QR Algorithm

Contents

$m \geq n$

Recap

Matrix w/ orthonormal columns

$$Q = [\vec{q}_1 \mid \vec{q}_2 \mid \cdots \mid \vec{q}_n] \in \mathbb{R}^{m \times n}$$

(tall rectangle)

- orthonormal columns means $Q^T Q = I$.
- $\|Q\vec{x}\|_2 = \|\vec{x}\|_2$
- $\|Q\|_2 = 1$

Orthogonal matrix

$$Q = [\vec{q}_1 \mid \vec{q}_2 \mid \cdots \mid \vec{q}_m] \in \mathbb{R}^{m \times m}$$

(square)

- $Q^T Q = I$
- $\|Q\vec{x}\|_2 = \|\vec{x}\|_2$
- $\|Q\|_2 = 1$.
- $Q^{-1} = Q^T$

An orthogonal matrix is invertible.

nonsingular

Q is orthogonal.

$\Longrightarrow$ Q is invertible (because Q^{-1} exists and is equal to Q^T)

$\Longleftrightarrow$ Q is nonsingular

$\Longleftrightarrow$ $\det(Q) \neq 0$

$\Longleftrightarrow$ $Q\vec{x} = \vec{b}$ has a unique solution.

$\Longleftrightarrow$ Columns of Q are linear independent.

Projection and Reflection Operators (cont')

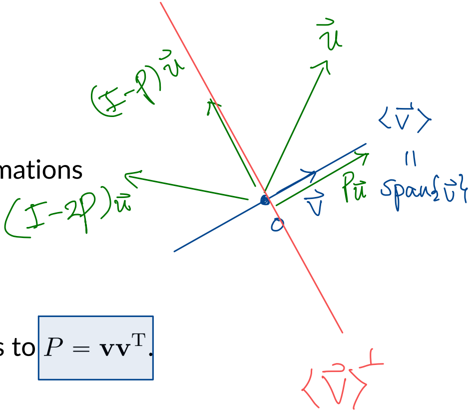
From Monday (Lec. 20)

Summary: for given $\mathbf{v} \in \mathbb{R}^m$, a nonzero vector, let

$$P = \frac{\mathbf{v}\mathbf{v}^{\mathrm{T}}}{\mathbf{v}^{\mathrm{T}}\mathbf{v}} \in \mathbb{R}^{m \times m}.$$

Then the following matrices carry out geometric transformations

- Projection onto $\langle \mathbf{v} \rangle$: P
- Projection onto $\langle \mathbf{v} \rangle$: $I - P$
- Reflection across $\langle \mathbf{v} \rangle^{\perp}$: $I - 2P$



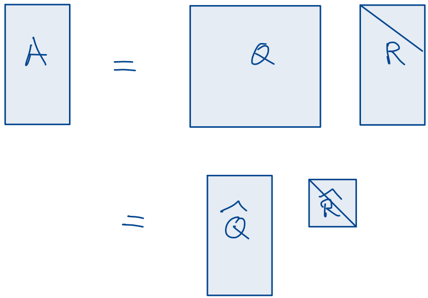
Note. If $\mathbf{v}$ were a unit vector, the definition of P simplifies to $\boxed{P = \mathbf{v}\mathbf{v}^{\mathrm{T}}}$.

$\Downarrow$ $\qquad\qquad\qquad\qquad$ $\Nearrow$

$\vec{v}^{T}\vec{v} = \|\vec{v}\|_2^2 = 1$

QR Factorization and Least Squares

$A \in \mathbb{R}^{m \times n}$



(Thick QR)

- $Q \in \mathbb{R}^{m \times m}$ orthogonal
- $R \in \mathbb{R}^{m \times n}$ upper-Δ

(Thin QR)

- $\hat{Q} \in \mathbb{R}^{m \times n}$ orthonormal columns
- $\hat{R} \in \mathbb{R}^{n \times n}$ upper-Δ

