GMRES — A, nonsingular.

- Solve $AU = F$, initial guess u^0
- $u^k = u^0 + Q_k \underline{y}_k$
- $Q_k = [q_1 \; q_2 \; \cdots \; q_k]$, an orthonormal basis for $\underbrace{\{r_0, Ar_0, \ldots, A^{k-1}r^0\}}_{K_k(r^0, A)}$.
- $Q_k e_1 = Q_{k+1} e_1 = \dfrac{r_0}{\|r_0\|}$.
- We will see how to get Q_k using the Arnoldi process later.
- Assume for now we have u^0, Q_k. GMRES chooses $\underline{y}_k$ to minimize the $\|r^k\|_2$ where
- $r^k = r^0 - A Q_k \underline{y}_k$
- $e^k = e^0 - Q_k \underline{y}_k$

__Finding $\underline{y}_k$:__

To minimize $(r^k)^T r^k$ or $\|r^k\|_2$, we choose $\underline{y}_k$ to be the least squares solution to the problem

$$AQ_k \underline{y}_k \approx r^0$$

OR

$$(AQ_k)^T AQ_k \underline{y}_k = (AQ_k)^T \underline{r}^0$$

$$Q_k^T A^T A Q_k \underline{y}_k = Q_k^T A^T \underline{r}^0 \quad (1)$$

$$\boxed{\underline{y}_k = (Q_k^T A^T A Q_k)^{-1} Q_k^T A^T r^0}$$

Theoretical result. We will simplify this later

So, $$\boxed{r^k = (I - AQ_k (Q_k^T A^T A Q_k)^{-1} Q_k^T A^T) r^0} \quad (2)$$

This last equation shows that

$$r^k = (I - P)r^0 \quad \text{where}$$

$P = P^2 = AQ_k(Q_k^TA^TAQ_k)^{-1}Q_k^TA^T$ is a projector. $\Rightarrow$

(3)

$$\boxed{\begin{array}{l}\text{If } r^0 \in \text{Range}(P) = \text{range}(AQ_k), \text{ then} \\ r^0 = AQ_k z \text{ for some } z, \text{ and } r^k \equiv 0. \\ r^k \perp \text{range}(AQ_k)\end{array}}$$

(4)

Likewise $\boxed{e^k = \left(I - Q_k(Q_k^TA^TA\,Q_k)^{-1}Q_k^TA^TA\right)e^0}$

and $e^k = (I - \mathbb{P})e^0$ where $\mathbb{P} = \mathbb{P}^2 = Q_k(Q_k^TA^TAQ_k)^{-1}Q_k^TA^TA$ is a projector.

(5)

$$\Rightarrow \boxed{\begin{array}{l}\text{If } e^0 \in \text{range}(\mathbb{P}) = \text{range}(Q_k), \text{ then} \\ e^0 = Q_k z \text{ for some } z, \text{ and } e^k \equiv 0. \\ e^k \perp \text{range}(A^TA\,Q_k)\end{array}}$$

The Arnoldi process gives,

(6) $$\boxed{AQ_k = Q_{k+1}\tilde{H}}$$

$$Q_{k+1} = [Q_k \quad q_{k+1}]$$

$$\tilde{H}_k = \begin{bmatrix} H_k \\ \cdots\cdots \\ h_{k+1,k}\, e_k^T \end{bmatrix}_{(k+1,\,k)}$$

or

(7) $$\boxed{AQ_k = Q_k H_k + h_{k+1,k}\, q_{k+1} e_k^T}$$

(8) $$\tilde{H} = \begin{bmatrix} h_{11} & h_{12} & \cdots & h_{1k} \\ h_{21} & h_{22} & \cdots & h_{2k} \\ & h_{32} & \ddots & \\ & & h_{k,k-1} & h_{kk} \\ \hline 0 & 0 & \cdots\ 0 & h_{k+1,k} \end{bmatrix}$$

H_k

last row is $h_{k+1,k}\, e_k^T$

$e_k^T = (0 \ 0 \ \cdots \ 1)$ ↑ kth position.

