^n$, and $\mathcal{V} \perp \mathcal{W}$, then \mathcal{V} and \mathcal{W} are **orthogonal complements** of each other.

$$\mathcal{V}^\perp = \mathcal{W} \text{ or } \mathcal{W}^\perp = \mathcal{V}; \quad (\mathcal{V}^\perp)^\perp = \mathcal{V}$$

Orthogonal Projection onto Subspaces



Orthogonal Projection onto Subspaces

$\|\mathbf{e}\|$ is the distance of the point \mathbf{b} from the line along \mathbf{a} . This distance is shortest when, $\mathbf{e} \perp \mathbf{a}$.

$$\mathbf{a}^\top (\mathbf{b} - \mathbf{p}) = \mathbf{a}^\top (\mathbf{b} - \alpha \mathbf{a}) = \mathbf{a}^\top \mathbf{b} - \alpha \mathbf{a}^\top \mathbf{a} = 0$$

$$\alpha = \frac{\mathbf{a}^\top \mathbf{b}}{\mathbf{a}^\top \mathbf{a}} \implies \mathbf{p} = \frac{\mathbf{a}^\top \mathbf{b}}{\mathbf{a}^\top \mathbf{a}} \mathbf{a}$$

$$\mathbf{p} = \frac{\mathbf{a}^\top \mathbf{b}}{\mathbf{a}^\top \mathbf{a}} \mathbf{a} = \mathbf{a} \frac{\mathbf{a}^\top \mathbf{b}}{\mathbf{a}^\top \mathbf{a}} = \frac{\mathbf{a} \mathbf{a}^\top}{\mathbf{a}^\top \mathbf{a}} \mathbf{b} = \mathbf{P} \mathbf{b}$$

Orthogonal Projection onto Subspaces

- ▶ We can project vectors onto high dimensional subspaces.
- ▶ Consider the subspace $\mathcal{S} \subseteq \mathbb{R}^n$ spanned by the orthonormal basis $\{\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_r\}$.
- ▶ We want to project a vector $\mathbf{b} \in \mathbb{R}^n$ onto \mathcal{S}
 $\mathbf{b}_{\mathcal{S}}$ – the orthogonal projection of \mathbf{b} onto \mathcal{S} is given by the following,

$$\mathbf{b}_{\mathcal{S}} = \mathbf{U}\mathbf{U}^{\top}\mathbf{b}; \quad \mathbf{U} = [\mathbf{u}_1 \quad \mathbf{u}_2 \quad \dots \quad \mathbf{u}_r]$$

$$\text{Projection matrix } \mathbf{P}_{\mathcal{S}} = \mathbf{U}\mathbf{U}^{\top}$$

- ▶ A projection matrix is **idempotent**, i.e. $\mathbf{P}^2 = \mathbf{P}$. What does this mean in terms of projecting a vector on to a subspace?

Orthogonal Projection onto Subspaces

- ▶ Consider two matrices $\mathbf{U}_1, \mathbf{U}_2$ whose columns form an orthonormal basis of the subspace $\mathcal{S} \subseteq \mathbb{R}^m$, $\mathcal{C}(\mathbf{U}_1) = \mathcal{C}(\mathbf{U}_2)$.
- ▶ The projection matrix onto the subspace \mathcal{S} , $\mathbf{U}_1 \mathbf{U}_1^\top = \mathbf{U}_2 \mathbf{U}_2^\top$. We get the same projection matrix irrespective of which orthonormal basis one uses.

Orthogonal Projection onto Subspaces

- ▶ Two subspaces $\mathcal{X}, \mathcal{Y} \subset \mathbb{R}^n$ are said to be **complementary subspaces** of \mathbb{R}^n , when

$$\mathcal{X} + \mathcal{Y} = \mathbb{R}^n \quad \text{and} \quad \mathcal{X} \cap \mathcal{Y} = \{\mathbf{0}\}$$

- ▶ For complementary subspaces $\mathcal{X}, \mathcal{Y} \subset \mathbb{R}^n$, then any vector $\mathbf{v} \in \mathbb{R}^n$ can be uniquely represented as,

$$\mathbf{v} = \mathbf{v}_{\mathcal{X}} + \mathbf{v}_{\mathcal{Y}}, \quad \mathbf{v}_{\mathcal{X}} \in \mathcal{X}, \quad \mathbf{v}_{\mathcal{Y}} \in \mathcal{Y}$$

$\mathbf{v}_{\mathcal{X}}, \mathbf{v}_{\mathcal{Y}}$ are the components of \mathbf{v} in \mathcal{X} and \mathcal{Y} , respectively.

- ▶ When $\mathcal{X} \perp \mathcal{Y}$, then $\mathbf{v}_{\mathcal{X}}^{\top} \mathbf{v}_{\mathcal{Y}} = 0$; $\mathbf{v}_{\mathcal{X}}, \mathbf{v}_{\mathcal{Y}}$ are orthogonal components.

