

Lecture 4

Orthonormal sets of vectors and QR factorization

- orthonormal set of vectors
- Gram-Schmidt procedure, QR factorization
- orthogonal decomposition induced by a matrix

Orthonormal set of vectors

set of vectors $\{u_1, \dots, u_k\} \subset \mathbf{R}^n$ is

- *normalized* if $\|u_i\| = 1$, $i = 1, \dots, k$
(u_i are called *unit vectors* or *direction vectors*)
- *orthogonal* if $u_i \perp u_j$ for $i \neq j$
- *orthonormal* if both

slang: we say ' u_1, \dots, u_k are orthonormal vectors' but orthonormality (like independence) is a property of a *set* of vectors, not vectors individually

in terms of $U = [u_1 \ \cdots \ u_k]$, orthonormal means

$$U^T U = I_k$$

- an orthonormal set of vectors is independent
(multiply $\alpha_1 u_1 + \alpha_2 u_2 + \cdots + \alpha_k u_k = 0$ by u_i^T)
- hence $\{u_1, \dots, u_k\}$ is an orthonormal basis for

$$\text{span}(u_1, \dots, u_k) = \mathcal{R}(U)$$

- **warning:** if $k < n$ then $UU^T \neq I$ (since its rank is at most k)
(more on this matrix later . . .)

Geometric properties

suppose columns of $U = [u_1 \cdots u_k]$ are orthonormal

if $w = Uz$, then $\|w\| = \|z\|$

- multiplication by U does not change norm
- mapping $w = Uz$ is *isometric*: it preserves distances
- simple derivation using matrices:

$$\|w\|^2 = \|Uz\|^2 = (Uz)^T(Uz) = z^T U^T U z = z^T z = \|z\|^2$$

- *inner products* are also preserved: $\langle Uz, U\tilde{z} \rangle = \langle z, \tilde{z} \rangle$
- if $w = Uz$ and $\tilde{w} = U\tilde{z}$ then

$$\langle w, \tilde{w} \rangle = \langle Uz, U\tilde{z} \rangle = (Uz)^T (U\tilde{z}) = z^T U^T U \tilde{z} = \langle z, \tilde{z} \rangle$$

- norms and inner products preserved, so *angles* are preserved:
 $\angle(Uz, U\tilde{z}) = \angle(z, \tilde{z})$
- thus, multiplication by U preserves inner products, angles, and distances

Orthonormal basis for \mathbf{R}^n

- suppose u_1, \dots, u_n is an orthonormal *basis* for \mathbf{R}^n
- then $U = [u_1 \cdots u_n]$ is called **orthogonal**: it is square and satisfies $U^T U = I$

(you'd think such matrices would be called *orthonormal*, not *orthogonal*)

- it follows that $U^{-1} = U^T$, and hence also $U U^T = I$, *i.e.*,

$$\sum_{i=1}^n u_i u_i^T = I$$

Expansion in orthonormal basis

suppose U is orthogonal, so $x = UU^T x$, *i.e.*,

$$x = \sum_{i=1}^n (u_i^T x) u_i$$

- $u_i^T x$ is called the *component* of x in the direction u_i
- $a = U^T x$ *resolves* x into the vector of its u_i components
- $x = Ua$ *reconstitutes* x from its u_i components
- $x = Ua = \sum_{i=1}^n a_i u_i$ is called the (u_i) *expansion* of x

the identity $I = UU^T = \sum_{i=1}^n u_i u_i^T$ is sometimes written (in physics) as

$$I = \sum_{i=1}^n |u_i\rangle\langle u_i|$$

since

$$x = \sum_{i=1}^n |u_i\rangle\langle u_i|x\rangle$$

(but we won't use this notation)

Geometric interpretation

if U is orthogonal, then transformation $w = Uz$

- preserves *norm* of vectors, *i.e.*, $\|Uz\| = \|z\|$
- preserves *angles* between vectors, *i.e.*, $\angle(Uz, U\tilde{z}) = \angle(z, \tilde{z})$

examples:

- rotations (about some axis)
- reflections (through some plane)

