(1) Direct methods require $O(m^3)$ work

→ You get the answer in finite number of steps!

(2) Iterative method require infinite number of iterations to get the exact answer but for practical purposes we can terminate the iterations using certain tolerance criteria. This reduces computational cost specifically when dealing with sparse matrices arising for discretization of partial different equations!

$$x \to \boxed{\text{Black box}} \to Ax \text{ or } A^T x \quad ✓$$

Krylov Subspace methods :-

Given a matrix $\underset{\sim}{A}$ and a vector $\underset{\sim}{b}$, the associated Krylov sequence is the set of vectors $\underset{\sim}{b}, \underset{\sim}{A}\underset{\sim}{b}, \underset{\sim}{A}^2\underset{\sim}{b}, \underset{\sim}{A}^3\underset{\sim}{b}, \ldots$

Heart of most iterative methods rely on projection into Krylov subspace!

Arnoldi Iteration :-

In phase I, we saw the reduction of $\underset{\sim}{A} \in \mathbb{R}^{m\times m}$ to upper Hessenberg form by choosing reflectors.

$$\boxed{\underset{\sim}{A} = \underset{\sim}{Q}\,\underset{\sim}{H}\,\underset{\sim}{Q}^T}$$

$$\Rightarrow \boxed{\underset{\sim}{A}\,\underset{\sim}{Q} = \underset{\sim}{Q}\,\underset{\sim}{H}} \quad — (1)$$

Now we will consider "n" columns of

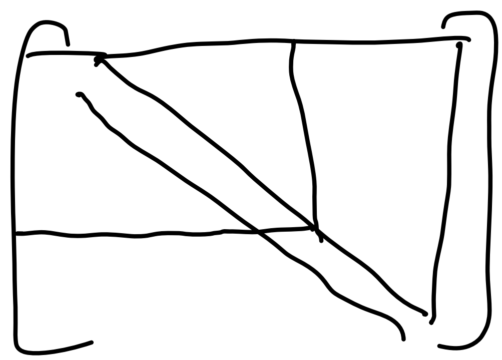
$$AQ = QH$$

Let $\hat{Q}_n$ be the $m \times n$ matrix whose columns are the first 'n' columns of Q:

$$\hat{Q}_n = \underbrace{\left[\, q_1 \,\middle|\, q_2 \,\middle|\, \cdots \,\middle|\, q_n \,\right]}$$

Let $\tilde{H}_n$ be the $(n+1) \times n$ upper left section of H is also Hessenberg matrix

$$\tilde{H}_n = \begin{bmatrix} h_{11} & \cdots & \cdots & h_{1n} \\ h_{21} & h_{22} & & \vdots \\ & \ddots & \ddots & \vdots \\ & & h_{n,n-1} & h_{nn} \\ & & & h_{n+1,n} \end{bmatrix}$$



$$\boxed{AQ = \underbrace{QH}}$$

$\hat{Q}_n$; $\tilde{H}_n$

Then we have

$$\boxed{A\hat{Q}_n = \hat{Q}_{n+1}\tilde{H}_n} \quad \text{— (2)}$$

The n^{th} column of Equation (2) can be written as follows:-

$$\boxed{\underset{\sim}{A}\,\underset{\sim}{q}_n = h_{1n}\underset{\sim}{q}_1 + h_{2n}\underset{\sim}{q}_2 + \cdots h_{n+1,n}\underset{\sim}{q}_{n+1}} \quad \text{— (3)}$$

$\underset{\sim}{q}_{n+1}$ satisfies $(n+1)$-term recurrence relation involves itself and previous vectors $\underset{\sim}{q}_1, \underset{\sim}{q}_2, \ldots \underset{\sim}{q}_n$.

Arnoldi iteration is essentially iterative procedure which implements (3) above.

<u>Algorithm</u>:-

$$\underset{\sim}{b} = \text{arbitrary}$$

$$\underset{\sim}{q}_1 = \frac{\underset{\sim}{b}}{\|\underset{\sim}{b}\|}$$

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

$$\boxed{\underset{\sim}{v} = \underset{\sim}{A}\,\underset{\sim}{q}_1}$$

for $j = 1$ to n

$$h_{jn} = q_j^T v$$

$$v = v - h_{jn} q_j$$

$$h_{n+1,n} = \|v\|$$

$$q_{n+1} = \frac{v}{h_{n+1,n}}$$

$$\boxed{A q_1 = h_{11} q_1 + h_{21} q_2}$$

$$*$$

$$K_n = \langle q_1, q_2, \ldots q_n \rangle = \langle b, Ab, A^2 b, \ldots A^{n-1} b \rangle$$

