Iterative methods for solving $Ax = b$ where A is non-symmertric.

GMRES $\left(\text{Generalited Minimum Residual}\right)$ method

The kth iteration of GMRES is the solution x_k
to the least squares problem

$$\min_{x \in x_0 + K_k} \left\| b - Ax \right\|_2^2 \Rightarrow \nabla \left\| b - Ax \right\|_2^2 = 2A^T \left(Ax - b \right) = 0$$

Step2 in CG $\Rightarrow \underbrace{\left(b - Ax_k\right)}_{r_k}^T A \underset{\in K_k}{J} = 0 \Rightarrow r_k$ is nolonger $\perp$ to K_k

Step3 in CG $\overset{x_{k+1}=x_k+\alpha_{k+1}p_{k+1}}{\Rightarrow} \alpha_{\mathrm{k}}\left(JAp_{k+1}\right) = J\left(r_k - r_{k+1}\right) \neq 0$

$\Rightarrow$ no A-orthoganoal property for p_{k+1}

Consider $y \in K_k$ and $K_k = span\left\{v_1 \cdots v_k\right\} = V_k$

One must have $x_k = x_0 + V_k \cdot y$ for some y(coefficient vector)

The minimization problem can be rewritten as following:

$$\min_{x \in x_0 + K_k} \left\| b - Ax \right\|_2 \equiv \min_{y \in R^k} \left\| b - A\left(x_0 + V_k y\right) \right\|$$

$$\equiv \min_{y \in R^k} \left\| r_0 - AV_k \cdot y \right\|$$

This ia a standard least Square problem.

One can solve it by QR or the Gram-Schmidt orthogonalization.

Gram-Schmidt orthogonalization procedure:

(Arnoldi process) $V_K = span\{v_1, v_2, \cdots, v_k\}$

1. Define $r_0 = b - Ax_0,\ v_1 = \dfrac{r_0}{\|r_0\|_2}$

2. For $i = 1 \sim k-1$, (restart with new $r_0 = b - Ax_k$ when needed)

$$v_{i+1} = \frac{Av_i - \sum_{j=1}^{i} \overbrace{\left[(Av_i)^T v_j \right]}^{h_{j,i}} \cdot v_j}{\underbrace{\left\| Av_i - \sum_{j=1}^{i} \left[(Av_i)^T v_j \right] \cdot v_j \right\|_2}_{h_{i+1,i}}}$$

(the algorithm breaks down when $h_{i+1,i} = 0$ $\Rightarrow$ restart is needed)

$$\Rightarrow A_{n\times n} V_{n\times k-1} = V_{n\times k} \cdot H_{k\times k-1};\ \text{H}=\begin{bmatrix} * & & & h_{1,i} & * & * \\ * & \ddots & & \vdots & * & * \\ & \ddots & \ddots & \vdots & & * \\ & & \ddots & \vdots & & \vdots \\ & & & h_{i+1,i} & * & * \\ & & & & * & * \\ & & & & 0 & * \end{bmatrix}_{k\times k-1}$$

$\leftarrow$ upper hessenberg matrix.

Now suppose we are at *kth* step. We have

$$\|r_k\|_2 = \|b - Ax_k\|_2 = \left\|A\left(x - x_0 + x_0 - x_k\right)\right\|_2$$

$$= \left\| r_0 - A\underbrace{\left(x_k - x_0\right)}_{=V_k y} \right\|_2$$

Since $r_0 = \beta v_1 e_1$, $\beta = \|r_0\|_2$,and V_i is an orthonormal basis

$$\|r_k\|_2 = \left\|V_k^T \left(r_0 - AV_k y\right)\right\|_2$$

$$= \left\|\beta e_1 - V_k^T \cdot V_{k+1} H_{k+1\times k} y\right\|_2 = \left\| \beta e_1 - \underset{\substack{\| \\ \bar{H}_k}}{\left[H\right]_{[1:k]\times[1:k]}} y \right\|$$

