Exercises: Line search and trust region methods

Optimisation - Fall 2023 Jaime Sánchez Salazar

Exercise 1

Although the exercise asks us to start by demonstrating that p_k is a descent direction we will start computing the first 5 starts of the descent algorithm due to the importance of it.

$$k = 0; \quad x_1 = x_0 + \alpha_0 p_0 = x_0 + \alpha_0 (-sign(x_0)) = 2 + (2 + \frac{3}{2})(-1) = -\frac{3}{2}$$

$$k = 1; \quad x_2 = x_1 + \alpha_1 p_1 = x_1 + \alpha_1 (-sign(x_1)) = -\frac{3}{2} + (2 + \frac{3}{2^2})(1) = \frac{5}{4}$$

$$k = 2; \quad x_3 = x_2 + \alpha_2 p_2 = x_2 + \alpha_2 (-sign(x_2)) = \frac{5}{4} + (2 + \frac{3}{2^3})(-1) = -\frac{9}{8}$$

$$k = 3; \quad x_4 = x_3 + \alpha_3 p_3 = x_3 + \alpha_3 (-sign(x_3)) = -\frac{9}{8} + (2 + \frac{3}{2^4})(1) = \frac{17}{16}$$

$$k = 4; \quad x_5 = x_4 + \alpha_4 p_4 = x_4 + \alpha_4 (-sign(x_4)) = \frac{17}{16} + (2 + \frac{3}{2^5})(-1) = -\frac{33}{32}$$

Looking at the iterations, one can see that denominator is always a power of 2 and the numerator a power of 2 plus 1 and also we can see that the sign of x_k is always changing. With all this, one propose the following formula:

$$x_k = (-1)^k \frac{2^k + 1}{2^k}$$

Let's prove that, in fact, this formula expresses the same as the x_k given by the descent algorithm. We will proceed to show it using induction. When k=0, the initial case, $x_0=1\cdot\frac{2^0+1}{2^0}=2$, which matches the initial value. Let's suppose the statement true until to a certain k and let's prove that's also true for k+1. Note that

$$x_{k+1} - x_k = (-1)^{k+1} \frac{2^{k+1} + 1}{2^{k+1}} - (-1)^k \frac{2^k + 1}{2^k} = \frac{(-1)^{k+1} (2^{k+1} + 1 + 2^{k+1} + 2)}{2^{k+1}} = \frac{(-1)^{k+1} (2^{k+2} + 3)}{2^{k+1}} = (-1)^{k+1} (2 + 3(2^{-k-1}).$$

Also, from the descent algorithm we have that

$$x_{k+1} - x_k = \alpha_k p_k = (2 + 3(2^{-k-1}))(-sign(x_k))$$

but, as $x_k = (-1)^k \frac{2^k + 1}{2^k}$ we have that $sign(x_k) = (-1)^k$. Thus, substituting this in the previous expression we obtain

$$x_{k+1} - x_k = (2 + 3(2^{-k-1}))(-(-1)^k) = (2 + 3(2^{-k-1}))(-1)^{k+1}.$$

Therefore, we've proved the statement for n = k + 1 and then both formulas are equivalent.

With this, proving that $f(x_{k+1}) < f(x_k)$ is a straightforward computation. In fact,

$$f(x_{k+1}) = [(-1)^{k+1} \frac{2^{k+1}+1}{2^{k+1}}]^2 < [(-1)^k \frac{2^k+1}{2^k}]^2 = f(x_k) \iff (\frac{2^{k+1}+1}{2^{k+1}})^2 < (\frac{2^k+1}{2^k})^2 \iff 2^k - 2^{k+1} - \frac{3}{4} < 0 \iff 2^k > -\frac{3}{4}$$

But the last expression is always satisfied as $k \in \mathbb{Z}$.

Finally, let's answer section 3. It's easy to see that the minimum of $f(x) = x^2$ is reached at x = 0. However as k goes to infinity, in the expression $x_k = (-1)^k \frac{2^k+1}{2^k}$, we can see that the fraction tends to 1 but the term $(-1)^k$ will be changing between 1 and -1 constantly. So, it's obvious that this descent will not converge. Regarding to the Wolfe conditions, only one of them is being violated. Let's see it. Note that both conditions can be reformulated in the following way:

$$f(x_k + \alpha_k p_k) < f(x_k) + c_1 \alpha_k (\nabla f(x_k))^T p_k \iff f(x_{k+1}) - f(x_k) < -2c_1 \alpha_k |x_k| (\nabla f(x_k + \alpha_k p_k))^T p_k \ge c_2 (\nabla f(x_k))^T p_k \iff |x_{k+1}| \ge -c_2 |x_k|$$

Where we have used that $x_{k+1} = x_k + \alpha_k p_k$, $|x_k| = x_k (sign(x_k))$, $sign(x_k) = -sign(x_{k+1})$ and that $\nabla f(x_k) = 2x_k$.