Intuitive proof:

$$q_1 = \frac{b}{\|b\|}$$

$$p = \beta_1 q_1 + \beta_2 q_2$$

$$= \beta_1 \frac{b}{\|b\|} + \frac{\beta_2}{h_{21}} \left(A q_1 - h_{11} q_1 \right)$$

$$= \beta_1 \frac{b}{\|b\|} + \frac{\beta_2}{h_{21}} \left(A \frac{b}{\|b\|} - h_{11} \frac{b}{\|b\|} \right)$$

$$= b \underbrace{\left[\frac{\beta_1}{\|b\|} - \frac{\beta_2 h_{11}}{h_{21} \|b\|} \right]} + A b \left(\frac{\beta_2}{h_{21} \|b\|} \right)$$

$$= b \alpha_1 + A b \alpha_2 = \alpha_1 b + \alpha_2 A b$$

$n=3$

$$\bar{p} = \beta_1 q_1 + \beta_2 q_2 + \beta_3 q_3$$
$$= \alpha_1 b + \alpha_2 A b + \alpha_3 A^2 b$$

$$K_n = \hat{Q}_n \hat{R}_n$$

$$K_n = \begin{pmatrix} | & | & | & & | \\ b & Ab & A^2 b & \cdots & A^{n-1} b \\ | & | & | & & | \end{pmatrix}$$

Projection onto Krylov subspace :-

$$x \to \boxed{\begin{array}{c}\text{Black box} \\ Ax,\ A^T x\end{array}} \to Ax$$
$$A \to$$

$$A \hat{Q}_n = Q_{n+1} \tilde{H}_n$$

$$\underset{n \times m}{\hat{Q}_n^T} \ \underset{m \times (n+1)}{\hat{Q}_{n+1}} = \begin{bmatrix} 1 & \cdots & & & & 0 \\ & 1 & & & & 0 \\ & & 1 & & & 0 \\ & 0 & & 1 & & 0 \\ & & & & 1 & 0 \end{bmatrix}_{m \times (n+1)}$$

$$\tilde{H}_n = \begin{bmatrix} h_{11} & \cdots & & h_{1n} \\ h_{21} & h_{22} & & \\ & \ddots & \ddots & h_{nn} \\ & & h_{n\,n-1} & \\ & & & h_{n+1\,n} \end{bmatrix}$$

$$\boxed{\hat{Q}_n^T \hat{Q}_{n+1} \tilde{H}_n = H_n}$$

H_n is actually $n \times n$ Hessenberg matrix obtained by removing the last row of $\tilde{H}_n$

$$H_n = \hat{Q}_n^T \hat{Q}_{n+1} \tilde{H}_n$$

$$A \hat{Q}_n = \hat{Q}_{n+1} \tilde{H}_n$$

$$\hat{Q}_n^T A \hat{Q}_n = \hat{Q}_n^T \hat{Q}_{n+1} \tilde{H}_n = H_n$$

$$\boxed{\underset{\sim}{H}_n = \hat{\underset{\sim}{Q}}_n^T \underset{\sim}{A} \hat{\underset{\sim}{Q}}_n}$$

This matrix $\underset{\sim}{H}_n$ can be interpreted as the representation of the orthogonal projection of matrix $\underset{\sim}{A}$ onto the subspace spanned by the basis $\{\underset{\sim}{q}_1, \underset{\sim}{q}_2, \dots \underset{\sim}{q}_n\}$ in terms of the same basis vectors $\{\underset{\sim}{q}_1, \underset{\sim}{q}_2, \dots \underset{\sim}{q}_n\}$

$$\underset{\sim}{A}_p = \underset{\sim}{P}\,\underset{\sim}{A} \qquad \underset{\sim}{P} = \hat{Q}_n \hat{Q}_n^T$$

$$\underset{\sim}{A}_p = \hat{Q}_n \hat{Q}_n^T \underset{\sim}{A} \quad \text{---} (*) \qquad \hat{Q}_n = [\underset{\sim}{q}_1 | \underset{\sim}{q}_2 \dots | \underset{\sim}{q}_n]$$

$$\boxed{m\times m} \quad \boxed{m\times n} \quad \boxed{n\times m} \quad \boxed{m\times m}$$

We have to express $\underset{\sim}{A}p$ in the basis of $K_n = [\underset{\sim}{q}_1 | \underset{\sim}{q}_2 | \cdots | \underset{\sim}{q}_n]$

i.e $$\tilde{A}_{p_{ij}} = \underset{\sim}{q}_i^T \underset{\sim}{A}_p \underset{\sim}{q}_j$$

$$\Rightarrow \underset{\sim}{\tilde{A}}_p = \underset{\sim}{\hat{Q}}_n^T \underset{\sim}{A}_p \underset{\sim}{\hat{Q}}_n$$

