

## Orthogonal matrices & Gram-Schmidt

Two goals in this SES:

Goal 1: See how orthogonal matrices make calculations of  $\hat{x}$ ,  $\underline{p}$ ,  $\underline{P}$  easier

Goal 2: See how to obtain orthogonal matrices (Gram-Schmidt process)

### Orthonormal vectors

**DEF** The vectors  $\underline{z}_1, \underline{z}_2, \dots, \underline{z}_n$  are orthonormal if

$$\underline{z}_i^T \underline{z}_j = \begin{cases} 0 & \text{if } i \neq j & \text{(orthogonal)} \\ 1 & \text{if } i = j & \text{(unit vectors } \|\underline{z}_i\| = 1) \end{cases}$$

Note: orthonormal vectors are always indep.

### Orthonormal matrices

$Q$  is an orthonormal matrix if its cols are orthonormal vectors  
( $Q$  can be rectangular)

**Fact** For orthonormal matrix  $Q$

$$Q^T Q = I$$

Reason:

$$Q^T Q = \begin{bmatrix} -\underline{\underline{\delta_1^T}} & & \\ & \ddots & \\ & & -\underline{\underline{\delta_n^T}} \end{bmatrix} \begin{bmatrix} 1 & & & & \\ & \delta_1 & & & \\ & & \dots & & \\ & & & \delta_n & \\ & & & & 1 \end{bmatrix}$$
$$= \begin{bmatrix} 1 & & & \\ & \ddots & & \\ & & \dots & \\ & & & 1 \end{bmatrix}$$

Note: If  $Q$  is square, we call it  
*orthogonal matrix*

In this case,

$$Q^T Q = I \Rightarrow Q^{-1} = Q^T \text{ (transpose = inverse)}$$

To repeat:  $Q^T Q = I$  even when  $Q$  is  
rectangular ( $Q^T$  is only a left inverse)

For square  $Q$ ,  $Q$  has full rank

$\Rightarrow Q^{-1}$  exist

$\Rightarrow Q^T$  is two-sided inverse  $\Rightarrow Q^{-1} = Q^T$

$\Rightarrow Q^T$  is also the right inverse

$\Rightarrow$  we also have  $Q Q^T = I$

( $Q$  also has orthonormal rows)

Important classes of matrix introduced

so far: triangular, diagonal, permutation  
symmetric, reduced row echelon,  
projection, and orthogonal matrices

Ex: Rotation matrix

$$Q = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}$$

orthogonal + unit vector  
( $\cos^2 \theta + \sin^2 \theta = 1$ )

$$Q^T = \begin{bmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{bmatrix} = \begin{bmatrix} \cos(-\theta) & -\sin(-\theta) \\ \sin(-\theta) & \cos(-\theta) \end{bmatrix}$$

$= Q^{-1}$  (rotate  $\theta$ ) (rotate  $-\theta$  back)

Ex: Permutation matrix (always orthogonal matrix)

$$Q = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}, \quad Q^T = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$$

(both  $Q$  &  $Q^T$  are orthogonal matrices  
&  $QQ^T = I$ ,  $Q^TQ = I$ )

Ex:  $\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$  NOT orthogonal matrix

orthogonal but NOT unit vector

normalize & get  $\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} = Q_1$

Ex: Hadamard matrices

$$Q = \frac{1}{2} \begin{bmatrix} \boxed{\begin{matrix} 1 & 1 \\ 1 & -1 \end{matrix}} & \boxed{\begin{matrix} 1 & 1 \\ -1 & -1 \end{matrix}} \\ \boxed{\begin{matrix} 1 & 1 \\ -1 & -1 \end{matrix}} & \boxed{\begin{matrix} 1 & -1 \\ -1 & 1 \end{matrix}} \end{bmatrix} = \frac{1}{2} \begin{bmatrix} Q_1 & Q_1 \\ Q_1 & -Q_1 \end{bmatrix}$$

$$\text{Ex: } \begin{bmatrix} 1 & -2 \\ 2 & -1 \\ 2 & 2 \end{bmatrix} \text{ (rectangular)}$$

orthogonal but NOT unit vector

normalize & get

$$Q = \frac{1}{3} \begin{bmatrix} 1 & -2 \\ 2 & -1 \\ 2 & 2 \end{bmatrix} \text{ (not square)}$$

we can add a 3<sup>rd</sup> col.

$$Q = \frac{1}{3} \begin{bmatrix} 1 & -2 & 2 \\ 2 & -1 & -2 \\ 2 & 2 & 1 \end{bmatrix} \text{ (orthogonal matrix)}$$

**Fact** If  $Q$  has orthonormal cols ( $Q^T Q = I$ )  
it leaves length unchanged, i.e.,

$$\|Q \underline{x}\| = \|\underline{x}\| \quad \forall \underline{x} \quad \text{--- ①}$$

$Q$  also preserves dot products, i.e.,

$$(Q \underline{x})^T (Q \underline{y}) = \underline{x}^T \underline{y} \quad \text{--- ②}$$

