Iterative Methods – May 17, 2005

Note Title 5/17/2006

GMRES

Generalized Minimum Residual

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

$$Q_k = [q_1, \ldots, q_k] \qquad Q_k^T Q_k = I_k$$

$$\tilde{H}_k = \begin{bmatrix} h_{11} & h_{12} & \cdots & h_{1k} \\ h_{21} & h_{22} & \cdot & h_{2k} \\ 0 & \ddots & & \\ \vdots & & \ddots & \\ 0 & & \cdots & h_{k+1,k} \end{bmatrix}_{k+1,k} \qquad r_0 = (b - A x_0)$$

$$\underset{\sim}{x}_k = \underset{\sim}{x}_0 + Q_k \underset{\sim}{y}_k$$

$$\| \underset{\sim}{b} - A(\underset{\sim}{x}_0 + Q_k \underset{\sim}{y}_k) \|_2$$

$$= \| (\underset{\sim}{b} - A\underset{\sim}{x}_0) - A Q_k \underset{\sim}{y}_k \|_2$$

$$= \| \underset{\sim}{r}_0 - Q_{k+1} \tilde{H}_k \underset{\sim}{y}_k \|_2$$

$$= \| Q_{k+1}^T \underset{\sim}{r}_0 - \tilde{H}_k \underset{\sim}{y}_k \|_2$$

$$Q^T \underset{\sim}{r}_0 = \rho \underset{\sim}{e}_1 \qquad = \| \rho \underset{\sim}{e}_1 - \tilde{H}_k \underset{\sim}{y}_k \|_2$$

$$\underset{\sim}{y}_k = \rho \tilde{H}_k^{+} \underset{\sim}{e}_1$$

$$J_{k,k+1} = \begin{pmatrix} 1 & & & & & \\ & \ddots & & & 0 & \\ & & \cos\theta & \sin\theta & & \\ & & -\sin\theta & \cos\theta & & \\ & 0 & & & \ddots & \\ & & & & & 1 \end{pmatrix} \begin{matrix} \\ \\ \leftarrow k \\ \leftarrow k+1 \\ \\ \\ \end{matrix}$$

$$J_{k,k+1}^T \cdot J_{k,k+1} = I$$

$$J_{12} \begin{pmatrix} h_{11} \\ h_{21} \\ 0 \\ \vdots \\ 0 \end{pmatrix} = \pm \sqrt{h_{11}^2 + h_{21}^2} \cdot e_1$$

$$\underbrace{J_{k+1,k} \cdots J_{23} J_{12}}_{Z} \tilde{H}_{k+1,k} = \begin{pmatrix} R \\ 0 \end{pmatrix}$$

$$\| \rho \underset{\sim}{e}_1 - \tilde{H}_{k+1,k} \, y_k \|$$

$$\| \rho Z e_1 - R \, y_k \|_2 = h_{k+1,k}$$

Continue until $h_{k+1,k} \doteq \varepsilon$

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1) Storage "enforces" restarts.
2) Stagnation & "prove theorems"
3) Orthogonalization

Can be very useful but should be used with caution.

$$M \underset{\sim}{x} = \underset{\sim}{x}$$

$$(M - I)\underset{\sim}{x} = \underset{\sim}{0}$$

$\lambda_1 = 0$ $\sigma_1 = 0$

Chen Greif (UBC)

$$A = A^T$$

$$A := MAM^T$$

$$A \neq A^T$$

$$A \underset{\sim}{x} = \underset{\sim}{b}$$

$$\underbrace{\left(M_1^{-1} A M_2^{-1}\right)}_{\tilde{A}} M_2 \underset{\sim}{x} = M_1^{-1} \underset{\sim}{b}$$

$$\tilde{A} \underset{\sim}{y} = \underset{\sim}{c}$$

$$\underset{\sim}{x} = M_2^{-1} \underset{\sim}{y}$$

<u>non-symmetric Lanczos</u>

$$A = A^T = \begin{pmatrix} \alpha_1 & \beta_1 & & 0 \\ \beta_1 & \ddots & \ddots & \\ & \ddots & \ddots & \beta_{n-1} \\ 0 & & \beta_{n-1} & \alpha_n \end{pmatrix}, \quad A \neq A^T$$

$$Q^{-1} A Q = T = \begin{pmatrix} \alpha_1 & \gamma_1 & & 0 \\ \beta_1 & \ddots & \ddots & \\ & \ddots & \ddots & \gamma_{n-1} \\ 0 & & \beta_{n-1} & \alpha_n \end{pmatrix}$$

$$T := D T D^{-1}$$

$$\boxed{\gamma_i \beta_i > 0} \quad \text{for } i = 1, 2, \dots, n-1$$

$$Q = (q_1, \dots, q_n)$$

$$Q^{-T} = P = [p_1, \dots p_n]$$

✓ $Q P^T = I$

$$\boxed{A Q = Q T}$$

$$Q^{-1} A = T Q^{-1}$$

$$A^T Q^{-T} = Q^{-T} T^T$$

$$A^T P = P T^T$$

$$\boxed{A^T P = P T^T}$$

$$A[\underset{\sim}{q}_1, \ldots, \underset{\sim}{q}_n] = [\underset{\sim}{q}_1, \ldots, \underset{\sim}{q}_n] \begin{bmatrix} \alpha_1 & \gamma_1 & & 0 \\ \beta_1 & \ddots & \ddots & \\ & \ddots & \ddots & \gamma_{n-1} \\ 0 & & \beta_{n-1} & \alpha_n \end{bmatrix}$$

