Last class: Linear Least Squares Problem

$$A\underline{x} \approx \underline{b} \qquad A \in \mathbb{R}^{m\times n} \qquad m > n.$$

$\Rightarrow$ find $\underline{x} \in \mathbb{R}^n$ that minimizes $\|A\underline{x} - b\|_2$.

The normal equation method:

Solve $\underbrace{A^TA}_{n\times n}\,\underbrace{\underline{x}}_{n\times 1} = \underbrace{A^Tb}_{n\times 1}$. using Cholesky Factorization.

Issue: The conditioning of the normal equation is worse than the original problem, i.e.

$$\text{cond}(A^TA) = \text{cond}(A)^2$$

how to define this quantity?

Today
- Conditioning of $A\underline{x} \approx \underline{b}$.
- QR Transformation
- Householder Transformation

Condition Number of $A \in \mathbb{R}^{m\times n}$ (rectangular matrix).

For a square matrix $\text{cond}(A) = \|A\| \cdot \underbrace{\|A^{-1}\|}$.

For a rectangular matrix A, A^{-1} is not defined.

Def: The pseudo inverse A^+ of an $m\times n$ matrix, $A \in \mathbb{R}^{m\times n}$ with $m > n$ is $\underbrace{A^+}_{n\times m} = \underbrace{(A^TA)}_{n\times n}{}^{-1}\underbrace{A^T}_{n\times m}$

Notice that $\underbrace{A^+}_{n\times m}\underbrace{A}_{m\times n} = \underbrace{(A^TA)^{-1}A^TA} = \underbrace{I}_{n\times n}$

Q: Is it true that $\underbrace{AA^+}_{m\times m} = I$? $\qquad AA^+ = A(A^TA)^{-1}A^T$

Observation. $\underline{A^T A}\, \underline{x} = A^T \underline{b}$ — normal equation

$$\underline{x} = \underbrace{(A^T A)^{-1} A^T}\, \underline{b}.$$

$$\underline{x} = A^+ \underline{b}$$

Def: For a rectangular matrix $A \in \mathbb{R}^{m\times n}$ with $m > n$.

$$\text{cond}(A) = \|A\| \cdot \|A^+\| \quad \text{if } \text{rank}(A) = n.$$

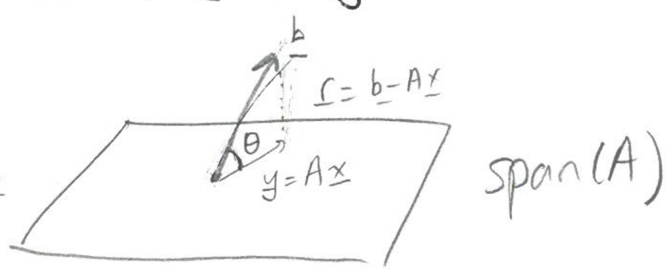
$$\text{cond}(A) = \infty \quad \text{if } \text{rank}(A) < n$$

Sensitivity of $A\underline{x} \approx \underline{b}$

Unlike in the square system $A\underline{x} = \underline{b}$, $A \in \mathbb{R}^{n\times n}$, the conditioning of the system $A\underline{x} \approx \underline{b}$ $A \in \mathbb{R}^{m\times n}$. depends on both A and $\underline{b}$.

We use θ to represent the angle betwen $\underline{b}$ and $\underline{y} = A\underline{x}$

Closest point to $\underline{b}$ in span(A)



Then $\cos(\theta) = \dfrac{\text{adj}}{\text{hyp}} = \dfrac{\|A\underline{x}\|_2}{\|\underline{b}\|_2}$

If we perturb $\underline{b}$ by $\Delta\underline{b}$ and obtain the perturbed solution $\underline{x} + \Delta\underline{x}$.

from the normal equation → $A^TA(\underline{x}+\Delta\underline{x}) = A^T(\underline{b}+\Delta\underline{b})$

$$A^TA\,\Delta\underline{x} = A^T\Delta\underline{b}$$ because $A^TA\underline{x} = A^T\underline{b}$

$$\Delta\underline{x} = (A^TA)^{-1}A^T\Delta\underline{b}$$

$$= A^+\Delta\underline{b}$$

take norm

relative error

$$\frac{\|\Delta\underline{x}\|_2}{\|\underline{x}\|_2} \le \frac{\|A^+\|_2\,\|\Delta\underline{b}\|_2}{\|\underline{x}\|_2}$$

