

ECE/MATH 520, Spring 2008

Homework Problems 3

Solutions (version: March 6, 2008, 17:42)

10.1 Let Q be a real symmetric positive definite $n \times n$ matrix. Given an arbitrary set of linearly independent vectors $\{p^{(0)}, \dots, p^{(n-1)}\}$ in \mathbb{R}^n , the *Gram-Schmidt* procedure generates a set of vectors $\{d^{(0)}, \dots, d^{(n-1)}\}$ as follows:

$$\begin{aligned} d^{(0)} &= p^{(0)} \\ d^{(k+1)} &= p^{(k+1)} - \sum_{i=0}^k \frac{p^{(k+1)T} Q d^{(i)}}{d^{(i)T} Q d^{(i)}} d^{(i)} \end{aligned}$$

Show that the vectors $d^{(0)}, \dots, d^{(n-1)}$ are Q -conjugate.

Ans.: We proceed by induction to show that for $k = 0, \dots, n-1$, the set $\{d^{(0)}, \dots, d^{(k)}\}$ is Q -conjugate. We assume that $d^{(i)} \neq 0$, $i = 1, \dots, k$, so that $d^{(i)T} Q d^{(i)} \neq 0$ and the algorithm is well defined.

For $k = 0$, the statement trivially holds. So, assume that the statement is true for $k < n-1$, i.e., $\{d^{(0)}, \dots, d^{(k)}\}$ is Q -conjugate. We now show that $\{d^{(0)}, \dots, d^{(k+1)}\}$ is Q -conjugate. For this, we need only to show that for each $j = 0, \dots, k$, we have $d^{(k+1)T} Q d^{(j)} = 0$. To this end,

$$\begin{aligned} d^{(k+1)T} Q d^{(j)} &= \left(p^{(k+1)T} - \sum_{i=0}^k \frac{p^{(k+1)T} Q d^{(i)}}{d^{(i)T} Q d^{(i)}} d^{(i)T} \right) Q d^{(j)} \\ &= p^{(k+1)T} Q d^{(j)} - \sum_{i=0}^k \frac{p^{(k+1)T} Q d^{(i)}}{d^{(i)T} Q d^{(i)}} d^{(i)T} Q d^{(j)}. \end{aligned}$$

By the induction hypothesis, $d^{(i)T} Q d^{(j)} = 0$ for $i \neq j$. Therefore

$$d^{(k+1)T} Q d^{(j)} = p^{(k+1)T} Q d^{(j)} - \frac{p^{(k+1)T} Q d^{(j)}}{d^{(j)T} Q d^{(j)}} d^{(j)T} Q d^{(j)} = 0.$$

In the above, we have assumed that the vectors $d^{(k)}$ are nonzero (so that $d^{(k)T} Q d^{(k)} \neq 0$ and the algorithm is well defined). To prove that this assumption holds, we use induction to show that $d^{(k)}$ is a (nonzero) linear combination of $p^{(0)}, \dots, p^{(k)}$ (which immediately implies that $d^{(k)}$ is nonzero because of the linear independence of $p^{(0)}, \dots, p^{(k)}$).

For $k = 0$, we have $\mathbf{d}^{(0)} = \mathbf{p}^{(0)}$ by definition. Assume that the result holds for $k < n - 1$; i.e., $\mathbf{d}^{(k)} = \sum_{j=0}^k \alpha_j^{(k)} \mathbf{p}^{(j)}$, where the coefficients $\alpha_j^{(k)}$ are not all zero. Consider $\mathbf{d}^{(k+1)}$:

$$\begin{aligned} \mathbf{d}^{(k+1)} &= \mathbf{p}^{(k+1)} - \sum_{i=0}^k \beta_i \mathbf{d}^{(i)} \\ &= \mathbf{p}^{(k+1)} - \sum_{i=0}^k \beta_i \sum_{j=0}^i \alpha_j^{(k)} \mathbf{p}^{(j)} \\ &= \mathbf{p}^{(k+1)} - \sum_{j=0}^k \sum_{i=j}^k \beta_i \alpha_j^{(k)} \mathbf{p}^{(j)}. \end{aligned}$$

So, clearly $\mathbf{d}^{(k+1)}$ is a nonzero linear combination of $\mathbf{p}^{(0)}, \dots, \mathbf{p}^{(k+1)}$.

