Chap 6+7: Iterative Methods

Part 7: Krylov Subspace Methods (KSMs)

GMRES and Conjugate Gradients

Given y_1 form $y_2 = Ay_1 \cdots y_i = Ay_{i-1} = A^{i-1}y_1$

$$\text{span}\{y_1, \ldots, y_k\} = \text{span}\{y_1, Ay_1, \ldots A^{k-1}y_1\}$$
$$= \mathcal{K}_k(A, y_1)$$

$$K = [y_1, y_2, \ldots y_n] = QR$$

$$\mathcal{K}_k(A, y_1) = \text{span}\underbrace{\{q_1, q_2, \ldots q_k\}}_{\text{Arnoldi vectors}}$$

$$Q = [\underset{\text{known}}{Q_k}, \underset{\text{unknown}}{Q_u}] \qquad Q_k = [q_1, \ldots, q_k]$$

$$H = Q^T A Q = [Q_k, Q_u]^T A [Q_k, Q_u]$$
$$= \begin{bmatrix} Q_k^T A Q_k & Q_k^T A Q_u \\ Q_u^T A Q_k & Q_u^T A Q_u \end{bmatrix}$$

after k steps of Arnoldi

$$= \left[\begin{array}{c|c} H_k & H_{uk} \\ \hline H_{ku} & H_u \end{array}\right] = \left[\begin{array}{c|c} H_k & \\ \hline O & \end{array}\right]$$

$$\underbrace{\phantom{H_{ku}}}_{\text{known}} \quad \underbrace{}_{\text{unknown}}$$

if $A = A^T \Rightarrow H = H^T = T$ tridiagonal

$$= \begin{bmatrix} \alpha_1 & \beta_1 & & O \\ \beta_1 & \alpha_2 & \beta_2 & \\ & \beta_2 & \ddots & \ddots \\ O & & \ddots & \alpha_n \end{bmatrix}$$

Goal: Solve $Ax = b$, Given Q_k

$= [q_1, \ldots, q_k]$

Find "best" approximate solution

x_k in span(Q_k)

Possible different definitions of "best"

(1) choose x_k to minimize $\|x_k - x\|_2$ where $Ax = b$; not enough info

(2) choose x_k to minimize

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

2 algorithms:

if $A = A^T$, use MINRES

if A general use <u>GMRES</u>

(3) Choose x_k so r_k orthogonal to $K_k(A,b)$ i.e. $r_k^T Q_k = 0$

called "orthogonal residual property" or Galerkin condition, by analogy to finite elements.

$A = A^T \Rightarrow$ use SYMMLQ

A general $\Rightarrow$ variation of GMRES

(4) When A is spd, it defines a norm $\|r\|_{A^{-1}} = (r^T A^{-1} r)^{1/2}$

"best" solution minimizes $\|r_k\|_{A^{-1}}$

$$
\begin{aligned}
\|r_k\|_{A^{-1}}^2 &= r_k^T A^{-1} r_k \\
&= (b - Ax_k)^T A^{-1} (b - Ax_k) \\
&= (Ax - Ax_k)^T A^{-1} (Ax - Ax_k) \\
&= (x - x_k)^T A^T A^{-1} A (x - x_k) \\
&= (x - x_k)^T A (x - x_k)
\end{aligned}
$$

$= \|x - x_k\|_A^2$

Algorithm called Conjugate Gradients (CG)

Thm When A s.p.d. defs (3) and (4) of "best" are equivalent.

Cost: computing x_k costs
- one multiplication by A
- a few dot products, "saxpys" ($y = \alpha \cdot x + y$)
- only need to keep 3 vectors in memory

Generally choice of algorithm depends on A (Fig 6.8)

