20 points

Convergence of Steepest Descent

In this problem we will bound the error of the steepest descent iterates for the following function

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

where $\mathbf{Q} \in \mathbb{R}^{n\times n}$ is symmetric and positive definite. Recall the steepest descent algorithm starts with an initial guess $\mathbf{x}_0 \in \mathbb{R}^n$ and proceeds to compute successive approximations

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha_k \nabla f(\mathbf{x}_k)$$

where α_k is a line search parameter found by solving the following minimization problem

$$\alpha_k = \underset{\alpha_k}{\operatorname{argmin}} f(\mathbf{x}_k - \alpha_k \nabla f_k),$$

where $\nabla f_k = \nabla f(\mathbf{x}_k)$. To simplify the notation, we denote $||\mathbf{x}||_{\mathbf{Q}}^2 = \mathbf{x}^T\mathbf{Q}\mathbf{x}$ and $\mathbf{x}^*$ minimizes $f(\mathbf{x})$. Please do the following parts.

1. Show that,

$$\alpha_k = \frac{||\nabla f_k||_2^2}{||\nabla f_k||_{\mathbf{Q}}^2}.$$

2. Show that,

$$f(\mathbf{x}_{k+1}) = f(\mathbf{x}_k) - \frac{||\nabla f_k||_2^4}{2||\nabla f_k||_{\mathbf{Q}}^2}.$$

(*Hint:* $\nabla f_k = \mathbf{Q}\mathbf{x}_k - \mathbf{b}$)

3. Show that,

$$\frac{1}{2}||\mathbf{x} - \mathbf{x}^*||_{\mathbf{Q}}^2 = f(\mathbf{x}) - f(\mathbf{x}^*).$$

(*Hint:* $\mathbf{x}^*$ *is the solution to* $\mathbf{Q}\mathbf{x} = \mathbf{b}$)

4. Show that,

$$f(\mathbf{x}_k) = f(\mathbf{x}^*) + \frac{1}{2}||\nabla f_k||_{\mathbf{Q}^{-1}}^2.$$

5. Use the expressions in previous parts to show that,

$$||\mathbf{x}_{k+1} - \mathbf{x}^*||_{\mathbf{Q}}^2 = \left(1 - \frac{||\nabla f_k||_2^4}{||\nabla f_k||_{\mathbf{Q}}^2 ||\nabla f_k||_{\mathbf{Q}^{-1}}^2}\right)||\mathbf{x}_k - \mathbf{x}^*||_{\mathbf{Q}}^2.$$

6. Finally, show that,

$$||\mathbf{x}_{k+1} - \mathbf{x}^*||_{\mathbf{Q}}^2 \leq \left(\frac{\lambda_n - \lambda_1}{\lambda_n + \lambda_1}\right)^2 ||\mathbf{x}_k - \mathbf{x}^*||_{\mathbf{Q}}^2,$$

where λ_1 and λ_n are the smallest and largest eigenvalues of $\mathbf{Q}$ respectively.
Hint: Use Kantorovich's Inequality. For positive reals $v_1, v_2, \dots, v_n$ such that $v_1 \leq v_2 \leq \dots \leq v_n$ and for non-negative reals $w_1, w_2, \dots, w_n$ such that $w_1 + w_2 + \cdots w_n = 1$, we have,

$$(\sum w_i v_i)(\sum w_i v_i^{-1}) \leq \frac{(v_1 + v_n)^2}{4 v_1 v_n}.$$

Be sure to show all your work and provide justifications for every step to receive full credit.

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- write your response out by hand, scan it, and upload it as a PDF.

  We will not accept unprocessed pictures taken with your phone.

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  If you're looking for an easy-ish way to type math, check out TeXmacs (http://texmacs.org/) or LyX (http://www.lyx.org/). Both are installed in the virtual machine. (Under "Applications / Accessories / GNU TeXmacs editor" and "Applications / Office / LyX document processor" respectively.)

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NOTE: Please make sure your solutions are legible and easy to follow. If they are not, we may deduct up to five points *per problem*.

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Your answer is correct.

