## Numerical linear algebra III

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$$U = \begin{bmatrix} \frac{1}{\lambda_1} A x_1 & \dots & \frac{1}{\lambda_n} A x_n \end{bmatrix} \begin{bmatrix} x_1 & \dots & x_n \end{bmatrix}^*$$

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$$UPx_i = Ax_i \Rightarrow A = UP$$

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$$\det P = \prod_{k=1}^n \lambda_k \leq \left(\frac{1}{n} \sum_{k=1}^n \lambda_k\right)^n \leq \left(\frac{1}{n} \operatorname{tr} P\right)^n = \left(\frac{1}{n} \sum_{k=1}^n b_k^* b_k\right)^n$$

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We compute  $\begin{bmatrix} A^n b_1 & \dots & A^n b_k \end{bmatrix}$ 



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 $B=Q_1^*AQ_1$ , apply the reasoning for an eigenpair of B A is similar with an upper triangular matrix  $\Rightarrow$  proof of Schur's lemma

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$$q^* = r^* A^{-1}$$

 $q^*$  is an iteration of the power method for  $A^{-1}$  starting from  $r^*$ 

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$$Q_1 Q_2 \dots Q_{k+1} R_{k+1} \dots R_2 R_1 = Q_1 Q_2 \dots Q_k A_{k+1} R_k \dots R_2 R_1 =$$

$$= Q_1 Q_2 \dots Q_k Q_k^* Q_{k-1}^* \dots Q_1^* A_1 Q_1 \dots Q_{k-1} Q_k R_k R_{k-1} \dots R_2 R_1 =$$

$$= A_1 Q_1 \dots Q_{k-1} Q_k R_k R_{k-1} \dots R_2 R_1 = A_1^{k+1}$$

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$$U_k = Q_1 \dots Q_k$$

$$T_k = R_1 \dots R_k$$

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$$= A_1 Q_1 \dots Q_{k-1} Q_k R_k R_{k-1} \dots R_2 R_1 = A_1^{k+1}$$

$$U_k=Q_1\ldots Q_k$$

$$T_k = R_1 \dots R_k$$

$$A_k = U_k^* A_1 U_k, \ U_k T_k = A_1^k$$

We want to show  $A_k \approx R$  upper triangular as  $k \to \infty$ 

$$A = A_1 = V \Lambda V^{-1}, \ U_k T_k = A_1^k = V \Lambda^k V^{-1}$$

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$$A_k = T_k V \Lambda^k V^{-1} A_1 V \Lambda^{-k} V^{-1} T_k^{-1} = T_k V \Lambda V^{-1} T_k^{-1}$$

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$$A_k = T_k V \Lambda V^{-1} T_k^{-1} = T_k A T_k^{-1}$$

$$A = A_{1} = V \Lambda V^{-1}, \ U_{k} T_{k} = A_{1}^{k} = V \Lambda^{k} V^{-1}$$

$$U_{k} = V \Lambda^{k} V^{-1} T_{k}^{-1}, \ U_{k}^{*} = T_{k} V \Lambda^{-k} V^{-1}$$

$$A_{k} = T_{k} V \Lambda^{k} V^{-1} A_{1} V \Lambda^{-k} V^{-1} T_{k}^{-1} = T_{k} V \Lambda V^{-1} T_{k}^{-1}$$

$$A_{k} = T_{k} V \Lambda V^{-1} T_{k}^{-1} = T_{k} A T_{k}^{-1}$$

$$A_{k} T_{k} = T_{k} A$$

Assume:

$$\lambda_1 > \lambda_2 > \ldots > \lambda_n > 0$$

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 $A = Q\Lambda Q^*$  the eigenvalue decomposition of A, A positive-definite

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$$(\Lambda^{k}L\Lambda^{-k})_{ij} = \begin{cases} I_{ij} \left(\frac{\lambda_{i}}{\lambda_{j}}\right)^{k}, & i > j \\ 1, & i = j \\ 0, & i < j \end{cases}$$