Example: rotation by θ in \mathbf{R}^2 is given by

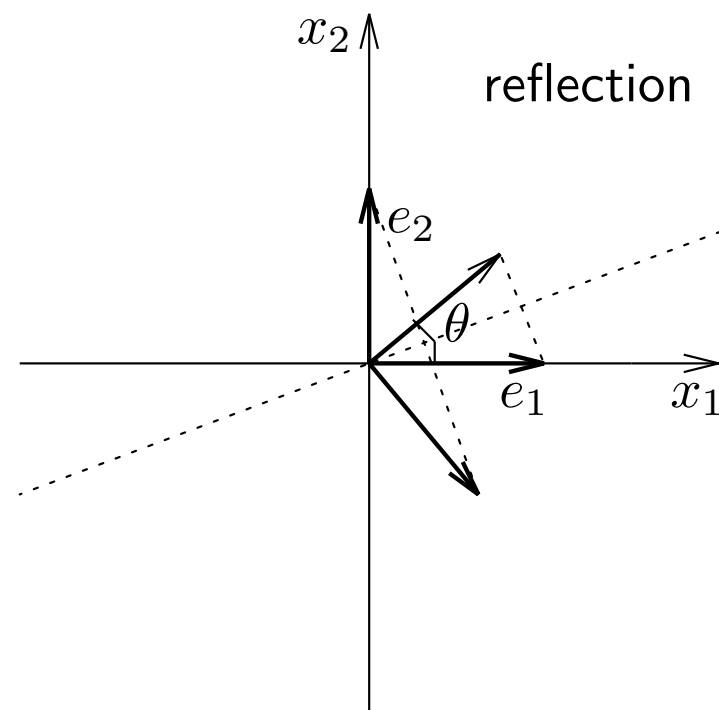
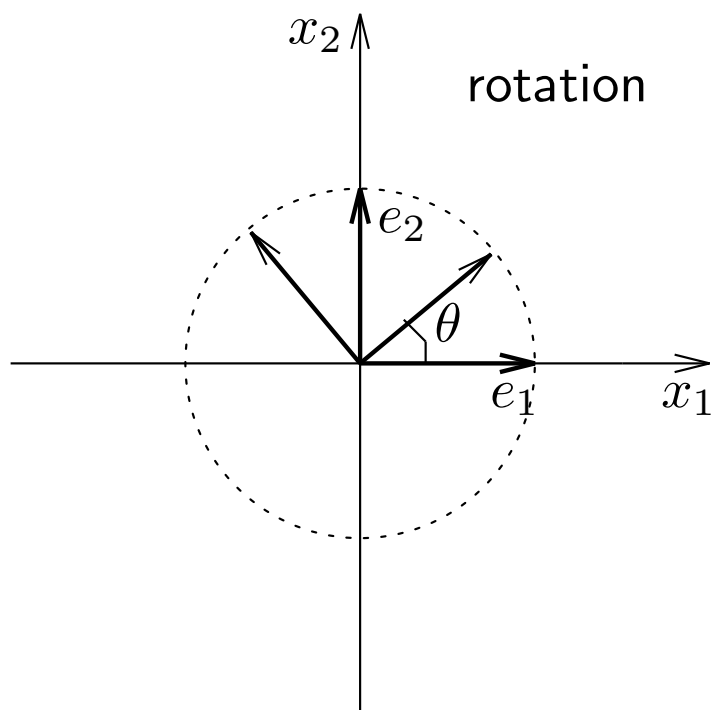
$$y = U_\theta x, \quad U_\theta = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}$$

since $e_1 \rightarrow (\cos \theta, \sin \theta)$, $e_2 \rightarrow (-\sin \theta, \cos \theta)$

reflection across line $x_2 = x_1 \tan(\theta/2)$ is given by

$$y = R_\theta x, \quad R_\theta = \begin{bmatrix} \cos \theta & \sin \theta \\ \sin \theta & -\cos \theta \end{bmatrix}$$

since $e_1 \rightarrow (\cos \theta, \sin \theta)$, $e_2 \rightarrow (\sin \theta, -\cos \theta)$



can check that U_θ and R_θ are orthogonal

Gram-Schmidt procedure

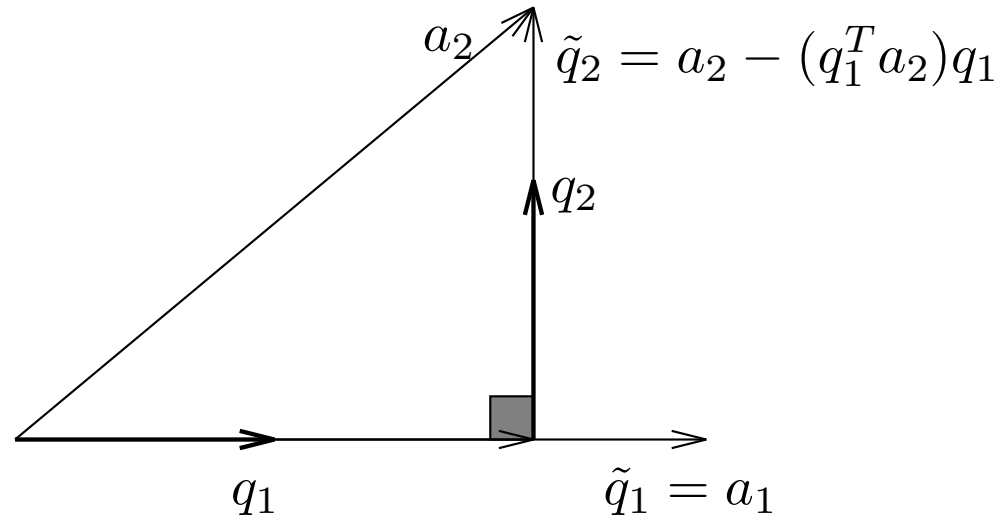
- given independent vectors $a_1, \dots, a_k \in \mathbf{R}^n$, G-S procedure finds orthonormal vectors q_1, \dots, q_k s.t.