$$= \|A^+\|_2\,\frac{\|A\|_2}{\|A\|_2}\,\frac{\|\underline{b}\|_2}{\|\underline{b}\|_2}\,\frac{\|\Delta\underline{b}\|_2}{\|\underline{x}\|_2}$$

$$= \text{cond}(A)\cdot\frac{\|\underline{b}\|}{\|A\|_2\|\underline{x}\|_2}\,\frac{\|\Delta\underline{b}\|_2}{\|\underline{b}\|_2}$$ rel change in $\underline{b}$

$$\le \text{cond}(A)\,\frac{\|\underline{b}\|}{\|A\underline{x}\|_2}\,\frac{\|\Delta\underline{b}\|_2}{\|\underline{b}\|_2}$$

$$\underbrace{\frac{\|\Delta\underline{x}\|_2}{\|\underline{x}\|_2}}_{\text{relative error in computed solution.}} \le \underbrace{\text{cond}(A)\cdot\frac{1}{\cos(\theta)}}_{\text{condition num. of the problem } A\underline{x}\approx\underline{b}}\cdot\underbrace{\frac{\|\Delta\underline{b}\|_2}{\|\underline{b}\|_2}}_{\text{relative error in } \underline{b}}$$

⇒ small when both

- cond(A) small and
- $\cos(\theta) \approx 1 \rightarrow$ (θ large)

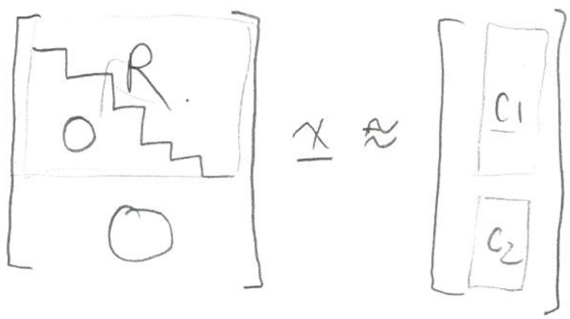
QR ~~Transformation~~ Factorization

Key idea: Use ~~som~~ a similar idea to G.E.

to reduce the system $A\underline{x} \approx \underline{b}$. to

another system $\begin{array}{c} n\times n \rightarrow \\ (m-n)\times n \rightarrow \end{array} \underbrace{\begin{bmatrix} R \\ O \end{bmatrix}}_{m\times n} \underbrace{\underline{x}}_{n\times 1} \approx \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} \begin{array}{l} \}\, n\times 1 \\ \}\, (m-n)\times 1. \end{array}$ with $A = Q\begin{bmatrix} R \\ 0 \end{bmatrix}$;

(where R upper triangular), with the same solution $\underline{x}$.



If we have such a system then:

$R\underline{x} = \underline{c_1}$ can be solved exactly

$O\underline{x} = \underline{c_2}$ cannot be solved

($A\underline{x} \approx \underline{b}$ is not solvable, and to minimize $\| A\underline{x} - \underline{b} \|_2$, we set $\underline{x}$ to be the solution to $R\underline{x} = c_1$)

in particular $\| A\underline{x} - \underline{b} \|_2 = \| c_2 \|_2$

Because if $R\underline{x} = \underline{c_1}$ then $\begin{bmatrix} R \\ 0 \end{bmatrix} \underline{x} = \begin{bmatrix} \underline{c_1} \\ \underline{0} \end{bmatrix}$. $\left\| \begin{bmatrix} \underline{c_1} \\ \underline{0} \end{bmatrix} - \begin{bmatrix} \underline{c_1} \\ \underline{c_2} \end{bmatrix} \right\|_2$

$= \| c_2 \|_2$

Q: can we use Gauss Elimination to factorize

$$A = Q\begin{bmatrix} R \\ 0 \end{bmatrix} \ ?$$

A: No. We need Q to <u>preserve norms</u>.

We are trying to minimize $\|A\underline{x} - \underline{b}\|_2$

So we want:

$$\left\| Q\begin{bmatrix} R \\ 0 \end{bmatrix} - \underline{b} \right\|_2 = \left\| \begin{bmatrix} R \\ 0 \end{bmatrix} - Q^{-1}\underline{b} \right\|_2 .$$

We need another set of transformations that are norm-preserving. (Elementary elimination matrices are <u>not</u> norm preserving)

<u>Orthogonal Transformations</u>

<u>Def</u>: A square matrix Q is <u>orthogonal</u> if its columns are orthonormal, i.e. $Q^TQ = I$.