- Part 1:

  Note that

$$
\begin{aligned}
f(\mathbf{x}_k - \alpha_k \nabla f_k) &= \frac{1}{2}(\mathbf{x}_k - \alpha_k \nabla f_k)^T \mathbf{Q}(\mathbf{x}_k - \alpha_k \nabla f_k) - \mathbf{b}^T(\mathbf{x}_k - \alpha_k \nabla f_k) \\
&= \frac{1}{2}(\mathbf{x}_k^T \mathbf{Q}\mathbf{x}_k - \alpha_k \mathbf{x}_k^T \mathbf{Q}\nabla f_k - \alpha_k \nabla f_k^T \mathbf{Q}\mathbf{x}_k + \alpha_k^2 \nabla f_k^T \mathbf{Q}\nabla f_k) - \mathbf{b}^T \mathbf{x}_k + \alpha_k \mathbf{b}^T \nabla f_k \\
&= \frac{1}{2}(\mathbf{x}_k^T \mathbf{Q}\mathbf{x}_k - 2\alpha_k \nabla f_k^T \mathbf{Q}\mathbf{x}_k + \alpha_k^2 \nabla f_k^T \mathbf{Q}\nabla f_k) - \mathbf{b}^T \mathbf{x}_k + \alpha_k \mathbf{b}^T \nabla f_k \\
&= \frac{1}{2}(\alpha_k^2 \nabla f_k^T \mathbf{Q}\nabla f_k - 2\alpha_k(\nabla f_k^T \mathbf{Q}\mathbf{x}_k - \mathbf{b}^T \nabla f_k) + \mathbf{x}_k^T \mathbf{Q}\mathbf{x}_k - 2\mathbf{b}^T \mathbf{x}_k) \\
&= \frac{1}{2}(\alpha_k^2 \nabla f_k^T \mathbf{Q}\nabla f_k - 2\alpha_k(\nabla f_k^T \nabla f_k) + \mathbf{x}_k^T \mathbf{Q}\mathbf{x}_k - 2\mathbf{b}^T \mathbf{x}_k).
\end{aligned}
$$

  where the third equality follows from the fact that Q is symmetric and the fifth is from the fact that $\nabla f(\mathbf{x}) = \mathbf{Q}\mathbf{x} - \mathbf{b}$

  Note that since Q is positive definite we have that $\nabla f_k^T \mathbf{Q}\nabla f_k > 0$. Therefore the above expression is a quadratic polynomial with a positive leading coefficient. For a quadratic polynomial $ax^2 + bx + c$ with $a > 0$, minimum is when $x = -b/(2a)$.

  This results in the following,

$$
\alpha_k = \frac{\nabla f_k^T \nabla f_k}{\nabla f_k^T \mathbf{Q}\nabla f_k}
$$

- Part 2:

  Reusing our computations from Part 1, we have,

$$
\begin{aligned}
f(\mathbf{x}_{k+1}) &= \frac{1}{2}(\alpha_k^2 \nabla f_k^T \mathbf{Q}\nabla f_k - 2\alpha_k(\nabla f_k^T \nabla f_k) + \mathbf{x}_k^T \mathbf{Q}\mathbf{x}_k - 2\mathbf{b}^T \mathbf{x}_k) \\
&= \frac{1}{2}(\alpha_k^2 \nabla f_k^T \mathbf{Q}\nabla f_k - 2\alpha_k(\nabla f_k^T \nabla f_k) + 2f(x_k)) \\
&= \frac{1}{2}\left(\frac{||\nabla f_k||_2^4}{||\nabla f_k||_{\mathbf{Q}}^4}||\nabla f_k||_{\mathbf{Q}}^2 - 2\frac{||\nabla f_k||_2^2}{||\nabla f_k||_{\mathbf{Q}}^2}||\nabla f_k||_2^2 + 2f(x_k)\right) \\
&= f(\mathbf{x}_k) - \frac{||\nabla f_k||_2^4}{2||\nabla f_k||_{\mathbf{Q}}^2}.
\end{aligned}
$$

- Part 3:

  We will use the fact that the minimum $\mathbf{x}^*$ of $f(\mathbf{x})$ is the solution to the linear system $\mathbf{Q}\mathbf{x} = \mathbf{b}$. This is easily derived similarly to how we derived α_k in Part 1. Note that

$$
\begin{aligned}
\frac{1}{2}||\mathbf{x} - \mathbf{x}^*||_{\mathbf{Q}}^2 &= \frac{1}{2}(\mathbf{x} - \mathbf{x}^*)^T \mathbf{Q}(\mathbf{x} - \mathbf{x}^*) \\
&= \frac{1}{2}(\mathbf{x}^T \mathbf{Q}\mathbf{x} - 2\mathbf{x}^T \mathbf{Q}\mathbf{x}^* + \mathbf{x}^{*T} \mathbf{Q}\mathbf{x}^*) \\
&= \frac{1}{2}(\mathbf{x}^T \mathbf{Q}\mathbf{x} - 2\mathbf{x}^T \mathbf{b} + \mathbf{x}^{*T} \mathbf{b}) \\
&= f(\mathbf{x}) - f(\mathbf{x}^*).
\end{aligned}
$$

since

$$
\begin{aligned}
f(\mathbf{x}^*) &= \frac{1}{2}\mathbf{x}^{*T}\mathbf{Q}\mathbf{x}^* - \mathbf{b}^T\mathbf{x}^* \\
&= \frac{1}{2}\mathbf{x}^{*T}\mathbf{b} - \mathbf{b}^T\mathbf{x}^* \\
&= -\frac{1}{2}\mathbf{x}^{*T}\mathbf{b}.
\end{aligned}
$$

