

# Conjugate Gradient Method & Steepest Descent

15-859N  
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Goal: Solve  $Ax = b$  where  $A \text{ spd}$  &  $A\tilde{x} = b$

We start with Steepest Descent.

Consider "Elliptical Bowl"

$$M(u) = (\tilde{x} - x)^T A (\tilde{x} - x)$$

note  $\min_u M(x) = \tilde{x}$

The major axis are the eigenvectors of  $A$ .

Expand

$$\begin{aligned} M(\ ) &= \tilde{x}^T A \tilde{x} - 2 x^T A \tilde{x} + x^T A x \\ &\leftarrow \tilde{x}^T b - 2 x^T b + x^T A x \end{aligned}$$

constant

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

## Crash course on matrix calculus

Let  $G: \mathbb{R}^n \rightarrow \mathbb{R}$ , say  $G(x_1, \dots, x_n) = y$

Def:  $\nabla G = \left( \frac{\partial G}{\partial x_1}, \dots, \frac{\partial G}{\partial x_n} \right)$

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To Show:  $\nabla F = \frac{1}{2} \nabla u^T A u - \nabla u^T b$

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Claim:  $\frac{d u^T b}{d u_i} = b_i$

$$\begin{aligned} \text{Pf } \frac{d u^T b}{d u_i} &= \lim_{h \rightarrow 0} \frac{(u + h e_i)^T b - u^T b}{h} \\ &= \lim_{h \rightarrow 0} \frac{h e_i^T b}{h} = b_i \end{aligned}$$


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Check that

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$$\frac{d u^T A u}{d u_i} = 2(Au)_i \quad (A \text{ sym})$$

$$\lim_{h \rightarrow 0} \frac{(u + h e_i)^T A (u + h e_i) - u^T A u}{h}$$

$$= \lim_{h \rightarrow 0} \frac{\cancel{u^T A u} + 2h e_i^T A u + \cancel{h^2 e_i^T A e_i} - \cancel{u^T A u}}{h}$$

$$2e_i^T A u = 2(Au)_i$$

Thus  $\nabla F(u) = Au - b$

Set  $g = \nabla F(u)$

In general:  $d \in \mathbb{R}^n$

$$\frac{\partial F(u)}{\partial d} = d^T (Au - b) = d^T g$$

Note Richardson's Alg

$$x^{(n+1)} = x^{(n)} + \alpha(b - Ax^{(n)}) \quad \alpha=1$$

thus RA is steepest descent with step size  $\alpha=1$ .

The Extrapolated Method

is optimal fixed size method.

Goal: Find a variable size method.

Idea: Pick  $\alpha$  to minimize  $F(u^{(n)} - \alpha g)$

$$\text{Set } U = X^{(n)}$$

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- Let 1)  $u$  be some guess.  
 2)  $d$  a search direction  
 3)  $\alpha$  step size.  
 4)  $g$  gradient
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$$\text{Claim } \frac{\partial F(u + \alpha d)}{\partial d} = d^T g + \alpha d^T A d$$

Pf Set  $\bar{u} = u + \alpha d$

$$\begin{aligned} \text{We know } \frac{\partial F(\bar{u})}{\partial d} &= d^T(A\bar{u} - b) \\ &= d^T(A(u + \alpha d) - b) \\ &= d^T(Au - b) + \alpha d^T A d \\ &= d^T g + \alpha d^T A d \end{aligned}$$


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$$\text{Setting } \frac{\partial F}{\partial \lambda} = 0$$

$$d^T g + \alpha d^T A d = 0$$

$$\text{thus: } \alpha = \frac{-d^T g}{d^T A d}$$

## Steepest Descent

Input:  $A, b$     A spd

Init:  $u^{(0)} = 0$

$$x^{(n+1)} = x^{(n)} + \alpha g \text{ where}$$

$$g = Ax^{(n)} - b$$

$$\alpha = -\frac{g^T g}{g^T A g}$$


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Claim:  $\nabla F(u - \alpha d) \perp d \quad ?$

$$\stackrel{?}{=} d^T (A(u - \alpha d) - b)$$

$$d^T (Au - b) - \alpha d^T A d$$

$$d^T g - d^T g = 0$$

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## Convergence Rate!

