Lecture 22:

Recall:

Conjugate gradient method

Goal: Minimize a quadratic functional:

$$\vec{x}_* = \underset{\vec{x} \in \mathbb{R}^n}{\operatorname{argmin}} \varphi(\vec{x}) \quad ; \quad \varphi(\vec{x}) = \frac{1}{2} \vec{x}^T A \vec{x} - \vec{b}^T \vec{x}$$

where A = symmetric positive definite matrix in $M_{n \times n}(\mathbb{R})$ and $\vec{b} \in \mathbb{R}^n$.

Recall: $\nabla \varphi(\vec{x}) = A\vec{x} - \vec{b}$ and $\underbrace{\varphi''(\vec{x})}_{\text{Hessian}} = A$

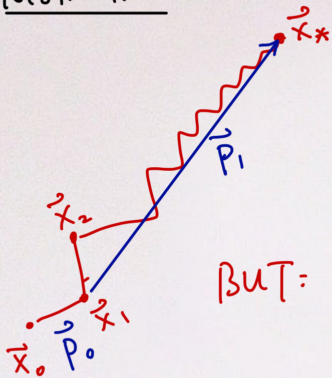
Minimizer $\vec{x}^*$ of $\varphi(\vec{x})$ satisfies $A\vec{x}^* = \vec{b}$ $\quad \left(\frac{\partial^2 \varphi}{\partial x_i \partial x_j}\right)$

Strategy: Given a current approximation $\vec{x}_k$, find a new approximation by:

$$\vec{x}_{k+1} = \vec{x}_k + \alpha_k \vec{p}_k \qquad \left(\begin{array}{l} \vec{p}_k = \text{search direction} \\ \alpha_k = \text{time step} \end{array} \right)$$

But we want to choose: time step α_k to be the optimal and search direction such that $\vec{p}_i \cdot A \vec{p}_j = 0$ for $i \neq j$.

Motivation:



For $A \in M_{2\times 2}(\mathbb{R})$, if $\vec{x}^* =$ sol of $A\vec{x} = \vec{b}$.

Ideally, we want to find $\vec{p}_1$ such that the direction allows us to move directly to $\vec{x}_*$.

$$\therefore \ \vec{p}_1 \parallel \vec{x}^* - \vec{x}_1 \ \Rightarrow \ \vec{p}_1 = c(\vec{x}^* - \vec{x}_1)$$

BUT: $$A\vec{p}_1 = \underset{\substack{\uparrow \\ \mathbb{R}}}{c}\,(\underbrace{A\vec{x}_*}_{\vec{b}} - A\vec{x}_1) = \underset{\substack{\uparrow \\ \mathbb{R}}}{c}\,(\vec{b} - A\vec{x}_1)$$

$$A\vec{p}_1 \cdot \vec{p}_0 = c\,\underbrace{(\vec{b} - A\vec{x}_1)}_{-\nabla\varphi(\vec{x}_1)} \cdot \vec{p}_0 = -c\,\nabla\varphi(\vec{x}_0 + \alpha_0\vec{p}_0)\cdot\vec{p}_0$$
$$= -c\,\frac{d}{d\alpha}\Big|_{\alpha=\alpha_0} \varphi(\vec{x}_0 + \alpha\vec{p}_0) = 0$$

$$\therefore \ A\vec{p}_1 \cdot \vec{p}_0 = 0$$

Get convergence in JUST 2 steps!!

Summary: Find search directions $\vec{p}_j$ $(j=0,1,2,\ldots)$ such that
(Goal:) $\vec{p}_j^{\,T} A \vec{p}_k = 0$ for $j \neq k$ and find optimal time step α_j.

Definition: We say that the set of directions $\{\vec{p}_j\}_{j=0}^{k-1}$ is a conjugate set of directions (with respect to A) if:

$$\vec{p}_j^{\,T} A \vec{p}_i = 0 \quad \text{for all } 1 \leq i, j \leq k-1 \text{ and } i \neq j.$$

Remark: $\because$ A is symmetric

$$\therefore \quad \vec{p}_j^{\,T} A \vec{p}_i = \vec{p}_i^{\,T} A^T \vec{p}_j = \vec{p}_i^{\,T} A \vec{p}_j$$

Notation: $W_k \stackrel{\text{def}}{:=} \operatorname{span}\{\vec{p}_0, \vec{p}_1, \ldots, \vec{p}_{k-1}\}$

Choice of time step α_k (Given $\vec{p}_0, \vec{p}_1, \ldots, \vec{p}_k$)