Our goal now is to find y that satisfies

$$\min_{x \in x_0 + K_k} \|b - Ax\| \equiv \min_{y \in R^k} \|r_0 - AV_k y\| \equiv \min_{y \in R^k} \left\| \beta e_1 - \bar{H}_k y \right\|_2 \quad -(+++)$$

Now the Gmres algorithm can be read as following

ALGORITHM 3.4.2. **gmresa**$(x, b, A, \epsilon, kmax, \rho)$

1. $r = b - Ax$, $v_1 = r/\|r\|_2$, $\rho = \|r\|_2$, $\beta = \rho$, $k = 0$
2. While $\rho > \epsilon\|b\|_2$ and $k < kmax$ do
   (a) $k = k + 1$
   (b) for $j = 1, \ldots, k$
   $h_{jk} = (Av_k)^T v_j$
   (c) $v_{k+1} = Av_k - \sum_{j=1}^{k} h_{jk} v_j$
   (d) $h_{k+1,k} = \|v_{k+1}\|_2$
   (e) $v_{k+1} = v_{k+1}/\|v_{k+1}\|_2$
   (f) $e_1 = (1, 0, \ldots, 0)^T \in R^{k+1}$
   Minimize $\|\beta e_1 - H_k y^k\|_{R^{k+1}}$ over R^k to obtain y^k.
   (g) $\rho = \|\beta e_1 - H_k y^k\|_{R^{k+1}}$.
3. $x_k = x_0 + V_k y^k$.

The convergence analysis is similar to the convergence analysis for CG. We leave the analysis to readers.

Theorem 1: Let $A = VAV^{-1}$ be a nonsingular diagnoalizable matrix and x_k be the *kth* GMRES iteration. Then for all $p_k \in P_k$

$$\frac{\|r_k\|_2}{\|r_r\|_2} \le K_2(v) \max_{z \in \sigma(A)} |p_k(z)|$$

$$\left(\begin{array}{l} \text{Remark1:} \\ \text{A is normal} \Rightarrow \text{ Vis orthonormal} \\ \qquad\qquad\qquad \Rightarrow \text{ the condition number } \mathrm{K}_2(v) = 1 \\ \text{If A is not normal, it is not clear how to estimate } \mathrm{K}_2(v) \end{array} \right)$$

Remark2: Proconditioning is generally needed to accerlatethe convergence rate. Moreover, due to possible lose of orthogonality in the Gram-Schmidt process.

$$\left(\begin{array}{l} \text{no guarantee that } Av_i \notin span\{v_1 \cdots v_n\} \Rightarrow \text{breakdown} \\ \Rightarrow \text{Arnoldi process can't generate } v_{i+1} \end{array} \right)$$

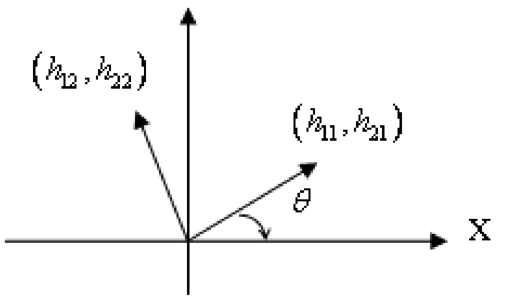
"Restart" is also generally needed in GMRES.

Remark3: The storage cost for the upper hessnberg martix H grows linearly with the number of iteration. Restarting strategy also can reduce the storage cost of H matrix.

