

Last time:  $A \in \mathbb{C}^{n \times n}$ , eigenvalues  $|\lambda_1| \geq |\lambda_2| \geq \dots \geq |\lambda_n|$   
 $v_1, v_2, \dots, v_n$

- Krylov subspaces

Given  $x_0 \in \mathbb{C}^n$ ,  $\|x_0\|_2 = 1$

$$K_k(A, x_0)$$

$$= \text{span}\{x_0, Ax_0, \dots, A^{k-1}x_0\}$$

$$= \{p(A)x_0 \in \mathbb{C}^n : p(A) = \sum_{l=0}^{k-1} t_l A^l \text{ is a polynomial of degree } \leq k-1\}$$

- Krylov matrix

$$K_k(A, x_0) = \begin{bmatrix} x_0 & Ax_0 & \dots & A^{k-1}x_0 \end{bmatrix} = Q_k R_k, \quad Q_k \in \mathbb{C}^{n \times k}$$

- Rayleigh-Ritz projection

$$B_k z = \tilde{\lambda} z$$

$$B_k = Q_k^* A Q_k \in \mathbb{C}^{k \times k}$$

$\tilde{\lambda}$  Ritz value,  $\tilde{v} = Q_k z$  Ritz vector

- Arnoldi's iteration

$$\begin{array}{ccccccc} x_0 & \rightarrow & Ax_0 & \rightarrow & A^2x_0 & \rightarrow & \dots \rightarrow A^{k-1}x_0 \\ \hline x_0 & & Aq_1 & & Aq_2 & & \dots & Aq_{k-1} \\ \downarrow & \nearrow & \downarrow & \nearrow & \downarrow & \nearrow & \dots & \nearrow \\ q_1 & & q_2 & & q_3 & & \dots & q_k \end{array}$$

Implementation:

Given  $x_0 \in \mathbb{C}^n$ ,  $k \geq 1$ ,

$$q_1 \leftarrow x_0 / \|x_0\|_2$$

For  $i = 1, \dots, k$

$$w_i \leftarrow Aq_i$$

For  $j = 1, \dots, i$

$$h_{ji} \leftarrow q_j^* w_i$$

$$w_i \leftarrow w_i - h_{ji} q_j$$

end

$$h_{i,i+1} = \|w_i\|_2$$

if  $h_{i,i+1} = 0$ , break.

$$q_{i+1} = w_i / \|w_i\|_2$$

end

Output:  $q_1, \dots, q_k, q_{k+1}, h_{ji}$

- Arnoldi decomposition:  $Q_k \in \mathbb{C}^{n \times k}$  orthonormal columns,  $H_k$  upper Hessenberg

$$A Q_k = Q_k H_k + h_{k+1,k} q_{k+1} e_k^*$$

$$q_{k+1}^* H_k = 0,$$

$$e_k = (0, \dots, 0, 1)^T$$

$$\Rightarrow Q_k^* A Q_k = H_k$$

- Special case: when  $A$  is Hermitian,  $Q_k^* A Q_k$  is Hermitian,

$\Rightarrow H_k$  is Hermitian  $\Rightarrow H_k$  is tridiagonal

$$\alpha_j \equiv h_{jj}, \quad \beta_j \equiv h_{j+1,j}$$

$$H_k = T_k = \begin{bmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \alpha_2 & \beta_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \beta_{k-2} & \alpha_{k-1} & \beta_{k-1} \\ & & & \beta_{k-1} & \alpha_k \end{bmatrix} \in \mathbb{C}^{k \times k}$$

Implementation: (Lanczos)