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

$\Rightarrow \|Q\underline{v}\|_2 = \|\underline{v}\|_2$ so Q is norm-preserving

<u>Claim</u>: A product of orthogonal matrices is orthogonal.

$$(Q_1Q_2)^T(Q_1Q_2) = Q_2^T \underbrace{Q_1^T Q_1}_{=I} Q_2 = Q_2^TQ_2 = I .$$

Idea: we will use orthogonal transforms to factor $A = Q\begin{bmatrix} R \\ 0 \end{bmatrix}$.

Just like in G.E, we will annhilate ~~to one~~ values in A below the diagonal one column at a time.

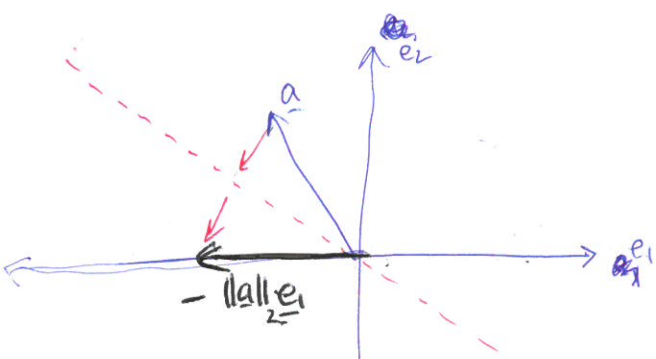
$A = \begin{bmatrix} | & | & \\ \underline{a}_1 & \underline{a}_2 & \cdots \\ | & | & \end{bmatrix}$, we will find. $Q_1\underline{a}_1 = \begin{bmatrix} \alpha \\ 0 \\ \vdots \\ 0 \end{bmatrix}$.

~~to anhilat~~

Then repeat for other columns ~~$\underline{a}_2, \underline{a}_3, \ldots$~~

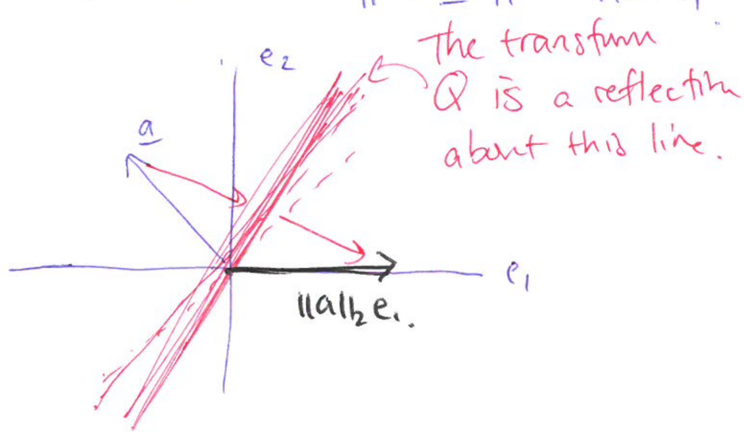
Householder Transformation

Idea: we seek an orthogonal transform that annihilates ~~the~~ all but the first component of a vector. $\underline{a} = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} \longrightarrow \begin{bmatrix} \alpha \\ 0 \end{bmatrix} = Q\underline{a}$.



Householder Transfer
$\Rightarrow$ reflection about the dotted line.

we want $\|Q\underline{a}\| = \|\underline{a}\|$



A Householder transformation or elementary reflector is a matrix of the form.

$$H = I - 2\frac{\underline{v}\underline{v}^T}{\underline{v}^T\underline{v}} \quad \text{with } \underline{v} \neq 0$$

In A3 Q6(g), you will show that $H = H^T = H^{-1}$, which means that H is orthogonal.

Given a vector $\underline{a}$, we can choose a vector $\underline{v}$ such that

$$H\underline{a} = \begin{bmatrix} \alpha \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \alpha \underline{e}_1 \sim \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

scalar

we need $\alpha \underline{e}_1 = H\underline{a} = \left(I - 2\frac{\underline{v}\underline{v}^T}{\underline{v}^T\underline{v}}\right)\underline{a} = \underline{a} - 2\underline{v}\frac{\underline{v}^T\underline{a}}{\underline{v}^T\underline{v}}$

$$\Rightarrow \quad \underline{v} = (\underline{a} - \alpha\underline{e}_1)\frac{\underline{v}^T\underline{v}}{2\underline{v}^T\underline{a}}$$

Since the norm of $\underline{v}$ divides out in the formula for H, we can take $\underline{v} = \underline{a} - \alpha\underline{e}_1$

To preserve norm, we need $\|\alpha \underline{e}_1\|_2 = \|\underline{a}\|_2$

So $\alpha = \pm\|a\|_2$

Choose the sign to avoid cancellation in $\underline{v} = \underline{a} - \alpha\underline{e}_1$ based on the first component of $\underline{a}$.

eg// $\underline{a} = \begin{bmatrix} 2 \\ 1 \\ 2 \end{bmatrix}$. we want an orthogonal transform that transforms $\underline{a}$ to $\begin{bmatrix} \alpha \\ 0 \\ 0 \end{bmatrix}$.