$n \times n$ $\quad$ $n \times m$ $\quad m \times m \quad m \times n$

$$\Rightarrow \underset{\sim}{\tilde{A}}_p = \underset{\sim}{\hat{Q}}_n^T \underset{\sim}{\hat{Q}}_n \underset{\sim}{\hat{Q}}_n^T \underset{\sim}{A} \underset{\sim}{\hat{Q}}_n$$

$$\boxed{\underset{\sim}{\tilde{A}}_p = \underset{\sim}{\hat{Q}}_n^T \underset{\sim}{A} \underset{\sim}{\hat{Q}}_n}$$

$$\boxed{\underset{\sim}{H}_n = \underset{\sim}{\hat{Q}}_n^T \underset{\sim}{A} \underset{\sim}{\hat{Q}}_n}$$

Since $\underset{\sim}{H}_n$ is a projection of $\underset{\sim}{A}$

onto K_n, there is a possibility that eigenvalues of $\underset{\sim}{H_n}$ is related to $\underset{\sim}{A}$ in a useful fashion!

$$\{\theta_j\} = \{\text{eigenvalues of } H_n\}$$

are called Arnoldi eigenvalue estimates (at step n) or Ritz values (with respect to K_n)

<u>Thm</u>:- The matrices $\hat{Q}_n$ generated by the Arnoldi iteration are reduced QR

factors of the Krylov matrix

$$\underset{\sim}{K}_n = \underset{\sim}{\hat{Q}}_n \underline{\hat{R}}_n$$

The Hessenberg matrices $\underset{\sim}{H}_n$ are the corresponding projections

$\underset{\sim}{H}_n = \underset{\sim}{\hat{Q}}_n^T \underset{\sim}{A} \underset{\sim}{\hat{Q}}_n$ and successive iterates are related by the formula $\underset{\sim}{A} \underset{\sim}{\hat{Q}}_n = \underset{\sim}{\hat{Q}}_{n+1} \underline{\tilde{H}}_n$

<u>How</u> do <u>we</u> compute <u>eigenvalues</u> of <u>$\underset{\sim}{A}$ using</u> Arnoldi <u>iteration</u>?

Project $A^{m\times m} \longrightarrow K_n$, you get projected matrix $\underset{\sim}{H}_n = \underset{\sim}{\hat{Q}}_n^T \underline{A} \underline{\hat{Q}}_n$

you can find eigenvalues of H_n by QR algorithm

Arnoldi iteration as a polynomial approximation :-

If $\underset{\sim}{x} \in K_n$, $K_n = \langle \underset{\sim}{b}, \underset{\sim}{A}\underset{\sim}{b}, \ldots A^{n-1}\underset{\sim}{b} \rangle$

$$\underset{\sim}{x} = c_0\underset{\sim}{b} + c_1\underset{\sim}{A}\underset{\sim}{b} + c_2\underset{\sim}{A}^2\underset{\sim}{b} + \ldots + c_{n-1}\underset{\sim}{A}^{n-1}\underset{\sim}{b} \quad -(4)$$

Introduce $q(z) = c_0 + c_1 z + c_2 z^2 + \ldots c_{n-1} z^{n-1}$, then

eqn (4) can be written as

$$\boxed{\underset{\sim}{x} = q(\underset{\sim}{A})\underset{\sim}{b}} \quad -(5)$$

Define $P^n = \{$monic polynomials of degree $n\}$

→ monic polynomials are those polynomials whose coefficient of Z^n is 1 (coefficient of term of degree n is 1)

<u>Arnoldi</u> <u>approximation</u> <u>problem</u> :-

Find $p^n \in P^n$ such that

$\boxed{\|p^n(\underset{\sim}{A})\,\underline{b}\|}$ is minimum.

<u>Thm</u>:- Let $\underset{\sim}{A} \in \mathbb{R}^{m\times m}$, $\underline{b} \in \mathbb{R}^m$ and P^n denotes the space of monic polynomial of degree n. If $K_n = \langle \underline{b}, \underset{\sim}{A}\underline{b}, \dots A^{n-1}\underline{b} \rangle$ is of full rank, the solution of

$$\boxed{\min_{p^n \in P^n} \|p^n(\underset{\sim}{A})\,\underline{b}\|}$$ is the

characteristic polynomial of $\underset{\sim}{H_n}$

$$p_{H^n}(z) = \det(z\underset{\sim}{I} - \underset{\sim}{H_n}) \text{ where}$$

$$\underset{\sim}{H_n} = \underset{\sim}{\hat{Q}_n}^T \underset{\sim}{A} \underset{\sim}{\hat{Q}_n} \text{ with}$$

$\hat{Q}_n = (\underset{\sim}{q_1}, \underset{\sim}{q_2} \dots q_n)$ constructed by Arnoldi iteration i.e

$$\boxed{p_{H_n} = \arg \min_{p^n \in P^n} \| p^n(A) \underset{\sim}{b} \|}$$

* The goal of Arnoldi iteration is to solve a polynomial approximation problem.

* If one's aim is to compute a monic polynomial p^n with the

property $\|p^n(\underset{\sim}{A})\underline{b}\|$ is small, we need to pick p^n such a way that it has zeros close to eigenvalues of $\underset{\sim}{A}$.