Relationship between the Four Fundamental Subspaces of A

- $\mathcal{C}(\mathbf{A}), \mathcal{N}(\mathbf{A}^\top) \subseteq \mathbb{R}^n$ are orthogonal complements.

$$\mathcal{C}(\mathbf{A}) \perp \mathcal{N}(\mathbf{A}^\top) \implies \mathcal{C}(\mathbf{A}) + \mathcal{N}(\mathbf{A}^\top) = \mathbb{R}^n$$

- $\mathcal{C}(\mathbf{A}^\top), \mathcal{N}(\mathbf{A}) \subseteq \mathbb{R}^m$ are orthogonal complements.

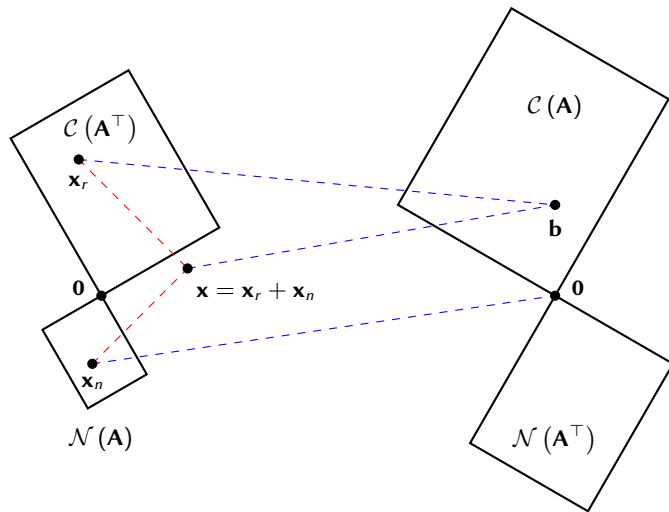
$$\mathcal{C}(\mathbf{A}^\top) \perp \mathcal{N}(\mathbf{A}) \implies \mathcal{C}(\mathbf{A}^\top) + \mathcal{N}(\mathbf{A}) = \mathbb{R}^m$$

Orthogonal Projection onto Subspaces

- An orthogonal projection matrix \mathbf{P}_S onto a subspace S represents a linear mapping, $\mathbf{P}_S : \mathbb{R}^n \rightarrow \mathbb{R}^n$. What are the four fundamental subspaces of \mathbf{P}_S ?

$$\begin{aligned}\mathcal{C}(\mathbf{P}_S) &= S; \quad \mathcal{N}(\mathbf{P}_S) = S^\perp \\ \mathcal{N}(\mathbf{P}_S^\top) &= S^\perp; \quad \mathcal{C}(\mathbf{P}_S^\top) = S\end{aligned}$$

Relationship between the Four Fundamental Spaces



Relationship between the Four Fundamental Spaces

- ▶ \mathbf{x}_r and \mathbf{x}_n are the components of $\mathbf{x} \in \mathbb{R}^m$ in the row space and nullspace of \mathbf{A} .

- ▶ **Nullspace** $\mathcal{N}(\mathbf{A})$ is mapped to $\mathbf{0}$.

$$\mathbf{A}\mathbf{x}_n = \mathbf{0}$$

- ▶ **Row space** $\mathcal{C}(\mathbf{A}^\top)$ is mapped to the **column space** $\mathcal{C}(\mathbf{A})$.

$$\mathbf{A}\mathbf{x}_r = \mathbf{A}(\mathbf{x}_r + \mathbf{x}_n) = \mathbf{A}\mathbf{x} = \mathbf{b}$$

- ▶ The mapping from the **row space** to the **column space** is invertible, i.e. every \mathbf{x}_r is mapped to a unique element in $\mathcal{C}(\mathbf{A})$
- ▶ What sort of mapping does \mathbf{A}^\top do?

Gram-Schmidt Orthogonalization

- ▶ Given a linearly independent set of vectors $\mathcal{B} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\}$, where $\mathbf{x}_i \in \mathbb{R}^m$, $\forall i \in \{1, 2, \dots, n\}$, how can we find an orthonormal basis $\{\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_n\}$ for $\text{span}(\mathcal{B})$? \longrightarrow **Gram-Schmidt Algorithm**
- ▶ Its an iterative procedure that can also detect if a given set \mathcal{B} is linearly dependent.