Normal eqn: $A^T A \vec{x} = A^T \vec{b}$

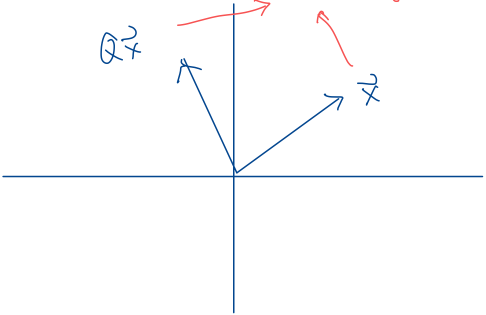
$$A^T A \vec{x} = A^T \vec{b} \;\xRightarrow{\text{thin QR}}\; \underbrace{\hat{R}\vec{x} = \hat{Q}^T \vec{b}}_{\text{Upper-}\Delta\text{ system}}$$

Householder Transformation

<u>Recall</u> Q orthogonal.

$$\|Q\vec{x}\|_2 = \|\vec{x}\|_2 \quad \text{(2-norm preserving)}$$

"same length"



- rotation $\longrightarrow$ Givens rotations
- reflection $\longrightarrow$ Householder transformation

Motivation

$$H\vec{z} = \begin{bmatrix} \star \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \|\star\|_2 \, \vec{e}_1$$

Problem

Given $\mathbf{z} \in \mathbb{R}^m$, find an orthogonal matrix $H \in \mathbb{R}^{m \times m}$ such that $H\mathbf{z}$ is nonzero only in the first element.

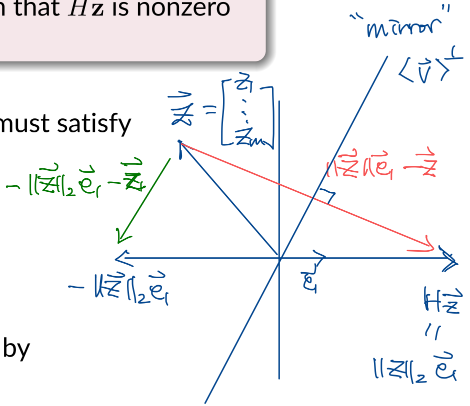
- Since orthogonal matrices preserve the 2-norm, H must satisfy

$$H\mathbf{z} = \begin{bmatrix} \pm \|\mathbf{z}\|_2 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \pm \|\mathbf{z}\|_2 \, \mathbf{e}_1 .$$

- The **Householder transformation matrix** H defined by

$$\boxed{H = I - 2\frac{\mathbf{v}\mathbf{v}^{\mathrm{T}}}{\mathbf{v}^{\mathrm{T}}\mathbf{v}},} \quad \text{where } \mathbf{v} = \pm \|\mathbf{z}\|_2 \, \mathbf{e}_1 - \mathbf{z},$$

solves the problem. See Theorem 1 on the next slide.



Properties of Householder Transformation

Theorem 1

Let $\mathbf{v} = \|\mathbf{z}\|_2\, \mathbf{e}_1 - \mathbf{z}$ *and let* H *be the Householder transformation defined by*

$$H = I - 2\frac{\mathbf{v}\mathbf{v}^{\mathrm{T}}}{\mathbf{v}^{\mathrm{T}}\mathbf{v}}.$$

(reflection across $\langle \vec{v} \rangle^{\perp}$)

Then

1. H *is symmetric;* ($H^T = H$)
2. H *is orthogonal;*
3. $H\mathbf{z} = \|\mathbf{z}\|_2\, \mathbf{e}_1$.

- H is invariant under scaling of $\mathbf{v}$.

$$I - 2\frac{(\alpha\vec{v})(\alpha\vec{v})^T}{(\alpha\vec{v})^T(\alpha\vec{v})} = I - 2\frac{\cancel{\alpha^2}\vec{v}\vec{v}^T}{\cancel{\alpha^2}\vec{v}^T\vec{v}} = I - 2\frac{\vec{v}\vec{v}^T}{\vec{v}^T\vec{v}}.$$

- If $\|\mathbf{v}\|_2 = 1$, then $H = I - \underset{2}{\wedge}\mathbf{v}\mathbf{v}^{\mathrm{T}}$.

