Eigenvalues / Eigenvectors – II
Improving the QR Iteration Efficiency

We want a 'real' version of the Schur Decomposition → impossible due to complex poles.

FACT (Real Schur Decomposition): If $A \in \mathbb{R}^{n\times n}$ then $\exists\ Q \in \mathbb{R}^{n\times n}$ s.t.

$$Q^T A Q = \begin{bmatrix} R_{11} & R_{12} & \cdots & R_{1m} \\ 0 & R_{22} & & R_{2m} \\ \vdots & & \ddots & \vdots \\ 0 & \cdots & 0 & R_{mm} \end{bmatrix}$$

where each R_{ii} is either a 1×1 matrix or a 2×2 matrix having complex conjugate eigenvalues.

Proof: Only real or Complex Conjugate eig. values are possible. Let there be k – complex conj. eigenvalues. We do induction on k.

True by Schur's thm for $k=0$. Now let $k \geq 1$. Let $\lambda = \nu + i\mu \in \lambda(A)$. Then $\exists\ y, z \in \mathbb{R}^n (z \neq 0)$ s.t. $A(y+iz) = (\nu + i\mu)(y+iz)$

i.e. $$A[y\ \ z] = [y\ \ z]\begin{bmatrix} \nu & \mu \\ -\mu & \nu \end{bmatrix}$$

By FACT above $(AX = XB)$ $sp\{y, z\}$ is a real invariant subspace of A & $\exists$ orthogonal $Q \in \mathbb{R}^{n\times n}$ s.t. $$Q^T A Q = \left[\begin{array}{c|c} T_{11} & T_{12} \\ \hline 0 & T_{22} \end{array}\right]$$

where $\lambda(T_{11}) = \{\nu + i\mu, \nu - i\mu\}$. Rest – exercise.

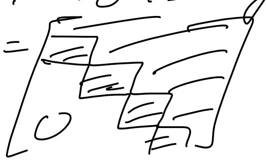
With this form in mind we set up the real analog of the QR iteration

```
Given $A \in \mathbb{R}^{n \times n}$ & orthogonal $Q_0$,
  Set $H_0 = Q_0^T A Q_0$
  for $K = 1, 2, \dots$
      $Q_K R_K = H_{K-1}$ (QR factorization)
      $H_K = R_K U_K$
  end
```

We can at best expect H_K to converge to the real schur form.

However, effort at each step is still $O(n^3)$

Solution: If Q_0 is chosen s.t. H_0 is upper Hessenberg, i.e. $Q_0^T A Q = H =$



Then the $QR = H$ i.e

$$R = Q^T H \equiv \underbrace{G_{n-1}^T \cdots G_1^T}_{n-1 \text{ Givens Rotations}} H \quad \sim O(n^2)$$

Similarly the $H_+ = RQ = R\underbrace{(G_1 \cdots G_{n-1})}_{\text{upper Hessenberg}} \rightsquigarrow O(n^2)$

Hence H_+ is also upper Hessenberg.

```
for $K = 1 : n-1$
    $[c_K, s_K] = \text{givens}(H(k,k), H(k+1,k))$
        $H(k:k+1, k:n) = \begin{bmatrix} c_K & s_K \\ -s_K & c_K \end{bmatrix}^T H(k:k+1, k:n)$
end
```

```
for k = 1 : n-1
    $H(1:k+1, k:k+1) = H(1:k+1, k:k+1)\begin{bmatrix} c_k & s_k \\ -s_k & c_k \end{bmatrix}$
end
```

Q. How to choose Q_0 s.t. $Q_0^T A Q$ is upper Hessenberg?

#: 1> Let $A = \begin{bmatrix} a_{11} & c^T \\ b & \hat{A} \end{bmatrix}$.

2> Choose a Householder reflector $\hat{Q}_1$ s.t.

$$\hat{Q}_1 b = [-\tau_1 \; 0 \; \cdots \; 0]^T; \quad |\tau_1| = \|b\|_2$$

& let $Q_1 = \begin{bmatrix} 1 & 0^T \\ 0 & \hat{Q}_1 \end{bmatrix}$

3> Then $A_{1/2} = Q_1 A = \left[\begin{array}{c|c} a_{11} & c^T \\ \hline -\tau_1 & \\ 0 & \hat{Q}_1 \hat{A} \\ \vdots & \\ 0 & \end{array}\right]$

& $$A_1 = A_{1/2} Q_1^T = \left[\begin{array}{c|c} a_{11} & c^T \\ \hline -\tau_1 & \\ 0 & \hat{Q}_1 \hat{A} \\ \vdots & \end{array}\right] \left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & \hat{Q}_1 \end{array}\right] \quad \left\{ \begin{array}{c} \text{Since} \\ Q_1^{-1} = Q_1^T \\ = Q_1 \end{array} \right\}$$

$$= \left[\begin{array}{c|c} a_{11} & c^T \hat{Q}_1 \\ \hline -\tau_1 & \\ 0 & \hat{Q}_1 \hat{A} \hat{Q}_1 \\ \vdots & \\ 0 & \end{array}\right]$$

Note: The right multiplication by Q_1 or Q_1^T would have destroyed a upper triangular structure if we tried that.