10.6 Consider the quadratic function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ given by

$$f(\mathbf{x}) = \frac{1}{2} \mathbf{x}^T \mathbf{Q} \mathbf{x} - \mathbf{x}^T \mathbf{b},$$

where $\mathbf{Q} = \mathbf{Q}^T > 0$. Let $\mathbf{D} \in \mathbb{R}^{n \times r}$ be of rank r , and $\mathbf{x}_0 \in \mathbb{R}^n$. Define the function $\phi : \mathbb{R}^r \rightarrow \mathbb{R}$ by

$$\phi(\mathbf{a}) = f(\mathbf{x}_0 + \mathbf{D}\mathbf{a}).$$

Show that ϕ is a quadratic function with a positive definite quadratic term.

Ans.: Expanding $\phi(\mathbf{a})$ yields

$$\begin{aligned} \phi(\mathbf{a}) &= \frac{1}{2} (\mathbf{x}_0 + \mathbf{D}\mathbf{a})^T \mathbf{Q} (\mathbf{x}_0 + \mathbf{D}\mathbf{a}) - (\mathbf{x}_0 + \mathbf{D}\mathbf{a})^T \mathbf{b} \\ &= \frac{1}{2} \mathbf{a}^T (\mathbf{D}^T \mathbf{Q} \mathbf{D}) \mathbf{a} + \mathbf{a}^T (\mathbf{D}^T \mathbf{Q} \mathbf{x}_0 - \mathbf{D}^T \mathbf{b}) + \left(\frac{1}{2} \mathbf{x}_0^T \mathbf{Q} \mathbf{x}_0 - \mathbf{x}_0^T \mathbf{b} \right). \end{aligned}$$

Clearly ϕ is a quadratic function on \mathbb{R}^r . It remains to show that the matrix in the quadratic term, $\mathbf{D}^T \mathbf{Q} \mathbf{D}$, is positive definite. Since $\mathbf{Q} > 0$, for any $\mathbf{a} \in \mathbb{R}^r$, we have

$$\mathbf{a}^T (\mathbf{D}^T \mathbf{Q} \mathbf{D}) \mathbf{a} = (\mathbf{D}\mathbf{a})^T \mathbf{Q} (\mathbf{D}\mathbf{a}) \geq 0$$

and

$$\mathbf{a}^T (\mathbf{D}^T \mathbf{Q} \mathbf{D}) \mathbf{a} = (\mathbf{D}\mathbf{a})^T \mathbf{Q} (\mathbf{D}\mathbf{a}) = 0$$

if and only if $\mathbf{D}\mathbf{a} = \mathbf{0}$. Since $\text{rank } \mathbf{D} = r$, $\mathbf{D}\mathbf{a} = \mathbf{0}$ if and only if $\mathbf{a} = \mathbf{0}$. Hence, the matrix $\mathbf{D}^T \mathbf{Q} \mathbf{D}$ is positive definite.

10.7 Let $f(\mathbf{x})$, $\mathbf{x} = [x_1, x_2]^T \in \mathbb{R}^2$, be given by

$$f(\mathbf{x}) = \frac{5}{2} x_1^2 + \frac{1}{2} x_2^2 + 2x_1 x_2 - 3x_1 - x_2$$

- a. Express $f(\mathbf{x})$ in the form of $f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T \mathbf{Q} \mathbf{x} - \mathbf{x}^T \mathbf{b}$.
- b. Find the minimizer of f using the conjugate gradient algorithm. Use a starting point of $\mathbf{x}^{(0)} = [0, 0]^T$.
- c. Calculate the minimizer of f analytically from \mathbf{Q} and \mathbf{b} , and check it with your answer in part b.

Ans.: a. We have $f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T \mathbf{Q} \mathbf{x} - \mathbf{b}^T \mathbf{x}$ where

$$\mathbf{Q} = \begin{bmatrix} 5 & 2 \\ 2 & 1 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} 3 \\ 1 \end{bmatrix}.$$

b. Since f is a quadratic function on \mathbb{R}^2 , we need to perform only two iterations. For the first iteration we compute

$$\begin{aligned} \mathbf{d}^{(0)} &= -\mathbf{g}^{(0)} = [3, 1]^T \\ \alpha_0 &= \frac{5}{29} \\ \mathbf{x}^{(1)} &= [0.51724, 0.17241]^T \\ \mathbf{g}^{(1)} &= [-0.06897, 0.20690]^T. \end{aligned}$$

For the second iteration we compute

$$\begin{aligned} \beta_0 &= 0.0047534 \\ \mathbf{d}^{(1)} &= [0.08324, -0.20214]^T \\ \alpha_1 &= 5.7952 \\ \mathbf{x}^{(2)} &= [1.000, -1.000]^T. \end{aligned}$$

c. The minimizer is given by $\mathbf{x}^* = \mathbf{Q}^{-1}\mathbf{b} = [1, -1]^T$, which agrees with part b.