GMRES: uses least structure of A

In GMRES, at each step choose x_k to minimize $\|r_k\|_2 = \|b - Ax_k\|_2$ where $x_k = Q_k y_k \in \mathcal{K}_k(A,b)$

$$\|r_k\|_2 = \|b - AQ_k y_k\|_2$$
$$= \|b - A[Q_k, Q_u] \cdot \begin{bmatrix} y_k \\ 0 \end{bmatrix}\|_2$$

$$= \| Q^T (\quad " \quad) \|_2$$

$$= \| \underbrace{Q^T b} - \underbrace{Q^T A Q}_{H} \begin{bmatrix} y_k \\ 0 \end{bmatrix} \|_2$$

$$= \| e_1 \|b\|_2 - \left[\begin{array}{c|c} H_k & H_{uk} \\ \hline H_{ku} & H_u \end{array} \right] \begin{bmatrix} y_k \\ 0 \end{bmatrix} \|_2$$

$$= \| e_1 \|b\|_2 - \begin{bmatrix} H_k \\ H_{ku} \end{bmatrix} y_k \|_2$$

$$= \| e_1 \cdot \|b\|_2 - \underbrace{\left[\begin{array}{c} H_k \\ \hline 0 \cdots 0 \; H(k+1,k) \end{array} \right]}_{k+1 \times k} y_k \|_2$$

solve least squares problem
using Givens rotations
cost $O(k^2)$ instead $O(k^3)$

CG: "best" in 2 senses

Lemma: A s.p.d. following equivalent

(3) Choose x_k so $r_k^T Q_k = 0$

(4) Choose x_k to minimize $\|r_k\|_{A^{-1}}$

$$= \| x - x_k \|_A$$

solved by $x_k = Q_k T_k^{-1} e_1 \|b\|_2$

where T_k is tridiagonal matrix computed by Arnoldi / Lanczos

$r_k = \pm \|r_k\|_2 \cdot q_{k+1}$

Proof: drop subscript k

so $Q = Q_k$, $T = T_k$

$x = Q T^{-1} e_1 \|b\|_2 \qquad r = b - Ax$

$T = Q^T A Q$ is s.p.d.

$$
\begin{aligned}
Q^T r &= Q^T (b - Ax) \\
&= Q^T b - Q^T A x \\
&= e_1 \|b\|_2 - \underbrace{Q^T A Q}\, T^{-1} e_1 \|b\|_2 \\
&= e_1 \|b\|_2 - \underbrace{T \quad T^{-1}}\, e_1 \|b\|_2 \\
&= e_1 \|b\|_2 - e_1 \|b\|_2 \\
&= 0
\end{aligned}
$$

Need to show x minimizes $\|r\|_{A^{-1}}$

try $x' = x + Qz \qquad r' = b - Ax' = r - AQz$

$$
\begin{aligned}
\|r'\|_{A^{-1}}^2 &= r'^T A^{-1} r' \\
&= (r - AQz)^T A^{-1} (r - AQz) \\
&= r^T A^{-1} r - 2 (AQz)^T A^{-1} r \\
&\quad + (AQz)^T A^{-1} (AQz) \\
&= r^T A^{-1} r - 2 z^T Q^T \overline{A A^{-1}} r \\
&\quad + (AQz)^T A^{-1} (AQz)
\end{aligned}
$$

$= r^T A^{-1} r - 2 z^T \underline{Q^T r} + (AQz)^T A^{-1} (AQz)$

$= r^T A^{-1} r + (AQz)^T A^{-1} (AQz)$

$= \|r\|_{A^{-1}}^2 + \|AQz\|_{A^{-1}}^2 \geq \|r\|_{A^{-1}}^2$

minimized when $z = 0$

$r_k = b - A \underset{\in \mathcal{K}_k}{\underline{x_k}} \in \mathcal{K}_{\underline{k+1}}$

$\Rightarrow r_k$ in span$\{q_1, \ldots, q_{k+1}\}$

r_k orthogonal to $q_1, \ldots q_k$

$\Rightarrow r_k$ parallel to q_{k+1}

$r_k = \pm \|r_k\|_2 \, q_{k+1}$ QED

Several ways to derive CG.

