LECTURE 29

GMRES - GENERAL MINIMAL RESIDUAL

(SOLUTION OF SPARSE LARGE LINEAR SYSTEMS)

Arnoldi iteration adopted for linear systems.

Let $A \in \mathbb{C}^{m \times m}$ where m is very large so that you cannot compute an LU factorization.

Basic Idea

Approximate the solution of

$$Ax = b$$

with the optimal solution of

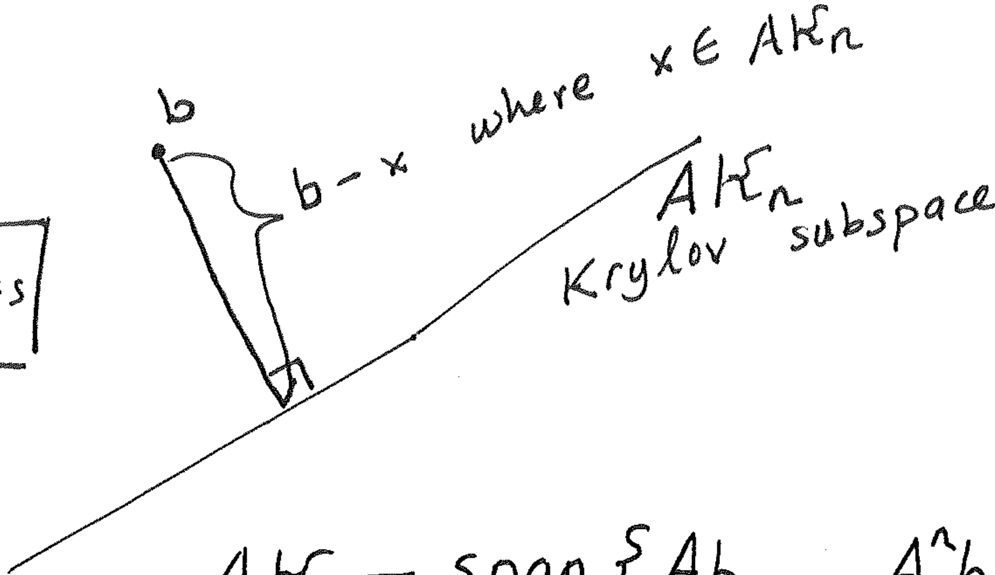
$$(*) \quad \underset{x \in \mathcal{K}_n}{\text{minimize}} \; \| Ax - b \|_2$$

where

$$\mathcal{K}_n = \text{span}\{b, Ab, \ldots, A^{n-1}b\}$$

with $n \ll m$

LEAST SQUARES VIEW



$$A\mathcal{K}_n = \text{span}\{Ab, \dots, A^n b\}$$

Consider problem (*) again

$$\underset{x \in \mathcal{K}_n}{\text{minimize}} \; \| Ax - b \|_2$$

$$= \left(\text{Recall if } K_n = Q_n R_n, \text{ then } AQ_n = Q_{n+1} \tilde{H}_n \right)$$

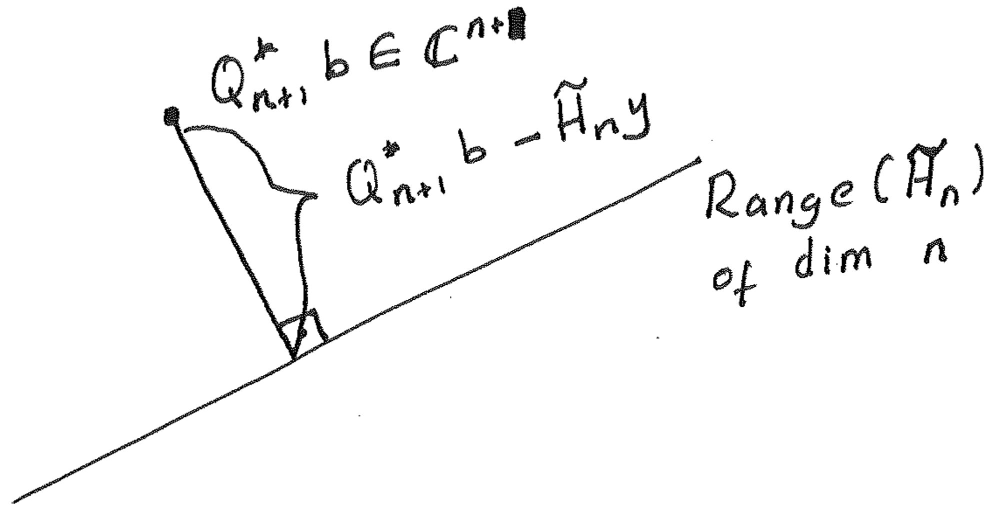
$$\underset{y \in \mathbb{C}^n}{\text{minimize}} \; \| A Q_n y - b \|_2$$

