CS532100 Numerical Optimization Homework 1

110062533 Yang, Jiun-Kai

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1. (45%) Consider a function $f(x_1, x_2) = x_1^3 x_2 - 2x_1 x_2^2 + x_1 x_2^3$.

   (a) Compute the gradient and Hessian of f.

   (b) Is $(x_1, x_2) = (1, 1)$ a local minimizer? Justify your answer.

   (c) What is the steepest descent direction of f at $(x_1, x_2) = (1, 2)$?

   (d) What is the Newton's direction of f at $(x_1, x_2) = (1, 2)$?

   (e) Compute the LDL decomposition of the Hessian of f at $(x_1, x_2) = (1, 2)$. (No pivoting)

   (f) Is the Newton's direction of f at $(x_1, x_2) = (1, 2)$ a descent direction? Justify your answer.

   (g) Modify the LDL decomposition computed in (d) such that all diagonal elements of D is larger than or equal to 1, and use the modified LDL decomposition to compute a modified Newton's direction at $(x_1, x_2) = (1, 2)$.

   (h) Suppose $\vec{x_0} = (1, 1)$ and $\vec{x_1} = (1, 2)$ and $B_0 = I$, compute the quasi Newton direction p_1 using SR1.

   (i) Suppose $\vec{x_0} = (1, 1)$ and $\vec{x_1} = (1, 2)$ and $B_0 = I$, compute the quasi Newton direction p_1 using BFGS.

   Answers are put here.

   (a) The Hessian H of f is

   $$\nabla f|_{x_1=x_2=1} = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} \end{bmatrix}^T = \begin{bmatrix} 3{x_1}^2 x_2 - 2{x_2}^2 + {x_2}^3 & {x_1}^3 - 4x_1 x_2 + 3x_1{x_2}^2 \end{bmatrix}^T$$

   $$H = \begin{bmatrix} \frac{\partial^2 f}{\partial {x_1}^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} \end{bmatrix} = \begin{bmatrix} 6x_1 x_2 & 3{x_1}^2 - 4x_2 + 3{x_2}^2 \\ 3{x_1}^2 - 4x_2 + 3{x_2}^2 & -4x_1 + 6x_1 x_2 \end{bmatrix}$$

   (b) Given $(x_1, x_2) = (1, 1)$, we have the gradient of f, ∇f, and the Hessian H:

   $$\nabla f|_{x_1=x_2=1} = \begin{bmatrix} 2 & 0 \end{bmatrix}^T$$

   $$H|_{x_1=x_2=1} = \begin{bmatrix} 6 & 2 \\ 2 & 2 \end{bmatrix}.$$

   Since all elements in H are positive, so we know that $\forall z \in \mathbb{R}^2, z^T H z > 0 \rightarrow$ H is a positive-definite matrix.
   However, $\nabla f \neq 0$, so $(x_1, x_2) = (1, 1)$ is not a local minimizer.

(c) The steepest descent direction of f is $-\nabla f$ at $(x_1, x_2) = (1, 2)$

$$[-\nabla f]_{x_1=1,x_2=2} = \begin{bmatrix} -6 & -5 \end{bmatrix}^T$$

(d) The Newton's direction of f at $(x_1, x_2) = (1, 2)$ is

$$[-H^{-1}\nabla f]_{x_1=1,x_2=2} = -\begin{bmatrix} 12 & 7 \\ 7 & 8 \end{bmatrix}^{-1} \begin{bmatrix} 6 \\ 5 \end{bmatrix} = -\frac{1}{47} \begin{bmatrix} 8 & -7 \\ -7 & 12 \end{bmatrix} \begin{bmatrix} 6 \\ 5 \end{bmatrix} = -\frac{1}{47} \begin{bmatrix} 13 \\ 18 \end{bmatrix}$$

(e) The LDL^T decomposition of Hessian H of f at $(x_1, x_2) = (1, 2)$:

$$H = \begin{bmatrix} 12 & 7 \\ 7 & 8 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 7/12 & 1 \end{bmatrix} \begin{bmatrix} 12 & 7 \\ 0 & 47/12 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 7/12 & 1 \end{bmatrix} \begin{bmatrix} 12 & 0 \\ 0 & 47/12 \end{bmatrix} \begin{bmatrix} 1 & 7/12 \\ 0 & 1 \end{bmatrix}$$

(f) We can check if $\vec{g_k}^T \vec{p_k} < 0$ where $\vec{g_k} = \nabla f$ and $\vec{p_k}$ is the Newton's direction of f.
At $(x_1, x_2) = (1, 2)$, we have

$$\vec{g_k}^T \vec{p_k} = -\frac{1}{47} \begin{bmatrix} 6 & 5 \end{bmatrix} \begin{bmatrix} 13 \\ 18 \end{bmatrix} < 0.$$

Therefore, we know that the Newton's direction of f at $(x_1, x_2) = (1, 2)$ is a descent direction.