We will take "direct" approach

using formula above, derive

recurrences for 3 sets of vectors:

x_k, r_k, p_k = "conjugate gradients"

(1) p_k's are called gradients because

each step of CG can be thought

of as moving x_{k-1} along

direction p_k ($x_k = x_{k-1} + \eta \cdot p_k$)

until x_k minimizes $\|r_k\|_{A^{-1}}$ over all

choices of η

(2) p_k's are called conjugate, or A-conjugate, orthogonal in inner product defined by A:

$$p_k^T A p_j = 0 \quad \text{if } k \neq j$$

CG sometimes derived by figuring out recurrences for x_k, r_k, p_k that satisify (1) and (2), and then showing they satisfy Lemma

We start with $x_k = Q_k T_k^{-1} e_1 \|b\|_2$

$T_k = Q_k^T A Q_k$ is spd and tridiagonal

Cholesky: $T_k = L_k' \cdot L_k'^T$ where L_k' is lower bidiagonal $\begin{bmatrix} \diagdown & 0 \\ 0 & \diagdown \end{bmatrix}$

$L_k' L_k'^T = L_k D_k L_k^T$ where L_k has 1s on diagonal, D_k diagonal $D_k(i,i) = L_k'(i,i)^2$

Lemma:

$$\begin{aligned} x_k &= Q_k T_k^{-1} e_1 \|b\|_2 \\ &= Q_k (L_k D_k L_k^T)^{-1} e_1 \|b\|_2 \\ &= \underbrace{(Q_k L_k^{-T})}_{= P_k'} \cdot \underbrace{(D_k^{-1} L_k^{-1} e_1 \|b\|_2)}_{y_k} \end{aligned}$$

where $P'_k = [p'_1, p'_2, \dots p'_k]$

eventually, conjugate gradients p_k will be scalar multiples of p'_k

Enough to prove (2) above

Lemma: p'_k s are A conjugate

$P_k'^T A P'_k$ is diagonal

proof: $P_k'^T A P'_k = (Q_k L_k^{-T})^T A (Q_k L_k^{-T})$

$$= L_k^{-1} \underbrace{Q_k^T A Q_k} L_k^{-T}$$

$$= L_k^{-1} \quad T_k \quad L_k^{-T}$$

$$= \underbrace{L_k^{-1} (L_k} D_k \underbrace{L_k^T) L_k^{-T}}$$

$$= D_k \quad \text{diagonal}$$

Next: derive recurrences for columns p'_k of P'_k and for components of $y_k \Rightarrow$ recurrence for x_k

P'_{k-1} is identical to leading $k-1$ columns of P'_k: $P'_k = [P'_{k-1}, p'_k]$

similarly: $y_{k-1} = \begin{bmatrix} s_1 \\ s_2 \\ \vdots \\ s_{k-1} \end{bmatrix}$ $\quad y_k = \begin{bmatrix} s_1 \\ s_2 \\ \vdots \\ s_{k-1} \\ s_k \end{bmatrix} = \begin{bmatrix} y_{k-1} \\ s_k \end{bmatrix}$

Assuming both, we get a recurrence for x_k

$$(R_x) \quad \underline{x_k} = P'_k y_k = [P'_{k-1}, p'_k] \begin{bmatrix} y_{k-1} \\ s_k \end{bmatrix}$$

$$= P'_{k-1} y_{k-1} + p'_k s_k$$

$$= \underline{x_{k-1}} + \underline{\underline{p'_k}}\,\underline{\underline{s_k}}$$

Since Lanczos construct T_k row by row, so T_{k-1} is leading $k-1 \times k-1$ submatrix of T_k, Similarly Cholesky computes row by row, so L_{k-1}, D_{k-1} factors of T_{k-1} are leading parts of L_k, D_k:

$$T_k = L_k D_k L_k^T$$

$$= \begin{bmatrix} L_{k-1} & 0 \\ 0 \cdots 0 \, \ell_{k-1} & 1 \end{bmatrix} \cdot \begin{bmatrix} D_{k-1} & 0 \\ 0 & d_k \end{bmatrix} \begin{bmatrix} L_{k-1} & 0 \\ 0 \cdots 0 \, \ell_{k-1} & 1 \end{bmatrix}^T$$

so $L_k^{-1} = \begin{bmatrix} L_{k-1}^{-1} & 0 \\ \text{stuff} & 1 \end{bmatrix}$

$$\underline{y_k} = D_k^{-1} L_k^{-1} e_1 \|b\|_2$$

$$= \begin{bmatrix} D_{k-1}^{-1} & 0 \\ 0 & d_k^{-1} \end{bmatrix} \cdot \begin{bmatrix} L_{k-1}^{-1} & 0 \\ \text{stuff} & 1 \end{bmatrix} \cdot e_1 \cdot \|b\|_2$$

$$= \begin{bmatrix} D_{k-1}^{-1} L_{k-1}^{-1} e_1 \cdot \|b\|_2 \\ s_k \end{bmatrix} = \begin{bmatrix} y_{k-1} \\ \hline s_k \end{bmatrix}$$