Given  $x_0 \in \mathbb{C}^n$ ,  $k \geq 1$ ,

$$q_1 \leftarrow x_0 / \|x_0\|_2, \quad \beta_0 = 0, \quad q_0 = 0$$

For  $i = 1, \dots, k$

$$w_i \leftarrow Aq_i$$

$$\alpha_i = q_i^* w_i$$

$$w_i \leftarrow w_i - \beta_i q_{i-1} - \alpha_i q_i$$

$$\beta_i = \|w_i\|_2 \quad \text{if } \beta_i = 0, \text{ break}$$

$$q_{i+1} = w_i / \beta_i$$

end

$$\bullet \text{ Cost} \approx (9n \text{ Flops} + \text{cost for } Aq) \times k$$

$$\bullet \text{ Storage} \approx kn \text{ for } Q_n$$

• What exactly are  $\tilde{\lambda}$  and  $\tilde{v} = Q_k z$ ?

Let  $\tilde{\lambda}, \tilde{v} = Q_k z$  be Ritz pair, i.e.  $H_k z = \tilde{\lambda} z, \|z\|_2 = 1$

$$\Rightarrow A \tilde{v} = \tilde{\lambda} \tilde{v} + h_{k+1,k} (e_k^* z) q_{k+1}$$

$$\Rightarrow (A + E) \tilde{v} = \tilde{\lambda} \tilde{v}, \quad \|\tilde{v}\|_2 = 1 \quad (*)$$

$$E = -h_{k+1,k} (e_k^* z) q_{k+1} \tilde{v}^*, \quad \|E\|_2 = |h_{k+1,k}| |z_k|, \quad z = (z_1, \dots, z_k)^T$$

The Ritz pairs are eigenpairs of a perturbed eigenvalue problem

Recall the following theorem from Lecture 11:

Thm (Bauer - Fike)

If  $\mu$  is an eig. val of  $A + E$  and

$$V^{-1} A V = D = \text{diag}(\lambda_1, \dots, \lambda_n) \quad (K_p(V) = \|V\|_p \|V^{-1}\|_p)$$

$$\text{then } \min_{1 \leq i \leq n} |\lambda_i - \mu| \leq K_p(V) \|E\|_p \quad \forall p \in [1, +\infty) \quad \square$$

Apply Bauer-Fike to (\*), we have

$$\text{Arnoldi: } \min_{1 \leq i \leq n} |\lambda_i - \tilde{\lambda}| \leq K_p(V) |h_{k+1,k}| |z_k|$$

$$\text{Lanczos: } \min_{1 \leq i \leq n} |\lambda_i - \tilde{\lambda}| \leq |\beta_k| |z_k|$$

Q: The approximation quality of  $H_k$ 's eigenvalues as a function of  $k$ ?

In the Hermitian setting, this can be made a little bit more precise.

Let  $\lambda_1 \geq \dots \geq \lambda_n$  be eig. val. of  $A$ .

$v_1, \dots, v_n$  be eig. vec. of  $A$ .

Thm (Kaniel-Paige-Saad) Let  $\|x_0\|_2 = 1$  in Krylov.

Suppose the Lanczos iteration are performed and  $T_k$

is obtained as a tridiagonal matrix. If  $\theta_1 = \lambda_1(T_k)$ , then

$$\lambda_1 \geq \theta_1 \geq \lambda_1 - (\lambda_1 - \lambda_n) \left( \frac{\tan(\phi_1)}{C_{k-1}(1+2\rho_1)} \right)^2$$

where  $\cos(\phi_1) = x_0^* v_1$ ,

$$\rho_1 = \frac{\lambda_1 - \lambda_2}{\lambda_2 - \lambda_n}$$

and  $C_{k-1}(x)$  is the Chebyshev polynomial of degree  $k-1$ .

$$C_k(x) = 2x C_{k-1}(x) - C_{k-2}(x), \quad C_0 = 1, \quad C_1 = x, \quad C_2 = 2x^2 - 1$$

Pf: We use the following characterization of the dominant eigenvalue of an Hermitian matrix

$$\theta_1 = \max_{z \neq 0} \frac{z^* T_k z}{z^* z} \quad \leftarrow \text{Rayleigh quotient}$$