(g) From the previous problem (e), we can see that all diagonal elements of D is larger or equal to 1, so we don't need to modify the LDL decomposition. The Newton's direction is same as (d).

(h) We have $\vec{x_0} = (1, 1)$, $\vec{x_1} = (1, 2)$, and the initial guess of Hessian $B_0 = I$.
$\because \nabla f(\vec{x_0}) = [2, 0]^T$ and $\nabla f(\vec{x_1}) = [6, 5]^T$
$\therefore y_0 = [4, 5]^T$
$\because \vec{x_0} = (1, 1)$, $\vec{x_1} = (1, 2)$
$\therefore \vec{s_0} = [0, 1]^T$
The quasi Newton's direction using SR1 is $\vec{p_1} = -B_1^{-1}\nabla f(\vec{x_1})$ where

$$B_1 = B_0 + \frac{(\vec{y_0} - B_0\vec{s_0})(\vec{y_0} - B_0\vec{s_0})^T}{(\vec{y_0} - B_0\vec{s_0})^T \vec{s_0}} = \begin{bmatrix} 5 & 4 \\ 4 & 5 \end{bmatrix}$$

Therefore, $\vec{p_1} = -\frac{1}{9} \begin{bmatrix} 5 & -4 \\ -4 & 5 \end{bmatrix} \begin{bmatrix} 6 \\ 5 \end{bmatrix} = -\frac{1}{9} \begin{bmatrix} 10 \\ 1 \end{bmatrix}$

(i) From the previous problem (h), we know that $\vec{s_0} = [0, 1]^T$, $y_0 = [4, 5]^T$, $\nabla f(\vec{x_1}) = [6, 5]^T$, and $B_0 = I$.
The quasi Newton's direction using BFGS is $\vec{p_1} = -B_1^{-1}\nabla f(\vec{x_1})$ where

$$B_1 = B_0 - \frac{B_0\vec{s_0}\vec{s_0}^T B_0}{\vec{s_0}^T B_0 \vec{s_0}} + \frac{\vec{y_0}\vec{y_0}^T}{\vec{y_0}^T \vec{s_0}} = I - \frac{\vec{s_0}\vec{s_0}^T}{\vec{s_0}^T \vec{s_0}} + \frac{\vec{y_0}\vec{y_0}^T}{\vec{y_0}^T \vec{s_0}} = \begin{bmatrix} 21/5 & 4 \\ 4 & 5 \end{bmatrix}$$

Therefore, $\vec{p_1} = -B_1^{-1}\nabla f(\vec{x_1}) = -\frac{1}{5} \begin{bmatrix} 5 & -4 \\ -4 & 21/5 \end{bmatrix} \begin{bmatrix} 6 \\ 5 \end{bmatrix} = \begin{bmatrix} -2 \\ 3/5 \end{bmatrix}$

2. (20%)

   (a) A set $S \subseteq R^n$ is a *convex* set if the straight line connecting any two points in S is also entirely in S. A function $f : S \rightarrow R$ is a *convex* function if S is a convex set. The following properties are equivalent:

      i. $S \subseteq R^n$ is a convex set, $f : S \rightarrow R$ is a convex function.

      ii. $f(\alpha\vec{x}+(1-\alpha)\vec{y}) \leq \alpha f(\vec{x})+(1-\alpha)f(\vec{y})$ for all $\alpha \in [0,1]$, $\vec{x}, \vec{y} \in S$.

      Prove that when f is a convex function, any local minimizer $\vec{x}^*$ is a global minimizer of f.
      (Hint: Suppose there is another point $\vec{z} \in S$ such that $f(\vec{z}) \leq f(\vec{x}^*)$, then $\vec{x}^*$ is not a local minimizer.)