Simplify solution for $\underline{y}_k$ based on ARNOLDI Process

$$\underline{y}_k = (Q_k^T A^T A Q_k)^{-1} Q_k^T A^T r^0 \qquad \text{from } (1).$$

$$\underline{Q_k^T A^T A Q_k} = (Q_{k+1}\tilde{H})^T (Q_{k+1}\tilde{H}) = \tilde{H}^T Q_{k+1}^T Q_{k+1}\tilde{H} = \underline{\underline{\tilde{H}^T \tilde{H}}}$$

$$Q_k^T A^T = (Q_{k+1}\tilde{H})^T = \tilde{H}^T Q_{k+1}^T$$

$$\underline{Q_k^T A^T r^0} = \tilde{H}^T Q_{k+1}^T r_0 = \tilde{H}^T * \begin{pmatrix} \frac{r_0^T r_0}{\|r_0\|} \\ 0 \\ \vdots \\ 0 \end{pmatrix} = \underline{\underline{\tilde{H}^T \cdot \|r_0\|\, e_1}}$$

So, 1 becomes,

$$\underline{y}_k = (\tilde{H}^T \tilde{H})^{-1} \tilde{H}^T \|r^0\| \underline{e}_1 \quad , \text{ or}$$

$$\boxed{(\tilde{H}^T \tilde{H}) \cdot \underline{y}_k = \tilde{H}^T \cdot \|r^0\| \underline{e}_1} \quad (9)$$

Like Normal equations.

This shows that $\underline{y}_k$ chosen to minimize

$$\| \tilde{H} \underline{y}_k - \|r^0\| \underline{e}_1 \|_2 \quad (10)$$

which is exactly $\|r^k\|_2 = \| r^0 - AQ_k \underline{y}_k \|_2$

$$= \cancel{\| \|r^0\| Q_{k+1} \tilde{H}}$$

$$= \| \|r^0\| Q_{k+1} \underline{e}_1 - Q_{k+1} \tilde{H} \underline{y}_k \|_2$$

$$= \| \|r^0\| e_1 - \tilde{H} \underline{y}_k \|_2 .$$

We learned in 584, not to solve the normal equations but instead solve (9) by first factoring

$$\underset{k+1,k}{\tilde{H}} = \bar{Q} \bar{R} = [\bar{Q}_k \; \bar{q}_{k+1}] \begin{bmatrix} R_k \\ 0 \end{bmatrix} = \bar{Q}_k R_k = qr(\tilde{H}, 0) \text{ in MATLAB}$$

$\bar{Q}$: square $(k+1)\times(k+1)$

$\bar{Q}_k$: $(k+1), k$

R_k: $k \times k$

So use $\tilde{H} = \bar{Q}_k R_k$ to get the

Solution of 9 or 10 to be

$$\boxed{\begin{array}{c} R_k \, \underline{y}_k = \bar{Q}_k^T \left(\|r^0\| \, \underline{e}_1 \right) \\ \nabla \; | = | \quad \text{solve by backsub.} \end{array}} \quad (11)$$

Once (11) is solved for $\underline{y}_k$, we find

$$\boxed{u^k = u^0 + Q_k \, \underline{y}_k}$$

Look at r^k and its norm:

From least squares we know,

$$r^k = Q_{k+1} \underbrace{\left(I - \bar{Q}_k \bar{Q}_k^T \right)}_{\text{projection}} \underbrace{\|r^0\| \underline{e}_1}_{\text{RHS of system}}$$

$\tilde{H} \, y_k \approx \|r^0\| \underline{e}_1$

$\tilde{H} = \bar{Q}_k R_k$

$\Rightarrow$

$$r^k = Q_{k+1} \left(\bar{q}_{k+1} \bar{q}_{k+1}^T \right) \|r^0\| \underline{e}_1 ,$$

$\tilde{H} = \bar{Q} \bar{R}$

$\bar{Q} \bar{Q}^T = I = \bar{Q}_k \bar{Q}_k^T + \bar{q}_{k+1} \bar{q}_{k+1}^T$

$\Rightarrow \bar{q}_{k+1} \bar{q}_{k+1}^T = I - \bar{Q}_k \bar{Q}_k^T$

So

$$\|r^k\|_2 = \| \bar{q}_{k+1} \bar{q}_{k+1}^T \underline{e}_1 \| \cdot \|r^0\|_2$$

$$\Rightarrow \boxed{\|r^k\|_2 = |\bar{q}_{k+1}^T e_1| \cdot \|r^0\|_2} \quad (12)$$