Having said that, note that if k goes to infinity as $x_k = (-1)^k \frac{2^k + 1}{2^k}$, we have that x_{k+1} and x_k will be 1 or -1. Suppose, without loss of generality, that $x_{k+1} = 1$ and $x_k = -1$, then $f(x_{k+1}) = f(x_k) = 1$ and from the first Wolfe condition we obtain:

$$0 < -2c_1\alpha_k$$

As $\alpha_k > 0$ the previous inequality is equivalent to $c_1 < 0$, but this can not be true, since we impose c_1 to be positive.

As for the second condition, note that as , $x_k \neq 0 \ \forall k \geq 0$, it can be rewritten as $c_2 \geq -\frac{|x_{k+1}|}{|x_k|}$ but this inequality will always be true because $c_2 > 0$.

Exercise 2

We want to minimise the function $m_k(p_k) = f_k + G_k \cdot p_k + \frac{1}{2}p_k^T \cdot B_k \cdot p_k$ subject to $||p_k|| < \delta$. In order to do that, we will prove the following:

1)
$$p_k^l := \arg \min_{p \in \mathbb{R}^n, ||p|| < \delta} (f_k + G_k \cdot p) = -\frac{\delta}{||G_k||} G_k$$

2)
$$\tau_k := \arg\min_{\tau \in \mathbb{R}, ||\tau p_k^l|| < \delta} (m_k(\tau p_k^l)) = \begin{cases} 1 & \text{if } G_k B_k G_k^T \leq 0 \\ \min\{1, \hat{\tau_k}\} & \text{otherwise} \end{cases}$$
 where $\hat{\tau_k} = \frac{||G_k||^3}{\delta G_k B_k G_k^T}$

Let's start proving the first statement.

$$\arg\min_{p\in\mathbb{R}^n,||p||<\delta}(f_k+G_k\cdot p)=\arg\min(G_k\cdot p)=\arg\min(||G_k||||p||\cos(\alpha_k))$$
$$=\arg\min(||p||\cos(\alpha_k))$$

We first delete the dependence of f_k because given x_{k-1} it's a fixed value. Then we have the scalar product between G_k and p, and we substitute it by its definition. Hence, α_k is the angle between G_k and p. Now, by the same reason than before we can delete $||G_k||$ and, in order to minimise the expression $||p||\cos(\alpha_k)$ we want the cosine to be as negative as possible and ||p|| as big as possible. Therefore, $\alpha_k = \pi(+2\pi n)$ that is, $p = -G_k$. Finally, the modulus of p can be, at most, δ , so in total, we have that $p = -\frac{\delta}{||G_k||}G_k$ as we wanted to show.

About the second statement:

$$\tau_k := \arg\min_{\tau \in \mathbb{R}, ||\tau p_k^l|| < \delta} (m_k(\tau p_k^l)) = \arg\min(f_k + \tau G_k \cdot p_k^l + \frac{\tau^2}{2} p_k^l \cdot B_k \cdot p_k^l) = \arg\min(\frac{-\tau \delta}{||G_k||} G_k^2 + \frac{\tau^2 \delta^2}{2} \frac{G_k \cdot B_k \cdot G_k^T}{||G_k||^2})$$

Again, we first deleted the dependence of f_k . Then we substitute the value of p_k^l by the previous value that we just proved. Note that now we have a second order equation as a function of τ . We know that the minimum of this equation will be at $\tau_{min} = \frac{-b}{2a}$, that is, at $\tau_{min} = \frac{\delta G_k^2 \cdot ||G_k||^2}{||G_k||\delta^2 G_k \cdot B_k \cdot G_k^T} = \frac{||G_k||^3}{\delta G_k \cdot B_k \cdot G_k^T}$ due to $G_k^2 = ||G_k||^2$.

We will now distinguish cases, if $G_k \cdot B_k \cdot G_k^T > 0$, then $\tau_{min} > 0$ but taking into account that from the conditions $||\tau p_k^l|| < \delta$ and $\tau_k > 0$, we obtain that $|\tau| < 1 \Longrightarrow 0 < \tau < 1$, so we obtain that τ_k will be the minimum number between τ_{min} and 1.

Otherwise, if $G_k \cdot B_k \cdot G_k^T \leq 0$ note that the expression that we want to minimise $\frac{-\tau \delta}{||G_k||} G_k^2 + \frac{\tau^2 \delta^2}{2} \frac{G_k \cdot B_k \cdot G_k^T}{||G_k||^2}$ is negative. So, if we want to minimise it we want τ to be as big as possible, that is $\tau = 1$ (In fact if $G_k \cdot B_k \cdot G_k^T < 0$ note that we

obtain a parabola that has a maximum, and not a minimum).

