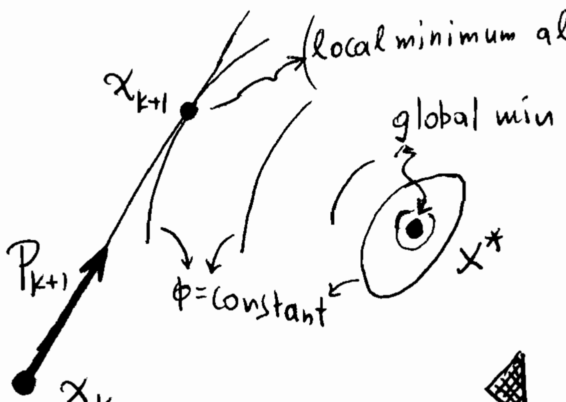
Solving $Ax=b$, A spd, by gradient methods:

» Conjugate Gradients «

⟨1.⟩ Solution of $Ax=b$ minimizes $\phi(x) = \frac{1}{2}x^TAx - x^Tb$ (1)

◀ Indeed, if $\bar{x} = x^* + d$ with $Ax^* = b$, A symmetric, positive definite (spd): $\phi(\bar{x}) = \phi(x) + \frac{1}{2}d^TAd \geq \phi(x)$ since $d^TAd > 0$ if $d \neq \underline{0}$ $\left[= \frac{1}{2}(x^*+d)^TA(x^*+d) - (x^*+d)^Tb = ?\right]$ ▶



⟨2.⟩ Let $x_k \in \mathbb{R}^n$; given direction p_{k+1}, choose α so x_{k+1} is at the minimum of ϕ along that direction.

◀ $x_{k+1} = x_k + \alpha p_{k+1}$: $\alpha = \dfrac{p_{k+1}^T r_k}{p_{k+1}^T A p_{k+1}}$ (2)

Def: Residual ($r(x) = b - Ax$)
$r_k = b - Ax_k$

For min: $0 = \left.\dfrac{\partial \phi}{\partial \alpha}\right|_{x_{k+1}} =$

$$= \frac{\partial}{\partial \alpha}\left\{\frac{1}{2}(x_k^T + \alpha p_{k+1}^T)A(x_k + \alpha p_{k+1}) - (x_k + \alpha p_{k+1})^T b\right\}$$

$$= \frac{\partial}{\partial \alpha}\left\{\frac{1}{2}\alpha^2 p_{k+1}^TAp_{k+1} + \alpha(p_{k+1}^TAx_k - p_{k+1}^Tb) - x_k^Tb\right\}$$

$$= p_{k+1}^T\{\alpha A p_{k+1} - r_k\} = 0$$ for minimum ((2) follows) (3) ▶

This suggests an algorithm for successive approximation of the solution:

* Step k: (given x_k (approx. solution); p_{k+1} (search direction))

$r_k = b - Ax_k$; $\alpha_{k+1} = p_{k+1}^T r_k / p_{k+1}^T A p_{k+1}$

$x_{k+1} = x_k + \alpha_{k+1} p_{k+1}$ [New search direction p_{k+2} ?]

How do we choose p_k ?

Two basic strategies for choosing p_k:
(i) Steepest descent, (ii) $\xrightarrow{A-}$ Conjugate directions

(i) <u>Steepest descent</u>: $p_{k+1} := -\nabla\phi|_{x_k} = b - Ax_k = r_k$

<u>Algorithm</u>: given x_0; $r_0 = b - Ax_0$
for $k=0,\ldots$ $\quad \alpha_{k+1} = r_k^T r_k / r_k^T A r_k \quad (p_{k+1} = r_k)^*$
$\quad x_{k+1} = x_k + \alpha_{k+1} r_k$
$\quad r_{k+1} = b - Ax_{k+1} = r_k - \alpha_{k+1} A r_k$
end

(*) This choice defines the method. It leads to steepest descent minimization which can be very slow if A is ill-conditioned.