Proof of ②: Since H is invariant under scaling of $\vec{v}$, assume that $\|\vec{v}\|_2 = 1$, so $H = I - 2\vec{v}\vec{v}^T$.

To show that H is orthogonal, we need to show $H^T H = I$.

$$
\begin{aligned}
H^T H &= (I - 2\vec{v}\vec{v}^T)^T (I - 2\vec{v}\vec{v}^T) \\
&= (I^T - 2(\vec{v}\vec{v}^T)^T)(I - 2\vec{v}\vec{v}^T) \\
&= (I - 2\vec{v}\vec{v}^T)(I - 2\vec{v}\vec{v}^T) \qquad \|\vec{v}\|_2^2 = 1 \\
&= I^2 - 2\vec{v}\vec{v}^T - 2\vec{v}\vec{v}^T + 4\vec{v}\boxed{\vec{v}^T\vec{v}}\vec{v}^T \\
&= I - \cancel{(2+2-4)}\vec{v}\vec{v}^T = I
\end{aligned}
$$

$\square$

Geometry Behind Householder Transformation

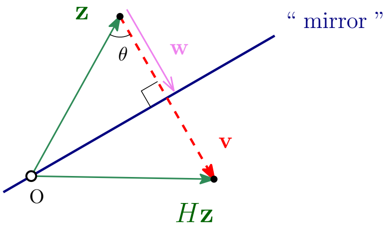
The Householder transformation matrix H is the reflector across $\langle \mathbf{v} \rangle^{\perp}$.

From any $\mathbf{z}$ to the "mirror":

$$\mathbf{w} = -\frac{\mathbf{z}^{\mathrm{T}}\mathbf{v}}{\sqrt{\mathbf{v}^{\mathrm{T}}\mathbf{v}}} \cdot \frac{\mathbf{v}}{\sqrt{\mathbf{v}^{\mathrm{T}}\mathbf{v}}} = -\mathbf{v}\frac{\mathbf{z}^{\mathrm{T}}\mathbf{v}}{\mathbf{v}^{\mathrm{T}}\mathbf{v}}\,.$$

From any $\mathbf{z}$ to its reflection:

$$H\mathbf{z} - \mathbf{z} = -2\mathbf{v}\frac{\mathbf{z}^{\mathrm{T}}\mathbf{v}}{\mathbf{v}^{\mathrm{T}}\mathbf{v}}\,.$$



Thus, for any $\mathbf{z}$,

$$H\mathbf{z} = \mathbf{z} - 2\mathbf{v}\frac{\mathbf{z}^{\mathrm{T}}\mathbf{v}}{\mathbf{v}^{\mathrm{T}}\mathbf{v}} = \left(I - 2\frac{\mathbf{v}\mathbf{v}^{\mathrm{T}}}{\mathbf{v}^{\mathrm{T}}\mathbf{v}}\right)\mathbf{z} \quad \Longrightarrow \quad H = I - 2\frac{\mathbf{v}\mathbf{v}^{\mathrm{T}}}{\mathbf{v}^{\mathrm{T}}\mathbf{v}}\,.$$

QR Factorization Algorithm

Office Hours (unusual schedule)

- M 4:45 ~ 6:15
- T 9:00 ~ 10:30
- Th 9:00 ~ 10:30 (for 3607 only)

