Today:

- Least squares
- QR
  - ↪ Gram-Schmidt
  - ↪ Householder
  - ↪ Givens

Announcements:

- Exam 1
- IEF debrief

Least-squares by Transformation

Want a matrix Q so that

$$QA\mathbf{x} \cong Q\mathbf{b}$$

has the same solution as

$$A\mathbf{x} \cong \mathbf{b}.$$

x s.t. $\|Ax-b\|_2$ is minimized

I.e. want

$$\|Q(A\mathbf{x}-\mathbf{b})\|_2 = \|A\mathbf{x}-\mathbf{b}\|_2 .$$

What type of matrix does that? Any invertible one?

orthogonal matrices

Orthogonal Matrices

What's an *orthogonal (=orthonormal) matrix*?

One that satisfies $Q^TQ = I$ and $QQ^T = I$.

Are orthogonal projectors orthogonal?

Nope, not in general.

Now what about that norm property?

$$\|\underline{Q\mathbf{v}}\|_2^2 = (Q\mathbf{v})^T(Q\mathbf{v}) = \mathbf{v}^T\underbrace{Q^TQ}_{I}\mathbf{v} = \mathbf{v}^T\mathbf{v} = \underline{\|\mathbf{v}\|_2^2}.$$

Simpler Problems: Triangular

$A = QR = QR$

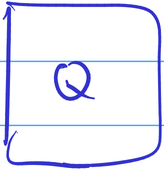
Would we win anything from transforming a least-squares system to upper triangular form?

$Q^TQ = I \qquad QQ^T = I$

$QA \to \begin{pmatrix} R_{top} \\ 0 \end{pmatrix} \vec{x} \cong \begin{pmatrix} (Q^Tb)_1 \\ (Q^Tb)_2 \end{pmatrix} \to \vec{x} = R_{top}^{-1}(Q^Tb)_{top}$

If so, how would we minimize the residual norm?

$$Q Q^T = I = Q Q^T$$



$$\|Qv\|_2 = \|v\|_2$$

$$\underset{m \times n}{A} = \underset{m \times m}{Q} \begin{bmatrix} R \\ 0 \end{bmatrix}$$

$$\|\underset{QR}{A}x - b\|_2 = \|Q^T(QRx - b)\|_2 = \|Rx - Q^T b\|_2$$

Computing QR

- Gram-Schmidt
- Householder Reflectors
- Givens Rotations

Latter two similar to LU:

- Successively zero out below-diagonal part
- But: using orthogonal matrices

Demo: Gram-Schmidt–The Movie
Demo: Gram-Schmidt and Modified Gram-Schmidt
Demo: Keeping track of coefficients in Gram-Schmidt

Seen: Even modified Gram-Schmidt still unsatisfactory in finite precision arithmetic because of roundoff

$$\begin{pmatrix} 1 & \varepsilon \end{pmatrix} \begin{pmatrix} 1 \\ \varepsilon \end{pmatrix}$$

$$A = \underbrace{Q}_{} \underbrace{R}_{}$$

Householder Transformations

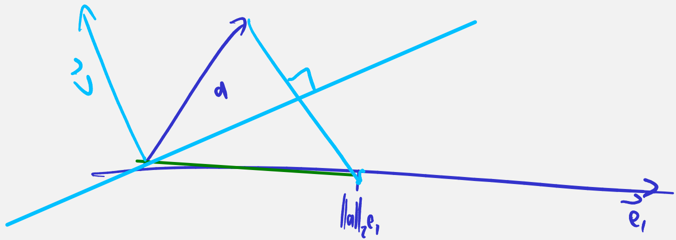
Reflectors

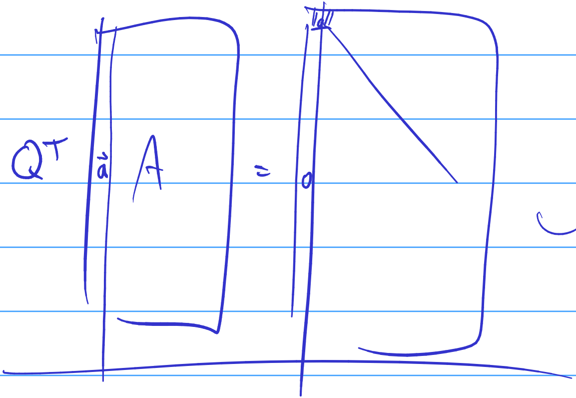
first col of A

$H \begin{bmatrix} \\ \\ \end{bmatrix} = \begin{bmatrix} * \\ 0 \\ \end{bmatrix}$

$\|Hv\|_2 = \|v\|_2$

Find an *orthogonal* matrix Q to zero out the lower part of a vector $\mathbf{a}$.





$\hookrightarrow Q^T A = R$

$A = QR$

$B^T A B$

Householder Reflectors: Properties

Seen from picture (and easy to see with algebra):

$$H\mathbf{a} = \mathbf{e}_1.$$

Remarks:

- Q: What if we want to zero out only the $i+1$th through nth entry?
  A: Use $\mathbf{e}_i$ above.
- A product $H_n \cdots H_1 A = R$ of Householders makes it easy (and quite efficient!) to build a QR factorization.
- It turns out $\mathbf{v}' = \mathbf{a} + \|\mathbf{a}\|_2 \mathbf{e}_1$ works out, too–just pick whichever one causes less cancellation.
- H is symmetric
- H is orthogonal

Demo: 3x3 Householder demo

Givens Rotations

If reflections work, can we make rotations work, too?

Demo: 3x3 Givens demo

In-Class Activity: QR

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