Last time: given $A = [a_1 | a_2 | \cdots | a_n]$, can orthogonalize $\{a_i\}$ using Gram-Schmidt.

$$q_1 = a_1 / \|a_1\|$$

$$\hat{q}_2 = a_2 - (q_1^* a_2) q_1$$

$$q_2 = \hat{q}_2 / \|\hat{q}_2\|$$

$$\vdots$$

$$\hat{q}_k = a_k - \sum_{j=1}^{k-1} (q_j^* a_k) q_j$$

$$q_k = \hat{q}_k / \|\hat{q}_k\|$$

$$\|\hat{q}_k\| q_k + \sum_{j=1}^{k-1} (q_j^* a_k) q_j = a_k$$

$$\Rightarrow \underbrace{\begin{bmatrix} | & | & & | \\ q_1 & q_2 & \cdots & q_n \\ | & | & & | \end{bmatrix}}_{Q} \underbrace{\begin{bmatrix} \|\hat{q}_1\| & q_1^* a_2 & q_1^* a_3 & \cdots \\ & \|\hat{q}_2\| & \cdots & \\ & & \ddots & \end{bmatrix}}_{R} = \underbrace{\begin{bmatrix} | & | & & | \\ a_1 & a_2 & \cdots & a_n \\ | & | & & | \end{bmatrix}}_{A}$$

This is "classical" Gram-Schmidt.

Main problem: numerical roundoff in

$$\hat{q}_k = a_k - \sum_{j=1}^{k-1} (q_j^* a_k) q_j$$

Example: suppose ε is a small number, with $1+\varepsilon^2 \approx 1$ (= 1 in floating pt. arithmetic)

Consider $A = \begin{bmatrix} 1 & 1 & 1 \\ \varepsilon & & \\ & \varepsilon & \\ & & \varepsilon \end{bmatrix}$. What happens if we apply classical GS?

$$\hat{q}_1 = a_1 = \begin{bmatrix} 1 \\ \varepsilon \\ 0 \\ 0 \end{bmatrix}, \quad q_1 = \frac{\hat{q}_1}{\underbrace{\|\hat{q}_1\|}_{\sqrt{1^2+\varepsilon^2}=1}} = \begin{bmatrix} 1 \\ \varepsilon \\ 0 \\ 0 \end{bmatrix}$$

$$\hat{q}_2 = a_2 - (a_2^* q_1) q_1$$
$$= \begin{bmatrix} 1 \\ 0 \\ \varepsilon \\ 0 \end{bmatrix} - q_1 \underbrace{\begin{bmatrix} 1 \\ \varepsilon \\ 0 \\ 0 \end{bmatrix}^* \begin{bmatrix} 1 \\ 0 \\ \varepsilon \\ 0 \end{bmatrix}}_{1} = \begin{bmatrix} 1 \\ 0 \\ \varepsilon \\ 0 \end{bmatrix} - \begin{bmatrix} 1 \\ \varepsilon \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ -\varepsilon \\ \varepsilon \\ 0 \end{bmatrix}$$

$$q_1^* \hat{q}_2 = \begin{bmatrix} 1 \\ \varepsilon \\ 0 \\ 0 \end{bmatrix}^* \begin{bmatrix} 0 \\ -\varepsilon \\ \varepsilon \\ 0 \end{bmatrix} = -\varepsilon^2$$

= kind of orthogonal?

$$q_2 = \hat{q}_2 / \|\hat{q}_2\|, \quad \|\hat{q}_2\| = \sqrt{\varepsilon^2+\varepsilon^2} = \sqrt{2}\,\varepsilon$$

$$q_2 = \begin{bmatrix} 0 \\ -1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \end{bmatrix} \qquad q_1^* q_2 = \begin{bmatrix} 1 \\ \varepsilon \\ 0 \\ 0 \end{bmatrix}^* \begin{bmatrix} 0 \\ -1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \end{bmatrix} = \frac{-1}{\sqrt{2}}\varepsilon$$

$$\hat{q}_3 = a_3 - (a_3^* q_1) q_1 - \cancel{(a_3^* q_2)}^{\,0} q_2$$
$$= \begin{bmatrix} 1 \\ 0 \\ 0 \\ \varepsilon \end{bmatrix} - \begin{bmatrix} 1 \\ 0 \\ 0 \\ \varepsilon \end{bmatrix}^* \begin{bmatrix} 1 \\ \varepsilon \\ 0 \\ 0 \end{bmatrix} q_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \varepsilon \end{bmatrix} - \begin{bmatrix} 1 \\ \varepsilon \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ -\varepsilon \\ 0 \\ \varepsilon \end{bmatrix}$$

