# Iterative Methods

## Part 3: Arnoldi for Linear Sys. (GMRES)

Recap

Arnoldi generates ONB $Q_n$ s.t.

ONB for Krylov Subspace

$$\underbrace{\begin{bmatrix} | & | & & | \\ x & Ax & \cdots & A^{n-1}x \\ | & | & & | \end{bmatrix}}_{K_n} = \underbrace{\begin{bmatrix} | & | & & | \\ q_1 & q_2 & \cdots & q_n \\ | & | & & | \end{bmatrix}}_{Q_n} \underbrace{\begin{bmatrix} \; \end{bmatrix}}_{R_n}$$

Arnoldi Decomp.

$$A \underbrace{\begin{bmatrix} | & & | \\ q_1 & \cdots & q_n \\ | & & | \end{bmatrix}}_{Q_n} = \underbrace{\begin{bmatrix} | & & | \\ q_1 & \cdots & q_n \\ | & & | \end{bmatrix}}_{Q_n} \underbrace{\begin{bmatrix} \; \end{bmatrix}}_{H_n} + h q_{n+1} e_n^T$$

$$\Rightarrow \quad H_n = Q_n^* A Q_n$$

## Approximating Eigenvalues

$\theta_1, \ldots, \theta_n$ eigenvalues of $H_n$ are roots of the minimizing polynomial

$$\|p_n(A)x\|_2 = \overset{\text{minimum over}}{\text{all}} \; p_n \in \underset{\text{deg. } n \text{ poly's}}{\underline{P_n}}$$

$\Rightarrow$ As $n$ increases, $p_n$ tends to place roots near extremal eigenvalues of $A$.

$\Rightarrow$ Can be much more efficient than power iterations/simultaneous iterations.

## Generalized Minimal Residuals (GMRES)

The Arnoldi iteration also produces powerful approximations to the solns of linear systems.

Solve $Ax = b \quad \Rightarrow \quad x_* = A^{-1}b$ Exact soln.

Krylov Subspace $\quad K_n(A,b) = \mathrm{span}\{b, Ab, A^2 b, \dots, A^{n-1}b\}$

Idea: choose $x_n \in K_n(A,b)$ to minimize the residual norm

$$x_n = \underset{x \in K_n(A,b)}{\mathrm{argmin}} \|Ax - b\|_2$$

$\Rightarrow$ This is just a Least-Squares problem!

## Arnoldi & Least-Squares

Approach 1: write $A\underbrace{K_n c}_{x \in K_n(A,b)}$ to get

$$x_n = \underset{c \in \mathbb{R}^n}{\operatorname{argmin}} \|AK_n c - b\|_2$$

Solve w/ QR factorization of tall skinny mat

$$\begin{bmatrix} | & | & & | \\ Ax & A^2x & \cdots & A^n x \\ | & | & & | \end{bmatrix}$$

$\Rightarrow$ ill-conditioned least-squares problem

Approach 2: write $A\underbrace{Q_n y}_{x \in K_n(A,b)}$ to get

$$x_n = \underset{Q_n y \in \mathbb{R}^n}{\operatorname{argmin}} \|AQ_n y - b\|_2$$

Use Arnoldi decomp $AQ_n = Q_{n+1}\tilde{H}_n$

$$\|AQ_n y - b\|_2 = \|Q_{n+1}\tilde{H}_n y - b\|_2$$

b/c $Q_{n+1}\tilde{H}_n y - b \in K_n(A,b)$ $\rightarrow = \|\tilde{H}_n y - Q_{n+1}^* b\|_2$

Since $q_1 = b/\|b\|$, we need to solve

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1) $y_n = \underset{y \in \mathbb{R}^n}{\operatorname{argmin}} \; \| \tilde{H}_n y - \|b\| e_1 \|_2$

2) $x_n = Q_n y_n$

$\Rightarrow$ Avoids ill-conditioning of $K_n$.

$\Rightarrow$ Special structure of $\tilde{H}_n$ allows us to update Least-Squares soln. $y_n$ fast as we build up $\tilde{H}_n$ column-by-column with Arnoldi iterations.