QR Factorization Algorithm via Triangularization

- The Gram-Schmidt orthogonalization (thin QR factorization) is unstable in floating-point calculations.
- **Stable alternative:** Find orthogonal matrices $H_1, H_2, \ldots, H_n$ so that

$$\underbrace{H_n H_{n-1} \cdots H_2 H_1}_{=:Q^{\mathrm{T}}} A = R\,.$$

$$Q^T A = R$$

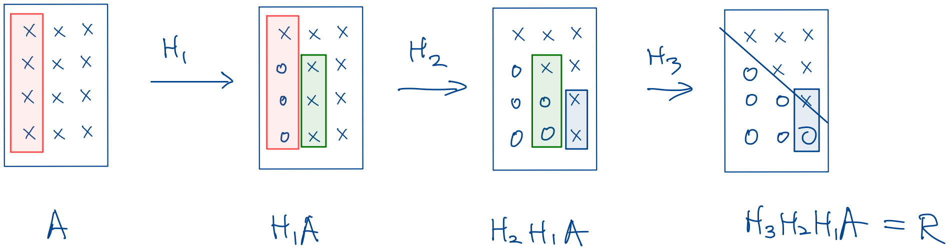
$$\underbrace{Q Q^T}_{= Q Q^{-1} = I} A = QR$$

introducing zeros one column at a time below diagonal terms. Householder matrices will do.

- As a product of orthogonal matrices, Q^{T} is also orthogonal and so $(Q^{\mathrm{T}})^{-1} = Q$. Therefore,

$$A = QR\,.$$

4x3 Illustration



$$H_2 = \left[\begin{array}{c|ccc} 1 & 0 & 0 & 0 \\ \hline 0 & & & \\ 0 & & \boxed{\text{Householder}} & \\ 0 & & & \end{array}\right], \quad H_3 = \left[\begin{array}{cc|cc} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ \hline 0 & 0 & \multicolumn{2}{c}{\boxed{\text{Householder}}} \\ 0 & 0 & & \end{array}\right]$$

Examples

1. Find an orthogonal matrix H such that

$$H \underbrace{\begin{bmatrix} 3 \\ -2 \\ 1 \end{bmatrix}}_{\vec{z}} = \underbrace{\begin{bmatrix} \sqrt{14} \\ 0 \\ 0 \end{bmatrix}}_{\|\vec{z}\|_2 \, \vec{e}_1}$$

Soln H is the Householder transformation obtained by

$$H = I - 2 \frac{\vec{v}\vec{v}^T}{\vec{v}^T\vec{v}}$$

where

$$\vec{v} = \|\vec{z}\|_2 \vec{e}_1 - \vec{z}$$

Side

- Note: $\|\vec{z}\|_2^2 = 3^2 + (-2)^2 + 1^2$

$$= 9 + 4 + 1$$

$$= 14$$

$$\Longrightarrow \|\vec{z}\|_2 = \sqrt{14}$$

- $\vec{e}_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \in \mathbb{R}^3$

Note that

$$\vec{v} = \begin{bmatrix} \sqrt{14} \\ 0 \\ 0 \end{bmatrix} - \begin{bmatrix} 3 \\ -2 \\ 1 \end{bmatrix} = \begin{bmatrix} \sqrt{14}-3 \\ 2 \\ -1 \end{bmatrix},$$

so

$$H = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} - \frac{2}{28-6\sqrt{14}} \begin{bmatrix} (\sqrt{14}-3)^2 & 2(\sqrt{14}-3) & -(\sqrt{14}-3) \\ 2(\sqrt{14}-3) & 4 & -2 \\ -(\sqrt{14}-3) & -2 & 1 \end{bmatrix}$$

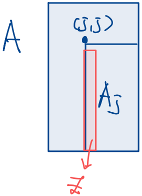
Scratch

$$\vec{v}^T\vec{v} = (\sqrt{14}-3)^2 + (2)^2 + (-1)^2$$

$$= 14 - 6\sqrt{14} + 9 + 4 + 1$$

$$= 28 - 6\sqrt{14}$$

```
function [Q, R] = myqr(A)
  [m, n] = size(A);
  A0 = A;
  Q = eye(m);
  for j = 1:min(m,n)
      Aj = A(j:m, j:n);
      z = Aj(:, 1);
      v = z + sign0(z(1))*norm(z)*eye(length(z), 1);
      Hj = eye(length(v)) - 2/(v'*v) * v*v';
(*)   Aj = Hj*Aj;
      H = eye(m);
      H(j:m, j:m) = Hj;
(**)  Q = Q*H;
      A(j:m, j:n) = Aj;
  end
  R = A;
end
```