Optimal α_k:

$$\varphi(\vec{x}_k + \alpha \vec{p}_k) = \varphi(\vec{x}_k) + \alpha \nabla\varphi(\vec{x}_k) \cdot \vec{p}_k + \frac{\alpha^2}{2} \vec{p}_k^{\,T} A \vec{p}_k$$

(Taylor expansion)

Minimum attained at $\alpha = \dfrac{-\nabla\varphi(\vec{x}_k) \cdot \vec{p}_k}{\vec{p}_k^{\,T} A \vec{p}_k}$

$\therefore$ we choose $\boxed{\alpha_k = \dfrac{-\vec{r}_k \cdot \vec{p}_k}{\langle \vec{p}_k, \vec{p}_k \rangle_A}}$

where $\vec{r}_k = A\vec{x}_k - \vec{b}$ and $\langle \vec{u}, \vec{v} \rangle_A \overset{\text{def}}{=} \vec{u} \cdot A\vec{v}$.

Choice of the search directions $\vec{p}_j$ $(j=0,1,2,\ldots)$

Suppose $\vec{p}_0, \vec{p}_1, \ldots, \vec{p}_{k-1}$ are known. Then, we proceed to find the search direction $\vec{p}_k$ in the form:

$$\vec{p}_k = -\vec{r}_k - \beta_{k-1}\vec{p}_{k-1} \quad \text{where } \beta_{k-1} = -\frac{\vec{p}_{k-1}^{\,T} A \vec{r}_k}{\vec{p}_{k-1}^{\,T} A \vec{p}_{k-1}}$$

$$\Rightarrow A\vec{p}_k = -A\vec{r}_k - \beta_{k-1} A\vec{p}_{k-1}$$

$$\Rightarrow \underbrace{\vec{p}_{k-1}^{\,T} A \vec{p}_k}_{=0} = -\vec{p}_{k-1}^{\,T} A \vec{r}_k - \beta_{k-1}\vec{p}_{k-1}^{\,T} A \vec{p}_{k-1}$$

$$\Rightarrow \beta_{k-1} = -\frac{\vec{p}_{k-1}^{\,T} A \vec{r}_k}{\vec{p}_{k-1}^{\,T} A \vec{p}_{k-1}}$$

Conjugate gradient method

(Solve : $A\vec{x} = \vec{b}$)

Given $\vec{x}_0 \in \mathbb{R}^n$, $\vec{p}_0 = -\vec{r}_0 \overset{\text{def}}{=} -(A\vec{x}_0 - \vec{b})$, find $\vec{x}_k$ and $\vec{p}_k$ ($k = 1, 2, \ldots$)

such that :

(a) $\vec{x}_{k+1} = \vec{x}_k + \alpha_k \vec{p}_k$

(b) $\alpha_k = - \dfrac{\vec{r}_k \cdot \vec{p}_k}{\langle \vec{p}_k, \vec{p}_k \rangle_A}$ $\left(= \dfrac{\vec{r}_k \cdot \vec{r}_k}{\langle p_k, p_k \rangle_A} \right)$

$\vec{r}_k = A\vec{x}_k - \vec{b}$

$\langle \vec{u}, \vec{v} \rangle_A = \vec{u} \cdot A\vec{v}$.

(c) $\vec{p}_{k+1} = -\vec{r}_{k+1} - \beta_k \vec{p}_k$

(d) $\beta_k = - \dfrac{\langle \vec{r}_{k+1}, \vec{p}_k \rangle_A}{\langle \vec{p}_k, \vec{p}_k \rangle_A}$ $\left(= - \dfrac{\vec{r}_{k+1} \cdot \vec{r}_{k+1}}{\vec{r}_k \cdot \vec{r}_k} \right)$

(Check)

Iteration converges in less than n iterations.

$(\vec{r}_i \cdot \vec{r}_j = 0 \quad \forall\, i \neq j)$

Example: Consider the linear system: $\underbrace{\begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}}_{A} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \underbrace{\begin{pmatrix} 1 \\ 0 \end{pmatrix}}_{\vec{b}}$.

Exact solution is: $\begin{pmatrix} \frac{2}{3} \\ \frac{1}{3} \end{pmatrix}$.

Start with $\vec{x}_0 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$.