(Kantorovich Lemmer)  $B$  spd

$\lambda_M \& \lambda_m$  for  $B$ . then

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

pf See SAAD Chap 5 page 132.

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

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$$x \perp_A y \text{ if } x^T A y = 0$$

$$\text{note } x^T A y = (A^{\frac{1}{2}} x)^T (A^{\frac{1}{2}} y)$$

$$x \perp_A y \text{ iff } A^{\frac{1}{2}} x \perp A^{\frac{1}{2}} y$$


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$$\text{Thm } A \text{ spd} \& \varepsilon^{(k)} = \tilde{u} - u^{(k)}$$

for steepest descent then

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

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

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

pf SAAD Chap 5 133p

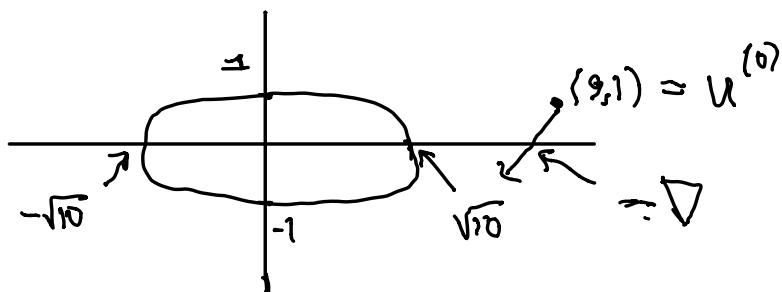
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## Steepest Descent an Example

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

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

"the Elliptical bowl"



$$\lambda = \frac{r^T r}{r^T A r} = \frac{|r|^2}{|Ar|^2} = \frac{181}{81+1000} = \frac{181}{1081}$$

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

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

we over shot  $y=0$ !

## Krylov Subspaces

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

Def:  $n$ th Krylov Subspace

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

If  $x^{(0)} \neq 0$  then consider affine space

$$x^{(0)} + \mathcal{K}_n \quad \text{Krylov Space}$$

We will assume that  $x^{(0)} = 0$ .

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

Claim: Given an iterative method of form

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

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

Pf Induction on  $n$

$$n=0 \quad x^{(0)} = b \in \langle b \rangle = \mathcal{K}_0$$

Claim  $x^{(n)} \in \mathcal{K}_n$  then  $Ax^{(n)} \in \mathcal{K}_{n+1}$

assume  $x^{(n)} = c_0b + c_1Ab + \dots + c_nA^n b$

$$Ax^{(n)} = c_0Ab + c_1A^2b + \dots + c_nA^{n+1}b$$

Thus  $Ax^{(n)} \in \mathcal{K}_{n+1}$

Thus all our method do in find  $x^{(n)} \in \mathcal{K}_n$ ! 12

The best would be to find

$$x^{(n)} = \underset{x \in \mathcal{K}_n}{\operatorname{Argmin}} \| \bar{x} - x \|_2$$

We do not know how to do this efficiently.

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Next best thing

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

$$\text{Recall } \|y\|_A = \sqrt{y^T A y}$$

This we can do! It is called  
Conjugate Gradient

Conjugate Gradient

Design Goals:

1) Step direction should  
be orthogonal

2) Step size should minimize  $F$ .

Alg: CG ( $Ax = b$ )

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Init:  $x_0 = 0$   $d_0 = -g_0 = b - Ax_0$

$$x_1 = x_0 + \alpha_0 d_0$$

$$\text{where } \alpha_0 = -\frac{g_0^T g_0}{g_0^T A g_0}$$

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For  $k \geq 1$  while  $g_k \neq 0$

$$g_k = Ax_k - b \quad (\text{gradient})$$

$$\beta_k = \frac{g_k^T A d_{k-1}}{d_{k-1}^T A d_{k-1}} \quad (\text{correction})$$