Repeating the same idea

$$\underbrace{(Q_1 \cdots Q_{n-2})^T}_{Q_0^T} A \underbrace{(Q_1 \cdots Q_{n-2})}_{Q_0} = \underset{\substack{\downarrow \\ \text{upper} \\ \text{Hessenberg}}}{H}$$

<u>Algo:</u>

```
for k = 1 : n-2
    $[v, \beta] = \text{house}(A(k+1:n, k))$
    $A(k+1:n, k:n) = (I - \beta v v^T) A(k+1:n, k:n)$
    $A(1:n, k+1:n) = A(1:n, k+1:n)(I - \beta v v^T)$
end
```

Requires $10n^3/3$ flops → but once.

Non-uniqueness of Hessenberg Decompositions

A Hessenberg matrix is said to be "unreduced" if it has no zero subdiagonal entry.

<u>Implicit Q-Theorem</u>: Let $A \in \mathbb{R}^{n\times n}$ Suppose $Q = [q_1 | \cdots | q_n]$ and $V = [v_1 | \cdots | v_n]$ are orthogonal matrices s.t. $Q^T A Q = H$ & $V^T A V = G$ are both upper Hessenberg. Let k denote the smallest no. for which $h_{k+1,k} = 0$. ($k = n$ if H is unreduced)

1> If $q_1 = v_1$, then $q_i = \pm v_i$ & $|h_{i,i-1}| = |g_{i,i-1}|$ for $i = 2:k$.

2> If $k < n$, then $g_{k+1,k} = 0$

<u>Proof</u>: Define orthogonal $W = [w_1 | \cdots | w_n] = V^T Q$.

Note: $GW = GV^T Q = V^T A Q = V^T Q Q^T A Q = WH$.

Comparing column $i-1$ for $i = 2:k$

$$h_{i,i-1} w_i + \sum_{j=1}^{i-1} h_{j,i-1} w_j = G_2 w_{i-1} \quad \text{---} \; ⓧ$$

$$- \left\{ \overset{W}{\begin{bmatrix} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{bmatrix}} \overset{H}{\begin{bmatrix} \underset{i-1}{|} \end{bmatrix}} = G_2 [w_1 \cdots w_{i-1} \cdots w_n] \right\}$$

Recall $w_1 = e_1$

$$, \begin{bmatrix} 1 & * & \\ 0 & * & \\ \vdots & x_1 & \\ \vdots & x_2 & \\ 0 & x_{n-2} & \end{bmatrix} \begin{bmatrix} a & * & \cdots \\ b & c & \\ 0 & d & \\ \vdots & 0 & \\ 0 & \vdots & \end{bmatrix} = \begin{bmatrix} p & * & \\ q & r & \\ 0 & s & \\ 0 & 0 & \\ \vdots & \vdots & \end{bmatrix} \begin{bmatrix} 1 & \\ 0 & \\ \vdots & \\ 0 & \end{bmatrix}$$

Compare the 3, 1 element : $0.a + x_1 b = 0.1 + s.0 + \cdots 0$

$\Rightarrow x_1 = 0$

Compare the 4, 1 element, $0.a + x_2 . b = 0 \Rightarrow x_2 = 0$

$\vdots$

$x_3 = \cdots = x_{n-2} = 0$

Hence

$$, \begin{bmatrix} 1 & * & & \\ 0 & * & & \\ 0 & 0 & * & \\ 0 & 0 & x_1 & \\ 0 & 0 & x_{n-3} & \end{bmatrix} \begin{bmatrix} a & * & \cdots \\ b & c & \\ 0 & d & \\ \vdots & 0 & \\ 0 & 0 & \end{bmatrix} = \begin{bmatrix} p & * & & \\ q & r & & \\ 0 & s & t & \\ 0 & 0 & w & \\ \vdots & \vdots & 0 & \end{bmatrix} \begin{bmatrix} 1 & & & \\ 0 & * & & \\ \vdots & 0 & & \\ 0 & 0 & & \end{bmatrix}$$