To summarise the information, we can conclude saying that:
$$\tau_k = \begin{cases} 1 & \text{if } G_k B_k G_k^T \leq 0 \\ min\{1, \tau_{min}\} & \text{otherwise} \end{cases} \text{ where } \tau_{min} = \frac{||G_k||^3}{\delta G_k B_k G_k^T}$$

Exercise 3

Let $f(x_1, x_2) = (1-x_1)^2 + 5(x_2-x_1^2)^2$ be the Rosenbrock function with a=1 and b=5. We will implement 2 steps of Cauchy point search for $f(x_1,x_2)$ starting at $x_0 = (-2, -2)$ and with the trust regions being balls of radius $\varepsilon = 0.5$. Just for notation we will rewrite the function as $f(x,y) = (1-x)^2 + 5(y-x^2)^2$, that is, we are setting $(x_1, x_2) = (x, y)$

Let's start computing the gradient and the hessian of f(x, y):

$$\nabla f(x,y) = (-2(1-x) - 20x(y-x^2), 10(y-x^2)$$
$$\nabla^2 f(x,y) = \begin{pmatrix} 2 - 20(y-3x^2) & -20x \\ -20x & 10 \end{pmatrix}$$

In order to solve this exercise we will use the results and the notation given in the previous exercise. To compute the first step we have that: $f_1 = f(-2, -2) =$

189,
$$G_1 = \nabla f(-2, -2)^T = (-246, -60), B_1 = \nabla^2 f(-2, -2) = \begin{pmatrix} 282 & 40 \\ 40 & 10 \end{pmatrix}$$

Hence, the function that we want to minimise is the following: $m_1(p_1) = (-246, -60)$

$$f_1 + G_1 p_1 + \frac{1}{2} p_1^T \begin{pmatrix} 282 & 40 \\ 40 & 10 \end{pmatrix} p_1$$

Let's find the point p_1^l and the scalar τ_1 defined in the previous exercise.

$$p_1^l = -\frac{0.5(-246, -60)^T}{||(-246, -60)||}$$

$$G_1 B_1 G_1^T = (-246, -60) \begin{pmatrix} 282 & 40 \\ 40 & 10 \end{pmatrix} (-246, -60)^T = 1.83 \cdot 10^7 > 0.$$

As for the scalar τ_1

$$\tau_1 = \begin{cases} 1 & \text{if } G_1 B_1 G_1^T \le 0 \\ \min\{1, \hat{\tau_1}\} & \text{otherwise} \end{cases}$$

$$\begin{split} \tau_1 &= \begin{cases} 1 & \text{if } G_1B_1G_1^T \leq 0 \\ \min\{1,\hat{\tau_1}\} & \text{otherwise} \end{cases} \\ \text{Where } \hat{\tau_1} &= \frac{||G_1||^3}{\delta G_1B_1G_1^T}, \text{ that is } \hat{\tau_1} &= \frac{||(-246,-60)||^3}{0.5\cdot 1,83\cdot 10^7} \approx 1,77; \text{ which implies that } \\ \tau_1 &= 1. \text{ Now, } p_1^C &= \tau_1 p_1^l. \end{split}$$

With this we have that $x_1 = x_0^T + p_1^C = (-2, -2)^T - \frac{0.5(-246, -60)^T}{||-246, -60)||} = (-1, 514; -1, 882)$ Let's compute the second step: $f_2 = f(x_1) = 93, 45$, $G_2 = \nabla f(x_1)^T = (-131, 43; -41, 74), B_2 = \nabla^2 f(x_1) = \begin{pmatrix} 177, 17 & 30, 28 \\ 30, 28 & 10 \end{pmatrix}$

Again, studying p_2^C :

$$p_2^l = -\frac{0.5(-131,43;-41,74)^T}{||(-131,43;-41,74)||} \text{ and } G_2 B_2 G_2^T = (-131,43;-41,74) \begin{pmatrix} 177,17 & 30,28 \\ 30,28 & 10 \end{pmatrix} = (-131,43;-41,74)^T = 3.41 \cdot 10^6 > 0. \text{ So we need to calculate } \hat{\tau_2}, \ \hat{\tau_2} = \frac{116(-131,43;-41,74)^T}{112} = \frac{112}{2} + \frac{112}$$

 $\frac{||(-131,43;-41,74)||^3}{0.5\cdot 3.41\cdot 10^6}\approx 1,54 \text{ which implies, again, that } \tau_2=1.$

Finally,
$$x_2 = x_1^T + p_2^C = (-1, 514; -1, 882)^T - \frac{0.5(-131, 43; -41, 74)^T}{||(-131, 43; -41, 74)||} = (-1, 037; -1, 731).$$
 Concluding, we have computed that $x_1 = (-1, 514; -1, 882)$ and $x_2 = (-1, 037; -1, 731)$.