2130711 0161 林子开

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1. Suppose that $A \in \mathbb{R}^{n\times n}$ is symmetric and positive definite. Let r_k be the residual vector at kth iterate produced by the steepest descent (SD) method when solving the linear system $Ax = b$. Show that if $r_{k+1} = 0$, then r_k is an eigenvector of A.

解: $r_k = b - Ax_k \iff Ax_k = b - r_k$

$x_{k+1} = x_k + \alpha \cdot r_k$

其中 $\alpha = \dfrac{r_k^T r_k}{r_k^T A r_k} \neq 0$

$r_{k+1} = b - Ax_{k+1} = 0$

$\Rightarrow b - A(x_k + \alpha r_k) = 0$

$\Rightarrow b - Ax_k - \alpha A r_k = 0$

$\Rightarrow b - (b - r_k) - \alpha A r_k = 0$

$\Rightarrow A r_k = \frac{1}{\alpha} r_k$

$\therefore$ r_k 是 A 的特征向量，特征值为 $\frac{1}{\alpha}$

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2. Suppose that $A \in \mathbb{R}^{n\times n}$ is symmetric and positive definite. Let x_k be the approximate solution at kth iterate when applying the steepest descent (SD) method to the linear system $Ax = b$. Show that

$$f(x_{k+1}) \leq \left(1 - \kappa^{-1}\right) f(x_k),$$

where $f(x) = x^\top Ax - 2b^\top x$ and $\kappa = \|A\|_2 \|A^{-1}\|_2$.

解: $f(x_{k+1}) - f(x_k)$

$= (x_k + \alpha r_k)^T A (x_k + \alpha r_k) - 2b^T(x_k + \alpha r_k)$

$\quad - x_k^T A x_k + 2b^T x_k$

$(r_k = b - Ax_k)$

$$= 2\alpha r_k^T A x_k + \alpha^2 r_k^T A r_k - 2\alpha b^T r_k$$

$$= 2 \cdot \frac{r_k^T r_k}{r_k^T A r_k} \cdot r_k^T (b - r_k) + \alpha^2 \cdot r_k^T A r_k - 2\frac{r_k^T r_k}{r_k^T A r_k} b^T r_k$$

$$= \frac{2 r_k^T r_k r_k^T b}{r_k^T A r_k} - \frac{2 r_k^T r_k r_k^T r_k}{r_k^T A r_k}$$

$$+ \frac{r_k^T r_k r_k^T r_k}{(r_k^T A r_k^T)^2} \cdot r_k^T A r_k - \frac{2 r_k^T r_k}{r_k^T A r_k} b^T r_k$$

$$= - \frac{(r_k^T r_k)^2}{r_k^T A r_k}$$

$$\therefore f(x_{k+1}) = f(x_k) - \frac{(r_k^T r_k)^2}{r_k^T A r_k}$$

$$\therefore f(x_{k+1}) = \left(1 - \frac{(r_k^T r_k)^2}{r_k^T A r_k} \cdot \frac{1}{f(x_k)}\right) f(x_k)$$

其中: $\frac{r_k^T A r_k}{r_k^T r_k} = \frac{r_k^T}{\|r_k\|} \cdot A \cdot \frac{r_k}{\|r_k\|} \in [\sigma_n, \sigma_1]$

$$\Rightarrow \frac{1}{\sigma_1} \leq \frac{r_k^T r_k}{r_k^T A r_k} \leq \frac{1}{\sigma_n} \quad (A > 0,\ \sigma_n > 0)$$

① 若 $f(x_k) \leq 0$, 又由 $f(x_{k+1}) - f(x_k) < 0$ 可知

$$f(x_{k+1}) \le f(x_k) \le (1-\kappa^{-1}) f(x_k)$$

已经成立

② 若 $f(x_k) > 0$

注意到：

$$r_k = b - Ax_k \Rightarrow x_k = A^{-1}(b - r_k)$$

$$\frac{f(x_k)}{r_k^T r_k} = \frac{x_k^T A x_k - 2b^T x_k}{r_k^T r_k}$$

$$= \frac{(b-r_k)^T A^{-1} A A^{-1}(b-r_k) - 2b^T A^{-1}(b-r_k)}{r_k^T r_k}$$

$$= \frac{r_k^T A^{-1} r_k - b^T A^{-1} b}{r_k^T r_k} \le \frac{r_k^T}{\|r_k\|} \cdot A^{-1} \cdot \frac{r_k}{\|r_k\|}$$

由 $f(x_k) > 0$ 可知：

$$\frac{r_k^T r_k}{f(x_k)} \geq \frac{1}{\frac{r_k^T}{\|r_k\|} \cdot A^{-1} \cdot \frac{r_k}{\|r_k\|}} \geq \sigma_n$$

