Nov 13, 2020

Problem: $Ax = b$ today: A symm. pos. def $A = A^T$ $\lambda_1 \geq \dots \geq \lambda_n > 0$

Approach: iterative Krylov subspace method

$$K_k(A, b) = \text{span}\{b, Ab, \dots, A^{k-1} b\}$$

$x_k \in K_k(A, b)$ $\quad x_1, x_2, x_3, \dots$ $\quad \|Ax_k - b\|$

$f(x) = \frac{1}{2} x^T A x - b^T x \qquad \nabla f(x) = Ax - b \Rightarrow \nabla f(x) = 0 \Leftrightarrow Ax = b$

$$\boxed{\begin{array}{l}\text{Conjugate gradient (CG) method:} \\ \qquad x_k = \arg\min_x f(x) \text{ s.t. } x_k \in K_k(A, b)\end{array}}$$

$\|\cdot\|_M \quad \|x\|_M = x^T M x \quad$ (M SPD)

$$\|r_\cdot\|_{A^{-1}} = \|Ax_\cdot - b\|_{A^{-1}} = (Ax-b)^T A^{-1} (Ax-b)$$
$$= (Ax-b)^T (x - A^{-1} b) = \underbrace{x^T A x - x^T b - b^T x}_{= 2f(x)} + \cancel{b^T A^{-1} b}$$

$$x_k = \arg\min_x \|Ax - b\|_{A^{-1}} \quad \|\cdot\|_2 \rightarrow \text{MINRES}$$
$$\text{s.t. } x_k \in K_k$$

Lanczos

Q_k orthonormal basis for K_k

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

$$\bar{T}_k = \begin{pmatrix} \alpha_1 & \beta_1 & & \beta_{k-1} \\ \beta_1 & \ddots & \beta_{k-1} & \alpha_k \\ & & & \beta_k \end{pmatrix}$$

$$Q_k^T A Q_k = T_k = \begin{pmatrix} \alpha_1 & \beta_1 & \cdots & \beta_{k-1} \\ \beta_1 & \cdots & \beta_{k-1} & \alpha_k \end{pmatrix}$$

$$\min \tfrac{1}{2} x^T A x - x^T b$$

s.t. $x \in K_k$ $\quad x = Q_k y$ $\quad q_1 \beta_0$

$$\min \tfrac{1}{2} y^T \underbrace{Q_k^T A Q_k}_{T_k} y - y^T \underbrace{Q_k b}_{e_1\beta_0}$$

$$\Rightarrow \quad T_k y_k = \beta_0 e_1$$

$$x_k = Q_k y_k$$

$$T_k = \underline{L_k D_k L_k^T} \qquad L_k = \begin{pmatrix} 1 & & \\ l_1 & \ddots & \\ & l_{k-1} & 1 \end{pmatrix}$$

$$LDz = \boxed{\beta_0 e_1} \qquad L^T z = y$$

$$\begin{pmatrix} 1 & & \\ l_1 & \ddots & \\ & l_{k-1} & 1 \end{pmatrix}\begin{pmatrix} d_1 & & \\ & \ddots & \\ & & d_k \end{pmatrix}\begin{pmatrix} z_1 \\ \vdots \\ z_k \end{pmatrix} = \begin{pmatrix} \beta_0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

$$z_1 = \beta_0 / d_1$$

$$l_{j-1} d_{j-1} z_{j-1} + d_j z_j = 0$$

$$\star \quad z_j = -\frac{1}{d_j} l_{j-1} d_{j-1} z_{j-1}$$

$$W_k L_k^T = Q_k$$

$$(w_1 \cdots w_k)\begin{pmatrix} 1 & l_1 & \cdots & l_{k-1} \\ & \ddots & & \\ & & & 1 \end{pmatrix} = (q_1 \cdots q_k)$$

$$w_1 = q_1$$

$$l_{j-1} w_{j-1} + w_j = q_j$$

$$\star \quad w_j = q_j - l_{j-1} w_{j-1}$$

$$L_k = \begin{pmatrix} L_{k-1} & 0 \\ 0^T\ l_k & 1 \end{pmatrix} \qquad D_k = \begin{pmatrix} D_{k-1} & \\ & d_k \end{pmatrix}$$