$$\text{span}(a_1, \dots, a_r) = \text{span}(q_1, \dots, q_r) \quad \text{for } r \leq k$$

- thus, q_1, \dots, q_r is an orthonormal basis for $\text{span}(a_1, \dots, a_r)$
- rough idea of method: first *orthogonalize* each vector w.r.t. previous ones; then *normalize* result to have norm one

Gram-Schmidt procedure

- step 1a. $\tilde{q}_1 := a_1$
- step 1b. $q_1 := \tilde{q}_1 / \|\tilde{q}_1\|$ (normalize)
- step 2a. $\tilde{q}_2 := a_2 - (q_1^T a_2)q_1$ (remove q_1 component from a_2)
- step 2b. $q_2 := \tilde{q}_2 / \|\tilde{q}_2\|$ (normalize)
- step 3a. $\tilde{q}_3 := a_3 - (q_1^T a_3)q_1 - (q_2^T a_3)q_2$ (remove q_1, q_2 components)
- step 3b. $q_3 := \tilde{q}_3 / \|\tilde{q}_3\|$ (normalize)
- etc.



for $i = 1, 2, \dots, k$ we have

$$\begin{aligned} a_i &= (q_1^T a_i)q_1 + (q_2^T a_i)q_2 + \cdots + (q_{i-1}^T a_i)q_{i-1} + \|\tilde{q}_i\|q_i \\ &= r_{1i}q_1 + r_{2i}q_2 + \cdots + r_{ii}q_i \end{aligned}$$

(note that the r_{ij} 's come right out of the G-S procedure, and $r_{ii} \neq 0$)

QR decomposition

written in matrix form: $A = QR$, where $A \in \mathbf{R}^{n \times k}$, $Q \in \mathbf{R}^{n \times k}$, $R \in \mathbf{R}^{k \times k}$:

$$\underbrace{\begin{bmatrix} a_1 & a_2 & \cdots & a_k \end{bmatrix}}_A = \underbrace{\begin{bmatrix} q_1 & q_2 & \cdots & q_k \end{bmatrix}}_Q \underbrace{\begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1k} \\ 0 & r_{22} & \cdots & r_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & r_{kk} \end{bmatrix}}_R$$

- $Q^T Q = I_k$, and R is upper triangular & invertible
- called **QR decomposition** (or factorization) of A
- usually computed using a variation on Gram-Schmidt procedure which is less sensitive to numerical (rounding) errors
- columns of Q are orthonormal basis for $\mathcal{R}(A)$

General Gram-Schmidt procedure

- in basic G-S we assume $a_1, \dots, a_k \in \mathbf{R}^n$ are independent
- if a_1, \dots, a_k are dependent, we find $\tilde{q}_j = 0$ for some j , which means a_j is linearly dependent on a_1, \dots, a_{j-1}
- modified algorithm: when we encounter $\tilde{q}_j = 0$, skip to next vector a_{j+1} and continue:

```
 $r = 0;$   
for  $i = 1, \dots, k$   
  {  
     $\tilde{a} = a_i - \sum_{j=1}^r q_j q_j^T a_i;$   
    if  $\tilde{a} \neq 0$  {  $r = r + 1; q_r = \tilde{a} / \|\tilde{a}\|;$  }  
  }
```


on exit,

- q_1, \dots, q_r is an orthonormal basis for $\mathcal{R}(A)$ (hence $r = \mathbf{Rank}(A)$)
- each a_i is linear combination of previously generated q_j 's

in matrix notation we have $A = QR$ with $Q^T Q = I_r$ and $R \in \mathbf{R}^{r \times k}$ in *upper staircase form*:

$$\begin{bmatrix} \times & & & & & & \\ & \times & & & & & \\ & & \times & & & & \\ & & & \times & & & \\ & & & & \times & & \\ & & & & & \times & \\ & & & & & & \times & \\ & & & & & & & \times & \\ & & & & & & & & \times & \\ & & & & & & & & & \times \end{bmatrix}$$

possibly nonzero entries

zero entries

‘corner’ entries (shown as \times) are nonzero

can permute columns with \times to front of matrix:

$$A = Q[\tilde{R} \ S]P$$

where:

