CG or PCG method for solving $Ax=b$, A or $-A$ is SPD.

PCG: preconditioning $Ax=b$

$\mathrm{cond}_2(PA) < \mathrm{cond}(A)$ $\quad PAx = Pb$

$\varphi(x) = \frac{1}{2}x^T A x - x^T b$

$\nabla\varphi = 0$

CG method:

x_0, $\quad r_0 = b - Ax_0$, $\quad r_0 \neq 0$, $p_0 = r_0$

b

$$\begin{cases} x_{k+1} = x_k + \alpha_k p_k \\ p_k^T r_{k+1} = p_k^T r_k - \alpha_k p_k^T A p_k \\ A p_{k+1} = A r_{k+1} + \beta_{k+1} A p_k \end{cases}$$

$$\alpha_k = \frac{p_k^T r_k}{p_k^T A p_k}$$

$$\beta_{k+1} = -\frac{r_{k+1}^T A p_k}{p_k^T A p_k}$$

Linear search. $r_{k+1}^T p_k = 0$

Let $x_k = x_k - x^*$, $\quad A$ is SPD

$A e_k = A(x_k - x^*)$
$= Ax_k - Ax^*$
$= Ax_k - b$
$= -r$

X $\|e_k\|_2$, $\quad \|e_k\|_{A^{\frac{1}{2}}}^{CG}$, $\quad \|e_k\|_A$ ✓

Not computable

$= \sqrt{e_k^T A e_k}$

$= \sqrt{(Ae_k)^T Ae_k}$

$= \sqrt{e_k^T r_k}$

$= \|r_k\|_2$

GMRES

Convergence

$$r_{k+1} = r_k - \alpha_k A p_k$$

α_k is chosen such that

$\|e_{k+1}\|_{A^{\frac{1}{2}}}$ is minimized

$$\|e_{k+1}\|_{A^{\frac{1}{2}}} \overset{?}{\underset{=}{<}} \|e_k\|_{A^{\frac{1}{2}}} \quad ?$$

$p_k \in K_k(r_0)$, $\quad r_k \in K_k(r_0)$

$\{A^{\frac{1}{2}} p_j\}$, $j = 0, 1, \dots k-1$, is an orthogonal set of $K_k(r_0)$ $\quad = \{r_0, Ar_0, \dots, A^k r_0\}$

$\longrightarrow$ A-conjugate.

Proof: $p_0 = r_0 = K_0(r_0)$,

Assum the conclusions are true

for $j = 1, 2, \ldots k$,

$p_{k+1} = r_{k+1} + \beta_{k+1} p_k$

$r_{k+1} = r_k - \alpha_k A \underline{\underline{p_k}}$ $= \{r_0, Ar_0, \ldots A^{k-1} r_0$

$\in K_k(r_0)$ $\in K_k(r_0)$

$r_{k+1} \in K_{k+1}(r_0)$ $\in K_{k+1}(r_0)$

$p_{k+1} = r_{k+1} + \beta_{k+1} p_k$ $\in K_k(r_0)$ $\in K_{k+1}(r_0)$

$\in K_{k+1}(r_0)$

We want orthogonal basis

$$K_k(r_0) = \{ r_0, Ar_0, \dots A^{k-1} r_0 \}$$

$$= \{ r_0, \underline{A^{\frac{1}{2}} p_0}, A^{\frac{1}{2}} p_1, \dots A^{\frac{1}{2}} p_k \}$$