$\rightarrow$ desired recurrence for y_k

Similarly:

$$P'_k = Q_k L_k^{-T}$$

$$= [Q_{k-1}, \underline{q_k}] \cdot \begin{bmatrix} L_{k-1}^{-T} & \text{stuff} \\ 0 & 1 \end{bmatrix}$$

$$= [Q_{k-1} \cdot L_{k-1}^{-T}, \ p'_k]$$

$$= [P'_{k-1}, \ \underline{p'_k}]$$

so to get a formula for p'_k

$$Q_k = P'_k \cdot L_k^T$$

equate last columns:

$$q_k = p'_k + p'_{k-1} \cdot \underline{L_k(k, k-1)}$$

$$(R_p) \quad p'_k = q_k - l_{k-1} \cdot p'_{k-1}$$

is desired recurrence for p'_k

Need a recurrence for r_k, use (Rx)

$$(Rr) \quad r_k = b - Ax_k$$
$$= b - A(x_{k-1} + p'_k \cdot s_k)$$
$$= r_{k-1} - \underline{Ap'_k} \cdot s_k$$

Putting all recurrences together:

$$(Rr) \quad r_k = r_{k-1} - A p'_k s_k$$
$$(Rx) \quad x_k = x_{k-1} + p'_k s_k$$
$$(Rp) \quad p'_k = q_k - \ell_{k-1} \cdot p'_{k-1}$$

substitute:

$$q_k = r_{k-1} / \| r_{k-1} \|_2 \qquad p_k = \| r_{k-1} \|_2 \cdot p'_k$$

$$(Rr') \quad r_k = r_{k-1} - Ap_k (s_k / \| r_{k-1} \|_2)$$
$$= r_{k-1} - Ap_k (z_k)$$

$$(Rx') \quad x_k = x_{k-1} + p_k z_k$$

$$(Rp') \quad p_k = r_{k-1} - (\| r_{k-1} \|_2 \cdot \ell_{k-1} / \| r_{k-2} \|_2) p_{k-1}$$
$$= r_{k-1} + \nu_k p_{k-1}$$

How to compute ν_k and ζ_k?

Several choices, some more stable than others! (text for details)

$$\zeta_k = r_{k-1}^T r_{k-1} / p_k^T A p_k$$

$$\nu_k = r_{k-1}^T r_{k-1} / r_{k-2}^T r_{k-2}$$

CG algorithm:

$$k=0, \quad x_0=0, \quad r_0=b, \quad p_1=b$$

repeat

$$k=k+1$$

$$z=Ap_k$$

$$\zeta_k = r_{k-1}^T r_{k-1} / p_k^T z$$

$$x_k = x_{k-1} + p_k \cdot \zeta_k$$

$$r_k = r_{k-1} - z \cdot \zeta_k$$

$$\nu_{k+1} = r_k^T r_k / r_{k-1}^T r_{k-1}$$

$$p_{k+1} = r_k + \nu_{k+1} \cdot p_k$$

until $\|r_k\|_2$ small enough

minimization property follows

from x_k minimizing $\|r_k\|_{A^{-1}}$ over all x_k in span (Q_k)

Convergence:

Thm: $\|r_k\|_{A^{-1}} / \|r_0\|_{A^{-1}}$

$$\leq \frac{2}{1 + \frac{2k}{\sqrt{\text{cond}(A) - 1}}}$$

$\Rightarrow$ cond(A) large $\Rightarrow O(\sqrt{\text{cond}(A)})$ steps to converge

Poisson: $n \times n$ mesh:
cond(A) $\sim O(n^2) \Rightarrow O(n)$ steps to converge