Convergence: Let $AQ = Q\Lambda$, write $r_k = Qs_k$. Then we have $\sum_{i=1}^{n}(1-\alpha_{k+1}\lambda_i)s_{k,i}^2 = 0$ (4)

$$\alpha_{k+1} = r_k^T r_k / r_k^T A r_k = s_k^T Q^T Q s_k / s_k^T Q^T A Q s_k = s_k^T s_k / s_k^T \Lambda s_k$$

<u>Corollary</u>: $1/\lambda_{max} \le \alpha_{k+1} \le 1/\lambda_{min}$ (say $\lambda_{max} = \lambda_1$; $\lambda_{min} = \lambda_n$). (5)

Substituting r_k in expression for r_{k+1}:
$$Qs_{k+1} = r_{k+1} = (I - \alpha_{k+1}A)Qs_k \Rightarrow \boxed{s_{k+1} = (I - \alpha_{k+1}\Lambda)s_k} \quad (6)$$

The i-th evector component of the residual, $s_{k,i}$, is multiplied by the factor $(1-\lambda_i\alpha_{k+1})$ to produce $s_{k+1,i}$.
Since (5) $1/\lambda_1 \le \alpha_{k+1} \le 1/\lambda_n$ it follows that $s_{k,1}$ and $s_{k,n}$ have largest negative & positive factors, respectively.

∴ Extreme **eigenvector components** govern **convergence**.

(ii) Conjugete directions: choose p_k (linearly independent) so that x_k minimizes $\phi(x)$ in $[p_0, p_1, \ldots, p_k]$. If this possible, then will get solution at n-th step (if exact arithmetic). Thus, want to choose set p_k so that solution to

$$\min_{\alpha} \phi(x_k + \alpha p_{k+1})$$

also gives $\min\limits_{\substack{x \in [p_1, \ldots, p_{k+1}] \\ \hookrightarrow (k+1)}} \phi(x)$. Now let $x = [p_0, \ldots, p_k]$

$$\Rightarrow x = P_{k-1} y + \alpha p_k \quad (P_{k-1}^{n \times (k-1)})$$

Then

$$\phi(x) = \frac{1}{2}\left[y^T P_{k-1}^T A P_{k-1} y + \alpha^2 p_k^T A p_k + 2\alpha y^T P_{k-1}^T A p_k \right]$$
$$- y^T P_{k-1}^T b - \alpha p_k^T b$$
$$= \phi(P_{k-1} y) + \alpha y^T \{P_{k-1}^T A p_k\} + \underbrace{\frac{\alpha^2}{2} p_k^T A p_k - \alpha p_k^T b}_{\phi(\alpha p_k)}$$

Hestenes & Stiefel (1952): Let $p_i A p_j = 0, \; i \neq j$. $\quad (7)^*$

Then two separate minimizations!

(i) Let $P_{k-1} y = X_{k-1}$ minimizer over $[p_1, \ldots, p_{k-1}]$

(ii) $\alpha = \alpha_k = p_k^T r_{k-1} / p_k^T A p_k$

$\therefore$ Must ensure $p_k^T A p_\ell = 0, \; k \neq \ell$; $p_k^T r_{k-1} \neq 0$.

(*) Condition (7) is the A-conjugacy condition that defines the method (still needs a unique specification!)

Since we are building the p_j "from scratch", we need to specify the space they are chosen from. Once that is fixed, the p_j are an A-orthogonal basis. It turns out that $[r_0, \ldots, r_{k-1}]$ is a reasonable choice. Then, selecting $p_{k+1} = r_k + \beta p_k$, turns that space into a Krylov space, $\mathcal{K}_n = [r_0, \ldots, r_{k-1}]$. Here is why:

Theorem: A spd, $r_k \neq 0$; let $p_0 = 0$. Then the recurrence $$p_{k+1} = r_k + \beta p_k, \quad k \geq 0 \qquad (8)$$ with $\beta \equiv \beta_{k+1}$ chosen so that $p_{k+1}^T A p_k = 0$ gives sequences $\{r_0, \dots, r_k, r_{k+1}, \dots\}$, $\{p_0, \dots, p_k, p_{k+1}, \dots\}$ $\{x_0, \dots, x_k, x_{k+1}\}$ that satisfy

(i) $p_k \in \mathcal{K}_k$ and $r_k \in \mathcal{K}_{k+1}$

where $\mathcal{K}_k = [r_0, \dots, r_{k-1}]$ is the Krylov space of r_0.

