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 $\{u_1, \ldots, u_k\}$ is an orthonormal basis for

$$\mathrm{span}(u_1, \ldots, u_k) = \mathcal{R}(U)$$

- **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 $u_1, \ldots, u_n$ 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 $UU^T = I$, *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

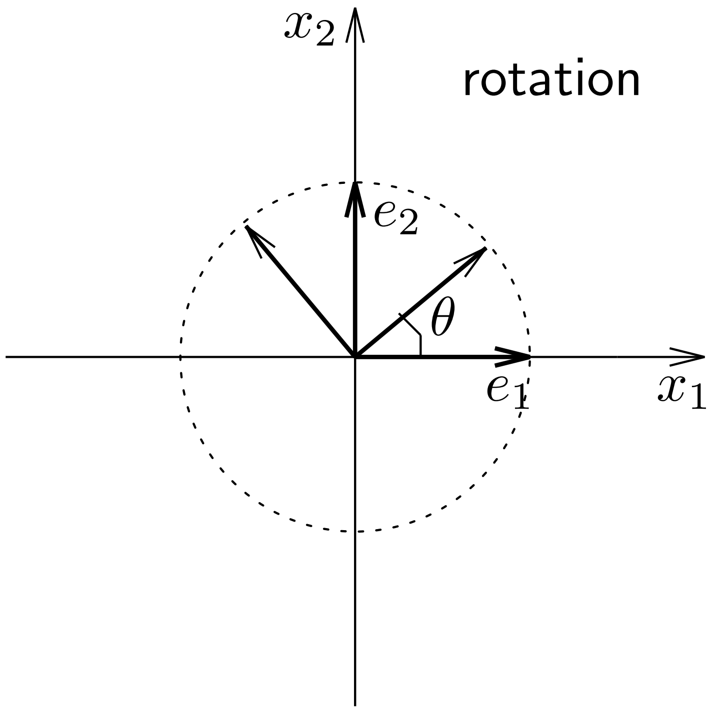
$$y = U_\theta x, \quad U_\theta = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$$

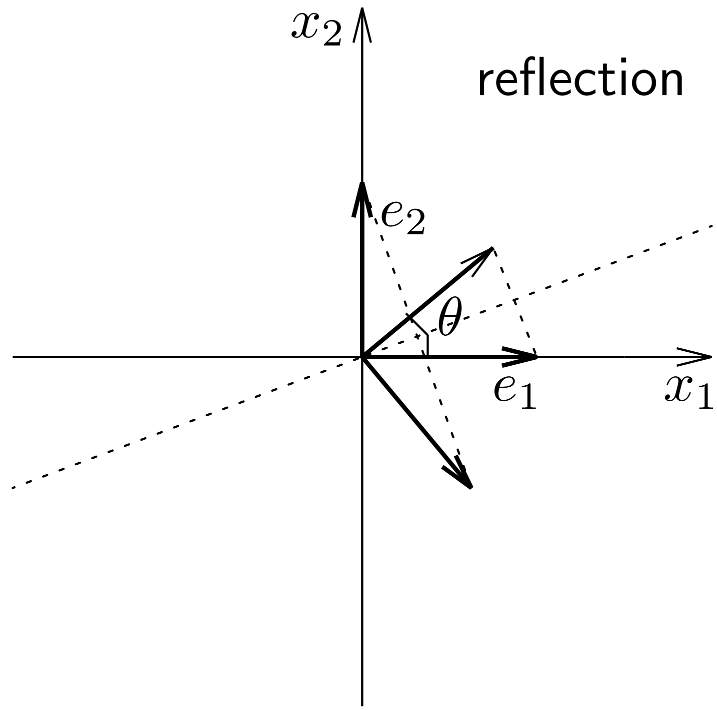
since $e_1 \to (\cos\theta, \sin\theta)$, $e_2 \to (-\sin\theta, \cos\theta)$

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 $e_1 \to (\cos\theta, \sin\theta)$, $e_2 \to (\sin\theta, -\cos\theta)$





