# QR factorization

(Gram-Schmidt orthogonalization)

① Least squares
Regression problem

② Eigenvalues and Eigenvectors of Large scale Symmetric/Hermitian matrices

③ SVD uses bi-diagonalization techniques and have an underlying EVP to solve.

④ Solve linear system of equations!

## Reduced QR factorization!

$$\underset{\sim}{A} = \begin{bmatrix} | & | & & | \\ \underset{\sim}{a_1} & \underset{\sim}{a_2} & \cdots & \underset{\sim}{a_n} \\ | & | & & | \end{bmatrix}_{m \times n}$$ and a full rank matrix

Spaces spanned by the columns of $\underset{\sim}{A}$ in succession

$$\underbrace{\langle a_1 \rangle} \subseteq \underbrace{\langle \underset{\sim}{a_1}, \underset{\sim}{a_2} \rangle} \subseteq \underbrace{\langle \underset{\sim}{a_1}, \underset{\sim}{a_2}, a_3 \rangle} \subseteq \cdots$$

are called successive column spaces of $\underset{\sim}{A}$

i.e $\langle \underset{\sim}{a}_1 \rangle$ is 1D space spanned by $\underset{\sim}{a}_1$ and $\langle \underset{\sim}{a}_1, \underset{\sim}{a}_2 \rangle$ is 2D space spanned by $\underset{\sim}{a}_1, \underset{\sim}{a}_2$ and so on.

The idea behind QR factorization is to successively construct orthonormal vectors $\underset{\sim}{q}_1, \underset{\sim}{q}_2, \ldots \underset{\sim}{q}_n$ that span these successive column spaces of $\underset{\sim}{A}$ as described before.

" Let $\underset{\sim}{A} \in \mathbb{R}^{m \times n}$ $(m \geq n)$ have full rank $n$, we want to find $\langle \underset{\sim}{q}_1, \underset{\sim}{q}_2, \ldots \underset{\sim}{q}_n \rangle$ orthonormal vectors such that

$$\langle \underset{\sim}{q}_1, \underset{\sim}{q}_2, \ldots \underset{\sim}{q}_j \rangle = \langle \underset{\sim}{a}_1, \underset{\sim}{a}_2, \ldots \underset{\sim}{a}_j \rangle$$

for $j = 1, 2, \ldots n$

$$\left.\begin{aligned}
\underset{\sim}{a}_1 &= r_{11} \underset{\sim}{q}_1 \\
\underset{\sim}{a}_2 &= r_{12} \underset{\sim}{q}_1 + r_{22} \underset{\sim}{q}_2 \\
\underset{\sim}{a}_3 &= r_{13} \underset{\sim}{q}_1 + r_{23} \underset{\sim}{q}_2 + r_{33} \underset{\sim}{q}_3
\end{aligned}\right\}$$

$\vdots$

$$\underset{\sim}{a_n} = r_{1n}\underset{\sim}{q_1} + r_{2n}\underset{\sim}{q_2} + \dots r_{nn}\underset{\sim}{q_n} \quad )$$

$$\begin{bmatrix} | & | & | & & | \\ \underset{\sim}{a_1} & \underset{\sim}{a_2} & a_3 & \cdots & a_n \\ | & | & | & & | \end{bmatrix} = \begin{bmatrix} | & | & & | \\ \underset{\sim}{q_1} & \underset{\sim}{q_2} & \cdots & \underset{\sim}{q_n} \\ | & | & & | \end{bmatrix} \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ & r_{22} & \cdots & r_{2n} \\ & & \ddots & \vdots \\ & & & r_{nn} \end{bmatrix}$$

$\underset{\sim}{A}$ $m \times n$ $\qquad \hat{Q}$ $m \times n$ $\quad \hat{R}$ $n \times n$

