Conjugate Gradient Method

Steepest Descent

Goal: Solve $Ax=b$ A spd $A\bar{u}=b$

We start with steepest descent

Consider "Eliptical Bowl"

$$G(u) = (\bar{u}-u)^T A (\bar{u}-u)$$

$$\min_u G(u) = \bar{u}$$

Major axises are eigenvector of A.

note $G(u) = \bar{u}^T A \bar{u} - 2u^T A \bar{u} + u^T A u$

$$= \underbrace{\bar{u}^T b}_{\text{constant}} - 2u^T b + u^T A u.$$

Suffice to min $F(u) = \frac{1}{2} u^T A u - u^T b$

> To be consistant with Trefethen & Bau
> $A^{m \times m}$ n is the step index.

Recall $\nabla F = \begin{pmatrix} \frac{dF}{du_1} \\ \vdots \\ \frac{dF}{du_m} \end{pmatrix}$ $\nabla F = \frac{1}{2} \nabla u^T A u - \nabla u^T b$

<u>Claim</u> $\frac{d u^T b}{du_i} = b_i$ pf $\lim_{h \to 0} \frac{(u+he_i)^T b - u^T b}{h}$

$$= \lim_{h \to 0} \frac{h e_i^T b}{h} = b_i$$

Check $\frac{d u^T A u}{du_i} = 2(Au)_i$ (A sym)

---

thus $\nabla F(u) = Au - b$ residual $r = b - Au$

<u>Note</u> Richardson Alg

$$u^{(n+1)} = u^{(n)} + \lambda (b - Au^{(n)}) \quad \lambda = 1$$

$\therefore$ RA is steepest descent, step size $\lambda = 1$

Goal: Pick λ minimize $F(u^{(n)}+\lambda r)$

Set $u = u^{(n)}$

$$F(u+\lambda r) = \frac{1}{2}(u+\lambda r)^T A (u+\lambda r) - b^T(u+\lambda r)$$

$$\frac{\partial F(u-\lambda r)}{\partial \lambda} = r^T A u + \lambda r^T A r - b^T r$$

$$= r^T \underbrace{(Au-b)}_{=-r} + \lambda r^T A r$$

$$= -r^T r + \lambda r^T A r$$

set $\frac{\partial F}{\partial \lambda} = 0$

$$-r^T r + \lambda r^T A r = 0$$

$$\lambda = \frac{r^T r}{r^T A r} \leftarrow \text{step size}$$

Steepest Descent Input A, b

Initial guess $u^{(0)} = 0$

$$u^{(n+1)} = u^{(n)} + \lambda r \quad \text{where}$$

$$r = b - Au$$

$$\lambda = r^T r / r^T A r$$

Convergence Rate

(Kantorovich Lemma) B spd (real) λ_M, λ_m for B

$$\frac{(x^T B x)(x^T B^{-1} x)}{(x^T x)^2} \leq \frac{(\lambda_M + \lambda_m)^2}{4 \lambda_M \lambda_m}$$

Pf See SAAD Chap 5 page 132

Def $\|x\|_A = (x^T A x)^{1/2}$

$x \perp_A y$ if $x^T A y = 0$

note $x^T A y = (A^{1/2} x)^T (A^{1/2} y)$

$x \perp_A y$ iff $(A^{1/2} x) \perp A^{1/2} y$

Thm A spd, error in steepest descent $\varepsilon^{(k)} = \bar{u} - u^{(k)}$ then

$$\|\varepsilon^{(k+1)}\|_A \le \left(\frac{\lambda_M - \lambda_m}{\lambda_M + \lambda_m}\right) \|\varepsilon^{(k)}\|_A$$

$$= \left(\frac{\kappa - 1}{\kappa + 1}\right) \|\varepsilon^{(k)}\|_A \qquad \kappa = \frac{\lambda_M}{\lambda_m}$$

