§5. The Conjugate Gradient method

Iterative solver for symm pos def systems

$Ax = b \qquad A \in \mathbb{R}^{n \times n}$ symm pos def

$$\Leftrightarrow \quad \min_{x \in \mathbb{R}^n} \frac{1}{2} x^T A x - x^T b = f(x)$$

$$\nabla f(x) = Ax - b$$
$$\nabla^2 f(x) = A$$

Gradient method:

$$x_{k+1} = x_k - \alpha_k \nabla f_k$$

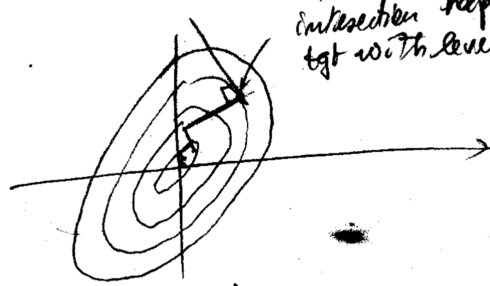
where α_k solves $\min_\alpha \varphi(\alpha) = f(x_k - \alpha \nabla f_k)$ i.e.:

$$\varphi'(\alpha) = -\nabla f(x_k - \alpha \nabla f_k)^T \nabla f_k$$
$$= -\nabla f_k^T A (x_k - \alpha \nabla f_k) + \nabla f_k^T b$$
$$= -\|\nabla f_k\|^2 + \alpha \nabla f_k^T A \nabla f_k$$

$$\varphi''(\alpha) > 0 \quad \leadsto \quad \boxed{\alpha_k = \frac{\|\nabla f_k\|^2}{\nabla f_k^T A \nabla f_k}}$$

Possible to show $\nabla f_k^T \nabla f_{k+1} = 0$. Method can take long to converge

"Zigg-zagging" 2D:



The linear conjugate gradient method

$x_{k+1} = x_k + \alpha_k p_k$, where α_k p_k is determined s.t.

x_{k+1} solves

$$\min_{x \in x_0 + \operatorname{span}\{p_0, \dots, p_{k-1}, r_k\}} \frac{1}{2} x^T A x - b^T x \qquad (1)$$

where $r_k = -\nabla f_k = b - Ax_k$

$(1) \Leftrightarrow (2) \quad \min \frac{1}{2}\hat{x}^T A \hat{x} - \hat{x}^T r_0$

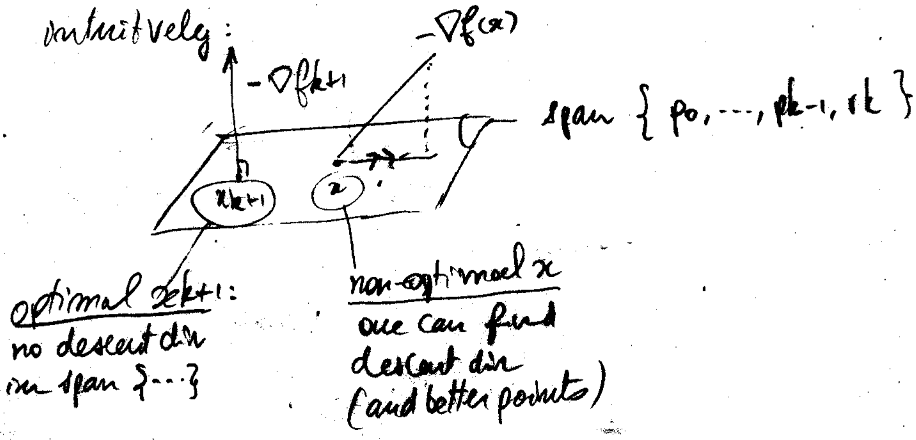
$\hat{x} \in \mathrm{span}\{p_0, \dots, p_{k-1}, r_k\}$ where $\hat{x} = x - x_0$

It can be shown that $\hat{x}_{k+1}$ solves (2) iff

$$(A\hat{x}_{k+1} - r_0)^T v = 0 \quad \forall v \in \mathrm{span}\{p_0, \dots, p_{k-1}, r_k\}.$$

$$\Leftrightarrow \quad (\underbrace{A x_{k+1} - b}_{-\nabla f_{k+1}})^T v = 0$$

($\sim$ Galerkin)



