LECTURE 28

ARNOLDI'S METHOD

(SOLUTION OF SPARSE LARGE EIGENVALUE PROBLEMS)

Let $A \in \mathbb{C}^{m \times m}$ where m is very large so that it is not even computationally feasible to reduce it to Hessenberg form by unitary similarity transformations.

$$Q^* A \underbrace{Q}_{\text{Unitary}} = \underbrace{H}_{\text{Hessenberg}} \quad - \text{ NOT FEASIBLE}$$

Consider the space $\mathcal{K}_n = \text{span}\{b, \dots, A^{n-1}b\}$ with $n \ll m$.

By subspace iteration you would expect $\mathcal{K}_n$ would capture the space spanned by dominant eigenvectors of A as n is getting larger.

Arnoldi iteration

(i) $\underbrace{\begin{bmatrix} b & Ab & \dots & A^{n-1}b \end{bmatrix}}_{K_n - m\times n} = \underbrace{Q_n}_{m\times n} \underbrace{R_n}_{n\times n}$ (REDUCED QR FACTOR)

(ii) $H_n = Q_n^{*} A Q_n$ ($\underline{\text{NOTE}}$ NOT A SIMILARITY TRANSFORMATION)

(Assuming Q_n approximates eigenvectors
H_n approximates eigenvalues)

TERMINOLOGY

(1) $\mathcal{K}_n = \text{span}\{b, \dots, A^{n-1}b\}$ is a <u>Krylov subspace</u>.

(2) $K_n = \begin{bmatrix} b & \dots & A^{n-1}b \end{bmatrix} \in \mathbb{C}^{m\times n}$ is a <u>Krylov matrix</u>.

(3) <u>Eigenvalues</u> of H_n are <u>Ritz values</u>.

Arnoldi iteration as above is numerically unstable (similar to the simultaneous iteration).

Numerically Stable Arnoldi Iteration

Let

$$Q_n = [q_1 \quad q_2 \quad \cdots \quad q_n] \in \mathbb{C}^{m \times n}$$

(see the QR factorization in (i)).

Then

$$\text{span}\{q_1\} = \mathcal{K}_1 = \text{span}\{b\}$$

$$\text{span}\{q_1, q_2\} = \mathcal{K}_2 = \text{span}\{b, Ab\}$$

$$\vdots$$

$$\text{span}\{q_1, q_2, \dots, q_n\} = \mathcal{K}_n = \text{span}\{b, \dots, A^{n-1}b\}$$

Use Gram-Schmidt to construct the orthonormal basis $\{q_1, \dots, q_n\}$ for $\mathcal{K}_n$ progressively.

(1) $q_1 = b / \|b\|$

(2) $\text{span}\{q_1, Aq_1\} = \text{span}\{b, Ab\}$

$$Aq_1 = h_{11} q_1 + h_{21} q_2$$

(3) $\text{span}\{q_1, q_2, Aq_2\} = \text{span}\{b, Ab, A^2b\}$

$$Aq_2 = h_{12} q_1 + h_{22} q_2 + h_{32} q_3$$

(n) $\operatorname{span}\{q_1, \dots, q_{n-1}, Aq_{n-1}\} = \operatorname{span}\{b, \dots, A^{n-1}b\}$

$$Aq_{n-1} = h_{1(n-1)}q_1 + h_{2(n-1)}q_2 + \dots + h_{n(n-1)}q_n$$

Combining the recurrence equations above

$$\underbrace{A}_{m\times m}\underbrace{\begin{bmatrix} q_1 & q_2 & \cdots & q_{n-1}\end{bmatrix}}_{m\times(n-1)} = \underbrace{\begin{bmatrix} q_1 & q_2 & \cdots & q_{n-1} & q_n\end{bmatrix}}_{m\times n}\underbrace{\begin{bmatrix} h_{11} & h_{12} & \cdots & h_{1(n-1)} \\ h_{21} & h_{22} & & \vdots \\ 0 & h_{32} & \ddots & h_{(n-1)(n-1)} \\ \vdots & \vdots & \ddots & \\ 0 & 0 & & h_{n(n-1)}\end{bmatrix}}_{\substack{\tilde{H}_{n-1}\in\mathbb{C}^{n\times(n-1)} \\ \text{Hessenberg}}}$$

that is

$$A\,Q_{n-1} = Q_n\,\tilde{H}_{n-1}$$

Multiply both sides above by Q_{n-1}^* from left to obtain

$$Q_{n-1}^*\,A\,Q_{n-1} = Q_{n-1}^*\,Q_n\,\tilde{H}_{n-1}$$

$$= \underbrace{\begin{bmatrix} 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 \\ \vdots & & \ddots & & \vdots & \vdots \\ 0 & 0 & \cdots & & 1 & 0\end{bmatrix}}_{(n-1)\times n}\tilde{H}_{n-1}$$

$$= \underbrace{\begin{bmatrix} h_{11} & h_{12} & \cdots & \cdots & h_{1(n-1)} \\ h_{21} & \ddots & & & h_{2(n-1)} \\ 0 & \ddots & \ddots & & \vdots \\ \vdots & & & & \\ 0 & & & h_{(n-1)(n-2)} & h_{(n-1)(n-1)}\end{bmatrix}}_{\substack{H_{n-1}\in\mathbb{C}^{(n-1)\times(n-1)} \\ \text{Hessenberg}}}$$

REMARKS

* H_{n-1} is obtained from $\tilde{H}_{n-1}$ by removing last row.

* H_{n-1} is the matrix on the left-hand side in (ii) (but with $n-1$ replaced by n)

* Eigenvalues of H_{n-1} are Ritz values.

Algorithm (Arnoldi Iteration)

$q_1 = b/\|b\|$

for $j = 1, \dots, n$

  $v = Aq_j$ } $2m^2$ FLOPS

  for $k = 1, \dots, j$

    $h_{kj} = v^* q_j$ } $2m$ FLOPS

    $v = v - h_{kj} \cdot q_k$ } $2m$ FLOPS

  end

  $h_{(j+1)j} = \|v\|$

  $q_{j+1} = v / h_{(j+1)j}$

end

Each iteration is $O(m^2)$.

Least Squares Point of View

Consider the polynomial $\hat{p}(z)$ of degree n (monic) with roots equal to the eigenvalues of H_n.

$\hat{p}(z)$ turns out to be the optimal solution for the following problem

$$(*) \quad \inf_{p \in P^n} \| p(A) b \|_2$$

where P^n is the set of all monic polynomials of degree n.

<u>THM</u> (Hamilton - Cayley)

Let $A \in \mathbb{C}^{m \times m}$ and

$$q(\lambda) = \det(A - \lambda I).$$

Then $q(A) = 0$.

<u>OBSERVATIONS</u>

* When $\|p(A)\|_2$ is small, so is $\|p(A)b\|_2$
* By Hamilton-Cayley thm $\|p(A)\|_2$ is small, if roots of p are close to eigenvalues of A.

* Since eigenvalues of H_n are optimal roots, they should capture eigenvalues of A.

Consider

$$\|p(A)b\|_2 = \| A^n b - \underbrace{(\alpha_{n-1} A^{n-1} b + \dots + \alpha_0 b)}_{\in \mathcal{K}_n} \|_2$$

$$= \|A^n b - Q_n y\| \quad \exists y \in \mathbb{C}^n$$

Consequently (*) could be posed as

$$\text{(LSP)} \quad \underset{y \in \mathbb{C}^n}{\text{minimize}} \; \|A^n b - Q_n y\|$$