Data: $\{\mathbf{x}_i\}_{i=1}^n$

Result: Return an orthonormal basis $\{\mathbf{u}_i\}_{i=1}^n$ if the set \mathcal{B} is linearly independent, else return nothing.

for $i = 1, 2, \dots, n$ **do**

1. $\tilde{\mathbf{q}}_i = \mathbf{x}_i - \sum_{j=1}^{i-1} (\mathbf{u}_j^\top \mathbf{x}_i) \mathbf{u}_j \longrightarrow$ (Orthogonalization step);

2. **If** $\tilde{\mathbf{q}}_i = \mathbf{0}$ **then return;**

3. $\mathbf{u}_i = \tilde{\mathbf{q}}_i / \|\tilde{\mathbf{q}}_i\| \longrightarrow$ (Normalization step);

end

return $\{\mathbf{u}_i\}_{i=1}^n$;

Gram-Schmidt Orthogonalization

- The algorithm can also be conveniently represented in a matrix form.

$$\mathcal{B} = \{\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n\}$$

Let $\mathbf{U}_1 = 0_{m \times 1}$ and $\mathbf{U}_i = [\mathbf{u}_1 \quad \mathbf{u}_2 \quad \dots \quad \mathbf{u}_{i-1}] \in \mathbb{R}^{m \times (i-1)}$

$$\mathbf{U}_i^\top \mathbf{x}_i = \begin{bmatrix} \mathbf{u}_1^\top \mathbf{x}_i \\ \mathbf{u}_2^\top \mathbf{x}_i \\ \vdots \\ \mathbf{u}_{i-1}^\top \mathbf{x}_i \end{bmatrix} \quad \text{and} \quad \mathbf{U}_i \mathbf{U}_i^\top \mathbf{x}_i = \sum_{j=1}^{i-1} (\mathbf{u}_j^\top \mathbf{x}_i) \mathbf{u}_j$$

$$\mathbf{u}_i = \frac{(\mathbf{I} - \mathbf{U}_i \mathbf{U}_i^\top) \mathbf{x}_i}{\|(\mathbf{I} - \mathbf{U}_i \mathbf{U}_i^\top) \mathbf{x}_i\|}$$

- ▶ Gram-Schmidt procedure leads us to another form of matrix decomposition – **QR decomposition**.

- ▶ Given a matrix $\mathbf{A} = [\mathbf{a}_1 \ \mathbf{a}_2 \ \cdots \ \mathbf{a}_n] \in \mathbb{R}^{n \times n}$, whose columns form a linearly independent set.

Gram-Schmidt algorithm produces an orthonormal basis $\{\mathbf{q}_1, \mathbf{q}_2, \cdots \mathbf{q}_n\}$ for $\mathcal{C}(\mathbf{A})$.

$$\mathbf{q}_1 = \frac{\mathbf{a}_1}{r_1} \quad \text{and} \quad \mathbf{q}_i = \frac{\mathbf{a}_i - \sum_{j=1}^{i-1} (\mathbf{q}_j^\top \mathbf{a}_i) \mathbf{q}_j}{r_i}$$

where, $r_1 = \|\mathbf{a}_1\|$ and $r_i = \left\| \mathbf{a}_i - \sum_{j=1}^{i-1} (\mathbf{q}_j^\top \mathbf{a}_i) \mathbf{q}_j \right\|$.

QR Decomposition

$$\mathbf{a}_1 = r_1 \mathbf{q}_1 \quad \text{and} \quad \mathbf{a}_i = r_i \mathbf{q}_i + \sum_{j=1}^{i-1} \left(\mathbf{q}_j^\top \mathbf{a}_i \right) \mathbf{q}_j$$

$$\begin{aligned} \mathbf{A} &= [\mathbf{a}_1 \quad \mathbf{a}_2 \cdots \mathbf{a}_n] \\ &= [\mathbf{q}_1 \quad \mathbf{q}_2 \cdots \mathbf{q}_n] \begin{bmatrix} r_1 & \mathbf{q}_1^\top \mathbf{a}_2 & \mathbf{q}_1^\top \mathbf{a}_3 & \cdots & \mathbf{q}_1^\top \mathbf{a}_n \\ 0 & r_2 & \mathbf{q}_2^\top \mathbf{a}_3 & \cdots & \mathbf{q}_2^\top \mathbf{a}_n \\ 0 & 0 & r_2 & \cdots & \mathbf{q}_3^\top \mathbf{a}_n \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & r_n \end{bmatrix} \\ &= \mathbf{QR} \end{aligned}$$

$$\mathbf{A} = \mathbf{QR}; \quad \mathbf{A}, \mathbf{Q} \in \mathbb{R}^{m \times n}, \quad \mathbf{R} \in \mathbb{R}^{n \times n}$$

- The columns of \mathbf{Q} form an orthonormal basis for $\mathcal{C}(\mathbf{A})$, and \mathbf{R} is upper-triangular.
- $\mathbf{A} = \mathbf{QR}$ can be used for used to solve $\mathbf{Ax} = \mathbf{b}$.

$$\mathbf{Ax} = \mathbf{QRx} = \mathbf{b} \implies \mathbf{Rx} = \mathbf{Q}^{-1}\mathbf{b} = \mathbf{Q}^{\top}\mathbf{b}$$