Compare the 4, 2 element $x_1 . d = 0 \Rightarrow x_1 = 0$

" " " 5, 2 elemt $x_2 . d = 0 \Rightarrow x_2 = 0$

$x_1 = x_2 = \cdots = x_{n-3} = 0$

Proceeding similarly, $[w_1 \cdots w_k]$ is upper triangular

Claim : $w_i = \pm e_i$ $(i = 2, \cdots, k)$

Proof:
$$\left\{ \begin{aligned} & w_1^T w_2 = [1 \; 0 \cdots 0] \begin{bmatrix} x_1 \\ x_2 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = 0 \Rightarrow x_1 = 0 \\ & \text{Moreover } \|w_2\| = 1 \quad \Rightarrow x_2 = \pm 1 \\ & \text{Similarly,} \quad w_i = \pm e_i \end{aligned} \right\}$$

$$w_i^o = V^T q_i^o \Rightarrow \pm e_i = V^T q_i \Rightarrow v_i^o = \pm q_i$$

Also, $h_{i,i-1} = w_i^{oT} G w_{i-1}$ (from $\circledast$)

$$= q_i^T V G V^T q_{i-1} = q_i^{oT} A q_{i-1}^o$$

$$|h_{i,i-1}| = |q_i^T A q_{i-1}| = |v_i^T A v_{i-1}| = |g_{i,i-1}| \quad i = 2:k$$

Remaining: Exercise

Q> How to accelerate convergence?

<u>Shifted QR</u>: Let $\mu \in \mathbb{R}$ and consider:

```
$H_0 = Q_0^T A Q_0$   (Hessenberg reduction)
for $k = 1, 2 \ldots$
    Determine $\mu$.   (strategies later)
    $Q_{k-1} R_{k-1} = (H_{k-1} - \mu I)$   (QR factorization)
    $H_k = R_{k-1} Q_{k-1} + \mu I$
end
```

$\#$ H_k ($\forall k$) is similar to A.

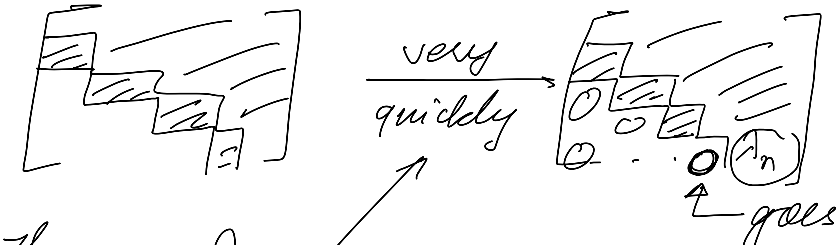
$$H_k = R_{k-1} Q_{k-1} + \mu I = Q_{k-1}^T Q_{k-1} \left[R_{k-1} Q_{k-1} + \mu I\right] Q_{k-1}^T Q_{k-1}$$

$$= Q_{k-1}^T \left[(H_{k-1} - \mu I) Q_{k-1} + \mu Q_{k-1}\right]$$

$$= Q_{k-1}^T \left[H_{k-1}\right] Q_{k-1}$$

But H_0 similar to A $\Rightarrow$ H_k sim. to A.

If we re-numbes the eigenvalues such that $|\lambda_1 - \mu| \geq \cdots\cdots \geq |\lambda_n - \mu|$



If $\mu \approx \lambda_n$ & if $|\lambda_n| \neq |\lambda_{n-1}|$ at the rate $\left|\frac{\lambda_n - \mu}{\lambda_{n-1} - \mu}\right|^k$

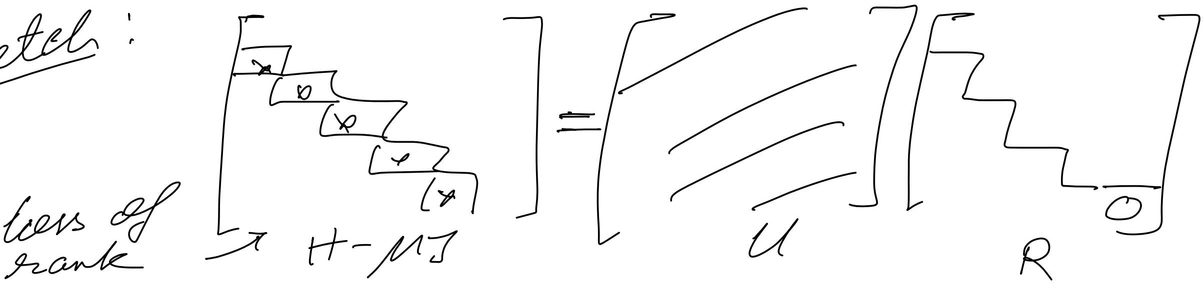
Q. How to choose μ? or How to Change from iteration to iteration?