## GMRES (Pseudocode)

$q_1 = b/\|b\|$

for $k = 1, 2, 3, \ldots$

- Step $n$ of Arnoldi adds $k^{th}$ column to $\tilde{H}_k$, $Q_k$
- Solve LS problem $y = \operatorname{argmin} \|\tilde{H}_k y - \|b\| e_1\|_2$ using fast QR update.
- Compute $x_k = Q_k y_k$

## GMRES : Polynomial Approx

Since $x_n \in K_n(A, b) = \operatorname{span}\{b, Ab, A^2 b, \ldots, A^{n-1} b\}$,

$$x_n = q_{n-1}(A) b = c_0 b + c_2 Ab + \cdots + c_{n-1} A^{n-1} b$$

We minimize the residual

$$r_n = b - Ax_n = b - A(c_0 b + c_2 Ab + \dots + c_{n-1}A^{n-1}b)$$

so $\quad r_n = p_n(A)b \quad$ where $p_n(z) = 1 - z\,q_{n-1}(z)$

is a degree $n$ polynomial w/ $p_n(0) = 1$.

<u>Thm</u> Over all degree $n$ polynomials with $p(0)=1$, GMRES constructs $p_n(z)$

s.t. $\qquad \|p_n(A)b\|_2 = \text{minimum}.$

<u>Convergence</u>

First, note that $\|r_{n+1}\| \leq \|r_n\|$ for all $n \geq 1$ b/c $K_n(A,b) \subset K_{n+1}(A,b)$.

Second, note that $\|r_m\| = 0$ since $K_m(A,b) = \mathbb{R}^m$ and $A$ is invertible: $A^{-1}b \in K_m(A,b)$

So $\|r_n\| \to 0$ monotonically (nonincreasing) in no more than $m$ steps.

We need $n \ll m$, so key question is how fast does $\|r_n\|$ decrease?

<u>Extremal problems in polynomial approx</u>

Denote $P_n^0 = \{$set of deg. $n$ poly with $p(0)=1\}$

$$\|r_n\| = \min_{p \in P_n^0} \|p(A)b\| \leq \|p(A)\| \, \|b\| \quad \text{for any } p \in P_n^0$$

$$\frac{\|r_n\|}{\|b\|} \leq \inf_{p \in P_n^0} \|p(A)\|$$

$A = V \Lambda V^{-1}$ diagonalizable, then

$$p(A) = V p(\Lambda) V^{-1} \Rightarrow \|p(A)\| \leq \underbrace{\|V\|\|V^{-1}\|}_{\kappa(V)} \underbrace{\|p(\Lambda)\|}_{\max_{1 \leq j \leq m} p(\lambda_j)}$$

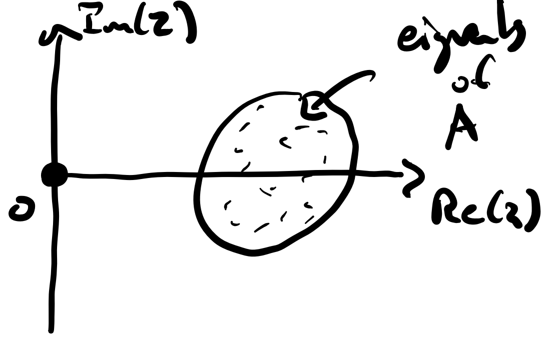
$$\therefore \quad \frac{\|r_n\|}{\|b\|} \leq \kappa(V) \min_{p \in P_n^0} \max_{1 \leq j \leq n} p(\lambda_j)$$

Min-max problem on spectrum of A.

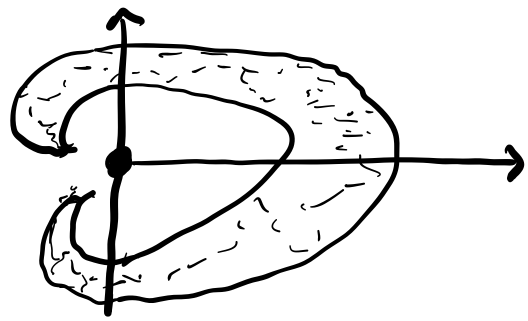
Note: Non-normality (large $\kappa(V)$) can degrade convergence of iterative methods like

Arnoldi & GMRES.

**Example 1**




**Example 2**



$p(0)=1$, how small can $p(z)$ be on spectrum of $A$?