$\{A^{\frac{1}{2}} p_j\}$ is orthogonal set $A = UDU^H$

$p_i^T A p_j = 0$, if $i \neq j$

$$A^{\frac{1}{2}} = U D^{\frac{1}{2}} U^H$$

$$U D^{\frac{1}{2}} U$$

$$= A^{\frac{1}{2}} A^{\frac{1}{2}}$$

$$x_{k+1} = x_k + \alpha_k p_k$$

b-

$$= x_{k-1} + \alpha_{k-1} p_{k-1} + \alpha_k p_k$$

$$\hat{x}_{k+1} = \hat{x}_0 + \sum_{j=0}^{k} \hat{\alpha}_j p_j$$

$$x_{k+1} - x_0 \in K_k(r_0)$$

$$r_{k+1} = r_0 - \sum_{j=0}^{k} \alpha_j A p_j \in K_{k+1}(r_0)$$

$$e_{k+1} = e_0 + \sum_{j=0}^{k} \alpha_j p_j$$

$$\|e_{k+1}\|_{A^{\frac{1}{2}}} = \min_{\{\bar{\alpha}_j\}} \left\| e_0 + \sum_{j=0}^{k} \bar{\alpha}_j p_j \right\|_{A^{\frac{1}{2}}}$$

$$= \min_{\{\bar{\alpha}_j\}} \sqrt{\left(e_0 + \sum_{j=0}^{k} \bar{\alpha}_j p_j\right)^T A \left(e_0 + \sum_{j=0}^{k} \bar{\alpha}_j p_j\right)}$$

$p_i^T A p_j = 0$ $i \neq j$

$$\bar{\alpha}_j = \alpha_j$$

$$= \min_{\{\bar{\alpha}_j\}} \sqrt{e_0^T A e_0 + \sum_{j=0}^{k} \bar{\alpha}_j^2 p_j^T A p_j}$$

$$\bar{\alpha}_j = \frac{-e_j^T A e_0}{p_j^T A p_j}$$

$$\|e_j\|_{A^{\frac{1}{2}}} = \sqrt{e_j^T A e_j}$$

Thm:

$$\|e_k\|_{A^{\frac{1}{2}}} \leq 2\|e_0\|_{A^{\frac{1}{2}}} \left(\frac{\sqrt{\kappa_2(A)} - 1}{\sqrt{\kappa_2(A)} + 1} \right)^k$$

Proof sketch:

$\kappa_2(A) = \text{cond}_2(A)$

$x_k = x_0 + \sum \alpha_j p_j \qquad \leq 1$

$e_k = e_0 + \sum_{j=0}^{k-1} \alpha_j p_j \qquad e_k = x^* - x_k$

$e_k = e_0 - \sum_{j=0}^{k-1} \nu_j A^j r_0 \quad \to K_{k-1}(r_0)$

$= e_0 - \sum_{j=0}^{k-1} \nu_j A^{j+1} e_0 \qquad e_1 = e_0 -$

$r_0 = b - Ax_0$

$= A(A^{-1}b - x_0)$

$e_k = \left(I - \sum_{j=0}^{k-1} \nu_j A^{j+1} \right) e_0$

$= p_k(A) e_0 \qquad p_k(0) = 1$

CG and GMRES

A SPD   Any A $Ax=b$

$e_k = A^{-1}b - x_k$

$Ae_k = r_k$

$$e_k = e_0 - \sum_{j=0}^{k-1} \alpha_j p_j$$

$$= e_0 - \sum_{j=0}^{k-1} \tilde{\alpha}_j A^j r_0$$

$$= e_0 - \sum_{j=0}^{k-1} \tilde{\alpha}_j A^{j+1} e_0$$

$r_0 = b - Ax_0$

$r_0 = A(A^{-1}b - x_0)$

$= Ae_0$

$$= \left(I - \sum_{j=0}^{k-1} \tilde{\alpha}_j A^{j+1}\right) e_0$$

$e_k = p_k(A) e_0$, $p_k(\lambda)$ is a polynomial of degree k. $p_k(0)=1$

The x_k from the CG method is the one that minimize $\|e_k\|_{A^{\frac{1}{2}}}$

$$\|e_k\|_{A^{\frac{1}{2}}} \le \min_{\substack{p_k \in P_k \\ p(0)=1}} \|p_k(A)\|_2 \, \|e_0\|_{A^{\frac{1}{2}}}$$

$$\|Ae_k\|_{A^{\frac{1}{2}}} = \|A\|_2 \|e_k\|_{A^{\frac{1}{2}}}$$

$$\sqrt{\lambda_{min}}\|x\|_2 \le \|x\|_{A^{\frac{1}{2}}} = \sqrt{x^T A x} \le \sqrt{\lambda_{max}(A)}\, \|x\|_2$$