$$\approx \left(1 - \frac{2}{\kappa}\right) \|\varepsilon^{(k)}\|_A$$

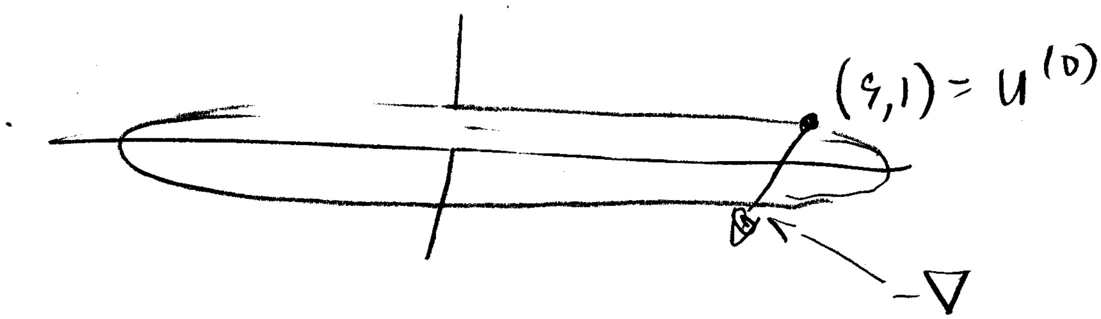
pf SAAD Chap 5 133 p.

Steepest Descent an example

$$A = \begin{pmatrix} 1 & 0 \\ 0 & 10 \end{pmatrix} \quad b = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad \bar{u} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad u^{(0)} = \begin{pmatrix} 9 \\ 1 \end{pmatrix}$$

$$r = b - Au^{(0)} = -\begin{pmatrix} 1 & 0 \\ 0 & 10 \end{pmatrix}\begin{pmatrix} 9 \\ 1 \end{pmatrix} = -\begin{pmatrix} 9 \\ 10 \end{pmatrix}$$

"Eliptical Bowl"



$$\lambda = \frac{r^T r}{r^T A r} = \frac{181}{81 + 1000} = \frac{181}{1081}$$

$$u^{(1)} = \begin{pmatrix} 9 \\ 1 \end{pmatrix} - \left(181/1081\right)\begin{pmatrix} 9 \\ 10 \end{pmatrix}$$

$$u_2^{(1)} = 1 - \frac{1810}{1081} = \frac{-729}{1081} \approx -3/4$$

We over shot!

Krylor Subspaces

$Ax=b$ & $A\bar{x}=b$ initial guess $x^{(0)}$

Def nth Krylov subspace

$$\mathcal{K}_n = \langle b, Ab, A^2b, \dots, A^{n-1}b \rangle$$

If $x^{(0)} \neq 0$ affine space $x^{(0)} + \mathcal{K}_n$ Krylov space

Why is $\mathcal{K}_n$ of interest?

assume $x^{(0)} = 0$

Claim Given an iterative method

$$x^{(n+1)} = \alpha_n x^{(n)} + \beta_n (b - A x^{(n)}) \text{ then}$$

$$x^{(n)} \in \mathcal{K}_n$$

pf Induction on n

$n=1$ then $x^{(1)} = \beta b \in \mathcal{K}_1$

<u>Claim</u> If $x^{(n)} \in \mathcal{K}_n$ then $Ax^{(n)} \in \mathcal{K}_{n+1}$

Assume $x^{(n)} = a_1 b + \cdots + a_{n-1} A^{n-1} b$

$$Ax^{(n)} = a_1 Ab + \cdots + a_{n-1} A^n b \in \mathcal{K}_{n+1}$$

$\therefore$ $x^{(n+1)} \in \mathcal{K}_{n+1}$

All our methods do is find $x^{(n)} \in \mathcal{K}_n$!

Best would be to find $\underset{x \in \mathcal{K}_n}{\mathrm{Argmin}} \|\bar{x} - x\|_2$

Not clear how to do this!

Next best thing

$$\underset{x^{(n)} \in \mathcal{K}_n}{\mathrm{Argmin}} \|\bar{x} - x^{(n)}\|_A$$

This we can do! It is called Conjugate Gradient.