Reason:

$$\text{For ①, } \|Q \underline{x}\|^2 = (Q \underline{x})^T (Q \underline{x}) = \underline{x}^T Q^T Q \underline{x} \\ = \underline{x}^T \underline{x} = \|\underline{x}\|^2$$

$$\text{For ②, } (Q \underline{x})^T (Q \underline{y}) = \underline{x}^T Q^T Q \underline{y} = \underline{x}^T \underline{y}$$

# Projection using orthonormal bases : Q replaces A

$$A^T A \hat{\underline{x}} = A^T \underline{b} \quad , \quad \underline{P} = A \hat{\underline{x}} \quad , \quad P = A(A^T A)^{-1} A^T$$

$\Downarrow$

$$Q^T Q \hat{\underline{x}} = Q^T \underline{b} \quad , \quad \underline{P} = Q \hat{\underline{x}} \quad , \quad P = Q(Q^T Q)^{-1} Q^T$$

$\Downarrow$

$$\hat{\underline{x}} = Q^T \underline{b} \quad , \quad \underline{P} = Q \hat{\underline{x}} \quad , \quad P = Q Q^T$$

$$(\hat{x}_i = \underline{\delta}_i^T \underline{b})$$

(projection is just

a dot product)

$$\underline{P} = \begin{bmatrix} | & & | \\ \underline{\delta}_1 & \dots & \underline{\delta}_n \\ | & & | \end{bmatrix} \begin{bmatrix} \underline{\delta}_1^T \underline{b} \\ \vdots \\ \underline{\delta}_n^T \underline{b} \end{bmatrix}$$

$$= \underline{\delta}_1 (\underline{\delta}_1^T \underline{b}) + \dots + \underline{\delta}_n (\underline{\delta}_n^T \underline{b})$$

Note : When Q is square, cols of Q span the entire space

$$\hat{\underline{x}} = Q^T \underline{b} \quad , \quad \underline{P} = Q \hat{\underline{x}} \quad , \quad P = Q Q^T$$

(least square sol.)  $\Downarrow$

$$\underline{x} = Q^{-1} \underline{b} \quad , \quad \underline{P} = Q Q^{-1} \underline{b} \quad , \quad P = I$$

(exact sol.)  $= \underline{b}$

or

$$\underline{P} = \underline{b} = \underline{\delta}_1 (\underline{\delta}_1^T \underline{b}) + \dots + \underline{\delta}_n (\underline{\delta}_n^T \underline{b})$$

(projection onto orthonormal basis & assemble it back)

(Foundation for Fourier series !)

# Gram-Schmidt process

Elimination  $\Rightarrow$  make matrix triangular

Gram-Schmidt  $\Rightarrow$  make matrix orthonormal

Step 1: construct orthogonal vectors

Step 2: normalize to get orthonormal vectors

Start with two indep. vectors  $\underline{a}$ ,  $\underline{b}$

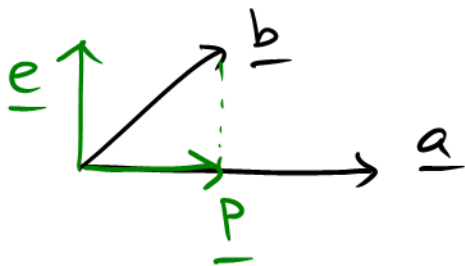


Find orthogonal vectors

$\underline{A}$ ,  $\underline{B}$  that span the same space

Q: How do we do that?

Set  $\underline{A} = \underline{a}$



$\underline{e} \perp \underline{P} \Rightarrow \underline{e} \perp \underline{a}$

Set  $\underline{B} = \underline{e}$

$$\Rightarrow \underline{B} = \underline{b} - \underline{P} = \underline{b} - \frac{\underline{A}^T \underline{b}}{\underline{A}^T \underline{A}} \underline{A}$$

$$(\text{chk: } \underline{A}^T \underline{B} = \underline{A}^T \underline{b} - \frac{\underline{A}^T \underline{A}}{\underline{A}^T \underline{A}} \underline{A}^T \underline{b} = 0)$$

(indeed orthogonal)

Q: What if we had 3<sup>rd</sup> indep. vector  $\underline{c}$ ?