- Note, that once $\tilde{H}$ has been QR factored into
$$\tilde{H} = \bar{Q}\bar{R}$$
we know $\bar{q}_{k+1}$. We already know $\|r^0\|_2$ and $\|r^k\|_2$ can be computed <u>WITHOUT</u> First finding $\underline{y}_k$ and doing $r^k = r^0 - AQ_k\underline{y}_k$ and then taking $\|r^k\|_2$.

- This is important since we <u>don't</u> have to compute $\underline{y}_k$ <u>unless</u> $\|r^k\|_2$ meets tolerance.

<u>GMRES</u>: (Solve $Au = F$)

- Choose u^0
- $r^0 = F - Au^0$
- Find $\|r^0\|_2$, $q_1 = r^0/\|r^0\|_2$.

For $k = 1, 2, \ldots$

- Do ARNOLDI ① TO get $Q_k, q_{k+1}, \tilde{H}$ so $AQ_k = Q_{k+1}\tilde{H}$
- Factor $\tilde{H} = \bar{Q}\bar{R} = [\bar{Q}_k \;\; \bar{q}_{k+1}]\begin{bmatrix} R_k \\ 0 \end{bmatrix}$ by QR-factoriz
- Compute $\|r^k\|_2 = |\bar{q}_{k+1}^T e_1| \cdot \|r^0\|_2$
  - If $\frac{\|r^k\|_2}{\|r^0\|_2} < tol$ then
    $u^k = u^0 + Q_k\underline{y}_k$ where
    $R_k\underline{y}_k = \bar{Q}_k^T(\|r^0\| e_1)$, backsub
    stop
  - .endif

endfor

Arnoldi Process

$$A Q_k = Q_{k+1} \tilde{H}$$

$$A[q_1 \; q_2 \; \cdots \; q_k] = [q_1 \; q_2 \; \cdots \; q_k \; q_{k+1}] \begin{bmatrix} h_{11} & h_{12} & \cdots & h_{1k} \\ h_{21} & h_{22} & \cdots & h_{2k} \\ & h_{32} & \ddots & \\ & & \ddots & h_{kk} \\ 0 & & & h_{k+1,k} \end{bmatrix}$$

$$q_1 = r^0 / \|r^0\|.$$

(1) $$A q_k = h_{1k} q_1 + h_{2k} q_2 + \cdots + h_{kk} q_k + h_{k+1,k} q_{k+1}$$

- Dot (1) with q_j, $j = 1, 2, \ldots, k$ to get

$$q_j^T A q_k = h_{jk}$$

- Solve (1) for $h_{k+1,k} q_{k+1} = A q_k - \sum_{j=1}^{k} h_{jk} q_j = v$

$$h_{k+1,k} = \|v\|_2, \quad q_{k+1} = v / \|v\|_2.$$

Algorithm (Computing Q_k, $Q_{k+1} = (Q_k \; q_{k+1})$, $\tilde{H}$)
(at step k find q_{k+1} and the kth colm of $\tilde{H}$)

$q_1 = r^0 / \|r^0\|_2$
For $k = 1, 2, \ldots$
  $v = A q_k$
  For $i = 1:k$
    $h_{ik} = q_i^T v$
    $v = v - h_{ik} q_i$
  end
  $h_{k+1,k} = \|v\|_2$
  $q_{k+1} = v / h_{k+1,k}$
end

(1) Computes q_{k+1} and the kth colm of $\tilde{H}$

Preconditioned GMRES

Solve $M^{-1}Au = M^{-1}F$, $\begin{cases} \hat{A} = M^{-1}A, & \hat{F} = M^{-1}F \\ \hat{u} = u \end{cases}$

Apply GMRES to system $\hat{A}\hat{u} = \hat{F}$ $(\hat{A}u = \hat{F})$

- $u^k = u^0 + Q_k \underline{y}_k$, Q_k orthonormal basis for $K_k(\hat{r}^0, \hat{A}) = \{\hat{r}^0, \hat{A}\hat{r}^{(0)}, (\hat{A})^2\hat{r}^{(0)}, \ldots, (\hat{A})^{k-1}\hat{r}^{(0)}\}$.