Conjugate Gradient Iteration

Init: $x_0 = 0 \quad r_0 = b \quad p_0 = r_0$

Iteration:

$\alpha_n = r_{n-1}^T r_{n-1} / p_{n-1}^T A p_{n-1}$ step length

$x_n = x_{n-1} + \alpha_n p_{n-1}$ approx solution

$r_n = r_{n-1} - \alpha_n A p_{n-1}$ residual

$\beta_n = r_n^T r_n / r_{n-1}^T r_{n-1}$ improvement

$p_n = r_n + \beta_n p_{n-1}$ search direction

Claim $r_n = b - Ax_n$

pf induct on n $n=0$

assume true for $n-1$

$$b - Ax_n = b - A(x_{n-1} + \alpha_n p_{n-1})$$

$$= (b - Ax_{n-1}) - \alpha_n A p_{n-1} \quad \text{induct}$$

$$= r_{n-1} - \alpha_n A p_{n-1} = r_n$$

Thm A CG for spd A for prob $Ax=b$ then while $r_{n-1} \neq 0$

$$\mathcal{K}_n = \langle x_1, \cdots, x_n \rangle = \langle p_0, \cdots, p_{n-1} \rangle$$

$$\langle r_0, \cdots, r_{n-1} \rangle = \langle b, Ab, \cdots, A^{n-1} b \rangle$$

& $r_n^T r_j = 0 \quad (j<n)$

& $p_n^T A p_j = 0 \quad (j<n)$

---

pf See Trefethen & Bau Chap 38

pf of 1)

By Thm A $\quad x_n \in \mathcal{K}_n$ where $x_0 = 0$

thus $x_n = Q_{n-1}(A)b$ some polynomial $Q_{n-1}(z)$

$\deg(Q_{n-1}(z)) \leq n-1$

Consider $P_n(z) = 1 - z \cdot Q(z) \qquad \deg(P_n) \leq n$

<u>Claim</u> $\varepsilon_n = P_n(A)\varepsilon_0$ where $\varepsilon_0 = \bar{x}$

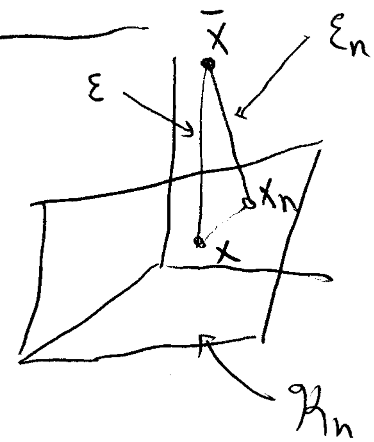
$$
\begin{aligned}
P_n(A)\varepsilon_0 &= (1 - A\,Q_{n-1}(A))\bar{x} \\
&= \bar{x} - Q_{n-1}(A)(A\bar{x}) \\
&= \bar{x} - Q_{n-1}(A)b \\
&= \bar{x} - x_n = \varepsilon_n
\end{aligned}
$$

<u>Thm B</u> $A^{m \times m} x = b$, A spd, CG

1) while $r_{n-1} \neq 0$ then x_n unique point in $\mathcal{K}_n$
minimizing $\| \varepsilon_n \|_A$ $\quad (\varepsilon_n = \bar{x} - x_n)$

2) $\| \varepsilon_n \|_A \leq \| \varepsilon_{n-1} \|_A$

3) $\exists n \leq m$ st $\varepsilon_n = 0$



<u>pf</u> $x_n \in \mathcal{K}_n$ by previous thm.

Let $x \in \mathcal{K}_n$ be arbitrary.

