Conjugate Gradients I: Setup

CS 205A:
Mathematical Methods for Robotics, Vision, and Graphics

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Time for Gaussian Elimination

$$A \in \mathbb{R}^{n \times n} \implies$$

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$$A \in \mathbb{R}^{n \times n} \implies O(n^3)$$

Common Case

"Easy to apply, hard to invert."

- Sparse matrices
- Special structure

New Philosophy

Iteratively improve approximation rather than solve in closed form.

For Today

$$A\vec{x} = \vec{b}$$

- Square
- Symmetric
- Positive definite

Variational Viewpoint

$$A\vec{x} = \vec{b}$$

$$\Updownarrow$$

$$\min_{\vec{x}} \left[\frac{1}{2}\vec{x}^\top A\vec{x} - \vec{b}^\top \vec{x} + c\right]$$

Gradient Descent Strategy

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2. Do line search to find

$$\vec{x}_k \equiv \vec{x}_{k-1} + \alpha_k \vec{d}_k.$$

Line Search Along $\vec{d}$ from $\vec{x}$

$$\min_{\alpha} g(\alpha) \equiv f(\vec{x} + \alpha \vec{d})$$

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$$\min_{\alpha} g(\alpha) \equiv f(\vec{x} + \alpha \vec{d})$$

$$\alpha = \frac{\vec{d}^\top (\vec{b} - A\vec{x})}{\vec{d}^\top A \vec{d}}$$

Gradient Descent with Closed-Form Line Search

$$\vec{d}_k = \vec{b} - A\vec{x}_{k-1}$$

$$\alpha_k = \frac{\vec{d}_k^\top \vec{d}_k}{\vec{d}_k^\top A \vec{d}_k}$$

$$\vec{x}_k = \vec{x}_{k-1} + \alpha_k \vec{d}_k$$

Convergence

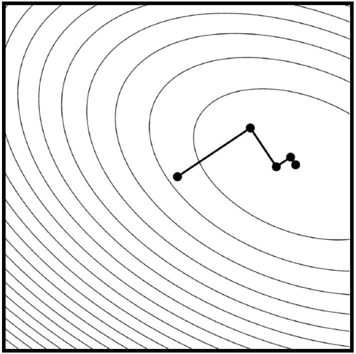
See book.

$$\frac{f(\vec{x}_k) - f(\vec{x}^*)}{f(\vec{x}_{k-1}) - f(\vec{x}^*)} \leq 1 - \frac{1}{\operatorname{cond} A}$$

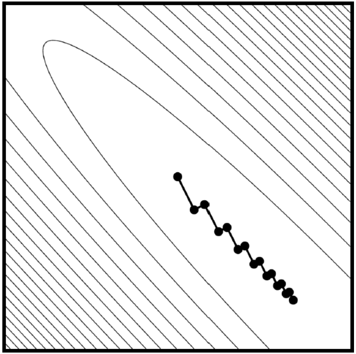
Conclusions:

- Conditioning affects speed *and* quality
- Unconditional convergence $(\operatorname{cond} A \geq 1)$

Visualization



Well conditioned A



Poorly conditioned A

Can We Do Better?

- **Can iterate forever:**
  Should stop after $O(n)$ iterations!
- **Lots of repeated work**
  when poorly conditioned

Observation

$$f(\vec{x}) = \frac{1}{2}(\vec{x} - \vec{x}^*)^\top A(\vec{x} - \vec{x}^*) + \text{const.}$$

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$$\implies f(\vec{x}) = \frac{1}{2}\|L^\top(\vec{x} - \vec{x}^*)\|_2^2 + \text{const.}$$

Substitution

$$\vec{y} \equiv L^\top \vec{x}, \vec{y}^* \equiv L^\top \vec{x}^*$$
$$\implies \bar{f}(\vec{y}) = \|\vec{y} - \vec{y}^*\|_2^2$$

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Proposition

Suppose $\{\vec{w}_1, \ldots, \vec{w}_n\}$ are orthogonal in $\mathbb{R}^n$. Then, $\bar{f}$ is minimized in at most n steps by line searching in direction $\vec{w}_1$, then direction $\vec{w}_2$, and so on.

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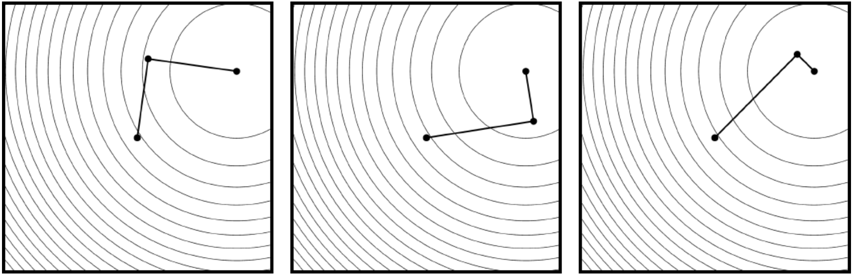

Any two orthogonal directions suffice!

Undoing Change of Coordinates

Line search on $\bar{f}$ along $\vec{w}$ is the same as line search on f along $(L^\top)^{-1}\vec{w}$.

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$$\begin{aligned} 0 = \vec{w}_i \cdot \vec{w}_j &= (L^\top \vec{v}_i)^\top (L^\top \vec{v}_j) \\ &= \vec{v}_i^\top (LL^\top) \vec{v}_j = \vec{v}_i^\top A \vec{v}_j \end{aligned}$$

Conjugate Directions

A-Conjugate Vectors

Two vectors $\vec{v}$ and $\vec{w}$ are A-conjugate if $\vec{v}^\top A\vec{w} = 0$.

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Corollary

Suppose $\{\vec{v}_1, \ldots, \vec{v}_n\}$ are A-conjugate. Then, f is minimized in at most n steps by line searching in direction $\vec{v}_1$, then direction $\vec{v}_2$, and so on.

High-Level Ideas So Far

- Steepest descent may not be fastest descent (surprising!)

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- Two inner products:

$$\vec{v} \cdot \vec{w}$$

$$\langle \vec{v}, \vec{w} \rangle_A \equiv \vec{v}^\top A \vec{w}$$

New Problem

Find n

A-conjugate directions.

Gram-Schmidt?

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- Potentially unstable

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- Storage increases with each iteration

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

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When performing gradient descent on f, $\operatorname{span}\{\vec{r}_0, \ldots, \vec{r}_k\} = \operatorname{span}\{\vec{r}_0, A\vec{r}_0, \ldots, A^k\vec{r}_0\}$.

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Krylov space?!

Gradient Descent: Issue

$$\vec{x}_k - \vec{x}_0 \neq \underset{\vec{v} \in \text{span}\{\vec{r}_0, A\vec{r}_0, \ldots, A^{k-1}\vec{r}_0\}}{\arg\min} f(\vec{x}_0 + \vec{v})$$

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But if this did hold...

Convergence in n steps!

Next