Problems for Conjugate Gradient Method in Solving Linear Systems

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1. Let $\{d_0, d_1, \ldots, d_{k-1}\}$ be a set of vectors which satisfy $d_i^T A d_j = \delta_{ij}$, where A is positive definite and δ_{ij} is the Kronecker delta. Suppose that we have searched the minimum value along each d_i sequentially(therefore we have a sequence of points $x_0, x_1, \cdots, x_{k-1}$). Let $g_j = Ax_j - b$ be the gradient of f at $x = x_j$, prove that $g_k^T d_j = 0, \quad j = 0, 1, \cdots, k-1$.

   Hint: if we do linear search along $x_{k-1} + t_{k-1} d_{k-1}$, then at the optimal t_{k-1}, we have $g_k^T d_{k-1} = 0$.

2. Let $\{d_0, d_1, \ldots, d_{k-1}\}$ be a set of vectors which satisfy $d_i^T A d_j = 0$ for any $0 \leqslant i < j \leqslant k-1$. $g_j = Ax_j - b$ is the gradient of f at $x = x_j$. Furthermore, suppose $d_0 = -g_0$. Let $d_k = -g_k + \sum_{j=0}^{k-1} a_j d_j$ be the searching direction at step k which satisfies $d_k^T A d_j = 0$ for all $j = 0, 1, \ldots, k-1$. Prove that $a_j = 0, \quad j = 0, 1, \ldots, k-2$.

3. Compute the optimal t_k and a_{k-1} at step k. Your results should have a simple form which only includes matrix-vector production and vector-vector production.

4. Implement the conjugate gradient algorithm for optimizing the quadratic function and test your program with the following examples.

   (a) $A \in \mathbb{R}^{n \times n}$, where $n = 60000$, and has the form

   $$A = \begin{pmatrix} 10 & 1 & & & \\ 1 & 10 & 1 & & \\ & 1 & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & 1 & 10 \end{pmatrix}$$

   b and x_0 can be chosen randomly.

   (b) $A = (a_{ij}) \in \mathbb{R}^{n \times n}$, where $n = 40$ and $a_{ij} = \frac{1}{i+j-1}$. $b = (b_i)$, where $b_i = \sum_{j=1}^{n} a_{ij}$. x_0 is chosen randomly. Obviously, the solution of $Ax = b$ is $x = (1, 1, \ldots, 1)^T$. Apply the Gaussian elimination with pivoting to solve the linear system again, and explain what you've observed.