Use  $T_k = Q_k^* A Q_k$ , we have

$$\theta_1 = \max_{z \neq 0} \frac{(Q_k z)^* A (Q_k z)}{(Q_k z)^* (Q_k z)}$$

$$= \max_{w \in K_k(A, x_0)} \frac{w^* A w}{w^* w}$$

$$= \max_{p \in \mathcal{P}_{k-1}(\mathbb{C})} \frac{x_0^* p(A) A p(A) x_0}{x_0^* p(A)^2 x_0}$$

maximize  $\rightarrow$  over polynomial degree  $\leq k-1$

Now let  $x_0 = d_1 v_1 + \dots + d_n v_n$  where  $d_i = x_0^* v_i$

$$\frac{x_0^* p(A) A p(A) x_0}{x_0^* p(A)^2 x_0} = \frac{\sum_{i=1}^n d_i^2 p(\lambda_i)^2 \lambda_i}{\sum_{i=1}^n d_i^2 p(\lambda_i)^2} \quad (**)$$

$$\begin{aligned} &\geq \frac{\lambda_1 d_1^2 p(\lambda_1)^2 + \lambda_n \sum_{i=2}^n d_i^2 p(\lambda_i)^2}{d_1^2 p(\lambda_1)^2 + \sum_{i=2}^n d_i^2 p(\lambda_i)^2} \\ &= \lambda_1 - (\lambda_1 - \lambda_n) \frac{\sum_{i=2}^n d_i^2 p(\lambda_i)^2}{d_1^2 p(\lambda_1)^2 + \sum_{i=2}^n d_i^2 p(\lambda_i)^2} \\ &\geq \lambda_1 - (\lambda_1 - \lambda_n) \frac{\sum_{i=2}^n d_i^2 p(\lambda_i)^2}{d_1^2 p(\lambda_1)^2} \end{aligned}$$

Now we pick

$$p(x) = C_{k-1} \left( -1 + 2 \frac{x - \lambda_n}{\lambda_2 - \lambda_n} \right)$$

want  $|p(\lambda_i)|$  small ( $i \geq 2$ )  
but  $|p(\lambda_1)|$  large  
so rescale  $[\lambda_n, \lambda_2]$  to  $[-1, 1]$

By the construction of Chebyshev,  $|C_k(x)| \leq 1, \forall x \in [-1, 1]$

Thus  $|p(\lambda_i)| \leq 1, \forall i = 2, 3, \dots, n$

and  $p(\lambda_1) = C_{k-1} (1 + 2\rho_1)$

$$\text{Thus } \sum_{i=2}^n d_i^2 p(\lambda_i)^2 \leq \sum_{i=2}^n d_i^2 = \sum_{i=1}^n d_i^2 - d_1^2 = 1 - d_1^2$$

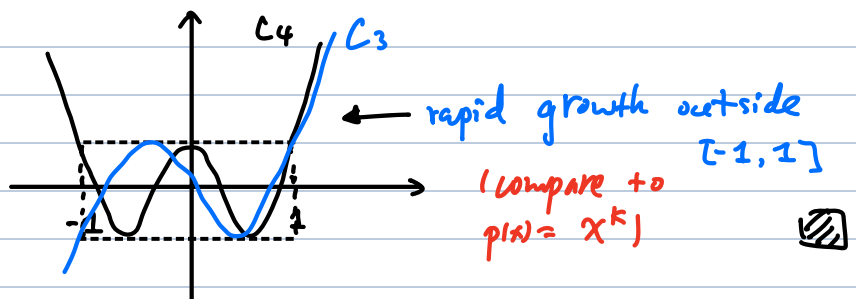
so we have

$$\theta_1 \geq \lambda_1 - (\lambda_1 - \lambda_n) \frac{1 - d_1^2}{d_1^2} \frac{1}{C_{k-1} (1 + 2\rho_1)}$$