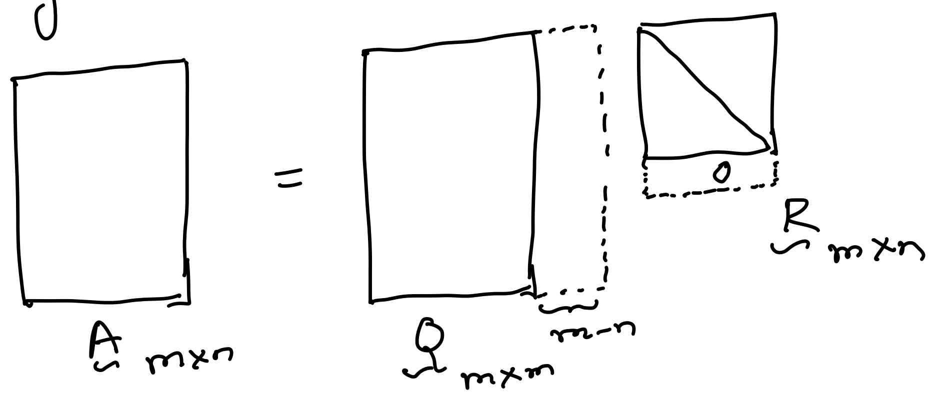
where $r_{kk} \neq 0$ for $k = 1 \dots n$

$\underset{\sim}{A} = \underset{\sim}{\hat{Q}}\,\underset{\sim}{\hat{R}}$ is called reduced QR factorization of $\underset{\sim}{A}$ where $\hat{Q} \in \mathbb{R}^{m \times n}$ matrix having $n$ orthonormal columns and $\hat{R} \in \mathbb{R}^{n \times n}$ is upper triangular matrix.

## Full $\underset{\sim}{Q}\underset{\sim}{R}$ factorization

A full QR factorization of $\underset{\sim}{A} \in \mathbb{R}^{m \times n}$

$(m \geq n)$ appends an additional $(m-n)$ orthonormal columns to $\hat{Q}$ to make it an $m \times m$ orthogonal matrix. $(m-n)$ rows of zeros are appended to $\hat{R}$ making it $m \times n$ matrix $\underset{\sim}{R}$




In full QR, the additional columns $\underset{\sim}{q_j}$ $(j > n)$ are orthogonal to range$(A)$

If $\underset{\sim}{A}$ had full rank, these additional are orthonormal basis for range$(A)^{\perp}$ (i.e the space orthogonal to range$(A)$ or equivalently to null$(A^T)$)

# Gram - Schmidt orthogonalization :-

Given $\underset{\sim}{a}_1, \underset{\sim}{a}_2, \dots \underset{\sim}{a}_n$ (linearly independent vectors)

and we want to build

$\underset{\sim}{q}_1, \underset{\sim}{q}_2, \dots \underset{\sim}{q}_n$ and entries

$r_{ij}$ by successive orthogonalization

At step $j$, we want a unit-vector

$\underset{\sim}{q}_j \in \langle \underset{\sim}{a}_1, \underset{\sim}{a}_2, \dots a_j \rangle \qquad j = 1 \dots n$

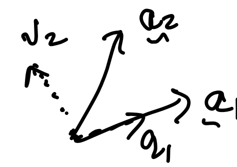
that is orthogonal to

$\langle \underset{\sim}{q}_1, \underset{\sim}{q}_2, \dots \underset{\sim}{q}_{j-1} \rangle$

Take a vector $\underset{\sim}{a}_j$

$$\underset{\sim}{V}_j = \underset{\sim}{a}_j - (\underset{\sim}{q}_1^T \underset{\sim}{a}_j)\, \underset{\sim}{q}_1 - (q_2^T a_j)\, \underset{\sim}{q}_2 \dots\dots$$

We divide $\underset{\sim}{V}_j$ by $\|V_j\|_2$ and we get our $\underset{\sim}{q}_j$




$$\underset{\sim}{q}_1 = \frac{\underset{\sim}{a}_1}{\|\underset{\sim}{a}_1\|}$$

$$\underset{\sim}{a}_2 = (\underset{\sim}{q}_1^T \underset{\sim}{a}_1)\, \underset{\sim}{q}_1 + \underset{\sim}{V}_2$$

$$\underset{\sim}{V}_2 = \underset{\sim}{a}_2 - (\underset{\sim}{q}_1^T \underset{\sim}{a}_2)\, \underset{\sim}{q}_1$$

$$\underset{\sim}{q}_2 = \frac{\underset{\sim}{V}_2}{\|\underset{\sim}{V}_2\|}$$

$$\underset{\sim}{q}_1 = \frac{\underset{\sim}{a}_1}{r_{11}} \; ; \; q_2 = \frac{\underset{\sim}{a}_2 - r_{12}\underset{\sim}{q}_1}{r_{22}} \; ;$$

