Numerical Optimization, Fall 2020
Homework 8

Due 14:59 (CST), Dec. 10, 2020
(NOTE: Homework will not be accepted after this due for any reason.)

Throughout this assignment, we focus on the following trust region subproblem, which reads

$$\begin{aligned} \min_{\boldsymbol{d}\in\mathbb{R}^n} \quad & m_k(\boldsymbol{d}) := f(\boldsymbol{x}_k) + \nabla f(\boldsymbol{x}_k)^T \boldsymbol{d} + \tfrac{1}{2}\boldsymbol{d}^T H_k \boldsymbol{d} \\ \text{s.t.} \quad & \|\boldsymbol{d}\| \le \Delta_k, \end{aligned} \tag{1}$$

where $\Delta_k > 0$ is the trust-region radius.

Note: Throughout this assignment, the notion of positive definiteness applies exclusively to symmetric matrices. Thus whenever we say that a matrix is positive (semi)definite, we implicitly assume that the matrix is symmetric.

1 Cauchy point calculation

[20pts] Please write down a closed-form expression of the Cauchy point. (Make sure you provided detailed proof; otherwise you won't earn marks.)

Specifically, first solve the a linear version of (1) to obtain vector $\boldsymbol{d}_k^s$, that is,

$$\boldsymbol{d}_k^s = \arg\min_{\boldsymbol{d}\in\mathbb{R}^n} f(\boldsymbol{x}_k) + \nabla f(\boldsymbol{x}_k)^T \boldsymbol{d} \qquad \text{s.t.} \quad \|\boldsymbol{d}\| \le \Delta_k. \tag{2}$$

Then, calculate the scalar $\tau_k > 0$ that minimizes $m_k(\tau \boldsymbol{d}_k^s)$ subject to the trust region bound, that is

$$\tau_k = \arg\min_{\tau\ge 0} \; m_k(\tau \boldsymbol{d}_k^s) \qquad \text{s.t.} \quad \|\tau \boldsymbol{d}_k^s\| \le \Delta_k. \tag{3}$$

Set $\boldsymbol{d}_k^c = \tau_k \boldsymbol{d}_k^s$.

Solution: First, it is easy to obtain the solution of (2), which reads

$$\boldsymbol{d}_k^s = -\frac{\Delta_k}{\|\nabla f(\boldsymbol{x}^k)\|}\nabla f(\boldsymbol{x}^k). \tag{4}$$

To obtain τ_k, we consider two cases

1. Suppose $\nabla f(\boldsymbol{x}^k)^T H_k \nabla f(\boldsymbol{x}^k) \le 0$. Then the function $m(\tau \boldsymbol{d}_k^s)$ decreases monotonically with τ whenever $\nabla f(\boldsymbol{x}^k) \neq \boldsymbol{0}$. Therefore, τ_k is simply the largest value that satisfies the trust-region bound, namely, $\tau_k = 1$.
2. Suppose $\nabla f(\boldsymbol{x}^k)^T H_k \nabla f(\boldsymbol{x}^k) > 0$. Then $m(\tau \boldsymbol{d}_k^s)$ is a convex quadratic in τ, so τ_k is either the unconstrained minimizer of this quadratic, $\|\nabla f(\boldsymbol{x}^k)\|^3/(\Delta_k \nabla f(\boldsymbol{x}^k)^T H_k \nabla f(\boldsymbol{x}^k))$, or the boundary value 1, whichever comes first.

   Overall, we have

$$\boldsymbol{d}_k^c = -\tau_k \frac{\Delta_k}{\|\nabla f(\boldsymbol{x}^k)\|}\nabla f(\boldsymbol{x}^k), \tag{5}$$

   where

$$\tau_k = \begin{cases} 1 & \text{if } \nabla f(\boldsymbol{x}^k)^T H_k \nabla f(\boldsymbol{x}^k) \le 0, \\ \min(1, \|\nabla f(\boldsymbol{x}^k)\|^3/(\Delta_k \nabla f(\boldsymbol{x}^k)^T H_k \nabla f(\boldsymbol{x}^k))) & \text{otherwise.} \end{cases}$$

2 Local convergence for trust region methods

[20pts] Given a step $\boldsymbol{d}_k$, consider the ratio (with positive denominator):

$$\rho_k := \frac{f(\boldsymbol{x}_k) - f(\boldsymbol{x}_k + \boldsymbol{d}_k)}{m_k(\boldsymbol{0}) - m_k(\boldsymbol{d}_k)}. \tag{6}$$

Show that if $\Delta_k \to 0$, then $\rho_k \to 1$. (This proves that for Δ_k sufficiently small, $m_k(\boldsymbol{d})$ approximates $f(\boldsymbol{x}_k + \boldsymbol{d}_k)$ well.)

