Dec 9, 2020 LLS: $\hat{x} = \arg\min_x \|Ax-b\|_2^2$ $\boxed{A}\boxed{x} = \boxed{b}$

Normal equations: $\nabla_x \; x^TA^TAx - 2x^TA^Tb + b^Tb = 0 \Rightarrow \underline{A^TAx} = \underline{A^Tb}$

Idea: A^TA SPD form $c = A^Tb$ use CG / MINRES

New idea: avoid A^TAx explicitly

$$\begin{pmatrix}0 & A\\ A^T & 0\end{pmatrix}\overset{Q_{2k}}{\begin{bmatrix}u_1 & 0 & \cdots & u_k & 0\\ 0 & v_1 & & 0 & v_k\end{bmatrix}} e_{2k} = \overset{Q_{2k+1}}{\begin{bmatrix}u_1 & 0 & \cdots & u_k & 0 & u_{k+1}\\ 0 & v_1 & & 0 & v_k & 0\end{bmatrix}} \bar{T}_{2k} e_{2k}$$

$$\begin{pmatrix}0 & A\\ A^T & 0\end{pmatrix}\begin{pmatrix}0\\ v_k\end{pmatrix} = \beta_{2k}\begin{pmatrix}u_k\\ 0\end{pmatrix} + \overset{0}{\cancel{\alpha_{2k}}}\begin{pmatrix}0\\ v_k\end{pmatrix} + \beta_{2k+1}\begin{pmatrix}u_{k+1}\\ 0\end{pmatrix}$$

$$Av_k = \underline{\beta_{2k}}\, u_k + \boxed{\beta_{2k+1}}\, u_{k+1}$$

$$\begin{pmatrix}0 & A\\ A^T & 0\end{pmatrix}\begin{pmatrix}u_{k+1}\\ 0\end{pmatrix} = \beta_{2k+1}\begin{pmatrix}0\\ v_k\end{pmatrix} + \overset{0}{\cancel{\alpha_{2k+1}}}\begin{pmatrix}u_{k+1}\\ 0\end{pmatrix} + \beta_{2k+2}\begin{pmatrix}0\\ v_{k+1}\end{pmatrix}$$

$$A^T u_{k+1} = \boxed{\beta_{2k+1}}\, v_k + \underline{\beta_{2k+2}}\, v_{k+1}$$

$\beta_{2k+1} \to \beta_k$ $\quad \beta_{2k} \to \alpha_k$

$A \cdot (A^TA)^{k-1} A^T b = (AA^T)^k b \in K_{k+1}(AA^T, b)$

$AV_k = U_{k+1}\bar{B}_k \quad \bar{B}_k = \begin{pmatrix} \alpha_1 & & \\ \beta_1 & \ddots & \\ & \ddots & \alpha_k \\ & \beta_{k-1} & \\ & & \beta_k \end{pmatrix} \to Av_k = \alpha_k u_k + \beta_k u_{k+1} \in K_{k+1}(AA^T, b)$

$A^TU_{k+1} = V_{k+1}B_{k+1}^T \quad B_{k+1}^T = \begin{pmatrix} \alpha_1 & \beta_1 & & \\ & \ddots & \ddots & \\ & & & \beta_k \\ & & & \alpha_{k+1} \end{pmatrix} \to A^Tu_{k+1} = \beta_k v_k + \alpha_{k+1} v_{k+1} \in K_{k+1}(A^TA, A^Tb)$

$A^T(AA^T)^k b$

$= (A^TA)^k A^T b \in K_{k+1}(A^TA, A^Tb)$

$\beta_0 b = u_1 \in K_1(AA^T, b)$

$\alpha_1 v_1 = A^T u_1 \in K_1(A^TA, A^Tb)$

- V_k is an orthobasis for $K_k(A^TA, A^Tb)$ ✓
  U_k $\quad K_k(AA^T, b)$ ✓

Eigensolvers

unsymm $\quad Q^TAQ = H = \begin{pmatrix} * & \cdots & * \\ \ddots & \ddots & \vdots \\ & \ddots & * \end{pmatrix}$

symm $\quad Q^TAQ = T = \begin{pmatrix} \ddots & \ddots & \\ \ddots & \ddots & \ddots \\ & \ddots & \ddots \end{pmatrix}$

SVD: $\quad A = U\Sigma V^T \quad A^TA = V\Sigma^2V^T$

$\begin{pmatrix} 0 & A \\ A^T & 0 \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} u \\ v \end{pmatrix}\Sigma \quad \bar{U}^TA\bar{V} = \begin{pmatrix} \ddots & \ddots \\ & \ddots \end{pmatrix}$