$$\underset{\sim}{q}_3 = \frac{\underset{\sim}{a}_3 - r_{13}\underset{\sim}{q}_1 - r_{23}\underset{\sim}{q}_2}{r_{33}}$$

$$\vdots$$

$$\underset{\sim}{q}_n = \frac{\underset{\sim}{a}_n - \sum_{i=1}^{n-1} r_{in}\underset{\sim}{q}_i}{r_{nn}}$$

where $\quad r_{ij} = \underset{\sim}{q}_i^T \underset{\sim}{a}_j \quad (i \neq j)$

$$|r_{jj}| = \|\underset{\sim}{a}_j - \sum_{\underbrace{i=1}}^{j-1} r_{ij}\underset{\sim}{q}_i\|$$

<u>Algo</u> :-

for $j = 1$ to $n$

$\quad \underset{\sim}{v}_j = \underset{\sim}{a}_j$

$\quad$ for $i = 1$ to $j-1$

$\quad\quad r_{ij} = \underset{\sim}{q}_i^T \underset{\sim}{a}_j$

$\quad\quad \underset{\sim}{v}_j = \underset{\sim}{v}_j - r_{ij}\underset{\sim}{q}_i$

$\quad r_{jj} = \|\underset{\sim}{v}_j\|_2 \; ; \; q_j = v_j / r_{jj}$

## Existence and uniqueness:-

**Thm:-** Every matrix $A \in \mathbb{R}^{m \times n}$ $(m \geq n)$ has a full QR factorization and hence also reduced QR factorization!

**Thm:-** Every $A \in \mathbb{R}^{m \times n}$ $(m \geq n)$ of full rank has a unique reduced QR factorization $A = \hat{Q}\hat{R}$ with $r_{jj} > 0$

## Solution of $Ax = b$ :-

$A \in \mathbb{R}^{m \times m}$ is non singular

$$Ax = b$$

Construct QR factorization of $A = QR$ $\Rightarrow$ $QRx = b$

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

Solve $Rx = y$ for $x$

$$\begin{bmatrix} * & \cdots & * \\ & \ddots & \vdots \\ & & * \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_m \end{bmatrix} = \begin{pmatrix} y_1 \\ \vdots \\ y_m \end{pmatrix}$$

GS algo is one of the algorithms for QR factorization!

$\underset{\sim}{A} \in \mathbb{R}^{m \times n}$ $(m \geq n)$ has full rank!

$$\underset{\sim}{q_1} = \frac{\underset{\sim}{a_1}}{r_{11}} \; ; \; \underset{\sim}{q_2} = \frac{\underset{\sim}{a_2} - r_{12} \underset{\sim}{q_1}}{r_{22}}$$

$$\underset{\sim}{q_3} = \frac{\underset{\sim}{a_3} - r_{13} \underset{\sim}{q_1} - r_{23} \underset{\sim}{q_2}}{r_{33}}$$

$$\vdots$$

$$\underset{\sim}{q_n} = \frac{\underset{\sim}{a_n} - \sum_{i=1}^{n-1} r_{in} \underset{\sim}{q_i}}{r_{nn}}$$

(1) $\underset{\sim}{q_1} = \frac{\underset{\sim}{a_1}}{r_{11}} = \frac{\underset{\sim}{P_1} \underset{\sim}{a_1}}{\| \underset{\sim}{P_1} \underset{\sim}{a_1} \|}$ where $\underset{\sim}{P_1} = \underset{\sim}{I}$

(2) $\underset{\sim}{q_2} = \frac{\underset{\sim}{a_2} - r_{12} \underset{\sim}{q_1}}{r_{22}} = \frac{\underset{\sim}{a_2} - (\underset{\sim}{q_1}^T \underset{\sim}{a_2}) \underset{\sim}{q_1}}{r_{22}}$

$$= \frac{\underset{\sim}{a_2} - (\underset{\sim}{q_1} \underset{\sim}{q_1}^T) \underset{\sim}{a_2}}{r_{22}}$$

$$= \frac{(\underset{\sim}{I} - \underset{\sim}{q_1} \underset{\sim}{q_1}^T) \underset{\sim}{a_2}}{r_{22}} = \frac{\underset{\sim}{P_2} \underset{\sim}{a_2}}{\| \underset{\sim}{P_2} \underset{\sim}{a_2} \|}$$

where $\underset{\sim}{P}_2 = \underset{\sim}{I} - \underset{\sim}{q}_1 \underset{\sim}{q}_1^T$