$\vec{v} = \vec{z} + \text{sign}(z_1)\,\|\vec{z}\|_2\,\vec{e}_1$

$\to$ Householder

$$H = \left[\begin{array}{c|c} I & 0 \\ \hline 0 & H_j \end{array}\right]$$

MATLAB Implementation: MYQR (cont')

Sine Sign

(continued from the previous page)

```
% local function
function sign0(x)
  y = ones(size(x));
  y(x < 0) = -1;
end
```

$$\text{sign0}(x) = \begin{cases} +1 & \text{if } x \geq 0 \\ -1 & \text{if } x < 0 \end{cases}$$

(signum)

- The MATLAB command `qr` works similar to, but more efficiently than, this.
- The function finds the factorization in $\sim (2mn^2 - n^3/3)$ flops asymptotically.

Explanation for (*), (**)

$$\underbrace{H_n \cdots H_2 H_1}_{=: Q^T} A = R$$

$$H_j = \left[\begin{array}{c|c} I & 0 \\ \hline 0 & \tilde{H}_j \end{array}\right]$$

Householder.

Note: $H_1, \cdots, H_n$ are all

① symmetric

② orthogonal

(*) : $A_j = H_j * A_j \longrightarrow R = A$

(**) : $Q = Q * H$

$$Q^T = H_n \cdots H_2 H_1$$

$$\Rightarrow Q = (Q^T)^T = (H_n \cdots H_1)^T = H_1^T H_2^T \cdots H_n^T = H_1 H_2 \cdots H_n$$

Suggestion for improvement (See exercise problems on OLS)

Note $A_j = H_j * A_j$

- mathematical ↓
- no subscript

$$A = H A$$

$$= \left(\underline{I} - 2\frac{\vec{v}\vec{v}^T}{\vec{v}^T\vec{v}} \right) \underline{A}$$

$$= A - \frac{2}{\vec{v}^T\vec{v}} \underbrace{\vec{v}}_{\text{vector}} \underbrace{\left(\underbrace{\vec{v}^T}_{\text{vec.}} \underbrace{A}_{\text{mat.}} \right)}_{\text{vector}}$$

Similarly for

$$Q = Q * H$$

Which Reflector Is Better?

Recall:

$$H = I - 2\frac{\mathbf{v}\mathbf{v}^{\mathrm{T}}}{\mathbf{v}^{\mathrm{T}}\mathbf{v}}, \quad \text{where } \mathbf{v} = \pm \|\mathbf{z}\|_2 \, \mathbf{e}_1 - \mathbf{z},$$

In `myqr.m`, the statement

```
v = z + sign0(z(1))*norm(z)*eye(length(z), 1);
```

defines $\mathbf{v}$ slightly differently, namely,

$$\mathbf{v} = \mathbf{z} \pm \|\mathbf{z}\|_2 \, \mathbf{e}_1.$$

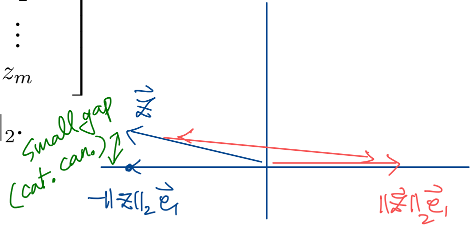
This does not cause any difference since H is invariant under scaling of $\mathbf{v}$; see p. 5.

Which Reflector Is Better? (cont')

The sign of $\pm\|\mathbf{z}\|_2$ is chosen so as to avoid possible catastrophic cancellation in forming $\mathbf{v}$:

$$\mathbf{v} = \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_m \end{bmatrix} + \begin{bmatrix} \pm\|\mathbf{z}\|_2 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \begin{bmatrix} z_1 \pm \|\mathbf{z}\|_2 \\ z_2 \\ \vdots \\ z_m \end{bmatrix}$$

Subtractive cancellation may arise when $z_1 \approx \pm\|\mathbf{z}\|_2$.



