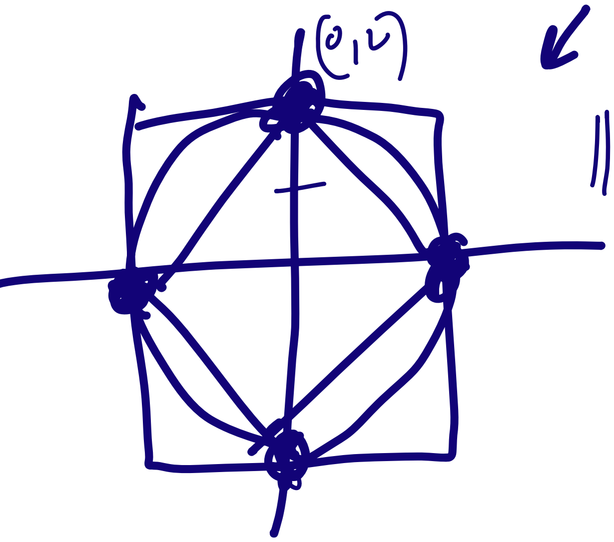
$\|A\|_2 = \sigma_1$

A

$A^T A$



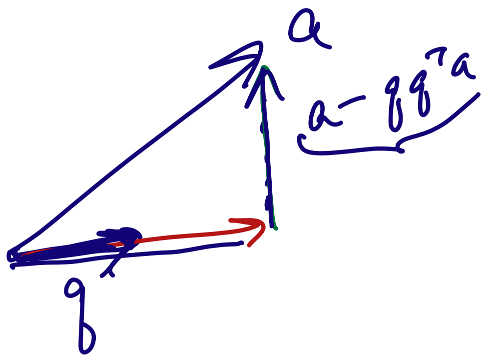
$\|v\| = 2 = 2\|\hat{v}\|$

QR decomposition

Gram-Schmidt orthogonalization

Householder QR

$\vec{a}$



$\boxed{(\vec{q}\,\vec{q}^T)\vec{a}}$

$\vec{q}\,\underbrace{(\vec{q}^T\vec{a})}$

$\underline{P = qq^T}$

$$a - qq^Ta = \boxed{\underbrace{(I - qq^T)}_{P^\perp}a} = \underbrace{P^\perp a}$$

$$q^T(P^\perp a) = q^T(I - qq^T)a \qquad q^Tq = 1$$

$$= (q^T - \underbrace{q^Tq}_{=1}q^T)a$$

$$= (q^T - q^T)a = 0 \checkmark$$

$$q \cdot (I - q\underline{q^T})a = 0$$

orthonormal basis for $\mathbb{R}^n$ $\{q_1, q_2, \ldots, q_n\}$

$$q_i \cdot q_j = \delta_{ij} = \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases}$$

$\vec{a}$

$$a = \underbrace{(q_1^T a)}\, q_1 + \underbrace{(q_2^T a)}\, q_2 + \cdots + \underbrace{(q_n^T a)}\, q_n$$

$$q \cdot (I - qq^T)a$$

$$\underline{q_1}^T \boxed{(I - \underline{q_1 q_1^T} - \underline{q_2 q_2^T})a} = 0$$

$$\underline{q_2}^T (\qquad\qquad)a = 0$$

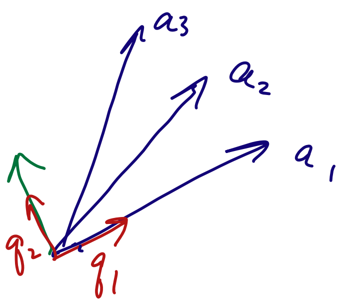
$$A = \begin{bmatrix} | & & | \\ a_1 & \cdots & a_n \\ | & & | \end{bmatrix}$$

$$Q = \begin{bmatrix} | & & | \\ q_1 & \cdots & q_n \\ | & & | \end{bmatrix}$$

$$\left\{\begin{array}{l} \to \operatorname{span}(q_1) = \operatorname{span}(a_1) \\ \to \operatorname{span}(q_1, q_2) = \operatorname{span}(a_1, a_2) \\ \quad \vdots \qquad\qquad\qquad \vdots \\ \to \operatorname{span}(q_1, \cdots q_n) = \operatorname{span}(a_1, \cdots, a_n) \end{array}\right.$$

$$q_i^T q_j = \delta_{ij} \qquad q_i \text{ orthonormal set}$$

$$\left.\begin{array}{ll} v_1 = a_1 & q_1 = \dfrac{v_1}{\|v_1\|} \\ v_2 = a_2 - (q_1^T a_2) q_1 & q_2 = \dfrac{v_2}{\|v_2\|} \\ v_3 = a_3 - (q_1^T a_3) q_1 - (q_2^T a_3) q_2 & q_3 = \dfrac{v_3}{\|v_3\|} \\ \vdots & \\ v_n = a_n - (q_1^T a_n) q_1 \cdots - (q_{n-1}^T a_n) q_{n-1} & q_n = \dfrac{v_n}{\|v_n\|} \end{array}\right\}$$