(3) $$\underset{\sim}{q}_3 = \frac{\underset{\sim}{a}_3 - r_{13}\underset{\sim}{q}_1 - r_{23}\underset{\sim}{q}_2}{r_{33}}$$

$$= \frac{\underset{\sim}{a}_3 - (\underset{\sim}{q}_1 \underset{\sim}{q}_1^T)\underset{\sim}{a}_3 - (\underset{\sim}{q}_2 \underset{\sim}{q}_2^T)\underset{\sim}{a}_3}{r_{33}}$$

$$= \frac{(\underset{\sim}{I} - \underset{\sim}{q}_1 \underset{\sim}{q}_1^T - \underset{\sim}{q}_2 \underset{\sim}{q}_2^T)\underset{\sim}{a}_3}{r_{33}} = \frac{\underset{\sim}{P}_3 \underset{\sim}{a}_3}{r_{33}}$$

$\vdots$

(4) $$\underset{\sim}{q}_n = \frac{\underset{\sim}{P}_n \underset{\sim}{a}_n}{\|\underset{\sim}{P}_n \underset{\sim}{a}_n\|}$$

$\underset{\sim}{P}_j = \underset{\sim}{I} - \hat{Q}_{j-1} \hat{Q}_{j-1}^T$ where

$$\hat{Q}_{j-1} = \left[\underset{\sim}{q}_1 \,\middle|\, \underset{\sim}{q}_2 \,\middle|\, \cdots \,\middle|\, \underset{\sim}{q}_{j-1}\right]$$

**Remark :-**

Each $\underset{\sim}{P}_j \in \mathbb{R}^{m\times m}$ is the matrix of rank $m-(j-1)$ that projects a vector in $\mathbb{R}^m$ onto a space orthogonal to $\langle \underset{\sim}{q_1}, \underset{\sim}{q_2}, \dots \underset{\sim}{q_{j-1}} \rangle$

Classical Gram-Schmidt is unstable numerically!

i.e loss of orthogonality occurs because of round off error accumulation!

<u>Algo for</u> CGS:-

Compute single orthogonal projection

$$\underset{\sim}{v_j} = \underset{\sim}{P_j}\, \underset{\sim}{a_j}$$

<u>Modified</u> GS :-

We get the same result by a sequence of $(j-1)$ projectors of rank $m-1$

$\underset{\sim}{P_{\perp q}}$ denotes $(m-1)$ rank orthogonal projector onto space orthogonal to non-zero vector $\underset{\sim}{q} \in \mathbb{R}^m$

$$\boxed{\underset{\sim}{v}_j = \underset{\sim}{P}_j \underset{\sim}{a}_j} \quad \text{— ① (CGS)}$$

$$\underset{\sim}{P}_j = P_{\perp q_{j-1}} \cdots P_{\perp q_3} P_{\perp q_2} P_{\perp q_1}$$

$$\boxed{\underset{\sim}{v}_j = P_{\perp q_{j-1}} \cdots P_{\perp q_3} P_{\perp q_2} P_{\perp q_1} \underset{\sim}{a}_j} \quad \text{— ② (MGS)}$$

① and ② are equivalent mathematically but sequence of arithmetic operations are different!

## MGS Algo

for $j = 1$ to $n$

$$\underset{\sim}{v}_j^{(1)} = \underset{\sim}{a}_j$$

$$\underset{\sim}{v}_j^{(2)} = P_{\perp q_1} \underset{\sim}{a}_j = \underset{\sim}{v}_j^{(1)} - \underset{\sim}{q}_1 \underset{\sim}{q}_1^T v_j^{(1)}$$

$$v_j^{(3)} = P_{\perp q_2} v_j^{(2)} = v_j^{(2)} - \underset{\sim}{q}_2 \underset{\sim}{q}_2^T v_j^{(2)}$$

$$\vdots$$

$$v_j = v_j^{(j)} = P_{\perp q_{j-1}} v_j^{(j-1)}$$

$$v_j = v_j^{(j-1)} - q_{j-1} q_{j-1}^T v_j^{(j-1)}$$

In finite precision arithmetic, you can show MGS algo introduces smaller errors than CGS algo!

$$q_1 = \frac{a_1}{r_{11}} \; ; \; q_2 = \frac{a_2 - (q_1^T a_2) q_1}{r_{22}} \; ; \; q_3 = \left(a_3 - (q_1^T a_3) q_1 - (q_2^T a_3) q_2\right) / r_{33}$$