Then:
$$\vec{p}_0 = -\vec{r}_0 = \vec{b} - A\vec{x}_0 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

$$\alpha_0 = \frac{-\vec{r}_0 \cdot \vec{p}_0}{\langle \vec{p}_0, \vec{p}_0 \rangle_A} = \frac{\begin{pmatrix} 1 \\ 0 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix}}{\begin{pmatrix} 1 \\ 0 \end{pmatrix} \cdot A \begin{pmatrix} 1 \\ 0 \end{pmatrix}} = \frac{1}{2} \quad \text{(optimal step size)}$$

$$\vec{x}_1 = \vec{x}_0 + \alpha_0 \vec{p}_0 = \begin{pmatrix} 0 \\ 0 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix}$$

$$\vec{r}_1 = A\vec{x}_1 - \vec{b} = \begin{pmatrix} 0 \\ -\frac{1}{2} \end{pmatrix}.$$

$$\beta_0 = -\frac{\langle \vec{r}_1, \vec{p}_0 \rangle_A}{\langle \vec{p}_0, \vec{p}_0 \rangle_A} = -\frac{1}{4}.$$

$$\vec{p}_1 = -\vec{r}_1 - \beta_0 \vec{p}_0 = \begin{pmatrix} \frac{1}{4} \\ 1/3 \end{pmatrix}$$

Second step: With $\vec{x}_1 = \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix}$, $\vec{p}_1 = \begin{pmatrix} \frac{1}{4} \\ \frac{1}{2} \end{pmatrix}$,

$$\alpha_1 = -\frac{\vec{r}_1 \cdot \vec{p}_1}{\langle \vec{p}_1, \vec{p}_1 \rangle_A} = \frac{2}{3}$$ (Optimal step size)

$$\vec{x}_2 = \vec{x}_1 + \alpha_1 \vec{p}_1 = \begin{pmatrix} \frac{2}{3} \\ \frac{1}{3} \end{pmatrix}.$$

$$\vec{r}_2 = A\vec{x}_2 - \vec{b} = \vec{0}$$ (exact solution).

Remark: For 2×2 linear system, conjugate gradient method converges in 2 iterations

For $n \times n$ linear system, conjugate gradient method converges in at most n iterations (usually faster!!)

Next: We need to show: with the above recursive scheme to obtain $\{\vec{p}_j\}_{j=0}^{\infty}$;

(i) $\{\vec{p}_j\}$ are conjugate to each others.

(ii) $\vec{r}_i \cdot \vec{r}_j = 0$ for $i \neq j$.

$(\vec{r}_i = A\vec{x}_i - \vec{b})$

If the above are true, then we have:

Theorem: Consider the iterative scheme:

$$\vec{x}_{k+1} = \vec{x}_k + \alpha_k \vec{p}_k \quad (k = 0, 1, 2, \ldots)$$

Suppose $\{\vec{r}_k\}_{k=0}^{\infty}$ are orthogonal to each others $(\vec{r}_i \cdot \vec{r}_j = 0$ for $i \neq j)$

Then, the iterative scheme converges to the sol $A\vec{x} = \vec{b}$ in less than or equal to n iterations.

Proof: Suppose $\vec{r}_0, \vec{r}_1, \dots, \vec{r}_n$ are all non-zero.

Then: $\{\vec{r}_0, \dots, \vec{r}_n\}$ form an orthogonal $\quad (\vec{r}_i \overset{\text{def}}{=} A\vec{x}_i - \vec{b})$

and lin. independent set in $\mathbb{R}^n$. Contradiction.

with $n+1$ elements

$\therefore \quad \vec{r}_i = 0$ for some $i \leq n$.

$\therefore \quad A\vec{x}_i - \vec{b} = \vec{0}$ for some $i \leq n$.

$\therefore \quad \vec{x}_i$ = sol of $A\vec{x} = \vec{b}$ for some $i \leq n$.

Theorem: In the conjugate gradient method,

(i) $\vec{r}_i \cdot \vec{r}_j = 0$ for $i \neq j$

(ii) $\langle \vec{p}_i, \vec{p}_j \rangle_A \overset{def}{=} \vec{p}_i \cdot A\vec{p}_j = 0$ for $i \neq j$.