   (b) Suppose $f(\vec{x}) = \vec{x}^T Q\vec{x}$, where Q is a symmetric positive semidefinite matrix, show that $f(\vec{x})$ is a convex function.
      (Hint: It might be easier to show $f(\vec{y} + \alpha(\vec{x} - \vec{y})) - \alpha f(\vec{x}) - (1 - \alpha)f(\vec{y}) \leq 0$.)

   Answers are put here.

   (a) Let $\vec{x}^*$ is the local minimizer of f.
      The point $\vec{x}^*$ is a local minimizer if there is a neighborhood N of $\vec{x}^*$ s.t. $f(x) \leq f(x)$, $\forall x \in N$.
      Suppose $\exists \vec{z} \in S$ s.t. $f(\vec{z}) < f(\vec{x}^*)$, which means $\vec{x}^*$ is not a global minimizer.
      By the second equivalent property, for $\vec{x}^*$ and $\vec{z}$, $\forall \alpha \in [0,1]$, $f(\alpha\vec{x}^* + (1-\alpha)\vec{z}) \leq \alpha f(\vec{x}^*) + (1-\alpha)f(\vec{z}) < \alpha f(\vec{x}^*) + (1-\alpha)f(\vec{x}) = f(\vec{x}^*)$.
      However, if $\alpha = 1$, $f(\vec{x}^*) < f(\vec{x}^*)$. That is a contracdiction!
      Therefore, when f is a convex function, any local minimizer $\vec{x}^*$ is a global minimizer of f.

   (b) By the second equivalent property, for $\vec{x}, \vec{y} \in S$, $\forall \alpha \in [0,1]$, $f(\alpha\vec{x} + (1-\alpha)\vec{y}) - [\alpha f(\vec{x}) + (1-\alpha)f(\vec{y})] \leq 0$. Given $f(\vec{x}) = \vec{x}^T Q\vec{x}$,

$$
\begin{aligned}
&f(\alpha\vec{x} + (1-\alpha)\vec{y}) - [\alpha f(\vec{x}) + (1-\alpha)f(\vec{y})] \\
&= (\alpha\vec{x} + (1-\alpha)\vec{y})^T Q(\alpha\vec{x} + (1-\alpha)\vec{y}) - \alpha\vec{x}^T Q\vec{x} - (1-\alpha)\vec{y}^T Q\vec{y} \\
&= \alpha^2\vec{x}^T Q\vec{x} + (1-\alpha)^2\vec{y}^T Q\vec{y} + 2\alpha(1-\alpha)\vec{x}^T Q\vec{y} - \alpha\vec{x}^T Q\vec{x} - (1-\alpha)\vec{y}^T Q\vec{y} \\
&= \alpha(\alpha-1)\vec{x}^T Q\vec{x} + \alpha(\alpha-1)\vec{y}^T Q\vec{y} + 2\alpha(1-\alpha)\vec{x}^T Q\vec{y} \\
&= \alpha(\alpha-1)[\vec{x}^T Q\vec{x} + \vec{y}^T Q\vec{y} - 2\vec{x}^T Q\vec{y}] \\
&= \alpha(\alpha-1)[(\vec{x}-\vec{y})^T Q(\vec{x}-\vec{y})]
\end{aligned}
$$

$$
\begin{aligned}
&\because Q \text{ is a symmetric positive semi-definite matrix and } \alpha \in [0,1] \\
&\therefore [(\vec{x}-\vec{y})^T Q(\vec{x}-\vec{y})] \geq 0, \alpha(\alpha-1) \leq 0 \\
&\Rightarrow f(\alpha\vec{x} + (1-\alpha)\vec{y}) - [\alpha f(\vec{x}) + (1-\alpha)f(\vec{y})] \leq 0
\end{aligned}
$$

      Therefore, Suppose $f(\vec{x}) = \vec{x}^T Q\vec{x}$, where Q is a symmetric positive semidefinite matrix, $f(\vec{x})$ is a convex function.

3. (20%) (Line search method) Suppose $\phi(\alpha) = f(\vec{x_k} + \alpha\vec{p_k}) = (\alpha - 1)^2$.