11.1 Given $f : \mathbb{R}^n \rightarrow \mathbb{R}$, $f \in \mathcal{C}^1$, consider the algorithm

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha_k \mathbf{d}^{(k)}$$

where $\mathbf{d}^{(1)}, \mathbf{d}^{(2)}, \dots$ are vectors in \mathbb{R}^n , and $\alpha_k \geq 0$ is chosen to minimize $f(\mathbf{x}^{(k)} + \alpha \mathbf{d}^{(k)})$; that is,

$$\alpha_k = \arg \min_{\alpha \geq 0} f(\mathbf{x}^{(k)} + \alpha \mathbf{d}^{(k)}).$$

Note that the above general algorithm encompasses almost all algorithms that we discussed in this part, including the steepest descent, Newton, conjugate gradient, and quasi-Newton algorithms.

Let $\mathbf{g}^{(k)} = \nabla f(\mathbf{x}^{(k)})$, and assume that $\mathbf{d}^{(k)T} \mathbf{g}^{(k)} < 0$.

- a. Show that $\mathbf{d}^{(k)}$ is a descent direction for f , in the sense that there exists $\bar{\alpha} > 0$ such that for all $\alpha \in (0, \bar{\alpha}]$,

$$f(\mathbf{x}^{(k)} + \alpha \mathbf{d}^{(k)}) < f(\mathbf{x}^{(k)}).$$

- b. Show that $\alpha_k > 0$.

- c. Show that $\mathbf{d}^{(k)T} \mathbf{g}^{(k+1)} = 0$.

- d. Show that the following algorithms all satisfy the condition $\mathbf{d}^{(k)T} \mathbf{g}^{(k)} < 0$, if $\mathbf{g}^{(k)} \neq \mathbf{0}$:

1. Steepest descent algorithm
2. Newton's method, assuming the Hessian is positive definite
3. Conjugate gradient algorithm
4. Quasi-Newton algorithm, assuming $\mathbf{H}_k > 0$

- e. For the case where $f(\mathbf{x}) = \frac{1}{2} \mathbf{x}^T \mathbf{Q} \mathbf{x} - \mathbf{x}^T \mathbf{b}$, with $\mathbf{Q} = \mathbf{Q}^T > 0$, derive an expression for α_k in terms of \mathbf{Q} , $\mathbf{d}^{(k)}$, and $\mathbf{g}^{(k)}$.

Ans.: a. Let

$$\phi(\alpha) = f(\mathbf{x}^{(k)} + \alpha \mathbf{d}^{(k)}).$$

Then, using the chain rule, we obtain

$$\phi'(\alpha) = \mathbf{d}^{(k)T} \nabla f(\mathbf{x}^{(k)} + \alpha \mathbf{d}^{(k)}).$$

Hence

$$\phi'(0) = \mathbf{d}^{(k)T} \mathbf{g}^{(k)}.$$

Since ϕ' is continuous, then, if $\mathbf{d}^{(k)T} \mathbf{g}^{(k)} < 0$, there exists $\bar{\alpha} > 0$ such that for all $\alpha \in (0, \bar{\alpha}]$, $\phi(\alpha) < \phi(0)$, i.e., $f(\mathbf{x}^{(k)} + \alpha \mathbf{d}^{(k)}) < f(\mathbf{x}^{(k)})$.

- b. By part a, $\phi(\alpha) < \phi(0)$ for all $\alpha \in (0, \bar{\alpha}]$. Hence,

$$\alpha_k = \arg \min_{\alpha \geq 0} \phi(\alpha) \neq 0$$

which implies that $\alpha_k > 0$.

- c. Now,

$$\mathbf{d}^{(k)T} \mathbf{g}^{(k+1)} = \mathbf{d}^{(k)T} \nabla f(\mathbf{x}^{(k)} + \alpha_k \mathbf{d}^{(k)}) = \phi'_k(\alpha_k).$$

Since $\alpha_k = \arg \min_{\alpha \geq 0} f(\mathbf{x}^{(k)} + \alpha \mathbf{d}^{(k)}) > 0$, we have $\phi'_k(\alpha_k) = 0$. Hence, $\mathbf{g}^{(k+1)T} \mathbf{d}^{(k)} = 0$.