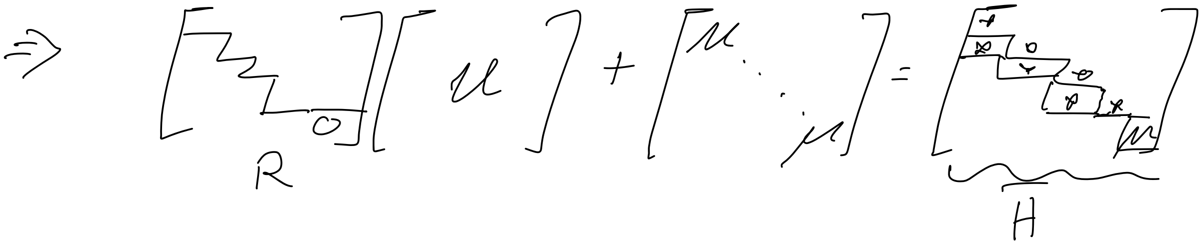
Clearly if $|\lambda_p| = |\lambda_{p+1}|$ then there is no convergence

$$\left|\frac{\lambda_{p+1} - \mu}{\lambda_p - \mu}\right|^k = 1$$

FACT: Let μ be an eigenvalue of a $n \times n$ unreduced Hessenberg matrise H.
If $\tilde{H} = RU + \mu I$
where $H - \mu I = UR$ is the QR fact,
then $\tilde{h}_{n,n-1} = 0$ & $\tilde{h}_{n,n} = \mu$.

Sketch:





$\Rightarrow$ μ is revealed in 1-step.

Deflation: Hessenberg $H = \begin{array}{c|cc} & p & n-p \\ \hline p & H_{11} & H_{12} \\ n-p & & H_{22} \end{array}$

Commonly used for $p = n-1$ or $p = n-2$

Single Shift Strategy

Assume h_{nn} at each step as our guess of μ.

```
for k = 1, 2, ...
    $\mu = H_{k-1}(n, n)$
    $Q_{k-1}, R_{k-1} = H_{k-1} - \mu I$
    $H_k = R_{k-1} Q_{k-1} + \mu I$
end
```

Double Shift Strategy

Above strategy faces problem if $G = \begin{bmatrix} h_{n-1,n-1} & h_{n-1,n} \\ h_{n,n-1} & h_{nn} \end{bmatrix}$ has complex eigenvalues say a_1 & a_2

Double shift :

a_1, a_2 are complex

$$U_1 R_1 = H - a_1 I \longrightarrow \text{QR fact}$$
$$H_1 = R_1 U_1 + a_1 I$$
$$U_2 R_2 = H_1 - a_2 I \longrightarrow \text{QR fact}$$
$$H_2 = R_2 U_2 + a_2 I$$

<u>Result</u>: From above (shifted QR derivation), $H_1 = U_1^* H U_1$

& $H_2 = U_2^* H_1 U_2$

$\Rightarrow H_2^* = [U_1 U_2]^* H [U_1 U_2]$

$\rho = 1$

$\tau = 2$

<u>Claim</u>: $(H - a_1 I)(H - a_2 I) = U_1 U_2 R_2 R_1$

<u>Proof</u>: Since $H_1 = U_1^* H U_1$

$\Rightarrow (H - a_2 I) U_1 = U_1 (H_1 - a_2 I)$ —— $\circledast$

Then : $(H - a_2 I)(H - a_1 I) = (H - a_2 I) U_1 R_1$

$= U_1 (H_1 - a_2 I) R_1$ (from $\circledast$)

$= U_1 (U_2 R_2) R_1$

\# If $a_1 = \overline{a_2}$, then $(H - a_1 I)(H - a_2 I) = M$ is real

clearly, $(H - a_1 I)(H - a_2 I) = H^2 + \underbrace{(a_1 + a_2)}_{\text{real}} H + \underbrace{a_1 a_2}_{\text{real}} I$

\# So $M = \underbrace{[U_1 U_2]}_{Q} \underbrace{[R_2 R_1]}_{R}$ is QR factorization of a real matrix

$\Rightarrow Q, R$ are both real.

$\Rightarrow H_2 = [U_1 U_2]^* H [U_1 U_2]$ is also real.

<u>Problem</u>: Because of round-off errors, exact return to reals is impossible.