Choose $\underline{v} = \underline{a} - \alpha \underline{e}_1$ $\qquad \alpha = \pm \| a \|_2 = \pm\sqrt{4+1+4} = \pm 3$

$$= \begin{bmatrix} 2 \\ 1 \\ 2 \end{bmatrix} - \alpha \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

$$= \begin{bmatrix} 2-\alpha \\ 1 \\ 2 \end{bmatrix}$$

to avoid cancellation choose $\alpha = -3$ since $2 > 0$.

$$= \begin{bmatrix} 5 \\ 1 \\ 2 \end{bmatrix}.$$

Verify $H\underline{a} = \underline{a} - 2\dfrac{\underline{v}^T\underline{a}}{\underline{v}^T\underline{v}} \cdot \underline{v}$

$$= \begin{bmatrix} 2 \\ 1 \\ 2 \end{bmatrix} - 2 \cdot \frac{\overbrace{2\cdot 5 + 1\cdot 1 + 2\cdot 2}^{15}}{\underbrace{5\cdot 5 + 1\cdot 1 + 2\cdot 2}_{30}} \cdot \begin{bmatrix} 5 \\ 1 \\ 2 \end{bmatrix}$$

$$= \begin{bmatrix} 2 \\ 1 \\ 2 \end{bmatrix} - \begin{bmatrix} 5 \\ 1 \\ 2 \end{bmatrix}$$

$$= \begin{bmatrix} -3 \\ 0 \\ 0 \end{bmatrix}.$$

eg// $A = \begin{bmatrix} 2 & 3 \\ 1 & 1 \\ 2 & 0 \end{bmatrix}$ We will reduce A to the form $\begin{bmatrix} R \\ 0 \end{bmatrix}$

$$\Rightarrow A = Q \begin{bmatrix} R \\ 0 \end{bmatrix}$$

<u>First step</u>: eliminate values below the diagonal in the first column.

We found $\underline{v}_1 = \begin{bmatrix} 5 \\ 1 \\ 2 \end{bmatrix}$. $H_1 \begin{bmatrix} 2 \\ 1 \\ 2 \end{bmatrix} = \begin{bmatrix} -3 \\ 0 \\ 0 \end{bmatrix}$

$$H_1 A = \begin{bmatrix} -3 & 2.\bar{3} \\ 0 & \boxed{-0.0\bar{6}} \\ 0 & \boxed{-2.1\bar{3}} \end{bmatrix}$$

$$H_1 \begin{bmatrix} 3 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 3 \\ 1 \\ 0 \end{bmatrix} - 2 \cdot \frac{\underline{v}_1^T \begin{bmatrix} 3 \\ 1 \\ 0 \end{bmatrix}}{\underline{v}_1^T \underline{v}_1} \cdot \underline{v}_1$$

$$= \begin{bmatrix} 3 \\ 1 \\ 0 \end{bmatrix} - 2 \frac{16}{30} \begin{bmatrix} 5 \\ 1 \\ 2 \end{bmatrix}$$

$$= \begin{bmatrix} 3 \\ 1 \\ 0 \end{bmatrix} - \frac{32}{30} \begin{bmatrix} 5 \\ 1 \\ 2 \end{bmatrix}$$

$$= \begin{bmatrix} 3 - \frac{16}{15} \cdot 5 \\ 1 - \frac{16}{15} \cdot \\ -\frac{16}{15} \cdot 2 \end{bmatrix} = \begin{bmatrix} 2.333 \\ -0.066 \\ -2.133 \end{bmatrix}$$

<u>Second step</u>

We will find an H_2 (or $\underline{v}_2$) that annihilates the 2nd position of vector $\begin{bmatrix} -0.0\bar{6} \\ -2.1\bar{3} \end{bmatrix}$

$$Q_2 \cdot Q_1 \cdot A = \begin{bmatrix} -3 & 2.\bar{3} \\ 0 & \alpha \\ 0 & 0 \end{bmatrix}$$

or $A = \underline{\underline{Q_1}}\, \underline{\underline{Q_2}} \begin{bmatrix} -3 & 2.\bar{3} \\ 0 & \alpha \\ 0 & 0 \end{bmatrix}$