- d.

- i. We have $\mathbf{d}^{(k)} = -\mathbf{g}^{(k)}$. Hence, $\mathbf{d}^{(k)T} \mathbf{g}^{(k)} = -\|\mathbf{g}^{(k)}\|^2$. If $\mathbf{g}^{(k)} \neq \mathbf{0}$, then $\|\mathbf{g}^{(k)}\|^2 > 0$, and hence $\mathbf{d}^{(k)T} \mathbf{g}^{(k)} < 0$.

ii. We have $\mathbf{d}^{(k)} = -\mathbf{F}(\mathbf{x}^{(k)})^{-1}\mathbf{g}^{(k)}$. Since $\mathbf{F}(\mathbf{x}^{(k)}) > 0$, we also have $\mathbf{F}(\mathbf{x}^{(k)})^{-1} > 0$. Therefore, $\mathbf{d}^{(k)T}\mathbf{g}^{(k)} = -\mathbf{g}^{(k)T}\mathbf{F}(\mathbf{x}^{(k)})^{-1}\mathbf{g}^{(k)} < 0$ if $\mathbf{g}^{(k)} \neq \mathbf{0}$.

iii. We have

$$\mathbf{d}^{(k)} = -\mathbf{g}^{(k)} + \beta_{k-1}\mathbf{d}^{(k-1)}.$$

Hence,

$$\mathbf{d}^{(k)T}\mathbf{g}^{(k)} = -\|\mathbf{g}^{(k)}\|^2 + \beta_{k-1}\mathbf{d}^{(k-1)T}\mathbf{g}^{(k)}.$$

By part c, $\mathbf{d}^{(k-1)T}\mathbf{g}^{(k)} = 0$. Hence, if $\mathbf{g}^{(k)} \neq \mathbf{0}$, then $\|\mathbf{g}^{(k)}\|^2 > 0$, and

$$\mathbf{d}^{(k)T}\mathbf{g}^{(k)} = -\|\mathbf{g}^{(k)}\|^2 < 0.$$

iv. We have $\mathbf{d}^{(k)} = -\mathbf{H}_k\mathbf{g}^{(k)}$. Therefore, if $\mathbf{H}_k > 0$ and $\mathbf{g}^{(k)} \neq \mathbf{0}$, then $\mathbf{d}^{(k)T}\mathbf{g}^{(k)} = -\mathbf{g}^{(k)T}\mathbf{H}_k\mathbf{g}^{(k)} < 0$.

e. Using the equation $\nabla f(\mathbf{x}) = \mathbf{Q}\mathbf{x} - \mathbf{b}$, we get

$$\begin{aligned} \mathbf{d}^{(k)T}\mathbf{g}^{(k+1)} &= \mathbf{d}^{(k)T}(\mathbf{Q}\mathbf{x}^{(k+1)} - \mathbf{b}) \\ &= \mathbf{d}^{(k)T}(\mathbf{Q}(\mathbf{x}^{(k)} + \alpha_k\mathbf{d}^{(k)}) - \mathbf{b}) \\ &= \alpha_k\mathbf{d}^{(k)T}\mathbf{Q}\mathbf{d}^{(k)} + \mathbf{d}^{(k)T}(\mathbf{Q}\mathbf{x}^{(k)} - \mathbf{b}) \\ &= \alpha_k\mathbf{d}^{(k)T}\mathbf{Q}\mathbf{d}^{(k)} + \mathbf{d}^{(k)T}\mathbf{g}^{(k)}. \end{aligned}$$

By part c, $\mathbf{d}^{(k)T}\mathbf{g}^{(k+1)} = 0$, which implies

$$\alpha_k = -\frac{\mathbf{d}^{(k)T}\mathbf{g}^{(k)}}{\mathbf{d}^{(k)T}\mathbf{Q}\mathbf{d}^{(k)}}.$$

11.6 Assuming exact line search, show that if $\mathbf{H}_0 = \mathbf{I}_n$ ($n \times n$ identity matrix), then the first two steps of the BFGS algorithm yield the same points $\mathbf{x}^{(1)}$ and $\mathbf{x}^{(2)}$ as conjugate gradient algorithms with the Hestenes-Stiefel, the Polak-Ribiere, as well as the Fletcher-Reeves formulas.