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$$\Lambda^k L \Lambda^{-k} \to I$$

$$Q\Lambda^k L\Lambda^{-k} \to Q$$

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$$Q = QI$$
 the QR factorization of  $Q$ 

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$$U_k \rightarrow Q$$

$$Q\Lambda^k L\Lambda^{-k} \to Q$$

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$$U_k \rightarrow Q$$

$$A_k = U_k^* A U_k \rightarrow Q^* A Q = \Lambda$$

B positive definite  $n \times n$  matrix

$$B_0 = B, \ B_k = C_k^* C_k, \ B_{k+1} = C_k C_k^*$$

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$$\widehat{B}_{ij} = \sum_{p=i}^{n} C_{ip} C_{pj}^* = \sum_{p=i}^{n} C_{ip} C_{jp}$$

B positive definite  $n \times n$  matrix The Cholesky iteration:

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$$\widehat{B}_{ij} = \sum_{p=i}^{n} C_{ip} C_{pj}^{*} = \sum_{p=i}^{n} C_{ip} C_{jp}$$

$$B_{kk} = \sum_{p=1}^{k} C_{kp}^{2}, \ \widehat{B}_{kk} = \sum_{p=k}^{n} C_{pk}^{2}$$

$$\sum_{k=1}^{m} B_{kk} = \sum_{k=1}^{m} \sum_{p=1}^{k} C_{kp}^{2} = \sum_{k=1}^{m} \sum_{p=1}^{m} C_{kp}^{2} = \sum_{i=1}^{m} \sum_{j=1}^{m} C_{ji}^{2}, \quad m \le n$$

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$$\sum_{k=1}^{m} \widehat{B}_{kk} - B_{kk} = \sum_{i=1}^{m} \sum_{j=1}^{n} C_{ji}^{2}$$

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$$m = n \Rightarrow \text{tr}(B) = \text{tr}(\widehat{B})$$

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$$m = n \Rightarrow \text{tr}(B) = \text{tr}(\widehat{B})$$

$$m < n \Rightarrow \sum_{k=1}^{m} \widehat{B}_{kk} \ge \sum_{k=1}^{m} B_{kk}$$

$$\operatorname{tr}(B) = \operatorname{tr}(B_0) = \ldots = \operatorname{tr}(B_k)$$

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$$\widehat{B}_{mm} - B_{mm} = \sum_{k=1}^{m} (\widehat{B}_{kk} - B_{kk}) - \sum_{k=1}^{m-1} (\widehat{B}_{kk} - B_{kk}) \ge 0$$

$$\operatorname{tr}(B) = \operatorname{tr}(B_0) = \ldots = \operatorname{tr}(B_k)$$

$$\widehat{B}_{mm} - B_{mm} = \sum_{k=1}^{m} (\widehat{B}_{kk} - B_{kk}) - \sum_{k=1}^{m-1} (\widehat{B}_{kk} - B_{kk}) \ge 0$$

 $(B_k)_{ii}$  is monotonous and bounded

$$\lim_{k\to\infty}(B_k)_{ii}=(B_\infty)_{ii}$$

$$\operatorname{tr}(B) = \operatorname{tr}(B_0) = \ldots = \operatorname{tr}(B_k)$$

$$\widehat{B}_{mm} - B_{mm} = \sum_{k=1}^{m} (\widehat{B}_{kk} - B_{kk}) - \sum_{k=1}^{m-1} (\widehat{B}_{kk} - B_{kk}) \ge 0$$

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For A positive definite

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The QR iteration for A is the Cholesky iteration for  $B \Rightarrow$  converges

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$$U_0 Q_0 R_0 = Q_0 R_0 U_0 \Rightarrow R_0 U_0 = Q_0^* U_0 Q_0 R_0$$

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# QR for Complex Eigenvalues

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For a general matrix with eigenvalues at his a chittle OP

For a general matrix with eigenvalues a + bi, a - bi the QR Algorithm goes towards  $A_{2k}$ ,  $A_{2k+1}$ 