Set $\Delta x = x_n - x$

$\varepsilon = \bar{x} - x = \varepsilon_n + \Delta x$

$$\| \varepsilon \|_A^2 = (\varepsilon_n + \Delta x)^T A (\varepsilon_n + \Delta x)$$

$$\varepsilon_n^T A \varepsilon_n + (\Delta x)^T A (\Delta x) + 2 \varepsilon_n^T A (\Delta x)$$

<u>note</u> $A \varepsilon_n = A(\bar{x} - x_n) = b - A x_n = r_n$ $2 \varepsilon_n^T A \Delta x = 2 r_n^T \Delta x = 0$ since $r_n \perp \mathcal{K}_n$

(thus) $\|\varepsilon\|_A^2 = \varepsilon_n^T A \varepsilon_n + (\Delta x)^T A (\Delta x)$

A spd $\Rightarrow$ $x \neq x_n$ then $\|\varepsilon\|_A^2 > \|\varepsilon_n\|_A^2$

---

2) $\mathcal{K}_n \subseteq \mathcal{K}_{n+1} \Rightarrow \|\varepsilon_n\|_A \leq \|\varepsilon_{n-1}\|_A$

---

3) For some $n \leq m$ $\tilde{x} \in \mathcal{K}_n$ and done.

CG & Polynomial Approx

Prob Find poly P_n, $P_m(0)=1$ $\deg(P_n) \le n$

minimizing $\| P_n(A)\, \varepsilon_0 \|_A$

Thm If $r_{n-1} \neq 0$ for CG then $\exists!\, P_n$, $P_n(0)=1$

1) X_n has error $\varepsilon_n = P_n(A)\, \varepsilon_0$ $\quad P_n(0)=1$

2) $$\frac{\|\varepsilon_n\|_A}{\|\varepsilon_0\|_A} = \inf_{P_n} \frac{\| P(A)\, \varepsilon_0\|_A}{\|\varepsilon_0\|_A} \le \inf_{P_n} \max_{\lambda \in \lambda(A)} |P(\lambda)|$$

---

pf 1) See page 12A.

2) $(=)$ follows from Thm B.

$(\le)$ Suppose $\varepsilon_0 = \sum_{j=1}^{m} a_j V_j$ (eigen expansion of A)

$V_j^T V_j = 1$

$$P(A)\, \varepsilon_0 = \sum a_j P_n(\lambda_j) V_j$$

$$\|\varepsilon_0\|_A = \sum_{j=1}^{m} a_j^2 \lambda_j \qquad \|e_n\|_A = \sum a_j^2 \, p_n(\lambda_j)^2 \lambda_j$$

$$\frac{\|\varepsilon_n\|_A}{\|\varepsilon_0\|_A} \le \max_j \frac{a_j^2 \, p(\lambda_j)^2 \lambda_j}{a_j^2 \lambda_j} = \max_j |p(\lambda_j)|$$

<u>Thm</u> CG to solve $Ax=b$, A spd

$$\frac{\|\varepsilon_n\|_A}{\|\varepsilon_0\|_A} \le 2\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^n$$

---

pf

$$\frac{\|\varepsilon_n\|_A}{\|\varepsilon_0\|_A} \le \max_{\lambda \in \lambda(A)} |P_n(A)| \le \max_{\lambda \in \lambda(A)} |p(x)|$$

any $p(x)$ st $\deg(p) \le n-1$

$p(0) = 1$

Call $Ax = b$ $\quad m = \lambda_m \leq \lambda(A) \leq \lambda_M = M$

$G_\alpha = (I - \alpha A) \qquad -\gamma \leq \lambda(G_\alpha) \leq \gamma$

$$\gamma = \frac{M-m}{M+m}$$

$$P(x) = T_n\left(\gamma^{-1} - \frac{2x}{M-m}\right) \Big/ T_n(\gamma^{-1}) \qquad T_n \equiv \text{Chebyshev Poly}$$

$$= T_n\left(\frac{M+m-2x}{M-m}\right) \Big/ T_n(\gamma^{-1})$$

Note $P(0) = 1 \qquad \deg(P) \leq n-1$

$P(x) \leq 1/T_n(\gamma^{-1})$ for $m \leq x \leq M$

Thus $P(\lambda) \leq 2\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^n \quad \forall \lambda \in \lambda(A)$

$\kappa = M/m$