(a) The sufficient decrease condition asks $\phi(\alpha) \leq \phi(0) + c_1\alpha\phi'(0)$, $\alpha \in [0, \infty)$. Suppose $c_1 = 0.1$, what is the feasible interval of α satisfying this condition ?

(b) The curvature condition asks $\phi'(\alpha) \geq c_2\phi'(0)$. Suppose $c_2 = 0.9$, what is the feasible interval of α satisfying this condition ?

Answers are put here.

(a) $\because \phi'(0) = 2(0-1) = -2$ and $\phi(0) = 1$
$\therefore \phi(\alpha) \leq 1 - 2c_1\alpha, \forall\alpha \in [0, \infty)$
Suppose $c_1 = 0.1$, $\phi(\alpha) \leq 1 - 0.2\alpha$.
$\Rightarrow \phi(\alpha) = (\alpha - 1)^2 \leq 1 - 0.2\alpha$
$\Rightarrow \alpha(\alpha - 1.8) \leq 0$
$\Rightarrow 0 \leq \alpha \leq 1.8$
$\because \alpha \in [0, \infty)$ and $0 \leq \alpha \leq 1.8$
$\therefore$ The feasible interval of α is $\alpha \in [0, 1.8]$.

(b) $\phi'(\alpha) = 2(\alpha - 1) \geq c_2 2(0-1)$.
Suppose $c_2 = 0.9$, $2(\alpha - 1) \geq -1.8$
$\Rightarrow \alpha \geq \frac{1}{2} \times 0.2 = 0.1$
$\Rightarrow$ The feasible interval of α is $\alpha \in [0.1, \infty)$

4. (15%) The conjugate gradient method for solving $Ax = b$ is given in Figure 1, where z_k is the approximate solution. In class we define $\alpha_k = (\vec{p_k}^T\vec{r_k})/(\vec{p_k}^TA\vec{p_k})$ and $\beta_k = (\vec{p_k}^TA\vec{r_{k+1}})/(\vec{p_k}^TA\vec{p_k})$. We need to modify $\beta_k = -(\vec{p_k}^TA\vec{r_{k+1}})/(\vec{p_k}^TA\vec{p_k})$ here since the direction of $\vec{p_{k+1}}$ in Figure 1 is opposite to the CG method we taught in slides, both versions are correct. Prove that the above formula of α_k and β_k are equivalent to the ones in step (3) and step (6). You may need the relations in step (4) and step (5), and the following properties:

(a) $\vec{r_i}^T\vec{r_j} = 0$ for all $i \neq j$.

(b) $\vec{p_i}^TA\vec{p_j} = 0$ for all $i \neq j$.

(c) $\vec{p_k}$ is a linear combination of $\vec{r_0}, \ldots.\vec{r_k}$, $\vec{p_k} = \sum_{i=1}^{k}\gamma_i\vec{r_i}$.
(which can be shown from step (7) by mathematical induction.)

Answers are put here.

Assume A in $Ax = b$ is a symmetric positive-definite matrix for solving CG algorithm.

Proof by Induction

Step 1: Verify that the desired result holds for k = 0.

(1)	Given $\vec{z}_0$. Let $\vec{p}_0 = \vec{b} - A\vec{z}_0$, and $\vec{r}_0 = \vec{p}_0$.
(2)	For $k = 0, 1, 2, \ldots$ until $\|\vec{r}_k\| \leq \epsilon$
(3)	$\quad \alpha_k = (\vec{r}_k^T \vec{r}_k)/(\vec{p}_k^T A\vec{p}_k)$
(4)	$\quad \vec{z}_{k+1} = \vec{z}_k + \alpha_k \vec{p}_k$
(5)	$\quad \vec{r}_{k+1} = \vec{r}_k - \alpha_k A\vec{p}_k$
(6)	$\quad \beta_k = (\vec{r}_{k+1}^T \vec{r}_{k+1})/(\vec{r}_k^T \vec{r}_k)$
(7)	$\quad \vec{p}_{k+1} = \vec{r}_{k+1} + \beta_k \vec{p}_k$

Figure 1: The CG algorithm.