---

$$q_1^T q_2 = \delta$$

$$q_1^T q_3 = \frac{1}{r_{33}} \left[ \cancel{q_1^T a_3} - \cancel{q_1^T a_3} - (q_2^T a_3) \underbrace{(q_1^T q_2)}_{\delta} \right]$$

$$= \frac{-1}{r_{33}} q_2^T a_3 \, \delta$$

$$q_2^T q_3 = - \frac{(q_1^T a_3) \delta}{r_{33}}$$

$$q_4 = \left[ a_4 - (q_1^T a_4) q_1 - (q_2^T a_4) q_2 - (q_3^T a_4) q_3 \right] \frac{1}{r_{44}}$$

$$q_1^T q_4 = \left[ -(q_2^T a_4) \delta + \frac{(q_3^T a_4)(q_2^T a_3) \delta}{r_{33}} \right] \frac{1}{r_{44}} .$$

$$q_2^T q_4 = \left[ -(q_1^T a_4) \delta + \frac{(q_3^T a_4)(q_1^T a_3) \delta}{r_{33}} \right] \frac{1}{r_{44}} ,$$

$$q_3^T q_4 = \left[\frac{(q_1^T a_4)(q_2^T a_3)\,\delta}{r_{33}} + \frac{(q_1^T a_3)(q_2^T a_4)\,\delta}{r_{33}}\right]\frac{1}{r_{44}}$$

In MGS :-

$$v_3^{(3)} = v_3$$

$$v_3^{(3)} = v_3^{(2)} - q_2 q_2^T v_3^{(2)}$$

$$= v_3^{(2)} - \left(q_2^T v_3^{(2)}\right) q_2$$

$$q_2^T v_3 = q_2^T v_3^{(2)} - q_2^T v_3^{(2)} = 0 \quad \checkmark$$

$$q_1^T v_3 = q_1^T\left[v_3^{(2)} - (q_2^T v_3^{(2)})\, q_2\right]$$

$$= q_1^T v_3^{(2)} - q_2^T v_3^{(2)}\,\delta$$

$$q_1^T v_3^{(2)} = q_1^T\left[v_3^{(1)} - q_1 q_1^T v_3^{(1)}\right] = 0$$

$$q_2^T v_3^{(2)} = q_2^T\left[v_3^{(1)} - q_1 q_1^T v_3^{(1)}\right]$$

$$= q_2^T v_3^{(1)} - q_1^T v_3^{(1)}\,\delta$$

$$q_1^T v_3 = -\left[q_2^T v_3^{(1)} - q_1 v_3^{(1)}\,\delta\right]\delta$$

$$= -\, q_2^T v_3^{(1)} \delta + O(\delta^2)$$

$q_1^T v_3$ is no worse than CGS but no error in $q_2^T v_3$

$$v_4 = v_4^{(4)} = v_4^{(3)} - q_3 q_3^T v_4^{(3)}$$

$q_3^T v_4 = 0$ ; $q_2^T v_4 = 0$ ; $q_1^T v_4 = O(\delta)$ !

Exercise

<u>Operation count of G.S:-</u>

Any of addition, subtraction, multiplication are counted as 1 flop

<u>Thm</u>:- G.S orthogonalization requires $\sim 2mn^2$ flops to compute QR factorization!

<u>Remark</u>:- Symbol $\sim$ has the meaning representing of asymptotic complexity

i.e $\displaystyle \lim_{m,n\to\infty} \frac{\text{number of flops}}{2mn^2} = 1$

for $j = 1$ to $n$

$\quad \underset{\sim}{v}_j = \underset{\sim}{a}_j$

$\quad$ for $i = 1$ to $j-1$

$$\left.\begin{aligned} r_{ij} &= \underset{\sim}{q}_i^T \underset{\sim}{a}_j \checkmark \\ \underset{\sim}{v}_j &= \underset{\sim}{v}_j - r_{ij}\underset{\sim}{q}_i \checkmark \end{aligned}\right\}$$