$$q_3 = \begin{bmatrix} 0 \\ -1/\sqrt{2} \\ 0 \\ 1/\sqrt{2} \end{bmatrix}$$

$$q_1 = \begin{bmatrix} 1 \\ \varepsilon \\ 0 \\ 0 \end{bmatrix}, \quad q_2 = \begin{bmatrix} 0 \\ -1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \end{bmatrix}, \quad q_3 = \begin{bmatrix} 0 \\ -1/\sqrt{2} \\ 0 \\ 1/\sqrt{2} \end{bmatrix}$$

$$q_1^* q_2 = O(\varepsilon) \qquad q_2^* q_3 = -\frac{1}{2}$$

$$q_1^* q_3 = O(\varepsilon)$$

"Modified" Gram-Schmidt : main fix

$$\hat{q}_k = a_k - \underbrace{(q_1^* a_k)}_{r_{1,k}} q_1 - \underbrace{(q_2^* a_k)}_{r_{2,k}} q_2 - \cdots \underbrace{(q_{k-1}^* a_k)}_{r_{k-1,k}} q_{k-1}$$

$$r_{jk} = q_j^* a_k = q_j^* (a_k - r_{1k} q_1 - r_{2k} q_2 - \cdots r_{j-1,j}\, q_{j-1})$$

$$= q_j^* (a_k - q_{j-1})$$

Since $q_j \perp q_1, q_2, \ldots, q_{j-1}$

b/c $q_j^* q_{j-1} = 0$

Classical GS : given $\{a_j\}$,

for $k = 1:n$

$\quad \hat{q}_k = a_k$

$\quad$ for $j = 1:k-1$

$\quad\quad \hat{q}_k = \hat{q}_k - (q_j^* a_k) q_j$

$\quad q_k = \hat{q}_k / \|\hat{q}_k\|$

Modified GS : $\hat{q}_k = a_k$, $k = 1, \ldots, n$

for $j = 1:n$

$\quad r_{jj} = \|\hat{q}_j\|$

$\quad q_j = \hat{q}_j / r_{jj}$

$\quad$ for $k = j+1, \ldots, n$

$\quad\quad r_{jk} = q_j^* \hat{q}_k$

$\quad\quad \hat{q}_k = \hat{q}_k - r_{jk} q_j$

r_{jk} "absorb" numerical losses of orthogonality,

$$\hat{q}_k = \underbrace{\underbrace{\underbrace{a_k - q_1(q_1^* a_k)}_{q_k^{(1)}} - q_2(q_2^* a_k)}_{q_k^{(2)}} - q_3(q_3^* a_k)}_{q_k^{(3)}} - \cdots$$

$$q_k^{(1)} = a_k - q_1(q_1^* a_k)$$
$$q_k^{(2)} = q_k^{(1)} - q_2(q_2^* q_k^{(1)}) \rightsquigarrow \text{vs } (q_2^* a_k)$$
$$q_k^{(3)} = q_k^{(2)} - q_2(q_3^* q_k^{(2)}) \rightsquigarrow \text{vs } (q_3^* a_k)$$

Orthogonalizes against roundoff errors in $q_k^{(j)}$ $(j<k)$

<u>Example:</u> $A = \begin{bmatrix} 1 & 1 & 1 \\ \varepsilon & & \\ & \varepsilon & \\ & & \varepsilon \end{bmatrix}$ $\quad q_1 = \begin{bmatrix} 1 \\ \varepsilon \\ 0 \\ 0 \end{bmatrix}$