Lemma: $\text{Span}\{\vec{p}_0, \dots, \vec{p}_{k-1}\} = \text{Span}\{\vec{r}_0, \dots, \vec{r}_{k-1}\}$

$= \text{span}\{\vec{r}_0, A\vec{r}_0, \dots, A^{k-1}\vec{r}_0\}$

Proof: (i) and (ii) are true for $i, j \leq 1$

($\vec{r}_0 \cdot \vec{r}_1 = 0$ because $0 = \frac{d}{d\alpha}\Big|_{\alpha=\alpha_0} \varphi(\vec{x}_0 + \alpha \underset{\substack{\| \\ -\vec{r}_0}}{\vec{p}_0}) = \underbrace{\nabla\varphi(\overbrace{\vec{x}_0 + \alpha_0\vec{p}_0}^{\vec{x}_1})}_{\substack{(A\vec{x}_1 - \vec{b}) \\ \| \\ \vec{r}_1}} \cdot \underbrace{\vec{p}_0}_{\substack{\| \\ -\vec{r}_0}}$

$\langle \vec{p}_1, \vec{p}_0 \rangle_A = 0$ follows from the definition)

Suppose the statement is true for $i, j \le k$. For $k+1$,

$\because$ $\text{Span}\{\vec{p}_0, \dots, \vec{p}_j\} = \text{Span}\{\vec{r}_0, \dots, \vec{r}_j\}$

$\therefore$ we get $\vec{r}_k \cdot \vec{p}_j = 0$ for $j = 0, 1, 2, \dots, k-1$ (By induction hypothesis)

$\vec{p}_j \in \text{Span}\{\vec{r}_0, \dots, \vec{r}_j\}$

Now, $\vec{r}_{k+1} = \vec{r}_k + \alpha_k A\vec{p}_k$

$$\left(\because A\vec{x}_{k+1} - \vec{b} = A\vec{x}_k - \vec{b} + \alpha_k A\vec{p}_k \right)$$

$$\Rightarrow \vec{r}_{k+1} \cdot \vec{p}_j = \cancelto{0}{\vec{r}_k \cdot \vec{p}_j} + \alpha_k \cancelto{0 \text{ (induction hypothesis)}}{\overbrace{A\vec{p}_k \cdot \vec{p}_j}^{\langle \vec{p}_k, \vec{p}_j \rangle_A}} = 0 \quad \text{for } j = 0, 1, 2, \dots, k-1$$

Also,

$$0 = \frac{d}{d\alpha}\bigg|_{\alpha=\alpha_0} \varphi(\vec{x}_k + \alpha\vec{p}_k) = \underbrace{\nabla\varphi(\overbrace{\vec{x}_k + \alpha\vec{p}_k}^{\vec{x}_{k+1}})}_{A\vec{x}_{k+1} - \vec{b} \,=\, \vec{r}_{k+1}} \cdot \vec{p}_k$$

All together, we get $\vec{r}_{k+1} \cdot \vec{p}_j = 0$ for $j = 0, 1, 2, \ldots, k$

$\because$ $\mathrm{Span}\{\vec{p}_0, \ldots, \vec{p}_k\} = \mathrm{Span}\{\vec{r}_0, \ldots, \vec{r}_k\}$

$\therefore$ $\vec{r}_{k+1} \cdot \vec{r}_j = 0$ for $j = 0, 1, 2, \ldots, k$

$\therefore$ (i) is true for the case $k+1$.

To show (ii) for the case $k+1$ (given the induction hypothesis),

note that: $\vec{r}_{j+1} = \vec{r}_j + \alpha_j A \vec{p}_j \Rightarrow A\vec{p}_j \in \mathrm{Span}\{\vec{r}_j, \vec{r}_{j+1}\}$

$$\therefore \quad \vec{r}_{k+1} \cdot \underbrace{A\vec{p}_j}_{\in\, \mathrm{Span}\{\vec{r}_j,\, \vec{r}_{j+1}\}} = \langle \vec{r}_{k+1}, \vec{p}_j \rangle_A = 0 \quad \text{for } j = 0, 1, 2, \ldots, k-1$$

Now, $\vec{p}_{k+1} \cdot A\vec{p}_j = -\cancelto{0}{\vec{r}_{k+1} \cdot A\vec{p}_j} - \beta_k \cancelto{0}{\vec{p}_k \cdot A\vec{p}_j}$

$\parallel$

$\langle \vec{p}_{k+1}, \vec{p}_j \rangle_A = 0$ for $j = 0, 1, 2, \dots, k-1$

Also, $\langle \vec{p}_{k+1}, \vec{p}_k \rangle_A = 0$ by definition.

$\therefore \langle \vec{p}_{k+1}, \vec{p}_j \rangle_A = 0$ for $j = 0, 1, 2, \dots, k$

$\therefore \langle \vec{p}_i, \vec{p}_j \rangle_A = 0$ for $i, j \le k+1$.

By M.I., the theorem is generally true!!