Solution: For the sake of simplicity, we use Pred_k and Ared_k to denote the predicted reduction (i.e., $m_k(\boldsymbol{0}) - m_k(\boldsymbol{d}_k)$) and the actual reduction (i.e., $f(\boldsymbol{x}_k) - f(\boldsymbol{x}_k + \boldsymbol{d}_k)$), respectively. Then, equivalently,

$$\rho_k = \frac{\text{Ared}_k}{\text{Pred}_k}. \tag{7}$$

Proof. Suppose $\lim\limits_{k\to\infty} \boldsymbol{d}_k = \boldsymbol{0}$. Then, we have

$$\begin{aligned}
|\rho_k - 1| &= \frac{\text{Ared}_k - \text{Pred}_k}{\text{Pred}_k} \\
&= \frac{o(\|\boldsymbol{d}_k\|) + O(\|\boldsymbol{d}_k\|^2 \|H_k\|)}{\text{Pred}_k} \\
&\le \frac{o(\|\boldsymbol{d}_k\|) + O(\|\boldsymbol{d}_k\|^2 \|H_k\|)}{\|\nabla f(\boldsymbol{x}^k)\| \min\{\Delta_k, \|\nabla f(\boldsymbol{x}^k)\|/\|H_k\|\}} \\
&\le \frac{o(\|\boldsymbol{d}_k\|)}{\Delta_k} \\
&\to 0,
\end{aligned} \tag{8}$$

where the first inequality holds due to the fact that $\text{Pred}_k \ge \frac{1}{2}\|\nabla f(\boldsymbol{x}^k)\| \min\{\Delta_k, \|\nabla f(\boldsymbol{x}^k)\|/\|H_k\|\}$ (e.g., see the proof in [1, Lemma 4.3]). Therefore

$$\lim_{k\to\infty} \rho_k = 1.$$

This completes the proof. □

3 Exact line search

[20pts] Consider minimizing the following quadratic function

$$\min_{\boldsymbol{x}\in\mathbb{R}^n} \quad f(\boldsymbol{x}) = \tfrac{1}{2}\boldsymbol{x}^T Q \boldsymbol{x} - \boldsymbol{b}^T \boldsymbol{x}, \tag{9}$$

where $Q \in \mathbb{R}^{n\times n}$ is positive definite and $\boldsymbol{b} \in \mathbb{R}^n$.

Let $\boldsymbol{d}_k$ be a descent direction at the kth iterate. Suppose that we search along this direction from $\boldsymbol{x}^k$ for a new iterate, and the line search are exact. Please find the stepsize α. This can be achieved exactly solving the following one-dimensional minimization problem

$$\min_{\alpha>0} \quad f(\boldsymbol{x}_k + \alpha \boldsymbol{d}_k). \tag{10}$$

Solution: Keep in mind that our goal is to choose $\alpha > 0$ to minimize $f(\boldsymbol{x}_{k+1})$. Toward achieving this, we let $g(\alpha) = f(\boldsymbol{x}_k + \alpha \boldsymbol{d}_k) = \frac{1}{2}(\boldsymbol{x}_k + \alpha \boldsymbol{d}_k)^T Q \boldsymbol{x}_k + \alpha \boldsymbol{d}_k - \boldsymbol{b}^T \boldsymbol{x}_k + \alpha \boldsymbol{d}_k$. It should be noticed that $g(\alpha)$ is quadratic and convex since Q is positive definite. Then, $g(\alpha) = a\alpha^2 + d\alpha + c$ with $a = \frac{1}{2}\boldsymbol{d}_k^T Q \boldsymbol{d}_k$, $d = (Q^T \boldsymbol{x}_k - b)^T \boldsymbol{d}_k$ and $c = \frac{1}{2}\boldsymbol{x}_k^T Q \boldsymbol{x}_k - \boldsymbol{b}^T \boldsymbol{x}_k$. Therefore, $-\frac{d}{2a} = \arg\min_{\alpha>0} g(\alpha)$. This leads to

$$\alpha = \frac{(\boldsymbol{b} - Q^T \boldsymbol{x}_k)^T \boldsymbol{d}_k}{\boldsymbol{d}_k^T Q \boldsymbol{d}_k}.$$

4 The conjugate gradient algorithm

[20pts] Let $A \in \mathbb{R}^{n\times n}$ be a positive definite matrix. Show that if the directions $\boldsymbol{d}_0, \ldots, \boldsymbol{d}_k \in \mathbb{R}^n$, $k \le n-1$, are A-conjugate, then they are linearly independent. (Hint: We say that a set of nonzero vectors $\boldsymbol{d}_1, \ldots, \boldsymbol{d}_m \in \mathbb{R}^n$ are A-conjugate if $\boldsymbol{d}_i^T A \boldsymbol{d}_j = 0, \ \forall i, j, \ \ i \neq j$.)