By applying rotation matrices to H, one can easily solve the above minimization problem.

$$\text{let } H = \begin{bmatrix} h_{1,1} & h_{1,2} & & & & \\ h_{2,1} & h_{2,2} & & & & \\ & h_{3,2} & h_{3,3} & & & \\ & & & \ddots & & \\ & & & & h_{k-1,k-1} & \\ & & & & h_{k,k-1} & h_{k,k} \\ & & & & & h_{k+1,k} \end{bmatrix}$$

observation:



$$\cos\theta = \frac{h_{11}}{\sqrt{h_{11}^2 + h_{21}^2}}$$

$$\sin\theta = \frac{h_{21}}{\sqrt{h_{11}^2 + h_{21}^2}}$$

$$\begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} h_{11} \\ h_{21} \end{bmatrix} = \begin{bmatrix} \sqrt{h_{11}^2 + h_{21}^2} \\ 0 \end{bmatrix}$$

From the block B_1, we can form $R_1 = \begin{bmatrix} c_1 & s_1 & \\ -s_1 & c_1 & \\ & & I \end{bmatrix}$, $\|R_1\| = 1$. We have $R_1 H = \begin{bmatrix} * & \widetilde{h_{12}} & & & \\ 0 & \widetilde{h_{22}} & \widetilde{h_{23}} & \cdots & \cdots \\ 0 & \widetilde{h_{32}} & h_{33} & \cdots & \cdots \\ \vdots & & & \ddots & \\ 0 & & & & \ddots \end{bmatrix}$

From the block B_2, we can obtain $R_2 = \left[\begin{array}{c|cc|c} & & & \\ \hline & c_2 & s_2 & \\ & -s_2 & c_2 & \\ \hline & & & I \end{array}\right]$, $\|R_2\| = 1$

By repeatly applying the rotation matrices, we have

$$\beta e_1 - H_k y = \underbrace{\overline{R_k}^*}_{\substack{rotation \\ matrices}} \cdot \underbrace{\left(\beta \overline{R_k} e_1 - \begin{bmatrix} \ddots & * \\ 0 & \ddots \end{bmatrix} y \right)}_{\substack{upper-triangular \\ linear\ \text{system}}}, \text{ here } \overline{R}_k = R_k R_{k-1} \cdots R_2 R_1$$

Now one can apply the backward substition to solve the upper triangular linear system.

Moreover,

$$\|\beta e_1 - H_k y\| = \left| \beta \underbrace{\left(\overline{R_k} e_1\right)_k}_{\text{(k+1)th component of } \overline{R_k} e_1} \right|,$$

the quantity can be used in checking the stopping tolerence.

The GMRES algorithm can be rewritten as following

ALGORITHM 3.5.1. gmres($x, b, A, \epsilon, kmax, \rho$)

1. $r = b - Ax$, $v_1 = r/\|r\|_2$, $\rho = \|r\|_2$, $\beta = \rho$,
   $k = 0$; $g = \rho(1, 0, \ldots, 0)^T \in R^{kmax+1}$

2. While $\rho > \epsilon\|b\|_2$ and $k < kmax$ do

   (a) $k = k + 1$

   (b) $v_{k+1} = Av_k$
   for $j = 1, \ldots k$
   i. $h_{jk} = v_{k+1}^T v_j$
   ii. $v_{k+1} = v_{k+1} - h_{jk}v_j$

   (c) $h_{k+1,k} = \|v_{k+1}\|_2$

   (d) Test for loss of orthogonality and reorthogonalize if necessary.

   (e) $v_{k+1} = v_{k+1}/\|v_{k+1}\|_2$

   (f) i. If $k > 1$ apply Q_{k-1} to the kth column of H.
   ii. $\nu = \sqrt{h_{k,k}^2 + h_{k+1,k}^2}$.
   iii. $c_k = h_{k,k}/\nu$, $s_k = -h_{k+1,k}/\nu$
   $h_{k,k} = c_k h_{k,k} - s_k h_{k+1,k}$, $h_{k+1,k} = 0$
   iv. $g = G_k(c_k, s_k)g$.

   (g) $\rho = |(g)_{k+1}|$.

3. Set $r_{i,j} = h_{i,j}$ for $1 \leq i, j \leq k$.
   Set $(w)_i = (g)_i$ for $1 \leq i \leq k$.
   Solve the upper triangular system $Ry^k = w$.

4. $x_k = x_0 + V_k y^k$.