- $\hat{r}^k = \hat{F} - \hat{A}u^k$

  $\hat{r}^k = M^{-1}F - M^{-1}Au^k = M^{-1}r^k$

$$r^k = F - Au^k = r^0 - AQ_k\underline{y}_k \quad ; \quad \hat{r}^k = M^{-1}r^0 - M^{-1}AQ_k\underline{y}_k$$

- Minimize $\|\hat{r}^k\|_2$. Choose $\underline{y}_k$ to solve the normal eqns,

$$(M^{-1}AQ_k)^T(M^{-1}AQ_k)\underline{y}_k = (M^{-1}AQ_k)^T \cdot M^{-1}r^0$$

$$\boxed{\left(Q_k^T A^T M^{-T} \underbrace{M^{-1}AQ_k}\right)\underline{y}_k = Q_k^T A^T M^{-T} M^{-1} r^0} \quad (1)$$

$\to$ Arnoldi process simplifies.

So, $$\boxed{\hat{r}^k = \left(I - M^{-1}AQ_k\left(Q_k^T A^T M^{-T} M^{-1} A Q_k\right)^{-1} Q_k^T A^T M^{-T}\right)\underbrace{M^{-1}r^0}_{\hat{r}^0}} \quad (2)$$

$\boxed{M\hat{r}^k = r^k}$

$$M\hat{r}^k = \left(M \cdot M^{-1}r^0 - AQ_k(Q_k^T A^T M^{-T} M^{-1} A Q_k)^{-1} Q_k^T A^T M^{-T} M^{-1} r^0\right)$$

$$\boxed{r^k = \left(I - AQ_k(Q_k^T A^T M^{-T} M^{-1} A Q_k)^{-1} Q_k^T A^T M^{-T} M^{-1}\right) r^0} \quad (3)$$

Arnoldi Process Produces

- $(M^{-1}A)Q_k = Q_{k+1}\tilde{H}$
- then the system ① for $\underline{y}_k$ becomes

$$(Q_{k+1}\tilde{H})^T Q_{k+1}\tilde{H}\cdot \underline{y}_k = (Q_{k+1}\tilde{H})^T\cdot M^{-1}r^0$$

$$\tilde{H}^T\tilde{H}\,\underline{y}_k = \tilde{H}^T Q_{k+1}^T \underbrace{(M^{-1}r^0)}_{\hat{r}^0} \qquad \cdot\ Q_{k+1}^T = \begin{bmatrix} q_1^T \\ q_2^T \\ \vdots \\ q_{k+1}^T \end{bmatrix}$$

$$\boxed{Q_{k+1}^T\hat{r}^0 = \begin{bmatrix} q_1^T\hat{r}^0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \begin{bmatrix} (\hat{r}^{0T}\hat{r}^0)/\|\hat{r}^0\| \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \|\hat{r}^0\|_2\cdot \underline{e}_1}$$

$$q_1 = \frac{\hat{r}^0}{\|\hat{r}^0\|} = \frac{M^{-1}r^0}{\|M^{-1}r^0\|}.$$

$$\Rightarrow \boxed{\tilde{H}^T\tilde{H}\,\underline{y}_k = \tilde{H}^T\cdot\|\hat{r}^0\|_2\,\underline{e}_1} \leftarrow$$

$\underline{y}_k$ chosen to $\min_{\underline{y}_k} \| \|\hat{r}^0\|_2\underline{e}_1 - \tilde{H}\underline{y}_k\|_2$

Factor $\tilde{H} = \bar{Q}\bar{R} = [\bar{Q}_k\ \bar{q}_{k+1}]\begin{bmatrix} R_k \\ 0 \end{bmatrix} \Rightarrow \boxed{R_k\underline{y}_k = \bar{Q}_k^T(\|\hat{r}^0\|_2\cdot e_1)}$

$$\hat{r}^k = Q_{k+1}\underbrace{(I - \bar{Q}_k\bar{Q}_k^T)}_{\bar{q}_{k+1}\bar{q}_{k+1}^T}\|\hat{r}^0\|_2\cdot\underline{e}_1$$

$\Rightarrow \|\hat{r}^k\|_2 = |\bar{q}_{k+1}^T e_1|\cdot\|\hat{r}^0\|_2$, can be found without finding $\underline{y}_k$ first.