Krylov bases

$AQ_k = Q_{k+1}\bar{H}_k$

$AQ_k = Q_{k+1}\bar{T}_k$

$AV_k = U_{k+1}\bar{B}_k$

$U_{k+1}^TA = B_kV_{k+1}^T$

LSQR

$$\hat{x}_k = \arg\min_x \|Ax-b\|_2^2 \quad \text{s.t.} \quad x \in K_k(A^TA, A^Tb)$$

$$\hat{x}_k = V_k \hat{y}_k$$

$$y_k = \arg\min_y \|AV_k y - b\|_2$$

$$= \overset{U_n^T}{\|} U_{k+1}\bar{B}_k y - b\|_2 \qquad \beta_0 b = u_1$$

$$= \left\| \begin{pmatrix} I \\ 0 \end{pmatrix} \bar{B}_k y - \begin{pmatrix} \beta_0 \\ \vdots \\ 0 \end{pmatrix} \right\|_2$$

$$= \|\bar{B}_k y - \beta_0 e_1\|_2$$

$$\bar{B}_k = \begin{pmatrix} \diagdown & \diagdown \end{pmatrix}$$

maintain
QR factorization
with Givens rotations

CG on NE

$$\min_x \frac{1}{2} x^T A^T A x - b^T A x \quad \text{s.t.} \quad x \in K_k(A^TA, A^Tb)$$

$$x = V_k y$$

$$\frac{1}{2} y^T V_k^T A^T A V_k y - y^T V_k^T A^T b$$

$$= \frac{1}{2} y^T \bar{B}_k^T \bar{B}_k y - y^T \bar{B}_k U_{k+1}^T b$$

$$= \frac{1}{2} y^T \bar{B}_k^T \bar{B}_k y - y^T \bar{B}_k^T \beta_0 e_1$$

LSQR is CG
on the NE
with better numerical
properties

LSMR is MINRES
on the NE
with better numerical properties

$$x_k = \arg\min_x \|A^TAx - A^Tb\|_2$$
$$\text{s.t. } x \in \mathcal{K}_k(A^TA, A^Tb)$$

$$x_k = V_k y_k$$

$$y_k = \arg\min_y \|A^TAVy - A^Tb\|_2 \qquad AV_k = U_{k+1}\bar{B}_k$$

$$= \|A^TU_{k+1}\bar{B}_k y - A^Tb\|_2 \qquad A^TU_{k+1} = V_k B_{k+1}^T$$

$$= V_k^T \, \|V_k B_{k+1}^T \bar{\bar{B}}_k y - A^Tb\|_2 \qquad \alpha_1 v_1 = A^Tu_1 = A^Tb/\beta_0$$

$$= \|B_{k+1}^T \bar{B}_k y - \alpha_1\beta_0 e_1\|_2$$

$$B_{k+1}^T\bar{B}_k = \begin{pmatrix} \bar{B}_k^T \\ e_{k+1}^T c_{k+1} \end{pmatrix}$$

$$\left\| \begin{pmatrix} \bar{B}_k^T \bar{\bar{B}}_k \\ e_{k+1}^T c_{k+1} \end{pmatrix} y - \alpha_1\beta_0 e_1 \right\|$$

maintain QR fact. of $\bar{B}_k$ with Givens

M. Saunders' notes for details

$$\| \boxed{A} \boxed{x} - \boxed{b} \| + \lambda \|x\|$$

$$(A, b) \to V_k, U_{k+1}^T, \bar{\bar{B}}_k$$

$$\left(\begin{pmatrix} A \\ \lambda I \end{pmatrix}, \begin{pmatrix} b \\ 0 \end{pmatrix} \right) \to V_k, \begin{pmatrix} U_{k+1}^T \\ 0 \end{pmatrix} \qquad \begin{pmatrix} A \\ \lambda I \end{pmatrix} V_k = \begin{pmatrix} U_{k+1} \\ 0 \end{pmatrix} \tilde{B}_k$$

$$G \begin{pmatrix} \bar{\bar{B}}_k \\ \lambda I \end{pmatrix} = \begin{pmatrix} \hat{B}_k \\ 0 \end{pmatrix}$$

LSQR

$$\left\| \begin{pmatrix} B_k \\ \lambda I \end{pmatrix} y - \beta_1 e_1 \right\|_2 = \| B_k y - \beta_1 e_1 \|_2 + \sqrt{\lambda} \|y\|_2$$

- rectangular  
- with or without regularization