$\quad r_{jj} = \|\underset{\sim}{v}_j\|_2$

$\quad \underset{\sim}{q}_j = \dfrac{\underset{\sim}{v}_j}{r_{jj}}$

$r_{ij} = \underset{\sim}{q}_i^T \underset{\sim}{a}_j$

$m$ multiplications $+ (m-1)$ additions

$\underset{\sim}{v}_j = \underset{\sim}{v}_j - r_{ij}\underset{\sim}{q}_i$

$m$ multiplications $+$ $m$ subtractions

Total work $\sim 4m$ flops

Total flops $\displaystyle \sim \sum_{j=1}^{n}\sum_{i=1}^{j-1} 4m$

$$\sim \sum_{j=1}^{n} (j-1)\,4m$$

$$\sim \left(\frac{n(n+1)}{2} - 1\right) 4m$$

$$\sim 2mn^2$$

# Householder triangularization :-

When it comes to produce orthogonality

how close $Q^T Q$ is close to identity

$\underbrace{\| \underset{\sim}{I} - \tilde{Q}^T \tilde{Q} \|}$

(a) CGS → usually poor orthogonality

(b) MGS → Dependeng on condition number of $\underset{\sim}{A}$ $K(\underset{\sim}{A})$

(c) Householder → good orthogonality better than MGS but dependents on $K(\underset{\sim}{A})$

→ Householder orthogonalization are popular for sequential dense matrices

→ Householder transformation has its application in algorithms for solving eigenvalue problem!

Key idea in Householder method is to apply succession of elementary orthogonal matrices $Q_K$ to the left of $A \in \mathbb{R}^{m \times n}$ so that resulting matrix is upper triangular.

$$\underbrace{Q_n \cdots Q_3 Q_2 Q_1}\, A = R \quad \text{upper triangular}$$

The product $Q = Q_1^T Q_2^T \cdots Q_n^T$ is orthogonal

$A = QR$ is full QR factorization of $A$

$$A = \begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix}_{5\times 3} \xrightarrow{Q_1} \begin{bmatrix} * & * & * \\ 0 & * & * \\ 0 & * & * \\ 0 & * & * \\ 0 & * & * \end{bmatrix}$$

$$Q_1 A$$

Orthogonal triangularization!

$$\Big\downarrow Q_2$$

$$\begin{bmatrix} \times & \times & * \\ & \times & * \\ & & * \\ & & 0 \\ & & 0 \end{bmatrix} \xleftarrow{Q_3} \begin{bmatrix} * & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \\ 0 & 0 & \times \\ 0 & 0 & \times \end{bmatrix}$$

$$Q_3 Q_2 Q_1 A \qquad\qquad Q_2 Q_1 A$$

Beginning of step 1, there are no zeros

" of step 2, block of zeros in first column

" of step 3, block of zeros in first 2 columns

⋮

step k, block of zeros in first (k-1) columns

After n steps, all entries below diagonal are zero!

<u>How to construct $Q_k$?</u>

Each $Q_k$ is chosen to be orthogonal matrix of the form

$$Q_k = \begin{bmatrix} I_{(k-1 \times k-1)} & 0 \\ 0 & F_{(m-k+1) \times (m-k+1)} \end{bmatrix}$$

$I_{(k-1)\times(k-1)} \rightarrow$ Identity matrix

$F \rightarrow (m-k+1) \times (m-k+1)$ orthogonal matrix

$\underset{\sim}{F}$ is chosen to be Householder reflector!

In our example before

$$\underset{\sim}{Q}_1 = \begin{bmatrix} \underset{\sim}{F} \end{bmatrix}_{5\times5}$$

$$\underset{\sim}{Q}_2 = \begin{bmatrix} 1 & 0 \\ 0 & \underset{\sim}{F}_{4\times4} \end{bmatrix}_{5\times5}$$

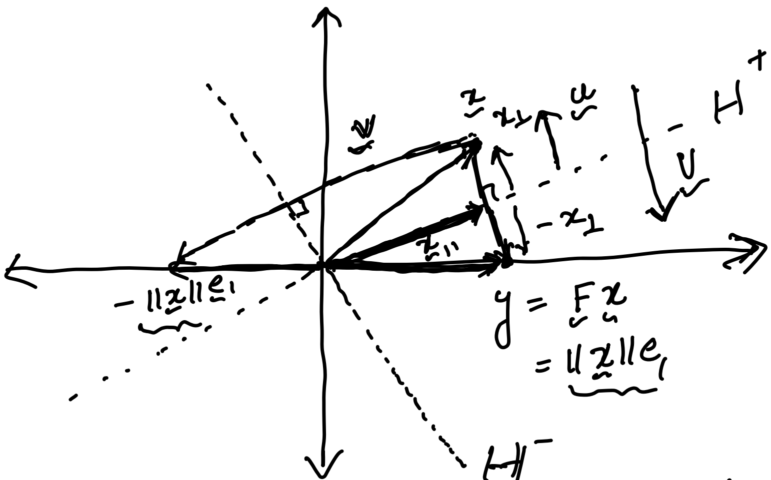
Suppose at beginning of step k the entries in the $k^{th}$ column $(k+1, \dots m)$ has to be zeroed