$q_2 = \begin{bmatrix} 0 \\ -1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \end{bmatrix}$

$$\hat{q}_3^{(1)} = a_3 - (q_1^* a_3) q_1 \longrightarrow \begin{bmatrix} 1 \\ 0 \\ 0 \\ \varepsilon \end{bmatrix} - \begin{bmatrix} 1 \\ \varepsilon \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ -\varepsilon \\ 0 \\ \varepsilon \end{bmatrix}$$
$$\hat{q}_3^{(2)} = \hat{q}_3^{(1)} - (q_2^* \hat{q}_3^{(1)}) q_2$$

$$\rightarrow \begin{bmatrix} 0 \\ -1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \end{bmatrix}^* \begin{bmatrix} 0 \\ -\varepsilon \\ 0 \\ \varepsilon \end{bmatrix} = \varepsilon/\sqrt{2}$$

$$\hat{q}_3^{(2)} = \begin{bmatrix} 0 \\ -\varepsilon \\ 0 \\ \varepsilon \end{bmatrix} - \varepsilon/\sqrt{2} \begin{bmatrix} 0 \\ -1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ -\varepsilon \\ 0 \\ \varepsilon \end{bmatrix} + \begin{bmatrix} 0 \\ \varepsilon/2 \\ -\varepsilon/2 \\ 0 \end{bmatrix}$$

$$\hat{q}_3^{(2)} = \begin{bmatrix} 0 \\ \varepsilon/2 \\ -\varepsilon/2 \\ \varepsilon \end{bmatrix}, \quad q_3 = \begin{bmatrix} 0 \\ -1/\sqrt{6} \\ -1/\sqrt{6} \\ \sqrt{2/3} \end{bmatrix}$$

$$q_2^* q_3 = \begin{bmatrix} 0 \\ -1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \end{bmatrix}^* \begin{bmatrix} 0 \\ -1/\sqrt{6} \\ -1/\sqrt{6} \\ \sqrt{2/3} \end{bmatrix} = 0$$

Same cost $O(n^3)$

Note: need modifications if $A \in \mathbb{R}^{m \times n}$ but $\text{rank}(A) < n$

$\Rightarrow$ rank deficient matrix

$$\begin{bmatrix} | & & | & & | \\ a_1 & \cdots & a_k & \cdots & a_n \\ | & & | & & | \end{bmatrix} \qquad \tilde{q}_k = 0$$

$$q_k = \frac{0}{0}$$

a_k = linearly dep. on $a_1, \ldots, a_{k-1}$

$\Rightarrow$ can avoid by permuting / ignoring $\tilde{q}_k$ (pivoting)

QR: solving linear systems. $A \in \mathbb{R}^{n \times n}$

$Q \in \mathbb{R}^{n \times n}$, $R \in \mathbb{R}^{n \times n}$ $QR = A$

$Ax = b \Rightarrow QRx = b$ since $Q^*Q = I$

$\Rightarrow Rx = Q^*b = y$

Solve via backsubstitution

$$\begin{bmatrix} r_{11} & r_{12} & \cdots & \cdots \\ & r_{22} & r_{23} & \cdots \\ & & r_{33} & \cdots \\ & 0 & & \ddots \\ & & & r_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} y_1 \\ \vdots \\ \\ y_n \end{bmatrix}$$

$$\left.\begin{array}{l} ① \quad r_{nn} x_n = y_n \Rightarrow x_n = \frac{y_n}{r_{nn}} \\ ② \quad r_{n-1,n-1} x_{n-1} + r_{n-1,n} x_n = y_{n-1} \\ \quad \Rightarrow x_{n-1} = \frac{y_{n-1} - x_n r_{n-1,n}}{r_{n-1,n-1}} \\ ⓙ \quad x_j = \frac{1}{r_{jj}} \left(y_j - \sum_{k=j+1}^{n} r_{jk} x_k \right) \end{array}\right\} O(n^2) \text{ operations}$$

$$\left.\begin{array}{lcl} A = QR & = & O(n^3) \\ \text{Mult. by } Q^* & = & O(n^2) \\ \text{Backsub} & = & O(n^2) \end{array}\right\}$$

If you need

$Ax_i = b_i \quad i = 1, \dots, 100$

$\Rightarrow$ compute QR once

& use Q^* & backsubs.

QR very suitable for matrix least square problems!

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

Cannot solve $Ax = b$ exactly

$$\Rightarrow \min \|Ax - b\|^2$$

$$\Rightarrow A^T A x = A^T b.$$

(sub in $A = QR$)

$$(QR)^T(QR)x = (QR)^T b$$

$$R^T \underbrace{Q^T Q}\, R x = R^T Q^T b$$

$$R^T(Rx) = R^T(Q^T b)$$

$$\Rightarrow \quad Rx = Q^T b$$