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With similar argument with the block LU factorization can be used Convergence is not guaranteed but the eigenvalues of the block upper triangular matrix converge to the real eigenvalues

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QR with explicit shifts is equivalent to the Inverse Power method

$$A_0 = A, A_k - \kappa_k I = Q_k R_k, A_{k+1} - \kappa_{k+1} I = R_k Q_k$$

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$$A_{k+1} - \kappa_{k+1} = (Q_0 \dots Q_k)^* (A_0 - \kappa_0 I)(Q_0 \dots Q_k)$$

$$Q_0 \dots Q_k R_k \dots R_0 = Q_0 \dots Q_{k-1} (A_k - \kappa_k I) R_{k-1} \dots R_0 =$$
  
=  $(A - \kappa_0 I) (Q_1 \dots Q_{k-1}) R_{k-1} \dots R_0 = (A - \kappa_0 I) \dots (A - \kappa_k I)$ 

$$A = \begin{bmatrix} B & h \\ g^* & \mu \end{bmatrix}$$

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 $\mu$  is the Rayleigh quotient of  $\emph{e}_{\emph{n}}$ 

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$$||f||_2^2 + \alpha^2 = ||e||_2^2 + \alpha^2 = 1 \Rightarrow ||f||_2^2 = ||e||_2^2$$

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#### **Error Bounds**

$$||f||_{2}^{2} + \alpha^{2} = ||e||_{2}^{2} + \alpha^{2} = 1 \Rightarrow ||f||_{2}^{2} = ||e||_{2}^{2}$$

$$g^{*} = e^{*}R \Rightarrow ||e||_{2} \leq ||R^{-1}||_{2}||g||_{2}$$

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$$|r| = |f^{*}h + \alpha(\mu - \kappa)| \leq |f^{*}h| + |\alpha||\mu - \kappa| \leq ||f||_{2}||h||_{2} + |\mu - \kappa|$$

 $|r| < ||R^{-1}||_2 ||g||_2 ||h||_2 + |\mu - \kappa|$ 

### Error Bounds

$$\begin{split} \|f\|_2^2 + \alpha^2 &= \|e\|_2^2 + \alpha^2 = 1 \Rightarrow \|f\|_2^2 = \|e\|_2^2 \\ g^* &= e^*R \Rightarrow \|e\|_2 \le \|R^{-1}\|_2 \|g\|_2 \\ \begin{bmatrix} P^* & e \\ f^* & \alpha \end{bmatrix} \begin{bmatrix} B - \kappa I & h \\ g^* & \mu - \kappa \end{bmatrix} = \begin{bmatrix} R & p \\ 0 & r \end{bmatrix} \end{split}$$

$$|r| = |f^*h + \alpha(\mu - \kappa)| \le |f^*h| + |\alpha||\mu - \kappa| \le ||f||_2 ||h||_2 + |\mu - \kappa|$$

 $f^*h + \alpha(\mu - \kappa) = r$ 

$$|r| \le ||R^{-1}||_2 ||g||_2 ||h||_2 + |\mu - \kappa|$$

$$\hat{g} = rg^* \Rightarrow \|\hat{g}\|_2 \le \|R^{-1}\|_2^2 \|g\|_2^2 \|h\|_2 + \|R^{-1}\|_2 \|g\|_2 |\mu - \kappa|$$

$$\|g_{k+1}\|_2 \le \|R_k^{-1}\|_2^2 \|g_k\|_2^2 \|h_k\|_2 + \|R_k^{-1}\|_2 \|g_k\|_2 |\mu_k - \kappa_k|$$

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Use a Rayleigh quotient shift  $\kappa_{\mathbf{k}}=\mu_{\mathbf{k}}$ 

$$\|g_{k+1}\|_2 \le \|R_k^{-1}\|_2^2 \|g_k\|_2^2 \|h_k\|_2 + \|R_k^{-1}\|_2 \|g_k\|_2 |\mu_k - \kappa_k|$$