(ii) $p_{k+1}^T A \xi = 0, \ \forall \xi \in \mathcal{K}_k \qquad (p_{k+1} \perp_A \mathcal{K}_k)$

(iii) $r_k^T \xi = 0, \ \forall \xi \in \mathcal{K}_k \qquad (r_k \perp \mathcal{K}_k)$

We have the following defining equations for the sequences $\{p_k\}_0^{n}$, $\{r_k\}_0^n$:

$$\begin{cases} p_0 = 0; \ x_0 \text{ arbitrary} \\ r_0 = b - A x_0 \end{cases}$$

for $k = 0, 1, \dots$: $p_{k+1} = r_k + \beta_{k+1} p_{k+1}$; ($\beta_{k+1}$ chosen to impose $p_{k+1}^T A p_k = 0$)

$r_{k+1} = r_k - \alpha_{k+1} A p_{k+1}$ $\qquad x_{k+1} = x_k + \alpha_{k+1} p_{k+1}$ where

$\alpha_{k+1} = p_{k+1}^T r_k / p_{k+1}^T A p_{k+1}$

(i) induction assumption: $p_{k-1} \in \mathcal{K}_{k-1}$; $r_k \in \mathcal{K}_{k+1}$; $\mathcal{K}_{k-1} \subset \mathcal{K}_k$

Then $p_{k+1} = r_k + \beta p_k \in \mathcal{K}_{k+1}$ while, since $\mathcal{K}_k$ is the k-th order Krylov space of r_0, then $A\mathcal{K}_k \subset \mathcal{K}_{k+1}$ and if

$p_{k+1} \in \mathcal{K}_{k+1} \Rightarrow A p_{k+1} \in \mathcal{K}_{k+2}$ i.e. $r_{k+1} = r_k - \alpha A p_{k+1} \in \mathcal{K}_{k+2}$

(ii) & (iii) Now the induction assumption is that

$$\left.\begin{array}{l} p_{\ell+1}^T A \xi = 0, \ \forall \xi \in \mathcal{K}_\ell \\ r_\ell^T \xi = 0, \ \forall \xi \in \mathcal{K}_\ell \end{array}\right\} \ \ell = 1, \dots, k-1;$$

We will show it is true for $\ell = k$

To show $p_{k+1}^T A \xi = 0, \; \xi \in \mathcal{K}_k$ we can show that

$p_{k+1}^T A r_\ell = 0, \; \ell = 0, \ldots, k-1$ (since by assumption the r_ℓ are mutually orthogonal and, so, independent

that is $\mathcal{K}_k = [r_0, \ldots, r_{k-1}]$ (9)

Now $p_{k+1}^T A r_\ell = r_k^T A r_\ell + \beta_{k+1} p_k^T A r_\ell$

(a) For $\ell \leq k-2$: $r_\ell \in \mathcal{K}_{\ell+1} \subset \mathcal{K}_{k-1}$

But $p_k \perp_A \mathcal{K}_{k-1} = [r_0, \ldots, r_{k-2}] \Rightarrow p_k^T A r_\ell = 0$

and $r_\ell \in \mathcal{K}_{k-1} \Rightarrow A r_\ell \in \mathcal{K}_k \perp r_k \Rightarrow r_k (A r_\ell) = 0$

$\Rightarrow p_{k+1}^T A r_\ell = 0, \quad \ell \leq k-2$

(b) We may choose β_{k+1} to make $p_{k+1}^T A r_{k-1} = 0$: this gives

$$0 = r_k^T A r_{k-1} + \beta_{k+1} p_k^T A r_{k-1} \Rightarrow \beta_{k+1} = -\frac{r_k^T A r_{k-1}}{p_k^T A r_{k-1}} \quad (10)$$

(11)

This establishes: $p_{k+1}^T A \xi = 0, \; \xi \in \mathcal{K}_k$

In particular, then: $p_{k+1}^T A p_k = 0$ since $p_k \in \mathcal{K}_k$

(as well as $p_{k+1}^T A p_\ell = 0, \; \ell = 0, \ldots, k$)