$$d_k = -g_k + \beta_k d_{k-1} \quad (\text{direction})$$

$$\alpha_k = -\frac{g_k^T d_k}{d_k^T A d_k} \quad (\text{step size})$$

$$x_{k+1} = x_k + \alpha_k d_k \quad (\text{new guess})$$

Thm A CG for solving  $Ax=b$  ( $A$  spd) then

while  $\mathcal{G}_{k-1} \neq 0$

$$\mathcal{X}_m = \langle x_1, \dots, x_k \rangle = \langle d_0, \dots, d_{k-1} \rangle$$

$$\langle g_0, \dots, g_{k-1} \rangle = \langle b, \dots, A^{k-1}b \rangle$$

$$g_k^T g_j = 0 \quad \forall j < k$$

$$d_k^T A d_j = 0 \quad \forall j < k$$


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The proof is much easier using  
the 1-Matrix-Vector form of CG.

Induct argument, see Trefethen & Bau  
Chap 38

# 1-Matrix-Vector CG

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Init:  $x_0 = 0$  &  $g_0 = -b$  &  $d_0 = g_0$

Iteration:

1)  $\alpha_n = g_{n-1}^T g_{n-1} / d_{n-1}^T A d_{n-1}$  (step size)

2)  $x_n = x_{n-1} + \alpha_n d_{n-1}$  (approx solution)

3)  $g_n = g_{n-1} + \alpha_n A d_{n-1}$  (gradient)

4)  $\beta_n = g_n^T g_n / g_{n-1}^T g_{n-1}$  (improvement)

5)  $d_n = g_n + \beta_n d_{n-1}$  (search direction)

Work per iteration

1-Matrix vector product  $A d_{n-1}$  used in 1) & 3)

2-Dot products  $g_n^T g_n$  &  $d_{n-1}^T A d_{n-1}$

lets try one proof:

Claim:  $g_n = Ax_n - b$

pf Induct on  $n$ ;  $n=0$   $g_0 = -b$  &  $x_0 = 0$  thus  $g_0 = Ax_0 - b$

Assume true for  $n-1$

$$\begin{aligned}
 Ax_n - b &= A(x_{n-1} + \alpha_n d_{n-1}) - b \\
 &= Ax_{n-1} - b + \alpha_n A d_{n-1} \\
 &= g_{n-1} + \alpha_n A d_{n-1} \\
 &= g_n
 \end{aligned}$$

Thm B Let  $A^{m \times m}x = b$ ,  $A$  spd, CG 16

1) While  $\mathcal{E}_{n-1} \neq 0$  then  $x_n$  is unique

point in  $\mathcal{K}_n$  minimizing  $\|\mathcal{E}_n\|_A$

$$(\mathcal{E}_n = \bar{x} - x_n)$$

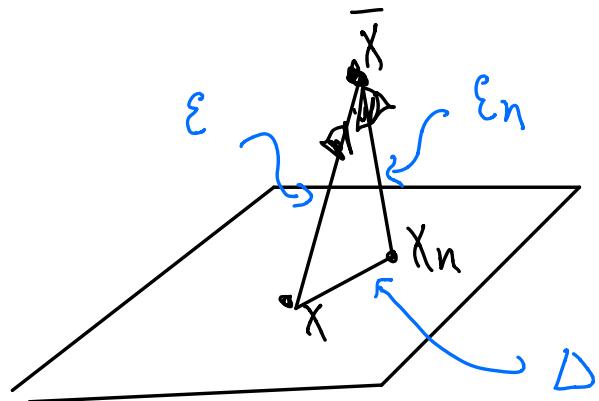
$$2) \|\mathcal{E}_n\|_A \leq \|\mathcal{E}_{n-1}\|_A$$

$$3) \exists n \leq m \text{ st } \mathcal{E}_n = 0$$

Pf 1) By Thm A  $x_n \in \mathcal{K}_n$

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

$$\text{Set } \Delta = x_n - x \quad \& \quad \mathcal{E} = \bar{x} - x = \mathcal{E}_n + \Delta$$



$$\|\mathcal{E}\|_A^2 = (\mathcal{E}_n + \Delta)^T A (\mathcal{E}_n + \Delta) =$$

$$\mathcal{E}_n^T A \mathcal{E}_n + \Delta^T A \Delta + 2 \mathcal{E}_n^T A \Delta$$