Double - Implicit Shift (in $O(n^2)$)

Impractical Method: (for getting real H_2 from H)

1) Calculate $M = H^2 - (a_1+a_2)H + a_1 a_2 I \sim O(n^3)$
2) Calculate real QR fact : $M = ZR \sim O(n^3)$
3) Set $H_2 = Z^T H Z$

Use implicit Q-theorem to get H_2 from H in $O(n^2)$ flops (Francis QR step)

1) Calculate $M = (H - a_1 I)(H - a_2 I)$ and consider $Me_1 \leftarrow$ 1st col of M.
2) determine a Householder matrix P_0 s.t. $P_0(Me_1) = \|Me_1\|_2 \, e_1$
3) Compute Householder matrices $P_1, \ldots, P_{n-2}$ s.t. $Z_1 = P_0 P_1 \cdots P_{n-2}$ s.t. $Z_1^T H Z_1$ is upper Hessenberg
4) Then Z_1 and Z are equal equal upto signs.

Claim: First column of Z = First col. of Z_1

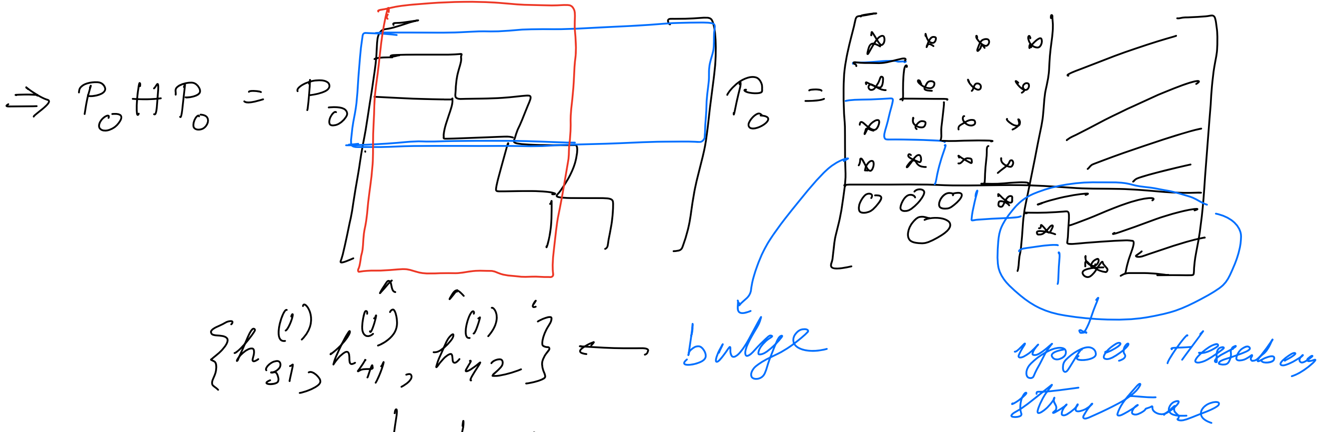
Proof: $$Me_1 = \begin{bmatrix} x \\ y \\ z \\ 0 \\ \vdots \\ 0 \end{bmatrix} \qquad \left\{ \begin{bmatrix} h_{11} & h_{12} & \cdots \\ h_{21} & h_{22} & \cdots \\ 0 & h_{32} & \cdots \\ & & \ddots \end{bmatrix} - a_1 I \right\} \left\{ \qquad \right\}$$

$x = h_{11}^2 + h_{12} h_{21} - (a_1 + a_2) h_{11} + a_1 a_2$

$y = h_{21}(h_{11} + h_{22} - (a_1 + a_2))$

$z = h_{21} h_{32}$

So $P_0(Me_1) = P_0 \begin{bmatrix} x \\ y \\ z \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \begin{bmatrix} x \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \Rightarrow P_0 = \left[\begin{array}{c|c} 3\times 3 & 0 \\ \hline 0 & \begin{matrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{matrix} \end{array}\right]$



[Due to pre-mult by P_0 1st three rows are affected. Due to post-mult by P_0, the 1st three col's are affected]

To calculate the original Z, we should calculate M, then factorize $M = ZR$

$$R = P_0^T M = \left[\begin{array}{cc|c} x & x & \\ 0 & r_{22} & \\ \vdots & r_{32} & \\ 0 & r_{42} & * \\ 0 & 0 & \\ \vdots & \vdots & \\ 0 & 0 & \end{array}\right]$$

Then from above derivation we can expect: $H_2 = Z^T H Z$

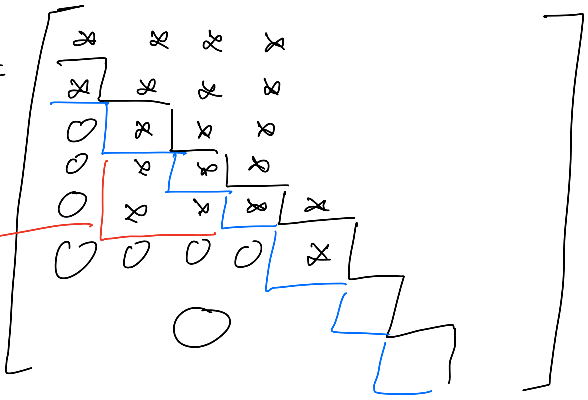
Not actually done

Then we should have found out P_1 s.t.