Similarly, for the residual

$$r_{k+1} = r_k - \alpha_{k+1} A p_{k+1}$$

(a) $r_{k+1}^T r_\ell = r_k^T r_\ell - \alpha_{k+1} p_{k+1}^T A r_\ell \; ; \; \ell = 0, \ldots, k-1$

$$\left.\begin{aligned} &\text{But } r_k^T r_\ell = 0 \text{ by assumption} \\ &p_{k+1}^T A r_\ell = 0 \text{ by above discussion (11)} \end{aligned}\right\} r_{k+1}^T r_\ell = 0 \quad (12)$$

Since $\mathcal{K}_k = \text{span}[r_0, \ldots, r_{k-1}]$, see above (9), i.e. $r_{k+1}^T \xi = 0$
$\forall \xi \in \mathcal{K}_k$.

Efficient Formulation: (minimize computation)

Lemma: $r_k \neq 0$, A spd. Then

$$\alpha_{k+1} = \|r_k\|_2^2 / \|p_{k+1}\|_A^2 \; ; \quad \beta_{k+1} = \frac{\|r_k\|_2^2}{\|r_{k-1}\|_2^2}$$

Use: $p_{k+1} = r_k + \beta_{k+1} p_k$; $r_{k+1} = r_k - \alpha_{k+1} A p_{k+1}$

So: $p_k^T A p_k = p_k^T A (r_{k-1} + \beta_k \underbrace{\cancel{p_{k-1}}}_{=0 \text{ (A-conjugacy)}}) = p_k^T A r_{k-1}$ (13)

$$p_k^T r_k = (r_{k-1}^T + \beta_k p_{k-1}^T) r_k = \underbrace{r_{k-1}^T r_k}_{=0} + \beta_k \underbrace{p_{k-1}^T r_k}_{=0} = 0 \quad (14)$$

$r_k \perp \mathcal{K}_k \supset \mathcal{K}_{k-1}$

$$p_{k+1}^T r_k = (r_k^T + \beta_{k+1} p_k^T) r_k = r_k^T r_k + \beta_{k+1} \cancel{p_k^T r_k} = \|r_k\|_2^2 \quad (15)$$

Then $$\alpha_{k+1} = \frac{p_{k+1}^T r_k}{p_{k+1}^T A p_{k+1}} \overset{\text{by (15)}}{=} \frac{\|r_k\|_2^2}{\|p_{k+1}\|_A^2} \quad (16)$$

Also $$r_k^T A r_{k-1} = r_k^T A (p_k - \beta_k p_{k-1}) = r_k^T A p_k = p_k^T A r_k \quad (17)$$

$$\left.\begin{aligned} (13) &\Rightarrow p_k^T A r_{k-1} = p_k^T A p_k = \|p_k\|_A^2 \overset{\text{by (16)}}{=} \|r_{k-1}\|_2^2 / \alpha_k \\ (17) &\Rightarrow r_k^T A r_{k-1} = r_k^T A p_k \\ &\|r_k\|^2 = r_k^T (r_{k-1} - \alpha_k A p_k) = -\alpha_k r_k^T A p_k \end{aligned}\right\} \Rightarrow r_k^T A r_{k-1} = -\frac{\|r_k\|^2}{\alpha_k}$$

So: $$\beta_{k+1} = -\frac{r_k A r_{k-1}}{p_k^T A r_{k-1}} = \frac{\|r_k\|_2^2}{\|r_{k-1}\|_2^2} \quad (18)$$

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x_0 arbitrary $r_0 = b - A x_0$ $p_0 = 0$ $p_1 = r_0$ $\alpha_1 = \|r_0\|_2^2 / \|r_0\|_A^2$	~~for k = 1, ...~~ $x_1 = x_0 + \alpha_1 p_1$ $r_1 = b - A x_1$	for $k = 2, \ldots$ $\beta_{k+1} = \|r_k\|_2^2 / \|r_{k-1}\|_2^2$ $p_{k+1} = r_k + \beta_{k+1} p_k$ $\alpha_{k+1} = \|r_k\|_2^2 / \|p_{k+1}\|_A^2$ $x_{k+1} = x_k + \alpha_{k+1} p_{k+1}$	$r_{k+1} = r_k - \beta_{k+1} A p_{k+1}$ or $r_{k+1} = b - A x_{k+1}$