Let the entries $k, \dots m$ for a vector $\underset{\sim}{x} \in \mathbb{R}^{m-k+1}$

$$\underset{\sim}{x} = \begin{bmatrix} x \\ x \\ \vdots \\ x \end{bmatrix}_{m-k+1} \xrightarrow{\underset{\sim}{F}} \underset{\sim}{F}\underset{\sim}{x} = \begin{bmatrix} * \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

$$= \begin{bmatrix} \|\underset{\sim}{x}\| \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

[ Recall $\underset{\sim}{F}$ is orthogonal matrix so it cannot change norm) $\|\underset{\sim}{x}\| \underset{\sim}{e}_1$




$$x + v = \|x\| e_1$$

$$\boxed{v = \|x\| e_1 - x}$$

$v$ = reflection vector

$$x = x_\parallel + x_\perp$$

$$x_\perp = u u^T x$$

$$x_\parallel - x_\perp = y$$

$$y = (x_\parallel + x_\perp) - 2 x_\perp$$

$$= x - 2 u u^T x$$

$$u = -\frac{v}{\|v\|}$$

$$y = F x = (I - 2 u u^T) x$$

$$\boxed{F = I - 2 u u^T} \Rightarrow \boxed{F = I - 2 \frac{v v^T}{\|v\|^2}}$$

Infact we can also construct $F$ such that

$$F x = - \|x\| e_1$$

$$x + v = - \|x\| e_1$$

$$v = - \|x\| e_1 - x$$

Which reflection do we pick?

We better pick the one that is not too close to $\underset{\sim}{x}$

Let us say $\underset{\sim}{x}$ is too close to $\|\underset{\sim}{x}\|\underset{\sim}{e}_1$ i.e angle b/w $H^+$ and $\underset{\sim}{e}_1$ axis is very small, then we would incur lot of round off error in computing $\underset{\sim}{v} = \|\underset{\sim}{x}\|\underset{\sim}{e}_1 - \underset{\sim}{x}$

If $\theta$ is angle between $\underset{\sim}{x}$ and $\underset{\sim}{y}$

$$\cos\theta = \frac{\underset{\sim}{x} \cdot \|\underset{\sim}{x}\|\underset{\sim}{e}_1}{\|x\| \, \|\underset{\sim}{x}\|} = \frac{x_1}{\|x\|}$$

Let us say $x_1 > 0$ i.e $\operatorname{sgn}(x_1) = +1$

then $\underset{\sim}{v} = -\|\underset{\sim}{x}\|\underset{\sim}{e}_1 - \underset{\sim}{x}$

$x_1 < 0$ i.e $\operatorname{sgn}(x_1) = -1$

$\underset{\sim}{v} = \|\underset{\sim}{x}\|\underset{\sim}{e}_1 - \underset{\sim}{x}$

$$\boxed{\underset{\sim}{v} = -\operatorname{sgn}(x_1)\|\underset{\sim}{x}\|\underset{\sim}{e}_1 - \underset{\sim}{x}}$$

$$\boxed{\underset{\sim}{v} = \operatorname{sgn}(x_1)\|\underset{\sim}{x}\|\underset{\sim}{e}_1 + \underset{\sim}{x}}$$

for $k = 1 : n$

$\underset{\sim}{x} = A(k:m, k)$

$\underset{\sim}{v}_k = \text{sgn}(x_1)\|\underset{\sim}{x}\|\underset{\sim}{e}_1 + \underset{\sim}{x}$

$\underset{\sim}{v}_k = \dfrac{\underset{\sim}{v}_k}{\|v_k\|_2}$

$A(k:m, k:n) = A(k:m, k:n) - 2\underset{\sim}{v}_k \underset{\sim}{v}_k^T A(k:m, k:n)$