- if $z_1 > 0$, use $z_1 + \|\mathbf{z}\|_2$;
- if $z_1 < 0$, use $z_1 - \|\mathbf{z}\|_2$;
- if $z_1 = 0$, either works.

For numerical stability, it is desirable to reflect $\mathbf{z}$ to the vector $s\|\mathbf{z}\|_2\,\mathbf{e}_1$ that is not too close to $\mathbf{z}$ itself. (Trefethen & Bau)

Appendix: Gram-Schmidt Orthogonalization

The Gram–Schmidt Procedure

Problem: Orthogonalization

Given $\mathbf{a}_1, \ldots, \mathbf{a}_n \in \mathbb{R}^m$, construct orthonormal vectors $\mathbf{q}_1, \ldots, \mathbf{q}_n \in \mathbb{R}^m$ such that

$$\operatorname{span}\{\mathbf{a}_1, \ldots, \mathbf{a}_k\} = \operatorname{span}\{\mathbf{q}_1, \ldots, \mathbf{q}_k\}, \quad \text{for any } k \in \mathbb{N}[1, n].$$

- **Strategy.** At the jth step, find a unit vector $\mathbf{q}_j \in \operatorname{span}\{\mathbf{a}_1, \ldots, \mathbf{a}_j\}$ that is orthogonal to $\mathbf{q}_1, \ldots, \mathbf{q}_{j-1}$.
- **Key Observation.** The vector $\mathbf{v}_j$ defined by

$$\mathbf{v}_j = \mathbf{a}_j - \left(\mathbf{q}_1^{\mathrm{T}}\mathbf{a}_j\right)\mathbf{q}_1 - \left(\mathbf{q}_2^{\mathrm{T}}\mathbf{a}_j\right)\mathbf{q}_2 - \cdots - \left(\mathbf{q}_{j-1}^{\mathrm{T}}\mathbf{a}_j\right)\mathbf{q}_{j-1}$$

  satisfies the required properties.

GS Algorithm

The Gram–Schmidt iteration is outlined below:

$$
\begin{aligned}
\mathbf{q}_1 &= \frac{\mathbf{a}_1}{r_{11}}, \\
\mathbf{q}_2 &= \frac{\mathbf{a}_2 - r_{12}\mathbf{q}_1}{r_{22}}, \\
\mathbf{q}_3 &= \frac{\mathbf{a}_3 - r_{13}\mathbf{q}_1 - r_{23}\mathbf{q}_2}{r_{33}}, \\
&\vdots \\
\mathbf{q}_n &= \frac{\mathbf{a}_n - \sum_{i=1}^{n-1} r_{in}\mathbf{q}_i}{r_{nn}},
\end{aligned}
$$

where

$$
r_{ij} = \begin{cases} \mathbf{q}_i^{\mathrm{T}}\mathbf{a}_j, & \text{if } i \neq j \\ \pm\left\|\mathbf{a}_j - \sum_{k=1}^{j-1} r_{kj}\mathbf{q}_k\right\|_2, & \text{if } i = j \end{cases} .
$$

GS Procedure and Thin QR Factorization

- The GS algorithm, written as a matrix equation, yields a **thin QR factorization**:

$$A = \underbrace{\begin{bmatrix} \\ \\ \mathbf{a}_1 & \cdots & \mathbf{a}_n \\ \\ \\ \end{bmatrix}}_{A} = \underbrace{\begin{bmatrix} \\ \\ \mathbf{q}_1 & \cdots & \mathbf{q}_n \\ \\ \\ \end{bmatrix}}_{\hat{Q}} \underbrace{\begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ 0 & r_{22} & \cdots & r_{2n} \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \cdots & r_{nn} \end{bmatrix}}_{\hat{R}} = \widehat{Q}\widehat{R}$$

- While it is an important tool for theoretical work, the GS algorithm is numerically unstable.