MA $A = UDU^{-1}$

Need $\gamma \delta\, 0$ to find the minimum. Chebyshev polynomials

Using Chebyshev approximation

Theorem, we can get

$$\|e_k\|_{A^{\frac{1}{2}}} \leq 2\left(\frac{\sqrt{\kappa_2(A)}-1}{\sqrt{\kappa_2(A)}+1}\right)^k \|e_0\|_{A^{\frac{1}{2}}}$$

<1

A is not an SPD

M 1. $A^T A x = A^T b$

$\text{Cond}(A^T A) = (\text{Cond}(A))^2$

GMRES:

$$x_k = x_0 + \sum_{j=0}^{k-1} \gamma_j A^j r_0$$

$$r_k = r_0 - \sum_{j=0}^{k-1} \gamma_j A^{j+1} r_0$$

Can not use $\|e_k\|_{A^{\frac{1}{2}}}$. Does not exist.

$$\|r_k\|_2 = \min_{p_k \in P_k,\ p(0)=1} \|p_k(A)\|_2 \|r_0\|_2$$

Need to find an orthogonal basis in $K_k(r_0)$. Only add one vector at one iteration.

Arnoldi process.

$r_0, Ar_0, \ldots A^{k-1} r_0$

$v_1 = r_0 / \|r_0\|_2$

$h_{21} v_2 = Av_1 - h_{11} v_1$

$v_2^T v_1 = 0$

$v_2^T v_2 = 1$

$(\quad 0 = v_1^T A v_1 - h_{11}$

$h_{11} = v_1^T A v_1$

$h_{21} = \| Av_1 - h_{11} v_1 \|_2$

Assume we have $v_1, v_2, \cdots, v_k$

$h_{k+1,k} v_{k+1} = Av_k - \sum_{j=1}^{k} h_{jk} v_j$

$v_i^T v_j = \begin{cases} 1 & i=j \\ 0 \end{cases}$

$h_{jk} = v_j^T A v_k, \quad h_{k+1,k} = \| Av_k - \sum_{j=1}^{k} h_{jk} v_j \|_2$

$$A[v_1\ v_2\ \cdots v_k] = [v_1\ v_2\ \cdots v_k\ v_{k+1}]_{n\times(k+1)}$$

$$\underline{AV_k = V_{k+1}H_k}$$

$$\begin{bmatrix} h_{11} & h_{12} & \cdots & h_{1k} \\ h_{21} & h_{22} & \cdots & h_{2k} \\ & & \ddots & \\ 0 & & & h_{kk} \\ & & & h_{k+1,k} \end{bmatrix}_{k+1,k}$$

GMRES

$$x_k = x_0 + \sum_{j=1}^{k} \tilde{\gamma}_j v_j$$

$$x_k = x_0 + V_k y_k \qquad \text{multiply by } A$$

$$\|r_k\|_2 = \|r_0 - V_{k+1}H_k y_k\|_2$$

The GMRES method, we choose y_k to minimize $\|r_k\|_2$

$$= \|V_{k+1}^{?}(V_{k+1}^{?} r_0 - H_k y_k)\|_2$$

$$= \|\, \|r_0\|_2 e_1 - H_k y_k\|_2$$

$$\begin{bmatrix} x & x & x & \cdots & x \\ x & x & x & x & x \\ & & & & \\ 0 & & & x & x \\ & & & x & x \end{bmatrix} \begin{bmatrix} y_1 \\ \vdots \\ \vdots \\ y_k \end{bmatrix} = \begin{bmatrix} \|r_0\|_2 \\ 0 \\ \vdots \\ \vdots \\ 0 \end{bmatrix}$$

least squares solution, $\to$ QR.

Given's rotation