can check that U_θ and R_θ are orthogonal

Gram-Schmidt procedure

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

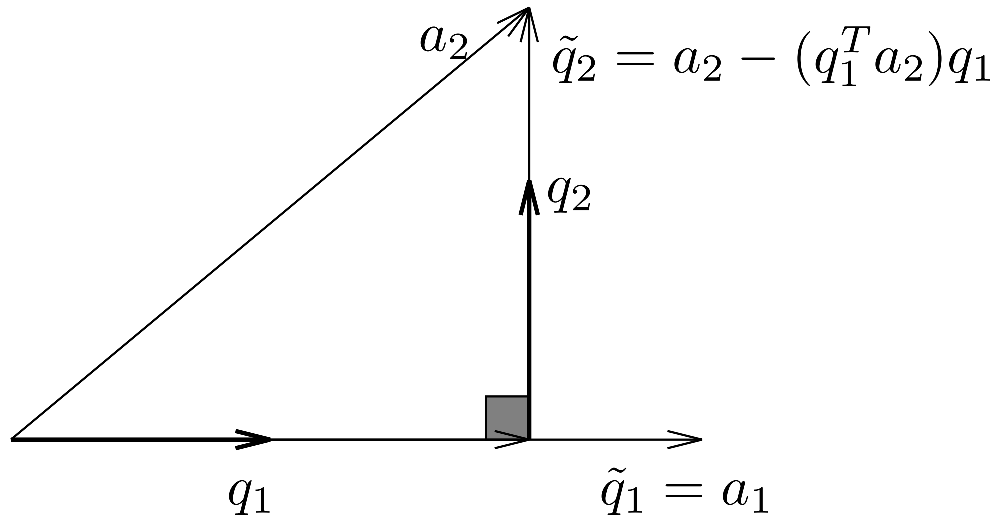
$$\mathrm{span}(a_1, \ldots, a_r) = \mathrm{span}(q_1, \ldots, q_r) \quad \text{for} \quad r \leq k$$

- thus, $q_1, \ldots, q_r$ is an orthonormal basis for $\mathrm{span}(a_1, \ldots, a_r)$

- 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 $i = 1, 2, \ldots, k$ 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 $A \in \mathbf{R}^{n\times k}$, $Q \in \mathbf{R}^{n\times k}$, $R \in \mathbf{R}^{k\times k}$:

$$\underbrace{\left[\begin{array}{cccc} a_1 & a_2 & \cdots & a_k \end{array}\right]}_{A} = \underbrace{\left[\begin{array}{cccc} q_1 & q_2 & \cdots & q_k \end{array}\right]}_{Q} \underbrace{\left[\begin{array}{cccc} r_{11} & r_{12} & \cdots & r_{1k} \\ 0 & r_{22} & \cdots & r_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & r_{kk} \end{array}\right]}_{R}$$

- $Q^TQ = I_k$, 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 $a_1, \ldots, a_k \in \mathbf{R}^n$ are independent

- if $a_1, \ldots, a_k$ are dependent, we find $\tilde{q}_j = 0$ for some j, which means a_j is linearly dependent on $a_1, \ldots, a_{j-1}$

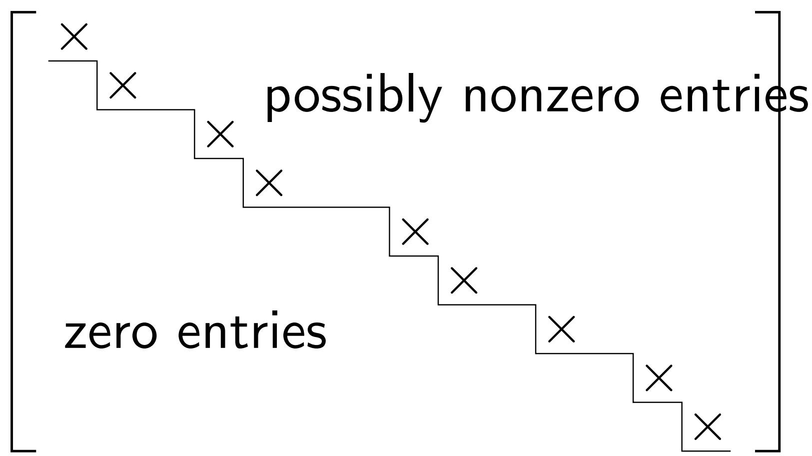
- modified algorithm: when we encounter $\tilde{q}_j = 0$, skip to next vector a_{j+1} and continue:

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

on exit,

- $q_1, \ldots, q_r$ 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*:



'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 $b \in \mathrm{span}(a_1, \ldots, a_k)$: 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 $p = 1, \ldots, k$:

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

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

$$A = \left[\begin{array}{cc} Q_1 & Q_2 \end{array} \right] \left[\begin{array}{c} R_1 \\ 0 \end{array} \right]$$

where $[Q_1 \ Q_2]$ 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. $[A \ \tilde{A}]$ has rank n (*e.g.*, $\tilde{A} = I$)
- apply general Gram-Schmidt to $[A \ \tilde{A}]$
- 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 $\mathbf{R}^k$:

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