- Part 4:

  To show this we will use the fact that $\mathbf{x}_k = \mathbf{Q}^{-1}(\nabla f_k + \mathbf{b})$. Plugging this in we have,

$$
\begin{aligned}
f(\mathbf{x}_k) - f(\mathbf{x}^*) &= \frac{1}{2}\langle \mathbf{x}_k, \mathbf{Q}\mathbf{x}_k\rangle - \langle \mathbf{x}_k, \mathbf{b}\rangle + \frac{1}{2}\mathbf{x}^{*T}\mathbf{b} \\
&= \frac{1}{2}\langle \mathbf{x}_k, \nabla f_k + \mathbf{b}\rangle - \langle \mathbf{x}_k, \mathbf{b}\rangle + \frac{1}{2}\langle \mathbf{x}^*, \mathbf{b}\rangle \\
&= \frac{1}{2}\langle \mathbf{x}_k, \nabla f_k\rangle - \frac{1}{2}\langle \mathbf{x}_k, \mathbf{b}\rangle + \frac{1}{2}\langle \mathbf{x}^*, \mathbf{b}\rangle \\
&= \frac{1}{2}\langle \mathbf{Q}^{-1}(\nabla f_k + \mathbf{b}), \nabla f_k\rangle - \frac{1}{2}\langle \mathbf{Q}^{-1}(\nabla f_k + \mathbf{b}), \mathbf{b}\rangle + \frac{1}{2}\langle \mathbf{Q}^{-1}\mathbf{b}, \mathbf{b}\rangle \\
&= \frac{1}{2}\langle \mathbf{Q}^{-1}(\nabla f_k + \mathbf{b}), \nabla f_k\rangle - \frac{1}{2}\langle \mathbf{Q}^{-1}\nabla f_k, \mathbf{b}\rangle \\
&= \frac{1}{2}\langle \mathbf{Q}^{-1}\nabla f_k, \nabla f_k\rangle
\end{aligned}
$$

  Last equality is because $\mathbf{Q}$ is symmetric $\implies \langle \mathbf{Q}^{-1}\mathbf{b}, \nabla f_k\rangle = \langle \mathbf{Q}^{-1}\nabla f_k, \mathbf{b}\rangle$

- Part 5:

  From part 3, the inequality we want to prove becomes

$$
f(\mathbf{x}_{k+1}) - f(\mathbf{x}^*) = \left(1 - \frac{(||\nabla f_k||_2^4}{||\nabla f_k||_{\mathbf{Q}}^2\,||\nabla f_k||_{\mathbf{Q}^{-1}}^2}\right)(f(\mathbf{x}_k) - f(\mathbf{x}^*))
$$

  From part 2, we have,

$$
\begin{aligned}
f(\mathbf{x}_{k+1}) - f(\mathbf{x}^*) &= f(\mathbf{x}_{k+1}) - f(\mathbf{x}_k) + f(\mathbf{x}_k) - f(\mathbf{x}^*) \\
&= -\frac{||\nabla f_k||_2^4}{2||\nabla f_k||_{\mathbf{Q}}^2} + f(\mathbf{x}_k) - f(\mathbf{x}^*) \\
&= \left(1 - \frac{(||\nabla f_k||_2^4}{2||\nabla f_k||_{\mathbf{Q}}^2(f(\mathbf{x}_k) - f(\mathbf{x}^*))}\right)(f(\mathbf{x}_k) - f(\mathbf{x}^*)) \\
&= \left(1 - \frac{(||\nabla f_k||_2^4}{||\nabla f_k||_{\mathbf{Q}}^2\,||\nabla f_k||_{\mathbf{Q}^{-1}}^2}\right)(f(\mathbf{x}_k) - f(\mathbf{x}^*)).
\end{aligned}
$$

  The second equality is from Part 2 and fourth equality is from Part 4.