This algo reduces $\underset{\sim}{A}$ to upper triangular form, the $\underset{\sim}{R}$ in $\underset{\sim}{Q}\underset{\sim}{R}$ factorization

$$\underset{\sim}{Q}^T = \underset{\sim}{Q}_n \underset{\sim}{Q}_{n-1} \cdots \underset{\sim}{Q}_2 \underset{\sim}{Q}_1$$

$$\underset{\sim}{A}\underset{\sim}{x} = \underset{\sim}{b}$$

$$\underset{\sim}{Q}\underset{\sim}{R}\underset{\sim}{x} = b$$

$$\Rightarrow \underset{\sim}{R}\underset{\sim}{x} = \underset{\sim}{Q}^T \underset{\sim}{b} \quad \text{(Back substitution)}$$

<u>Algo for $\underset{\sim}{Q}^T \underset{\sim}{b}$</u>

for $k = 1 : n$

$b(k:m) = b(k:m) - 2 v_k v_k^T b(k:m)$

Computational flops $\sim (2mn^2 - \frac{2}{3}n^3)$ flops!

## Stability of Householder triangularization :-

Householder triangularization is backward stable for all matrices A :

$\tilde{Q}\tilde{R} = \underset{\sim}{A} + \underset{\sim}{\delta A}$ where $\underset{\sim}{\delta A}$ is small

i.e $\frac{\|\delta A\|}{\|A\|} = O(\epsilon_m)$

i.e $\tilde{Q}\tilde{R}$ is exact QR factorization of the matrix which is perturbed by small $\delta A \in \mathbb{R}^{m \times n}$

$\tilde{R}$ is upper triangular matrix constructed by Householder triangularization in floating point arithmetic. (FPA)

And define

$\tilde{Q} = \tilde{Q}_1 \tilde{Q}_2 \cdots \tilde{Q}_n$ where $\tilde{Q}_k$

define exactly orthogonal matrix defined by $\tilde{v}_k$ which are obtained by FPA.

* Householder triangularization is backward stable but not always forward accurate, this means $\tilde{Q}$ and $Q$ may have large error depending on conditioning of matrix $\underset{\sim}{A}$.

* Is the accuracy of product of $\underset{\sim}{Q}\underset{\sim}{R}$ enough for application or do we need accuracy of $\underset{\sim}{Q}$ and $\underset{\sim}{R}$ individually! It turns out accuracy of product of $\underset{\sim}{Q}\underset{\sim}{R}$ is enough as seen below!

Algo solve $\underset{\sim}{A}\,\underset{\sim}{x} = \underset{\sim}{b}$ by QR factorization

(i) $\tilde{Q}\tilde{R} = \underset{\sim}{A}$ with $\tilde{Q}$ as represented as product of reflectors

(ii) $\tilde{y} = \tilde{Q}^T \underset{\sim}{b}$ Construct $\tilde{Q}^T \underset{\sim}{b}$ without explicitly building $\tilde{Q}$!

(iii) $\underset{\sim}{R}\,\tilde{\underset{\sim}{x}} = \tilde{\underset{\sim}{y}}$ ( Solve triangular s/m of eqns)!

Algo is backward stable i.e

$\tilde{x}$ is a solution $(\underset{\sim}{A} + \underset{\sim}{\delta A})\tilde{x} = \underset{\sim}{b}$

for some $\dfrac{\|\underset{\sim}{\delta A}\|}{\|\underset{\sim}{A}\|} = O(\varepsilon_M)$

because

(i) $\underset{\sim}{\tilde{Q}}\,\underset{\sim}{\tilde{R}} = \underset{\sim}{A}$ is backward stable

(ii) $\underset{\sim}{\tilde{y}} = \underset{\sim}{\tilde{Q}}^T \underset{\sim}{b}$ compute $\tilde{y}$ satisfies

$(\tilde{Q} + \delta Q)\,\tilde{y} = \underset{\sim}{b}$

for some $\|\delta Q\| = O(\varepsilon_M)$

(iii) Similarly

backward substitution is backward stable

compute $\tilde{x}$ satisfies $(\tilde{R} + \delta R)\,\tilde{x} = \tilde{y}$

for $\underset{\sim}{\delta R}$ satisfying

$\dfrac{\|\underset{\sim}{\delta R}\|}{\|\underset{\sim}{R}\|} = O(\varepsilon_M)$