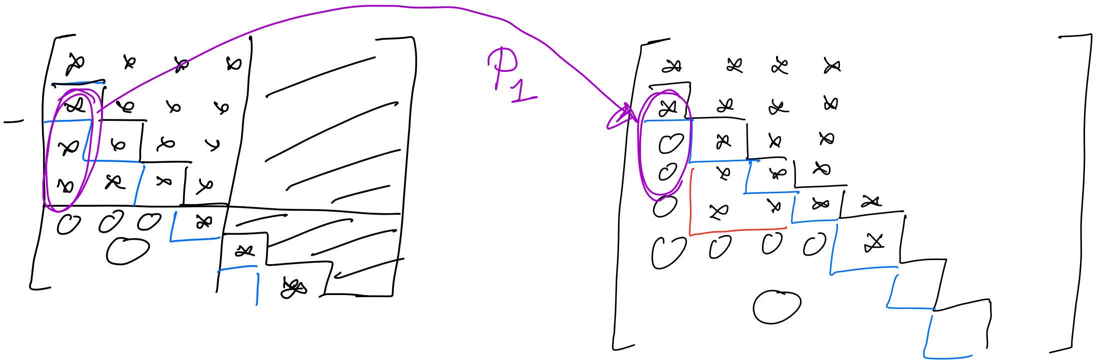
$$P_1^T P_0^T M = \left[\begin{array}{cc|c} x & x & \\ 0 & x & \\ \vdots & 0 & x \\ \vdots & \vdots & \\ 0 & 0 & \end{array}\right]$$

Instead we propose to find P_1 s.t.

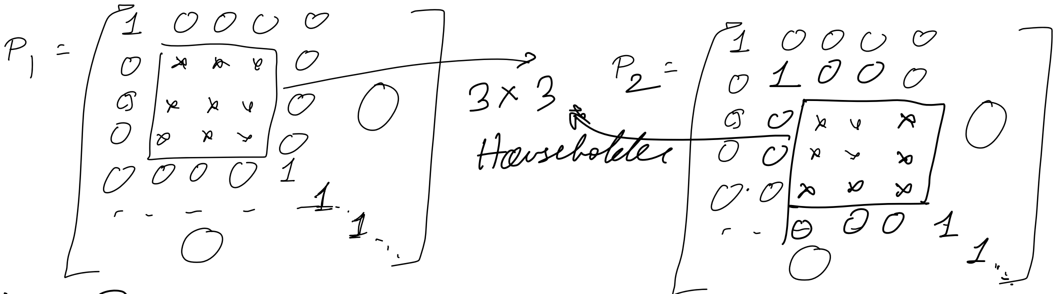
$P_1^T P_0^T H P_0 P_1^T =$



$\Rightarrow P_1$ is designed as a reflector that



So



$\Rightarrow P_k e_1 = e_1 \qquad k = 1 : n-2$

P_0 and Z have the same 1st col.

{ Since by design (recall Householder : QR) $P_0(Me_1) = \begin{bmatrix} x \\ 0 \\ \vdots \end{bmatrix}$, $Z(Me_1) = \begin{bmatrix} x \\ 0 \\ \vdots \\ 0 \end{bmatrix}$ $M = ZR$, $Z = Z^T$ }

Hence $Z_1 = P_0 P_1 \cdots P_{n-2}$

will have $\underset{P_0}{\begin{bmatrix} \boxed{\begin{matrix} x \\ x \\ x \\ x \end{matrix}} & \begin{matrix} x & x & \cdots & x \\ x & x & & x \\ & & & \\ x & x & & \end{matrix} \end{bmatrix}} \underset{P_1}{\left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & \end{array}\right]} \left[\begin{array}{c|c} 1 \; 1 & 0 \\ \hline 0 & x \end{array}\right]$

$- - - - - \cdot \quad P_{n-2} = Z_1$

$\begin{cases} \text{Clearly } 1^{st} \text{ col of } Z_1 = 1^{st} \text{ col of } P_0 \\ \text{But } 1^{st} \text{ col of } P_0 = 1^{st} \text{ col of } Z \end{cases}$

$\Rightarrow \quad Z_1 e_1 = Z e_1$

Then by the implicit Q-theorem, Z_1 & Z are equal upto signs if $Z^T H Z$ and $Z_1^T H Z_1$ are each unreduced.