- $Q^T Q = I_r$
- $\tilde{R} \in \mathbf{R}^{r \times r}$ is upper triangular and invertible
- $P \in \mathbf{R}^{k \times k}$ is a permutation matrix
(which moves forward the columns of a which generated a new q)

Applications

- directly yields orthonormal basis for $\mathcal{R}(A)$
- yields factorization $A = BC$ with $B \in \mathbf{R}^{n \times r}$, $C \in \mathbf{R}^{r \times k}$, $r = \mathbf{Rank}(A)$
- to check if $b \in \text{span}(a_1, \dots, a_k)$: apply Gram-Schmidt to $[a_1 \ \cdots \ a_k \ b]$
- staircase pattern in R shows which columns of A are dependent on previous ones

works incrementally: one G-S procedure yields QR factorizations of $[a_1 \ \cdots \ a_p]$ for $p = 1, \dots, k$:

$$[a_1 \ \cdots \ a_p] = [q_1 \ \cdots \ q_s] R_p$$

where $s = \mathbf{Rank}([a_1 \ \cdots \ a_p])$ and R_p is leading $s \times p$ submatrix of R

‘Full’ QR factorization

with $A = Q_1 R_1$ the QR factorization as above, write

$$A = \begin{bmatrix} Q_1 & Q_2 \end{bmatrix} \begin{bmatrix} R_1 \\ 0 \end{bmatrix}$$

where $\begin{bmatrix} Q_1 & Q_2 \end{bmatrix}$ is orthogonal, *i.e.*, columns of $Q_2 \in \mathbf{R}^{n \times (n-r)}$ are orthonormal, orthogonal to Q_1

to find Q_2 :

- find any matrix \tilde{A} s.t. $\begin{bmatrix} A & \tilde{A} \end{bmatrix}$ has rank n (*e.g.*, $\tilde{A} = I$)
- apply general Gram-Schmidt to $\begin{bmatrix} A & \tilde{A} \end{bmatrix}$
- Q_1 are orthonormal vectors obtained from columns of A
- Q_2 are orthonormal vectors obtained from extra columns (\tilde{A})

i.e., any set of orthonormal vectors can be *extended* to an orthonormal basis for \mathbf{R}^n

$\mathcal{R}(Q_1)$ and $\mathcal{R}(Q_2)$ are called *complementary subspaces* since

- they are orthogonal (*i.e.*, every vector in the first subspace is orthogonal to every vector in the second subspace)
- their sum is \mathbf{R}^n (*i.e.*, every vector in \mathbf{R}^n can be expressed as a sum of two vectors, one from each subspace)

this is written

- $\mathcal{R}(Q_1) \overset{\perp}{+} \mathcal{R}(Q_2) = \mathbf{R}^n$
- $\mathcal{R}(Q_2) = \mathcal{R}(Q_1)^\perp$ (and $\mathcal{R}(Q_1) = \mathcal{R}(Q_2)^\perp$)
(each subspace is the *orthogonal complement* of the other)

we know $\mathcal{R}(Q_1) = \mathcal{R}(A)$; but what is its orthogonal complement $\mathcal{R}(Q_2)$?

Orthogonal decomposition induced by A

from $A^T = \begin{bmatrix} R_1^T & 0 \end{bmatrix} \begin{bmatrix} Q_1^T \\ Q_2^T \end{bmatrix}$ we see that

$$A^T z = 0 \iff Q_1^T z = 0 \iff z \in \mathcal{R}(Q_2)$$

so $\mathcal{R}(Q_2) = \mathcal{N}(A^T)$

(in fact the columns of Q_2 are an orthonormal basis for $\mathcal{N}(A^T)$)

we conclude: $\mathcal{R}(A)$ and $\mathcal{N}(A^T)$ are *complementary subspaces*:

- $\mathcal{R}(A) \overset{\perp}{+} \mathcal{N}(A^T) = \mathbf{R}^n$ (recall $A \in \mathbf{R}^{n \times k}$)
- $\mathcal{R}(A)^\perp = \mathcal{N}(A^T)$ (and $\mathcal{N}(A^T)^\perp = \mathcal{R}(A)$)
- called *orthogonal decomposition (of \mathbf{R}^n) induced by $A \in \mathbf{R}^{n \times k}$*

- every $y \in \mathbf{R}^n$ can be written uniquely as $y = z + w$, with $z \in \mathcal{R}(A)$, $w \in \mathcal{N}(A^T)$ (we'll soon see what the vector z is . . .)
- can now prove most of the assertions from the linear algebra review lecture
- switching $A \in \mathbf{R}^{n \times k}$ to $A^T \in \mathbf{R}^{k \times n}$ gives decomposition of \mathbf{R}^k :

$$\mathcal{N}(A) \overset{\perp}{+} \mathcal{R}(A^T) = \mathbf{R}^k$$