因此，$f(x_k) > 0$ 时：

$$\frac{(r_k^T r_k)^2}{r_k^T A r_k} \cdot \frac{1}{f(x_k)} \geq \frac{\sigma_n}{\sigma_1} = \kappa^{-1}$$

也即：$f(x_{k+1}) \le (1-\kappa^{-1}) f(x_k)$

3. Let $A \in \mathbb{R}^{n\times n}$ be symmetric and positive definite, and $b \in \mathbb{R}^n$. Suppose that $\mathcal{V}$ is a subspace of $\mathbb{R}^n$. Show that

$$x_0 = \arg\min_{x\in\mathcal{V}} \|x - A^{-1}b\|_A$$

if and only if $b - Ax_0 \in \mathcal{V}^\perp$. (The orthogonal complement is defined using the standard inner product.)

解: ① 若: $b - Ax_0 \in V^\perp$

任取 $x \in V$, 记 $\Delta x = x - x_0 \in V$

即 $x = x_0 + \Delta x \in V$

$\| x - A^{-1}b \|_A^2$

$= \| x_0 + \Delta x - A^{-1}b \|_A^2$

$= \| x_0 - A^{-1}b + \Delta x \|_A^2$

$= \| x_0 - A^{-1}b \|_A^2 + \| \Delta x \|_A^2 + 2\Delta x A \cdot (x_0 - A^{-1}b)$

由于 $b - Ax_0 \perp V$, 且 $\Delta x \in V$

则 $\Delta x \cdot A(x_0 - A^{-1}b) = \Delta x (Ax_0 - b) = 0$

$\therefore \| x - A^{-1}b \|_A$

$= \| x_0 - A^{-1}b \|_A^2 + \| \Delta x \|_A^2 \geqslant \| x_0 - A^{-1}b \|_A^2$

当 $\| \Delta x \|_A^2 = 0$ 即 $\Delta x = 0$, $x = x_0$ 时取等号

$\therefore$ $b - Ax_0 \perp V$ 时,

$$\| x_0 - A^{-1}b \|_A = \min_{x\in V} \| x - A^{-1}b \|_A$$

② 若 $x_0 = \arg\min_{x \in V} \|x - A^{-1}b\|_A$

记 $x_* = A^{-1}b$

设 V 的一组标准正交基为 $\{v_1, \cdots, v_k\}$

定义：$W = \{z : z^TAx = 0,\ x \in V\}$

由于：$z \in W \iff z^TAV = 0 \iff V^TAz = 0$

由 $A \succ 0$ 可知

$$\operatorname{rank}(V^TA) = k$$

则 V^TAz 的解空间维数为：

$\dim(N(V^TAz)) = n-k$，即 $\dim W = n-k$

若 $\exists\ z \in W \cap V$

则 $z^TAz = 0$，由 A 正定可知 $z = 0$

即 $W \cap V = \{0\}$

那么，$\mathbb{R}^n = V \oplus W$

对 $x_* = A^{-1}b$ 作唯一分解：

$$x_* = x_1 + x_2,\quad x_1 \in V,\quad x_2 \in W$$

设 $x \in V$，那么：

$\|x - A^{-1}b\|_A^2 = \|x - x_1 - x_2\|_A^2$

由于 $x - x_1 \in V$， $x_2 \in W$

并且 $V^T A x_2 = 0$ (motivation)

则：

$$\|x - x_1 - x_2\|_A^2 = \|x - x_1\|_A^2 + \|x_2\|_A^2$$

要 $\|x - x_*\|_A^2$ 最小时，必有 $x = x_1 = VV^T A^{-1} b$

即 $x_0 = x_1 = \arg\min_{x \in V} \|x - x_*\|_A$

此时：$b - Ax_0$

$= b - A(x_* - x_2)$

$= b - b + Ax_2$

$= Ax_2$ 　其中 $x_2 \in W$

对于 $\forall x \in V$ 都有 $x(Ax_2) = 0$

即 $b - Ax_0 = Ax_2 \perp V$

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4. Derive the computational scheme of the preconditioned conjugate gradient (PCG) method.

解：

$x =$ random

$k = 0, \quad r = b - Ax$

while $(\sqrt{r^T r} > \varepsilon \|b\|_2)$ and $(k < k_{max})$

$z = M^{-1} r$

$k = k+1$

\# 先确定第k+1步的"下山"方向

if $k = 1$:

$p = z; \quad \rho = r^T z;$

else :

$\tilde{\rho} = \rho; \quad \rho = r^T z;$

$\beta = \frac{\rho}{\tilde{\rho}}; \quad p = z + \beta p$

end

\# 然后做一步"下山"，并计算第k+1步的残差 r_{k+1}

$w = Ap; \quad \alpha = \rho / p^T w;$

$x = x + \alpha p; \quad r = r - \alpha w;$

end