$$=$$

$$\underset{y \in \mathbb{C}^n}{\text{minimize}} \; \| \underbrace{Q_{n+1}}_{m \times (n+1)} \underbrace{\tilde{H}_n}_{(n+1) \times n} \underbrace{y}_{n \times 1} - \underbrace{b}_{m \times 1} \|_2$$

$$= \left(\text{By unitary invariance of 2-norm} \right)$$

$$(**) \quad \underset{y \in \mathbb{C}^n}{\text{minimize}} \; \| \tilde{H}_n y - Q_{n+1}^* b \|_2 \quad \left(\begin{array}{c} (n+1) \times n \\ \text{LSP} \end{array} \right)$$



Solve LSP in (**) using QR factor by Householder reflectors. (This can be done in $O(n^2)$ time, since $\tilde{H}_n$ is Hessenberg)

<u>Algorithm</u> (GMRES)

$q_1 = b/\|b\|$

for $j = 1, \dots, n$

  Generate $\tilde{H}_j$ and Q_{j+1} using Arnoldi iteration $\}$ $O(m^2)$ FLOPS

  Solve LSP $\min \|\tilde{H}_j y - Q_{j+1}^* b\|_2$ by Householder reflectors $\}$ $O(j^2)$ FLOPS

  Best approximate solution $\hat{x} = Q_j y$ $\}$ $O(j^2)$ FLOPS

end

REMARK

GMRES is guaranteed to converge after m iterations, since $\mathcal{K}_m = \mathbb{C}^m$ (assuming $\{b, Ab, \ldots, A^{m-1}b\}$ are linearly independent.)

Convergence

Original LSP $(*)$ was equivalent to

$$\underset{y \in \mathbb{C}^n}{\text{minimize}} \; \| A \underbrace{Q_n y}_{\alpha_{n-1} A^{n-1} b + \ldots + \alpha_0 b \;\; \exists \alpha_0, \ldots, \alpha_{n-1}} - b \|_2$$

$$=$$

$$\underset{q \in \hat{\mathbb{P}}_{n-1}}{\text{minimize}} \; \| \underbrace{A \, q(A) \, b}_{p(A) b} - b \|_2$$

for some polynomial p of degree n and constant term zero

$$=$$

$$(**) \quad \underset{p \in \mathbb{P}_n}{\text{minimize}} \; \| p(A) \, b \|_2$$

where

$\hat{\mathbb{P}}_{n-1}$: all polynomials of degree at most $(n-1)$

$\mathbb{P}_n$: all polynomials of degree at most n with constant term equal to 1.

OBSERVATIONS

* $\|p(A)b\|_2$ is small, whenever $\|p(A)\|_2$ is small.

* By Hamilton-Cayley thm the convergence is ~~small~~ faster if A has clustered eigenvalues.

  e.g. If A has 2 distinct eigenvalues and diagonalizable i.e.

$$A = V \begin{bmatrix} \lambda_1 I & 0 \\ 0 & \lambda_2 I \end{bmatrix} V^{-1},$$

then

$$p(A) = (A - \lambda_1 I)(A - \lambda_2 I) = 0$$

and GMRES would converge to the exact solution after 2 iterations.