Chebyshev polynomial

properties of Chebyshev:

$$|p(x)| \leq 1 \quad \forall x \in [-1, 1]$$



- Compare with power iteration:

In power iteration, at the  $k-1$ <sup>th</sup> stage,

$$x_{k-1} = A^{k-1} x_0 = \sum_{i=1}^n c_i \lambda_i^{k-1} v_i$$

and eig. val. estimator (Rayleigh quotient of  $x_{k-1}$ )

$$\gamma_1 = \frac{x_{k-1}^* A x_{k-1}}{x_{k-1}^* x_{k-1}}$$

corresponds to setting  $p(x) = x^{k-1}$  in (\*\*)

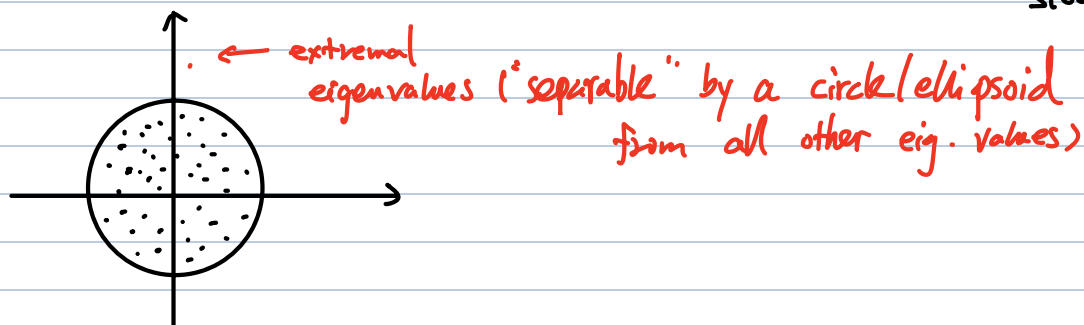
thus

$$\lambda_1 \geq \gamma_1 \geq \lambda_1 - (\lambda_1 - \lambda_n) \tan(\phi_1)^2 \left( \frac{\lambda_2}{\lambda_1} \right)^{2(k-1)}$$

Usually,  $C_{k-1} \left( 1 + 2 \frac{\lambda_1 - \lambda_n}{\lambda_2 - \lambda_n} \right) \gg \left( \frac{\lambda_2}{\lambda_1} \right)^{2(k-1)}$

- Remark: The idea can be applied to estimate interior eigenvalues, but the bound is less satisfactory. It is observed that Lanczos tends to approximate eigenvalues near the **edges** of spectrum with exp. rate in  $k$ .

Remark: For the non-Hermitian case, exponential convergence of Ritz values to "extremal" eigenvalues can also be proved. But convergence to "interior" eigenvalues can be much slower!



- Practical Arnoldi / Lanczos

Issues: 1) If  $k$  is large, the computation of  $q_{k+1}$  involves  $O(kn)$  flops in Arnoldi, and memory can quickly run out in both Arnoldi / Lanczos.

hope to: limit  $k$  in practice

but still want result be close to eigenvalues!

2) Arnoldi / Lanczos without reorthogonalization suffer from rounding error (orthogonality of  $\hat{Q}_k$  is lost)  $\Rightarrow$  many issues. such as ghost eigenvalues, i.e. single  $\lambda$  could repeat many times!

Solution: Restarting combine with other techniques. filtering (shifting).  $\Rightarrow$  implicitly restarting Arnoldi (ARPACK.jl)

- After  $k+p$  steps, throw out most of  $Q_{k+p}$ , keep only  $k$  "best" vectors so far, restart Arnoldi / Lanczos on step  $k$  with  $Q_k$  (reorthogonalized)

How to choose "best" vectors?

- want to satisfy the form of Arnoldi decomposition (See notes on restarting Arnoldi)
- Naive example: suppose we only want the dominant  $|\lambda|$ , just keep  $k=1$  vector. If  $p=0$ ,  $\approx$  power iteration