$$\alpha_0 = \frac{\vec{r_0}^T \vec{r_0}}{\vec{p_0}^T A\vec{p_0}} = \frac{\vec{p_0}^T \vec{r_0}}{\vec{p_0}^T A\vec{p_0}}$$

$$\beta_0 = \frac{\vec{r}_1^T \vec{r}_1}{\vec{r_0}^T \vec{r_0}} = \frac{(\vec{r}_0^T - \frac{\vec{r_0}^T \vec{r_0}}{\vec{p_0}^T A\vec{p_0}} A\vec{p}_0)^T \vec{r}_1}{\vec{r_0}^T \vec{r_0}} = \frac{\vec{r}_0^T \vec{r}_1}{\vec{r_0}^T \vec{r_0}} - \frac{\vec{p}_0^T A\vec{r}_1}{\vec{p}_0^T A\vec{p}_0}$$

$\because A$ is a symmetric positive-definite matrix and $\vec{r_i}^T \vec{r_j} = 0, \forall i \neq j$.

$$\therefore \beta_0 = -\frac{\vec{p}_0^T A\vec{r}_1}{\vec{p}_0^T A\vec{p}_0}$$

Step 2: Assume that the desired result holds for k = i.
Under this assumption,

$$\alpha_i = \frac{\vec{p}_i^T \vec{r}_i}{\vec{p}_i^T A\vec{p}_i}$$

$$\beta_i = -\frac{\vec{p}_i^T A\vec{r}_{i+1}}{\vec{p}_i^T A\vec{p}_i}$$

Step 3: Use the assumption from step 2 to show that the result holds for $k = (i+1)$.

$$\alpha_{i+1} = \frac{\vec{r}_{i+1}^T \vec{r}_{i+1}}{\vec{p}_{i+1}^T A \vec{p}_{i+1}} = \frac{(\vec{p}_{i+1} - \beta_i \vec{p}_i)^T \vec{r}_{i+1}}{\vec{p}_{i+1}^T A \vec{p}_{i+1}}$$

$\because \vec{p_k}$ is a linear combination of $\vec{r_0}, ...\vec{r_k}$, $\vec{p_k} = \sum_{i=1}^{k} \gamma_i \vec{r_i}$

$$\therefore \alpha_{i+1} = \frac{(\vec{p}_{i+1} - \beta_i \sum_{j=1}^{i} \gamma_j \vec{r_j})^T \vec{r}_{i+1}}{\vec{p}_{i+1}^T A \vec{p}_{i+1}}$$

$\because \vec{r_i}^T \vec{r_j} = 0$ for all $i \neq j$

$$\therefore \alpha_{i+1} = \frac{\vec{p}_{i+1}^T \vec{r}_{i+1}}{\vec{p}_{i+1}^T A \vec{p}_{i+1}}$$

$$\beta_{i+1} = \frac{\vec{r}_{i+2}^T \vec{r}_{i+2}}{\vec{r_{i+1}}^T \vec{r_{i+1}}} = \frac{(\vec{r}_{i+1} - \alpha_{i+1} A \vec{p}_{i+1})^T \vec{r}_{i+2}}{\vec{r_{i+1}}^T \vec{r_{i+1}}}$$

$\because \vec{r_i}^T \vec{r_j} = 0$ for all $i \neq j$

$$\therefore \beta_{i+1} = -\frac{(\alpha_{i+1} A \vec{p}_{i+1})^T \vec{r}_{i+2}}{\vec{r_{i+1}}^T \vec{r_{i+1}}}$$

$$\because \alpha_{i+1} = \frac{\vec{r}_{i+1}^T \vec{r}_{i+1}}{\vec{p}_{i+1}^T A \vec{p}_{i+1}}$$

$$\therefore \beta_{i+1} = -\frac{(\frac{\vec{r}_{i+1}^T \vec{r}_{i+1}}{\vec{p}_{i+1}^T A \vec{p}_{i+1}} A \vec{p}_{i+1})^T \vec{r}_{i+2}}{\vec{r_{i+1}}^T \vec{r_{i+1}}} = -\frac{\vec{p}_{i+1}^T A^T \vec{r}_{i+2}}{\vec{p}_{i+1}^T A \vec{p}_{i+1}}$$

$\because$ A is a symmetric matrix.

$$\therefore \beta_{i+1} = -\frac{\vec{p}_{i+1}^T A \vec{r}_{i+2}}{\vec{p}_{i+1}^T A \vec{p}_{i+1}}$$

Summarize the results

The above formula of α_k and β_k are equivalent to the ones in step (3) and step (6).