Francis QR step: Given unreduced upper Hessenberg $H \in \mathbb{R}^{n\times n}$ whose trailing 2x2 principal submatrise has eigenvalues a_1 & a_2, this algo overwrites

$H \leftarrow Z^T H Z$ $\quad \boxed{Z^T(H-a_1 I)(H-a_2 I) = \text{upper triangular}}$ $\quad H = \left[\begin{array}{c|c} & \\ \hline & \begin{matrix} x & x \\ x & x \end{matrix} \end{array}\right]$ $m = n-1$

$m = n-1$

$s = H(m,m) + H(n,n)$

$t = H(m,m) \cdot H(n,n) - H(m,n) \cdot H(n,m) \qquad H(m:n, m:n)$

$x = H(1,1) \cdot H(1,1) + H(1,2) \cdot H(2,1) - s \cdot H(1,1) + t$

$y = \cdot \; \cdot \; \cdot$

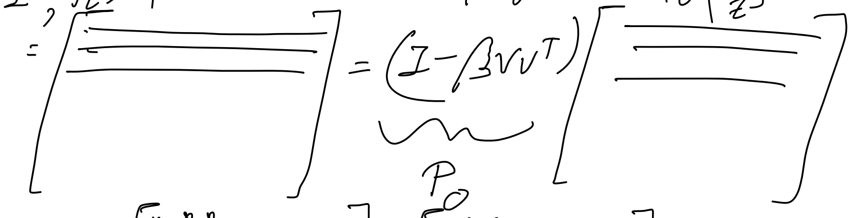
$z = \cdot \; \cdot$

```
for  $k = 0 : n-3$
    $[v, \beta] = house([x\ y\ z]^T)$
    $q = \max\{1, k\}$
    $H(k+1 : k+3, q : n) = (I - \beta v v^T) . H(k+1 : k+3, q : n)$  ——— ①
    $r = \min\{k+4, n\}$
    $H(1 : r, k+1 : k+3) = H(1 : r, k+1 : k+3) . (I - \beta v v^T)$  ——— ②
    $x = H(k+2, k+1)$
    $y = H(k+3, k+1)$
    if  $k < n-3$
        $z = H(k+4, k+1)$
    end
end
$[v, \beta] = house([x\ y]^T)$                                                   ⎫
$H(n-1 : n, n-2 : n) = (I - \beta v v^T)\ H(n-1 : n, n-2 : n)$   ⎬ ——— ①
$H(1 : n, n-1 : n) = H(1 : n, n-1 : n) . (I - \beta v v^T)$          ⎭
```

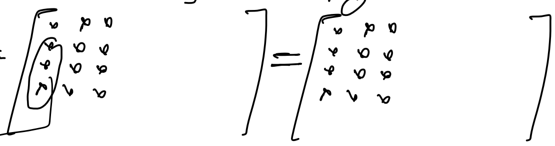
$k = 0, \quad q = 1, r = 4$

Recall P_0 was designed to make $P_0 \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x \\ 0 \\ 0 \end{bmatrix}$