Use a Rayleigh quotient shift  $\kappa_k = \mu_k$ 

$$||g_{k+1}||_2 \le \sigma^2 ||g_k||_2^2$$

For a proof for the bounds of  $||R^{-1}||_2^2$  and  $||h_k||_2^2$  see [4]

$$\|g_{k+1}\|_2 \le \|R_k^{-1}\|_2^2 \|g_k\|_2^2 \|h_k\|_2 + \|R_k^{-1}\|_2 \|g_k\|_2 |\mu_k - \kappa_k|$$

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The QR with Rayleigh quotient cannot produce complex eigenvalues

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Making both shifts at once = Francis' shift  $H^2 - 2\Re(\kappa)H + |\kappa|^2$  is hard to compute  $\mathcal{O}(n^3)$ 

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$$q_{k+1} = ||Aq_k - (h_{1k}q_1 + h_{2k}q_2 + \dots h_{kk}q_k)||_2$$



### Francis' Double Shift

Denote by c the first column of  $H^2-2\Re(\kappa)H+|\kappa|^2$ 

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Reduce  $H_1$  to Hessenberg form  $\hat{H}$ 

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 $\hat{Q}$  has to be the Hessenberg reduction of H to  $\hat{H}$ 

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Iterate this algorithm until close to Real Schur form



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There is an algorithm to reduce a complex Hessenberg matrix to a real one

Compute Hessenberg form of A

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Where  $Q_k$  is the matrix with the firs k columns of Q and

$$\hat{H} = \begin{bmatrix} h_{11} & h_{12} & \dots & h_{1n} \\ h_{21} & h_{22} & \dots & h_{2n} \\ 0 & h_{32} & \dots & h_{3n} \\ \dots & \dots & \dots & \dots \\ 0 & \dots & h_{n+1n-1} & h_{n+1n} \end{bmatrix}$$

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Similar construction with the implicit Q theorem

$$K_k(A, b) = \text{span}(b, Ab, A^2b, ..., A^{k-1}b)$$

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Arnoldi iteration isolates the information about the dominating eigenvalue via QR

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The Rayleigh Ritz quotient of the vectors  $q_i$  Main ideas of Arnoldi iteration

$$K_n = Q_n R_n$$
,  $H_n = Q_n^* A Q_n$ ,  $A Q_n = Q_{n+1} \overline{H_n}$ 



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As n increases  $H_n$  is closer to H so the eigenvalues of  $H_n$  are close to the eigenvalues of H

 $A = QHQ^*$  so the eigenvalues of A and H are the same Arnoldi iteration may give geometric convergence The algorithm breaks down when  $K_n$  is not of full rank

 $Q_nQp(H)Q^*b=0$   $\Rightarrow$  the first n elements of the first column of  $p_nH$  are 0

$$p_n(H_n)=0$$

From Cayley-Hamilton theorem  $p_n$  is the caracteristic polynomial of  $\overline{H_n}$ 

$$p_n(q_i^*Aq_i)=0, \quad i=\overline{1,n}$$

 $q_i^*Aq_i$  are the eigenvalues of  $H_n$ 

As n increases  $H_n$  is closer to H so the eigenvalues of  $H_n$  are close to the eigenvalues of H

 $A = QHQ^*$  so the eigenvalues of A and H are the same Arnoldi iteration may give geometric convergence The algorithm breaks down when  $K_n$  is not of full rank Arnoldi iteration is not fully understood (Trefethen)

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In any diagonal representation of A the number of positive eigenvalues is the same

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 $\Lambda_B^{-\frac{1}{2}} U^* A U \Lambda_B^{-\frac{1}{2}}$  is symmetric

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Repeat the process and denote

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By construction Q and Z simultaneously reduce A and B to Schur form

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The algorithm goes towards a diagonal form Only 4 entries are affected at each step  $\Rightarrow$  easy to compute in parallel

#### Pseudo-inverse

$$A = U\Sigma V^*$$

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