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Note:  $A\varepsilon_n = A(\bar{x} - x_n) = b - Ax_n = g_n$

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Thus  $2\varepsilon_n^T A \Delta = 2g_n^T \Delta = 0$  since  $g_n \perp K_n$

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Thus  $\|\varepsilon\|_A^2 = \varepsilon_n^T A \varepsilon_n + \Delta^T A \Delta$

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

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Pf 2  $K_n \subsetneq K_{n+1}$   $\|\varepsilon_n\|_A \geq \|\varepsilon_{n+1}\|_A$

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Pf 3 By (Cayley-Hamilton)

$\exists n \leq m$  st  $\bar{x} \in K_n$




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Polynomials:

Def  $P_n = \{P(z) \mid P(0)=1 \text{ & } \deg(P) \leq n-1\}$

# CG & Polynomial Approx

Prob: Find poly  $P_n$  st  $P_n(0)=1$  &  
 $\deg(P_n) \leq n$  to

$$\text{minimize } \|P_n(A)\|_A$$


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Thm C: While  $\mathcal{I}_{n-1} \neq \mathcal{D}$  for CG

$$\exists! P_n \in \mathcal{P}_{n+1} \text{ s.t.}$$

$$1) \quad \varepsilon_n = \tilde{x} - x_n = P_n(A) \varepsilon_0$$

$$2) \frac{\|\varepsilon_n\|_A}{\|\varepsilon_0\|_A} = \inf_{P \in \mathcal{P}_n} \frac{\|P(A) \varepsilon_0\|_A}{\|\varepsilon_0\|_A}$$

$$\leq \inf_{P \in \mathcal{P}_n} \max_{\lambda \in \lambda(A)} |P(\lambda)|$$

Pf of 1) thm C

By Thm A  $X_n \in \mathcal{H}_n$  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  $P_n(z) = I - z \cdot Q(z)$   $\deg(P_n) \leq n$

Claim  $\varepsilon_n = P_n(A)\varepsilon_0$  where  $\varepsilon_0 = \bar{x}$

$$P_n(A)\varepsilon_0 = (I - A Q_{n-1}(A))\bar{x}$$

$$= \bar{x} - Q_{n-1}(A)(A\bar{x})$$

$$= \bar{x} - Q_{n-1}(A)b$$

$$= \bar{x} - X_n = \varepsilon_n$$

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Pf Thm C 2)

(=) follows from Thm B

( $\Leftarrow$ )  $\varepsilon_0 = \sum a_j v_j$  (eigen expansion of A)  
 $v_i^T v_i = 1$

$$\forall \text{poly } P \quad P(A) \varepsilon_0 = \sum a_j P(\lambda_j) v_j$$

thus

$$\| \varepsilon_0 \|_A^2 = \sum a_j^2 \lambda_j$$

$$\| P(A) \varepsilon_0 \|_A^2 = \sum a_j^2 \lambda_j P(\lambda_j)^2$$

$$\text{thus } \frac{\| P(A) \varepsilon_0 \|_A^2}{\| \varepsilon_0 \|_A^2} = \frac{\sum a_j^2 \lambda_j P(\lambda_j)^2}{\sum a_j^2 \lambda_j}$$

$$\leq \max_{\lambda \in \sigma(A)} |P(\lambda)|^2$$

Thm CG to solve  $Ax=b$ ,  $A$  spd

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

Pf

$$\frac{\|\varepsilon_n\|_A}{\|\varepsilon_0\|_A} \leq \max_{\lambda \in \lambda(A)} |P_n(\lambda)| \leq \max_{\lambda \in \lambda(A)} |P(\lambda)|$$

Any  $P(x)$  st  $\deg(P) \leq n-1$   
 $P(0)=1$

Recall  $m = \lambda_{\min} \leq \lambda(A) \leq \lambda_{\max} = M$  22

$$G_\alpha = (\mathbb{I} - \alpha A) \quad -\gamma \leq \lambda(G) \leq \gamma$$

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

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

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

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

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

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

$$k = M/m$$