→ $$\begin{cases} A\underset{\sim}{q}_1 = \alpha_1 \underset{\sim}{q}_1 + \beta_1 \underset{\sim}{q}_2 \\ A\underset{\sim}{q}_k = \gamma_{k-1} \underset{\sim}{q}_{k-1} + \alpha_k \underset{\sim}{q}_k + \beta_k \underset{\sim}{q}_{k+1} \end{cases}$$

$$A^T P = P T^T$$

$$A^T \underset{\sim}{p}_1 = \alpha_1 \underset{\sim}{p}_1 + \gamma_1 \underset{\sim}{p}_2$$

$$A^T \underset{\sim}{p}_k = \beta_{k-1} \underset{\sim}{p}_{k-1} + \alpha_k \underset{\sim}{p}_k + \gamma_k \underset{\sim}{p}_{k+1}$$

$$\underset{\sim}{p}_k^T \underset{\sim}{q}_k = 1 \qquad \underset{\sim}{p}_r \underset{\sim}{q}_s = 0 \quad r \neq s.$$

$$\underset{\sim}{p}_k^T A \underset{\sim}{q}_k = \gamma_{k-1} \cancel{\underset{\sim}{p}_k^T \underset{\sim}{q}_{k-1}} + \alpha_k \underset{\sim}{p}_k^T \underset{\sim}{q}_k + \beta_k \cancel{\underset{\sim}{p}_k^T \underset{\sim}{q}_{k+1}}$$

$$\alpha_k = \underset{\sim}{p}_k^T A \underset{\sim}{q}_k$$

$$\beta_k \underset{\sim}{q}_{k+1} = \underbrace{(A - \alpha_k I) \underset{\sim}{q}_k - \gamma_{k-1} \underset{\sim}{q}_{k-1}} \equiv \underset{\sim}{r}_k$$

$$\gamma_k \underset{\sim}{p}_{k+1} = (A^T - \alpha_k I) \underset{\sim}{p}_k - \beta_{k-1} \underset{\sim}{p}_{k-1} \equiv s_k$$

$$\beta_k \gamma_k \underset{\sim}{q}_{k+1}^T \underset{\sim}{p}_{k+1} = (r_k^T, s_k)$$

$$\underset{\sim}{q}_{k+1}^T \underset{\sim}{p}_{k+1} = r_k^T s_k \mid \gamma_k \beta_k$$

q_1 & p_1 are given ; $q_1^T p_1 = 1$.

$$q_0 = 0, \quad r_0 = q_1$$

$$p_0 = 0 \qquad s_0 = p_1$$

while $(r_k \neq 0) \wedge (s_k \neq 0) \wedge (s_k^T r_k \neq 0)$

$$\beta_k = \| r_k \|_2$$

$$\gamma_k = s_k^T r_k / \beta_k$$

$$q_{k+1} = r_k / \beta_k$$

$$p_{k+1} = s_k / \gamma_k$$

$$k = k+1$$

$$\alpha_k = p_k^T A q_k$$

$$r_k = (A - \alpha_k I) q_k - \gamma_{k-1} q_{k-1}$$

$$s_k = (A - \alpha_k I)^T p_k - \beta_{k-1} p_{k-1}$$

end

$$r_k^T s_k = 0$$

$$T_k = \begin{bmatrix} \alpha_1 & \gamma_1 & & 0 \\ \beta_1 & \ddots & \ddots & \\ & \ddots & \ddots & \gamma_{k-1} \\ 0 & & \beta_{k-1} & \alpha_k \end{bmatrix}$$

$$T = \begin{pmatrix} \alpha_1 & \gamma_1 & & & 0 \\ \beta_1 & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \gamma_{n-1} \\ 0 & & & \beta_{n-1} & \alpha_n \end{pmatrix}$$

How to compute eigenvalues of T & not destroy the tri-diagonal property?

QR fills in tri-diagonal matrix when $T = T^T$.

$\delta_0 = 1$

$\delta_1 = (\alpha_1 - \lambda)$

$\det(T_k - \lambda I) = \delta_k$

$\delta_2 \quad (\alpha_1 - \lambda)(\alpha_2 - \lambda) - \gamma_1 \beta_1$

$$= (\alpha_2 - \lambda)\delta_1 - \gamma_1 \beta_1 \delta_0$$

complex arithmetic is needed.

Complications:

$$P^T A Q = \begin{bmatrix} M_1 & C_1^T & & & 0 \\ B_2 & M_2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & C_{r-1}^T \\ 0 & & & B_{r-1} & M_r \end{bmatrix}$$

$A: n \times n$, $pr = n$, $M_i : p \times p$

BLOCK LANCZOS.

LOOK AHEAD LANCZOS

p is not fixed

Parlett (Berkeley)