In previous step: $\hat{x}_k$ solves:

$$\min \frac{1}{2}\hat{x}^T A \hat{x} - \hat{x}^T r_0 \qquad \Rightarrow p_j^T (b - A x_k) = 0$$
$$\hat{x} \in \mathrm{span}\{p_0, \dots, p_{k-1}\} \qquad j = 0 \dots k-1$$

Since $x_{k+1} = x_k + \alpha_k p_k$:

$$0 = (A x_{k+1} - b)^T p_j = \overset{0}{\cancel{(A x_k - b)^T p_j}} + \alpha_k p_k^T A p_j$$

$\Rightarrow p_k$ is A-orthogonal (w.r.t. inner prod $(u,v)_A = u^T A v$) to previous k directions

$\rightsquigarrow$ get p_k using Gram-Schmidt orthogonalization, which will greatly simplify:

$$\begin{cases} p_0 = r_0 \\ \vdots \\ p_k = r_k - \displaystyle\sum_{j=0}^{k-1} \frac{r_k^T A p_j}{p_j^T A p_j} p_j \end{cases} \qquad \text{(GS)}$$

Now that we know in which direction to go, we can use gradient method to find

$$\boxed{\alpha_k = \arg\min_{\alpha} \phi(\alpha) = f(x_k + \alpha\, p_k) = \frac{r_k^T p_k}{p_k^T A p_k}}$$

problem w/ this preliminary version: # of operations grows linearly, storage } with iter

A closer look to the subspace used gives:

$$\begin{aligned} \text{span}\{p_0, \dots p_{k-1}, r_k\} &= \text{span}\{p_0, \dots p_{k-1}, p_k\} \\ &= \text{span}\{r_0, \dots, r_k\} \\ &= \mathcal{K}_{k+1}(A, r_0) \\ &:= \text{span}\{r_0, Ar_0, A^2 r_0, \dots, A^k r_0\} \\ &= \text{Krylov subspace} \end{aligned}$$

<u>why?</u>

$$r_0 = b - Ax_0 \in \mathcal{K}_1(A, r_0)$$

$$r_1 = b - Ax_1 = b - A(x_0 + \alpha(b - Ax_0)) \in \mathcal{K}_2(A, r_0)$$

etc...

<u>Why is this useful?</u>

optimality conditions:

$$r_{k+1}^T v = 0 \quad \forall v \in \mathcal{K}_{k+1}(A, r_0)$$

$$r_k^T v = 0 \quad \forall v \in \mathcal{K}_k(A, r_0)$$

take $p_i \in \mathcal{K}_{k-1}(A, r_0) \Rightarrow Ap_i \in \mathcal{K}_k(A, r_0)$

$$\Rightarrow r_k^T A p_i = 0 \quad i = 0 \dots k-2$$

thus (GS) reduces to:

$$p_k = r_k - \underbrace{\boxed{\frac{r_k^T A p_{k-1}}{p_{k-1}^T A p_{k-1}}}}_{= \beta_k} p_{k-1}$$

<u>Storage</u>: x_k, r_k, p_k, Ap_k

requires only knowledge of matrix-vector product

Can show:

$$\alpha_k = \frac{\|r_k\|^2}{p_k^T A p_k}$$

$$\beta_k = \frac{\|r_{k+1}\|^2}{\|r_k\|^2}$$

→ classical CG formulation (saves some MV prod)
see Algo 5.2 p 112.

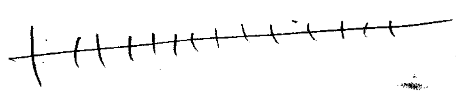
What happens if A is indefinite? ⇒ $\min x^T A x - x^T b$ has no sol

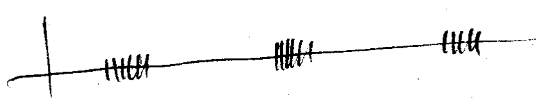
→ $\exists k$ for which $p_k^T A p_k < 0$

→ "negative curvature" direction → stop iterations

<u>Convergence results</u>: convergence properties determined by eigenvalues of A.

the fewer "clusters" the better

(S1)  many iterations

(S2)  few (~ 3) iterations.

<u>preconditioning</u> $Ax = b \Leftrightarrow MAx = Mb$

M = preconditioner
easy to compute
and somehow transforms
spectrum of A from
(S1) to (S2).