Subtract components in the direction of  $\underline{A}$  &  $\underline{B}$  from  $\underline{c}$

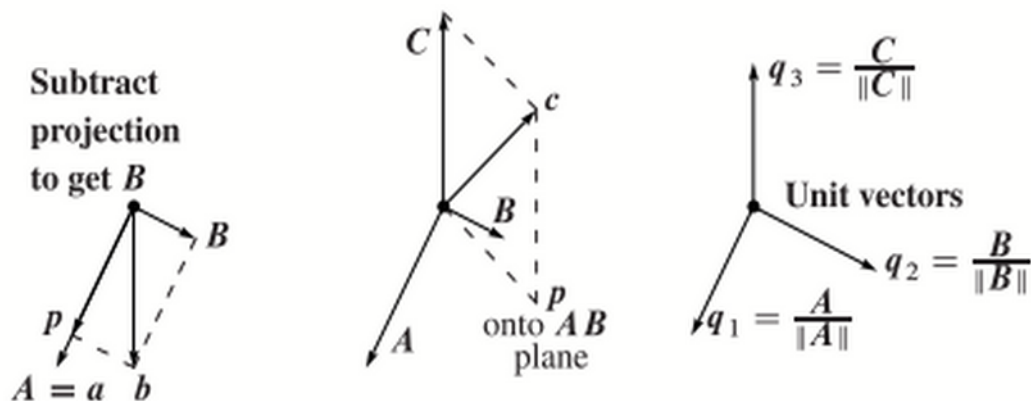


Figure 33: First project  $b$  onto the line through  $a$  and find the orthogonal  $B$  as  $b - p$ . Then project  $c$  onto the  $AB$  plane and find  $C$  as  $c - p$ . Divide by  $\|A\|$ ,  $\|B\|$ ,  $\|C\|$ .

$$\underline{C} = \underline{c} - \frac{\underline{A}^T \underline{c}}{\underline{A}^T \underline{A}} \underline{A} - \frac{\underline{B}^T \underline{c}}{\underline{B}^T \underline{B}} \underline{B} \quad \left( \begin{array}{l} \underline{C} \perp \underline{A} \\ \underline{C} \perp \underline{B} \end{array} \right)$$

$$\text{Step 2: } \underline{z}_1 = \frac{\underline{A}}{\|\underline{A}\|}, \quad \underline{z}_2 = \frac{\underline{B}}{\|\underline{B}\|}, \quad \underline{z}_3 = \frac{\underline{C}}{\|\underline{C}\|}$$

(we can keep doing this to construct more orthonormal vectors)

(read Ex 5 in textbook p. 235)

## QR decomposition

Recall: When we studied Elimination, use Elimination matrices to represent the process  $\Rightarrow$  leads to  $A = LU$

$$(EA = U \Rightarrow A = E^{-1}U = LU)$$

A similar eqn  $A = QR$  relates

$A$  to  $Q$  of the Gram-Schmidt process

$$(Q^T A = Q^T Q R = R \Rightarrow R = Q^T A)$$

$$\Rightarrow \begin{array}{ccc} A & Q & R \\ \left[ \begin{array}{ccc} \underline{a}_1 & \underline{a}_2 & \underline{a}_3 \\ | & | & | \\ | & | & | \end{array} \right] & = & \left[ \begin{array}{ccc} \underline{q}_1 & \underline{q}_2 & \underline{q}_3 \\ | & | & | \\ | & | & | \end{array} \right] \left[ \begin{array}{ccc} \underline{q}_1^T \underline{a}_1 & \underline{q}_1^T \underline{a}_2 & \underline{q}_1^T \underline{a}_3 \\ & \underline{q}_2^T \underline{a}_2 & \underline{q}_2^T \underline{a}_3 \\ & & \underline{q}_3^T \underline{a}_3 \end{array} \right] \end{array}$$

( $R$  is upper triangular since later  $\underline{q}$ 's are chosen to be orthogonal to earlier  $\underline{a}$ 's e.g.  $\underline{q}_2^T \underline{a}_1 = 0, \underline{q}_3^T \underline{a}_1 = 0 \dots$ )

This is Gram-Schmidt in a nutshell:

- $\underline{a}_1$  &  $\underline{q}_1$  are along a single line
- $\underline{a}_1, \underline{a}_2$  &  $\underline{q}_1, \underline{q}_2$  on the same plane  
( $\underline{a}_1, \underline{a}_2$  are comb. of  $\underline{q}_1, \underline{q}_2$ )
- $\underline{a}_1, \underline{a}_2, \underline{a}_3$  &  $\underline{q}_1, \underline{q}_2, \underline{q}_3$  in one subspace  
( $\dim = 3$ ) ( $\underline{a}_1, \underline{a}_2, \underline{a}_3$  are comb. of  $\underline{q}_1, \underline{q}_2, \underline{q}_3$ )

In general,  $\underline{a}_1, \dots, \underline{a}_k$  are comb. of  $\underline{q}_1, \dots, \underline{q}_k$  only  $\Rightarrow R$  is upper triangular



## Solving least squares problem

$$A\underline{x} = \underline{b} \quad (\text{no sol.})$$

$$A^T A \hat{\underline{x}} = A^T \underline{b} \quad (\text{using QR})$$

$$(QR)^T QR \hat{\underline{x}} = R^T Q^T \underline{b}$$

$$\Rightarrow R^T R \hat{\underline{x}} = R^T Q^T \underline{b} \quad \text{or} \quad R \hat{\underline{x}} = Q^T \underline{b}$$

$$\text{or} \quad \hat{\underline{x}} = R^{-1} Q^T \underline{b}$$

(can be easily solved  
using back sub.)