- Part 6:

  Consider the eigenvalue decompositions $\mathbf{Q} = \mathbf{V}\boldsymbol{\Lambda}\mathbf{V}^T$ and $\mathbf{Q}^{-1} = \mathbf{V}\boldsymbol{\Lambda}^{-1}\mathbf{V}^T$ and let $\mathbf{u} = \nabla f_k, \mathbf{y} = \mathbf{V}^T\mathbf{u}$

  Substituting these values in we have that

$$\frac{(\mathbf{u}^T\mathbf{u})^2}{(\mathbf{u}^T\mathbf{Q}\mathbf{u})(\mathbf{u}^T\mathbf{Q}^{-1}\mathbf{u})} = \frac{(\mathbf{y}^T\mathbf{y})^2}{(\mathbf{y}^T\mathbf{\Lambda}\mathbf{y})(\mathbf{y}^T\mathbf{\Lambda}^{-1}\mathbf{y})} = \frac{1}{(\frac{\mathbf{y}^T\mathbf{\Lambda}\mathbf{y}}{\mathbf{y}^T\mathbf{y}})(\frac{\mathbf{y}^T\mathbf{\Lambda}^{-1}\mathbf{y}}{\mathbf{y}^T\mathbf{y}})} = \frac{1}{(\frac{\sum y_i^2\lambda_i}{\sum y_i^2})(\frac{\sum y_i^2\lambda_i^{-1}}{\sum y_i^2})}$$

Let $w_i = \frac{y_i^2}{\sum y_i^2}$ and note that $0 \le w_i \le 1$ for all $i = 1, \ldots, n$ and $\sum_i^n w_i = 1$. And so

$$\frac{1}{(\frac{\sum y_i^2\lambda_i}{\sum y_i^2})(\frac{\sum y_i^2\lambda_i^{-1}}{\sum y_i^2})} = \frac{1}{(\sum w_i\lambda_i)(\sum w_i\lambda_i^{-1})}$$

From Kantorovich Inequality we get,

$$\frac{1}{(\sum w_i\lambda_i)(\sum w_i\lambda_i^{-1})} \ge \frac{4\lambda_1\lambda_n}{(\lambda_1+\lambda_n)^2}$$

Using the results of Part 2 we have that

$$\begin{aligned} ||\mathbf{x}_{k+1} - \mathbf{x}^*||_{\mathbf{Q}}^2 &= \left(1 - \frac{(\nabla f_k^T\nabla f_k)^2}{(\nabla f_k^T\mathbf{Q}\nabla f_k)(\nabla f_k^T\mathbf{Q}^{-1}\nabla f_k)}\right)||\mathbf{x}_k - \mathbf{x}^*||_{\mathbf{Q}}^2 \\ &\le \left(1 - \frac{4\lambda_n\lambda_1}{(\lambda_n+\lambda_1)^2}\right)||\mathbf{x}_k - \mathbf{x}^*||_{\mathbf{Q}}^2 \end{aligned}$$

With a bit of algebra, we see that

$$\begin{aligned} 1 - \frac{4\lambda_n\lambda_1}{(\lambda_n+\lambda_1)^2} &= \frac{(\lambda_n+\lambda_1)^2 - 4\lambda_n\lambda_1}{(\lambda_n+\lambda_1)^2} \\ &= \left(\frac{\lambda_n-\lambda_1}{\lambda_n+\lambda_1}\right)^2. \end{aligned}$$

- Proof of Kantorovich's inequality (you don't need to show this)

  For each i, define p_i and q_i as the solution to the following equations

$$\begin{cases} v_i = p_i v_n + q_i v_1 \\ v_i^{-1} = p_i v_n^{-1} + q_i v_1^{-1} \end{cases}$$

  Solving this system of equations will yield

$$p_i = \frac{v_i/v_1 - v_1/v_i}{v_n/v_1 - v_1/v_n} \ge 0$$

  Similarly, we can show $q_i \ge 0$. Then since

$$1 = v_i v_i^{-1} = (p_i v_n + q_i v_1)(p_i v_n^{-1} + q_i v_1^{-1}) = (p_i+q_i)^2 + p_i q_i (v_n - v_1)^2/(v_n v_1)$$

  we know $p_i + q_i \le 1$.

  Setting $p = \sum w_i p_i$ and $q = \sum w_i q_i$, we have

$$p + q = \sum w_i(p_i+q_i) \le \sum w_i = 1$$

  Then,

$$(\sum w_i v_i)(\sum w_i v_i^{-1}) = (pv_n + qv_1)(pv_n^{-1} + qv_1^{-1}) = (p+q)^2 + pq\frac{(v_n - v_1)^2}{v_n v_1}$$

Since $(p-q)^2 \geq 0 \implies 4pq \leq (p+q)^2$,

$$(p+q)^2 + pq\frac{(v_n - v_1)^2}{v_n v_1} \leq (p+q)^2\left[1 + \frac{(v_n - v_1)^2}{4v_n v_1}\right] = (p+q)^2\frac{(v_n + v_1)^2}{4v_n v_1} \leq \frac{(v_n + v_1)^2}{4v_n v_1}$$

Reference: https://www.jstor.org/stable/pdf/2311698.pdf#page=3