Ans.: The first step for both algorithms is clearly the same, since in either case we have

$$\mathbf{x}^{(1)} = \mathbf{x}^{(0)} - \alpha_0\mathbf{g}^{(0)}.$$

For the second step,

$$\begin{aligned} \mathbf{d}^{(1)} &= -\mathbf{H}_1\mathbf{g}^{(1)} \\ &= -\left(\mathbf{I}_n + \left(1 + \frac{\Delta\mathbf{g}^{(0)T}\Delta\mathbf{g}^{(0)}}{\Delta\mathbf{g}^{(0)T}\Delta\mathbf{x}^{(0)}}\right) \frac{\Delta\mathbf{x}^{(0)}\Delta\mathbf{x}^{(0)T}}{\Delta\mathbf{x}^{(0)T}\Delta\mathbf{g}^{(0)}} \right. \\ &\quad \left. - \frac{\Delta\mathbf{g}^{(0)}\Delta\mathbf{x}^{(0)T} + (\Delta\mathbf{g}^{(0)}\Delta\mathbf{x}^{(0)T})^T}{\Delta\mathbf{g}^{(0)T}\Delta\mathbf{x}^{(0)}}\right)\mathbf{g}^{(1)} \end{aligned}$$

$$\begin{aligned}
&= -\mathbf{g}^{(1)} - \left(1 + \frac{\Delta \mathbf{g}^{(0)T} \Delta \mathbf{g}^{(0)}}{\Delta \mathbf{g}^{(0)T} \Delta \mathbf{x}^{(0)}} \right) \frac{\Delta \mathbf{x}^{(0)} \Delta \mathbf{x}^{(0)T} \mathbf{g}^{(1)}}{\Delta \mathbf{x}^{(0)T} \Delta \mathbf{g}^{(0)}} \\
&\quad + \frac{\Delta \mathbf{g}^{(0)} \Delta \mathbf{x}^{(0)T} \mathbf{g}^{(1)} + \Delta \mathbf{x}^{(0)} \Delta \mathbf{g}^{(0)T} \mathbf{g}^{(1)}}{\Delta \mathbf{g}^{(0)T} \Delta \mathbf{x}^{(0)}}.
\end{aligned}$$

Since the line search is exact, we have

$$\Delta \mathbf{x}^{(0)T} \mathbf{g}^{(1)} = \alpha_0 \mathbf{d}^{(0)T} \mathbf{g}^{(1)} = 0.$$

Hence,

$$\begin{aligned}
\mathbf{d}^{(1)} &= -\mathbf{g}^{(1)} + \left(\frac{\Delta \mathbf{g}^{(0)T} \mathbf{g}^{(1)}}{\Delta \mathbf{g}^{(0)T} \Delta \mathbf{x}^{(0)}} \right) \Delta \mathbf{x}^{(0)} \\
&= -\mathbf{g}^{(1)} + \left(\frac{\mathbf{g}^{(1)T} \Delta \mathbf{g}^{(0)}}{\Delta \mathbf{g}^{(0)T} \mathbf{d}^{(0)}} \right) \mathbf{d}^{(0)} \\
&= -\mathbf{g}^{(1)} + \beta_0 \mathbf{d}^{(0)}
\end{aligned}$$

where

$$\beta_0 = \frac{\mathbf{g}^{(1)T} \Delta \mathbf{g}^{(0)}}{\mathbf{d}^{(0)T} \Delta \mathbf{g}^{(0)}} = \frac{\mathbf{g}^{(1)T} (\mathbf{g}^{(1)} - \mathbf{g}^{(0)})}{\mathbf{d}^{(0)T} (\mathbf{g}^{(1)} - \mathbf{g}^{(0)})}$$

is the Hestenes-Stiefel update formula for β_0 . Since $\mathbf{d}^{(0)} = -\mathbf{g}^{(0)}$, and $\mathbf{g}^{(1)T} \mathbf{g}^{(0)} = 0$, we have

$$\beta_0 = \frac{\mathbf{g}^{(1)T} (\mathbf{g}^{(1)} - \mathbf{g}^{(0)})}{\mathbf{g}^{(0)T} \mathbf{g}^{(0)}},$$

which is the Polak-Ribiere formula. Applying $\mathbf{g}^{(1)T} \mathbf{g}^{(0)} = 0$ again, we get

$$\beta_0 = \frac{\mathbf{g}^{(1)T} \mathbf{g}^{(1)}}{\mathbf{g}^{(0)T} \mathbf{g}^{(0)}},$$

which is the Fletcher-Reeves formula.