$x_k = Q_k y_k \qquad L_k^T y_k = z_k$

$$L_k D_k z_k = \beta_0 e_1$$

$$W_k L_k^T = Q_k$$

$$z_k = \begin{pmatrix} z_{k-1} \\ \eta_k \end{pmatrix}$$

$$W_k = [W_{k-1} \;\; w_k]$$

$$w_k = q_k - l_{k-1} W_{k-1} e_{k-1}$$

$$\begin{aligned}
x_k &= Q_k y_k \\
&= W_k L_k^T y_k \\
&= W_k z_k \\
&= (W_{k-1} \;\; w_k) \begin{pmatrix} z_{k-1} \\ \eta_k \end{pmatrix} \\
&= W_{k-1} z_{k-1} + w_k \eta_k \\
&= x_{k-1} + w_k \eta_k
\end{aligned}$$

CG

$O(n)$ storage $3n + O(1)$

Mat-vec:
1. Lanczos
2. residual

$x_0 = 0$

for $k = 1, 2, \ldots$

- Get q_k, β_{k-1}, α_k (Lanczos)
- Update T_k
- l_{k-1}, d_k
- η_k
- w_k

$x_k = x_{k-1} + w_k \eta_k$

~~if $\|Ax_k - b\|_2 \le \tau$~~
~~return x_k~~

if $|\beta_k \eta_k| \le \tau$
return x_k

Maintaining $\|r_k\|_2 = \|Ax_k - b\|_2$

$$
\begin{aligned}
r_k &= Ax_k - b \\
&= AQ_k y_k - b \\
&= Q_{k+1}\tilde{T}_k y_k - b \\
&= Q_{k+1}\left(\tilde{T}_k y_k - Q_{k+1}^T b\right) \\
&= Q_{k+1}\big(\underbrace{\tilde{T}_k y_k - \beta_0 \overset{\dim = k+1}{e_1}}_{t_{k+1}}\big)
\end{aligned}
$$

$$\|r_k\|_2 = \|Q_{k+1} t_{k+1}\|_2 = \|t_{k+1}\|_2$$

$$
t_{k+1} = \begin{pmatrix} T_k \\ 0^T \beta_k \end{pmatrix} y_k - \begin{pmatrix} \beta_0 \overset{\dim = k}{e_1} \\ 0 \end{pmatrix}
$$

$$
= \begin{pmatrix} \cancel{\beta_0 e_1} \\ \beta_k \underset{\psi_k}{\cancel{(y_k)_k}} \end{pmatrix} - \begin{pmatrix} \cancel{\beta_0 e_1} \\ 0 \end{pmatrix}
$$

$$\|r_k\|_2 = \|t_{k+1}\|_2 = |\beta_k|\,|\psi_k|$$

$$
z_k = L_k^T y_k = \begin{pmatrix} 1 & l_1 & \cdots & \\ & \ddots & \ddots & l_{k-1} \\ & & & 1 \end{pmatrix} \begin{pmatrix} \vdots \\ \psi_k \end{pmatrix}
$$

$$\psi_k = (z_k)_k = \eta_k$$

$$\Rightarrow \|r_k\|_2 = |\beta_k \eta_k|$$

All analysis in exact arithmetic

- Q_k becomes far from orthog w/ 3-term recurrence

  Need to re-orthog

Convergence

A $n \times n$, A full rank

$\Rightarrow A^{-1}b \in K_n$ $\quad O(n \cdot nnz(A))$

$O(nk)$ storage for full re-orthog.

$$\|x_{k+1} - x\| \leq \left(1 - \frac{1}{\kappa_2(A)}\right)^{1/2} \|x_k - x\|_2$$