Arnoldi Process for $M^{-1}AQ_k = Q_{k+1}\tilde{H}$.

$$M^{-1}A\underbrace{[q_1\ q_2\ \ldots\ q_k]}_{Q_k} = \underbrace{[q_1\ q_2\ \ldots\ q_k\ q_{k+1}]}_{Q_{k+1}} \underbrace{\begin{bmatrix} h_{11} & \cdots & & h_{1k} \\ h_{21} & h_{22} & \cdots & h_{2k} \\ & h_{32} & \ddots & \\ & & \ddots & h_{kk} \\ & & & h_{k+1,k} \end{bmatrix}}_{\tilde{H}}$$

- Q_k chosen to be orthonormal basis for $\{\hat{r}^0, M^{-1}A\hat{r}^0, (M^{-1}A)^2\hat{r}^0, \ldots, (M^{-1}A)^{k-1}\hat{r}^0\}$

- $q_1 = \hat{r}^0/(\|\hat{r}^0\|$

(1) $M^{-1}A\,q_k = h_{1k}q_1 + h_{2k}q_2 + \cdots + h_{kk}q_k + h_{k+1,k}q_{k+1}$

- Dot (1) with q_j, $j = 1, 2, \ldots, k$ to get

$$(q_j^T M^{-1}A\,q_k) = h_{ij} \qquad , j = 1, 2, \ldots, k$$

- Solve (1) for $h_{k+1,k}q_{k+1} = M^{-1}A\,q_k - \sum_{j=1}^{k} h_{jk}\,q_j = v$

$$h_{k+1,k} = \|v\|, \quad q_{k+1} = v/\|v\|_2$$

<u>Algorithm</u>: Arnoldi for $M^{-1}AQ_k = Q_{k+1}\tilde{H}$. Finds $Q_k, Q_{k+1}, \tilde{H}$ at step k.

$q_1 = \hat{r}^0/\|\hat{r}^0\|_2$

For $k = 1, 2, \ldots$

Extra solve per k-loop →

- Solve $M\underline{v} = Aq_k$ for v $\quad (v = M^{-1}Aq_k)$.
- For $i = 1:k$
  - $h_{ik} = q_i^T v$
  - $v = v - h_{ik}q_i$

  end
- $h_{k+1,k} = \|v\|_2$
- $q_{k+1} = v/h_{k+1,k}$

Finds kth colm of $\tilde{H}$ and q_{k+1}.

end

Preconditioned GMRES $\quad M^{-1}AU = M^{-1}F$

- Choose u^0
- $r^0 = F - Au^0$

extra solve $\rightarrow$

- $\hat{r}^0 = M^{-1}r^0$, solve $M\hat{r}^0 = r^0$ for $\hat{r}^0$.
- $q_1 = \hat{r}^0 / \|\hat{r}^0\|_2$.

For $k = 1, 2 \ldots$

- Do arnoldi process page ⑩: $Q_k, q_{k+1}, \tilde{H}$ (Find kth colm $\tilde{H}$ and q_{k+1}.) $\quad (M^{-1}AQ_k = Q_{k+1}\tilde{H})$
- Factor $\tilde{H} = \bar{Q}\bar{R} = [\bar{Q}_k \; \bar{q}_{k+1}]\begin{bmatrix} R_k \\ 0 \end{bmatrix} = \bar{Q}_k R_k$
- Compute $\dfrac{\|\hat{r}^k\|_2}{\|\hat{r}^0\|_2} = |\bar{q}_{k+1}^T e_1|$. $\cancel{\|\hat{r}^0\|_2}$
- If $\dfrac{\|\hat{r}^k\|}{\|\hat{r}^0\|_2} < tol$ then
    - $u^k = u^0 + Q_k \underline{y}_k$ where
    - $R_k \underline{y}_k = \bar{Q}_k^T(\|\hat{r}^0\| e_1)$ (do backsub)
    - STOP
- end if

end for