$$\boxed{\to q_1, q_2, \ldots, q_n}$$

$$\operatorname{span}(q_1) = \operatorname{span}(a_1)$$

$$\operatorname{span}(q_1, q_2) = \operatorname{span}(a_1, a_2)$$

$$\vdots$$

$$\operatorname{span}(q_1, \dots, q_n) = \operatorname{span}(a_1, \dots, a_n)$$

$$A = QR \; ?$$

R upper triangular

$$\begin{pmatrix} | & | & & | \\ a_1 & a_2 & \cdots & a_n \\ | & | & & | \end{pmatrix} = \begin{pmatrix} | & & | \\ q_1 & \cdots & q_n \\ | & & | \end{pmatrix} \begin{pmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ 0 & r_{22} & \cdots & r_{2n} \\ 0 & 0 & \ddots & \vdots \\ \vdots & & \ddots & r_{nn} \\ 0 & \cdots & 0 & \end{pmatrix}$$

$$\begin{pmatrix} | & & | \\ r_1 & \cdots & r_n \\ | & & | \end{pmatrix}$$

$$a_1 = Q r_1$$

$$\vdots$$

$$a_n = Q r_n$$

$$\begin{cases} a_1 = r_{11} q_1 \\ a_2 = r_{12} q_1 + r_{22} q_2 \end{cases}$$

$$\begin{cases} \vdots \\ a_n = r_{1n} q_1 + r_{2n} q_2 + \dots + r_{nn} q_n \end{cases}$$

$$\begin{cases} V_1 = a_1 & q_1 = \dfrac{V_1}{\|V_1\|} & \Rightarrow V_1 = r_{11} q_1 \\ V_2 = a_2 - (q_1^T a_2) q_1 & q_2 = \dfrac{V_2}{\|V_2\|} & V_2 = r_{22} q_2 \\ V_3 = a_3 - \underbrace{(q_1^T a_3) q_1 - (q_2^T a_3) q_2} & q_3 = \dfrac{V_3}{\|V_3\|} & \\ \vdots & & \\ V_n = a_n - (q_1^T a_n) q_1 \dots - (q_{n-1}^T a_n) q_{n-1} & q_n = \dfrac{V_n}{\|V_n\|} & V_n = r_{nn} q_n \end{cases}$$

$$a_1 = r_{11} q_1$$

$$a_2 = r_{22} q_2 + \underbrace{(q_1^T a_2)}_{= r_{12}} q_1$$

$$a_3 = r_{33} q_3 + \underbrace{(q_1^T a_3)}_{= r_{13}} q_1 + \underbrace{(q_2^T a_3)}_{r_{23}} q_2$$

$$\vdots$$

$$a_n = r_{nn} q_n + \underbrace{(q_1^T a_n)}_{r_{1n}} q_1 + \dots + \underbrace{(q_{n-1}^T a_n)}_{r_{n-1,n}} q_{n-1}$$

(Classical) Gram-Schmidt + QR

for $j = 1, \ldots, n$

$\quad v_j = a_j$

$\quad$ for $k = 1, \ldots, j-1$

$\quad\quad r_{kj} = q_k^T a_j$

$\quad\quad v_j \leftarrow v_j - r_{kj} q_k$

$\quad$ end

$\quad r_{jj} = \| v_j \|$

$\quad q_j = v_j / r_{jj}$

end

$$\boxed{A = QR}$$

uses:

