

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

$$K_k(A, x_0)$$

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

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

- 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
 $q_{k+1}^* H_k = 0$,
 $e_k = (0, \dots, 0, 1)^T$
 $A Q_k = Q_k H_k + h_{k+1,k} q_{k+1} e_k^*$
 $\Rightarrow Q_k^* A Q_k = H_k$

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- 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 $i = 1, \dots, k$

$$w_i \leftarrow A q_i$$

$$\alpha_i = q_i^* w_i$$

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

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

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

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 μ 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

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

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

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

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

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

$$\beta_1 = \frac{\lambda_1 - \lambda_2}{\lambda_2 - \lambda_n}$$

properties of Chebyshev:

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

but $|T_k(x)|$ grows rapidly outside $[-1, 1]$

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

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

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

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

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

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

maximize over polynomial degree $\leq k-1$ $\rightarrow p \in \mathcal{P}_{k-1}(A)$

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

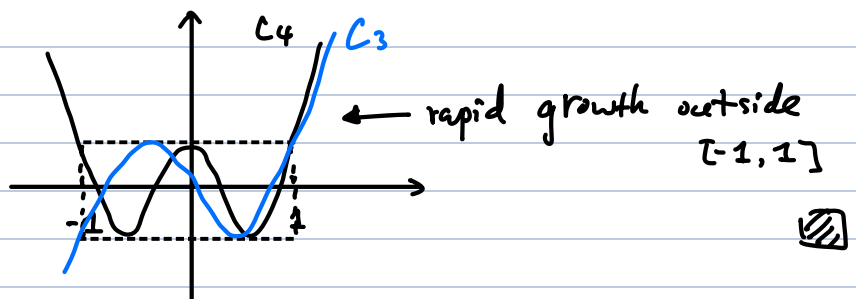
and $p(\lambda_1) = c_{k-1} (1 + 2\rho_1)$

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

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



- Compare with power iteration:

In power iteration, at the $k-1^{\text{th}}$ 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

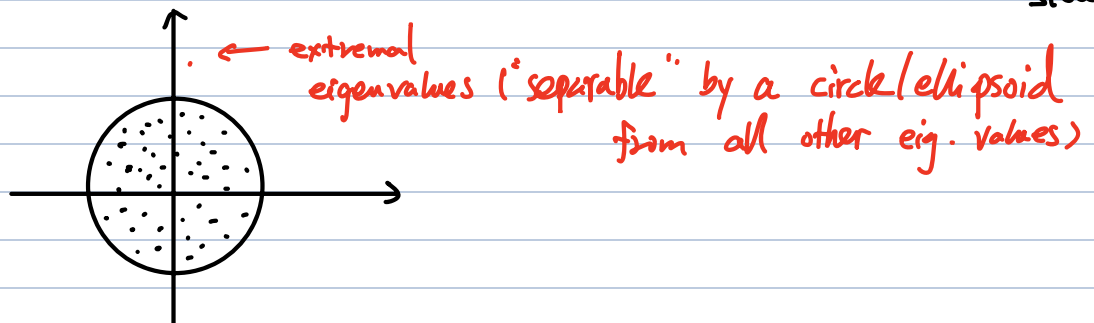
$$\lambda_1 \geq \gamma_1 \geq \lambda_1 - (\lambda_1 - \lambda_n) \tan(\phi_1)^2 \left(\frac{\lambda_2}{\lambda_1} \right)^{2(k-1)}$$

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 λ could repeat many times!

Solution: Restarting \Rightarrow implicitly restarting Arnoldi (combine with other techniques. ^{filtering (shifting).} 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
- Naive example: suppose we only want the dominant $|\lambda|$, just keep $k=1$ vector. If $p=0$, \approx power iteration