① $H(1:3, 1:n) =$ $= \underbrace{(I - \beta v v^T)}_{P_0}$



② $H(1:4, 1:3) =$ $=$ P_0

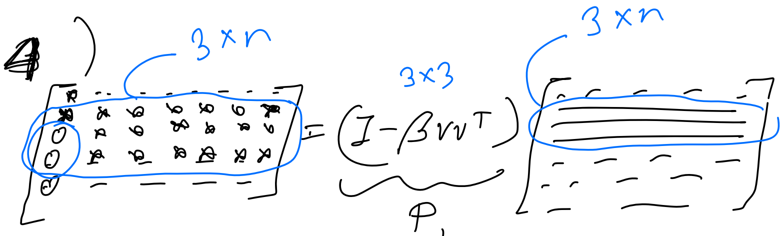


$x = H(2,1)$
$y = H(3,1)$
$z = H(4,1)$

$K = 1, q = 1, r = 5$

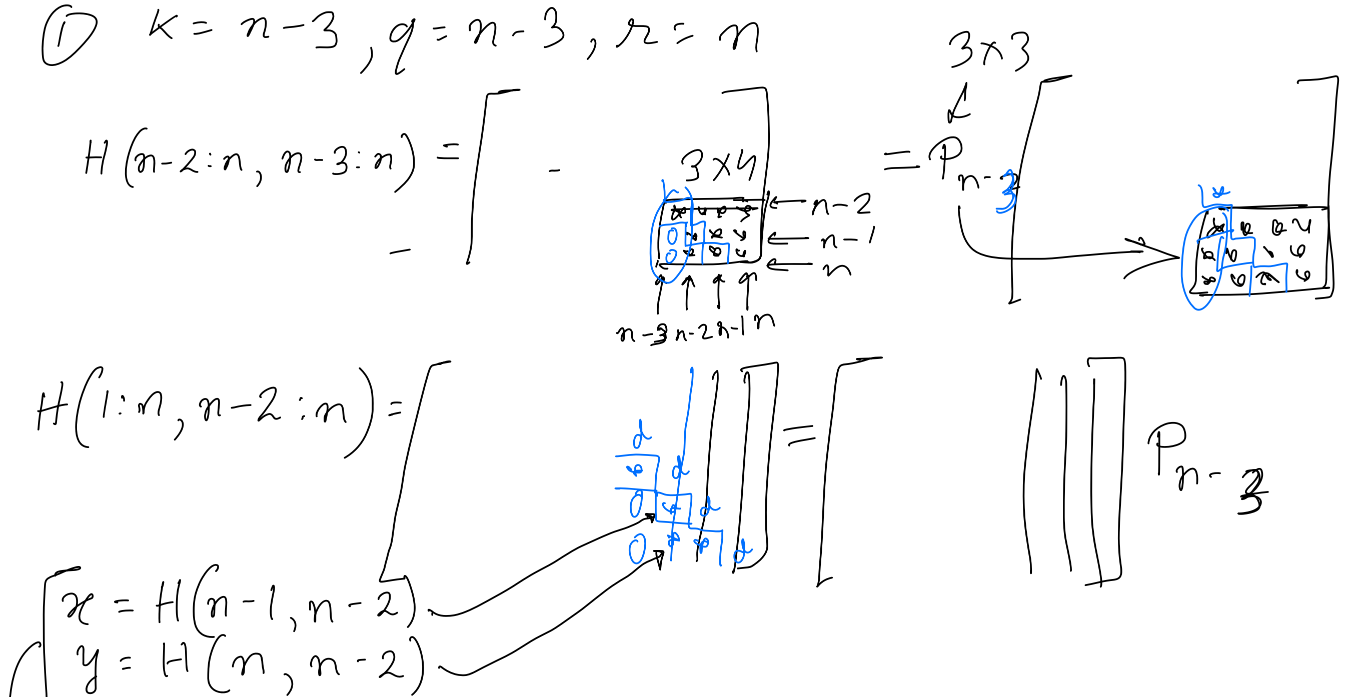
① $k = 1$ (2, …, $n-4$) same for

$q = 1, H(2:4, 1:n) =$ $= \underbrace{(I - \beta v v^T)}_{P_1}$



② $r = 5$, $H(1:5, 2:4) =$ $=$ $P_1 \rightarrow 3\times 3$

① $k = n-3$, $q = n-3$, $r = n$



→ used in the last "house" call outside the loop.

Overall QR with shifts

```
Compute Hessenberg reduction: $H = U_0^T A U_0$ where
    $U_0 = P_1 \cdots P_{n-2}$
while $q \leq n$
    Set to zero all sub-diagonal entries
    that satisfy
        $|h_{i,i-1}| \leq tol.(|h_{ii}| + |h_{i-1,i-1}|)$
    Find the largest q & smallest p s.t.
        $H = \begin{array}{cccc} H_{11} & H_{12} & H_{13} & p \\ 0 & H_{22} & H_{23} & n-p-q \\ 0 & 0 & H_{33} & q \\ p & n-p-q & q & \end{array}$
```

```
    where $H_{33}$ is upper quasi-triangular and
    $H_{22}$ is unreduced
    if $q < n$
        Perform a Francis QR step on
        $H_{22} = Z^T H_{22} Z$
    end
end
```

#if we don't do single-shifts in the F. QR step, then we need to separately upper triangularize the 2x2 blocks to get real eigenvalues.

Q. How to add to this code to get Q & H_{final}?

$$\boxed{H_{final} = Q^T H Q}$$

Computation of Eigenvectors of A (unsymmetric)

1> Hessenberg reduction : $U_0^T A U_0 = H$

2> QR Iteration → Calculate eigenvalues

3> For each computed λ, apply inverse iteration with shift $\mu = \lambda$ to produce $z \in \mathbb{R}^n$ s.t. $Hz = \mu z$

4> set $x = U_0 z$ ← eigenvector corr. to λ.