- least squares
- eigenvalue problems

modified Gram-Schmidt

for $j = 1, \ldots, n$

$\quad v_j = a_j$

$\quad$ for $k = 1, \ldots, j-1$

$\quad\quad r_{kj} = \cancel{q_k^T a_j}$ $q_k^T v_j$

$\quad\quad v_j \leftarrow v_j - r_{kj} q_k$

$\quad$ end

$\quad r_{jj} = \| v_j \|$

$\quad q_j = v_j / r_{jj}$

end

$$\left(I - q_1q_1^T - q_2q_2^T\right) a_3 \qquad q_j^T a_3$$

$$\left(I - q_2q_2^T\right)\underbrace{\left(I - q_1q_1^T\right) a_3}_{v_3}$$

* more numerically stable for larger, ill-conditioned A

Modified G-S

$V = A$

for $j = 1, \ldots, n$

$\quad r_{jj} = \|a_j\|$

$\quad q_j = v_j / r_{jj}$

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

$\quad\quad r_{jk} = \boxed{q_j^T v_k}$

$\quad\quad v_k \leftarrow v_k - r_{jk} q_j$

end

end

$$A = QR$$

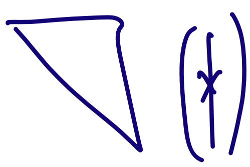
$$\boxed{Ax = b}$$

$$\boxed{QR}x = b \qquad Q^{-1} = Q^T$$

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

$$Rx = Q^T b$$

back substitution



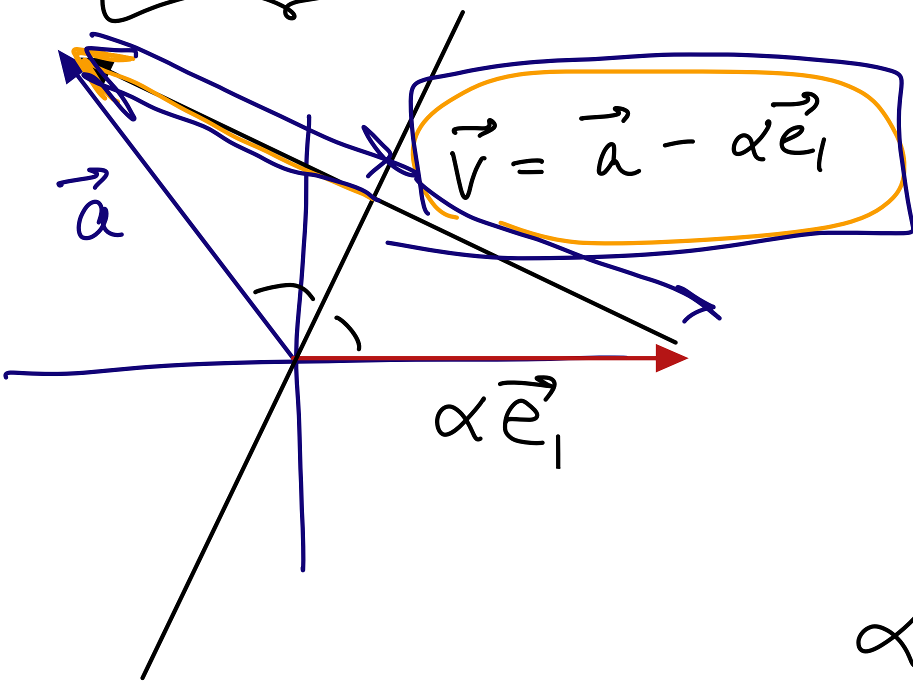
Householder reflections

Householder matrix

$$\underbrace{H^T H = I}$$

$$e_1 = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \qquad \alpha e_1 = \begin{pmatrix} \alpha \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

$$\alpha = \|\vec{a}\|$$

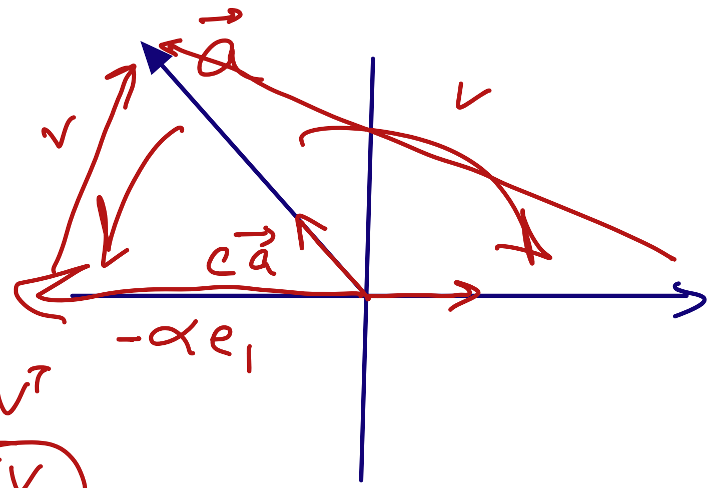


$$H\vec{a} = \alpha\vec{e}_1$$

$$H\vec{a} = \vec{a} - 2\left(\frac{\vec{v}\vec{v}^T}{\vec{v}^T\vec{v}}\right)\vec{a}$$

$$H\vec{a} = \underbrace{\left(I - 2\frac{\vec{v}\vec{v}^T}{\vec{v}^T\vec{v}}\right)}\vec{a}$$

$$\begin{cases} H \text{ orthogonal} & \checkmark \\ Ha = \alpha e_1 & \checkmark \end{cases}$$



practical points:

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

$$v = a - \alpha e_1$$

$$a^Ta$$

① $\vec{a} \leftarrow \boxed{\dfrac{\vec{a}}{\max_i |a_i|}}$ avoid overflow

② $\alpha = -\operatorname{sign}(a_1)$

avoid small $\vec{v}$