Solution:

Proof. We prove this by contradiction. Suppose this is not true. Then there exits $\alpha_0, \ldots, \alpha_k$ not all zeros such that

$$\alpha_0 \boldsymbol{d}_0 + \alpha_1 \boldsymbol{d}_1 + \ldots + \alpha_k \boldsymbol{d}_k = 0. \tag{11}$$

Without loss generality, we assume $\alpha_0 \neq 0$. Multiplying $\boldsymbol{d}_0^T A$ on both sides of (11), we have

$$\alpha_0 \boldsymbol{d}_0^T A \boldsymbol{d}_0 + \alpha_1 \boldsymbol{d}_0^T A \boldsymbol{d}_1 + \ldots + \alpha_k \boldsymbol{d}_0^T A \boldsymbol{d}_k = 0, \tag{12}$$

where all but the first term vanish becauseof A-conjugate. This implies

$$\alpha_0 \boldsymbol{d}_0^T A \boldsymbol{d}_0 = 0.$$

On the other hand, since $\boldsymbol{d}_0 \neq \mathbf{0}$ and A is positive definite, we have $\boldsymbol{d}_0^T A \boldsymbol{d}_0 > 0$. It therefore leads to $\alpha_0 \boldsymbol{d}_0^T A \boldsymbol{d}_0 \neq 0$. This contradiction completes the proof. □

5 Trust region subproblems

Consider the trust region subproblem (1), and H_k is positive definite. Let θ_k denote the angle between $\boldsymbol{d}_k$ and $-\nabla f(\boldsymbol{x}_k)$, defined by

$$\cos\theta_k = \frac{-\nabla f(\boldsymbol{x}_k)^T \boldsymbol{d}_k}{\|\nabla f(\boldsymbol{x}_k)\| \|\boldsymbol{d}_k\|}. \tag{13}$$

Show that

(i) [10pts] For sufficiently large Δ_k, the trust region subproblem (1) will be solved by the Newton step.

(ii) [10pts] When Δ_k approaches 0, the angle $\theta_k \to 0$.

Solution:

(i) The trust region subproblem is equivalent to an unconstrained subproblem

$$\min_{\boldsymbol{d}\in\mathbb{R}^n} \ f(\boldsymbol{x}_k) + \nabla f(\boldsymbol{x}_k)^T \boldsymbol{d}_k + \tfrac{1}{2} \boldsymbol{d}_k (H_k + \lambda I) \boldsymbol{d}_k \tag{14}$$

for some constant $\lambda \ge 0$ such that $H_k + \lambda I \succeq \mathbf{0}$. Therefore, $\boldsymbol{d}_k$ is a global solution of (1) if and only if for some $\lambda \ge 0$ we have

$$(H_k + \lambda I)\boldsymbol{d}_k = -\nabla f(\boldsymbol{x}^k) \tag{15a}$$
$$H_k + \lambda I \succeq \mathbf{0} \tag{15b}$$
$$\lambda(\|\boldsymbol{d}_k\| - \Delta_k) = 0. \tag{15c}$$

Note that $\|\boldsymbol{d}_k\| < \Delta_k$ for sufficiently large Δ_k. Then by (15a) and (15c), we know $\lambda = 0$, and consequently, $\boldsymbol{d}_k$ is the Newton direction. This completes the statement.

(ii) *Proof.* First, by (15a), it implies

$$\boldsymbol{d}_k = -(H_k + \lambda I)^{-1} \nabla f(\boldsymbol{x}^k) \tag{16}$$

It then follows from (16) that $\lambda \to \infty$ as $\Delta_k \to 0$.

Then, we show $\cos\theta_k \to 1$. To see this, we plug (16) into (13), and we have for $\lambda \to \infty$

$$\begin{aligned}
\cos\theta_k &= \frac{\langle \nabla f(\boldsymbol{x}^k), (H_k + \lambda I)^{-1} \nabla f(\boldsymbol{x}^k) \rangle}{\|\nabla f(\boldsymbol{x}^k)\| \|(H_k + \lambda I)^{-1} \nabla f(\boldsymbol{x}^k)\|} \\
&\geq \frac{\langle \nabla f(\boldsymbol{x}^k), (H_k + \lambda I)^{-1} \nabla f(\boldsymbol{x}^k) \rangle}{\|\nabla f(\boldsymbol{x}^k)\|^2 \|(H_k + \lambda I)^{-1}\|} \\
&\geq \frac{\lambda_{\min}((H_k + \lambda I)^{-1}) \|\nabla f(\boldsymbol{x}^k)\|^2}{\lambda_{\max}((H_k + \lambda I)^{-1}) \|\nabla f(\boldsymbol{x}^k)\|^2} \\
&= \frac{\lambda_{\min}((H_k + \lambda I)^{-1})}{\lambda_{\max}((H_k + \lambda I)^{-1})} \\
&= \frac{\lambda_{\max}(H_k) + \lambda}{\lambda_{\min}(H_k) + \lambda} \\
&\to 1.
\end{aligned} \tag{17}$$

This completes the proof. □

References

[1] J. Nocedal and S. Wright, *Numerical optimization*. Springer Science & Business Media, 2006.