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## Solutions to exercise set 3

1 Consider the quadratic function

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

where $Q \in \mathbb{R}^{d \times d}$ is a symmetric and positive definite matrix and $b \in \mathbb{R}^{d}$.
a) Compute the gradient and the Hessian of the function $f$, verify that $f$ is strictly convex, and find the unique global minimum of $f$.

Solution: $\nabla f=Q x-b$ and $\nabla^{2} f=Q$ from calculus. Since $Q$ is symmetric positive definite (SPD), it follows that $f$ is strictly convex on $\mathbb{R}^{d}$, and as such, there is at most one global minimum of $f$. Furthermore, this global minimum $x^{*}$ must be a stationary point satisfying $\nabla f\left(x^{*}\right)=0$. We conclude that $x^{*}=Q^{-1} b$, since $Q$ is invertible (all eigenvalues of $Q$ are positive, and hence, different from zero).
b) Let $x \in \mathbb{R}^{d}$, and let $p \in \mathbb{R}^{d}$ be a direction satisfying the inequality $\nabla f(x)^{\mathrm{T}} p<0$. Compute analytically the step length $\alpha_{x, p}$ that solves the (exact) linesearch problem $\min _{\alpha>0} f(x+\alpha p)$.

Solution: First of all, to avoid trivial cases let us note that $p \neq 0$ and $\nabla f(x)=$ $Q x-b \neq 0$ owing to the inequality $\nabla f(x)^{\mathrm{T}} p<0$.
Now, let us look at the first order necessary conditions for $\alpha_{x, p}$ to be a minimizer:

$$
\frac{\mathrm{d}}{\mathrm{~d} \alpha} f\left(x+\alpha_{x, p} p\right)=p^{\mathrm{T}} \nabla f\left(x+\alpha_{x, p} p\right)=p^{\mathrm{T}}\left[Q\left(x+\alpha_{x, p} p\right)-b\right]=0
$$

or

$$
\alpha_{x, p}=-\frac{p^{\mathrm{T}}[Q x-b]}{p^{\mathrm{T}} Q p}>0,
$$

since $p^{\mathrm{T}} Q p>0$ owing to $Q$ being positive definite, and $p^{\mathrm{T}}[Q x-b]=p^{\mathrm{T}} \nabla f(x)<$ 0 by our assumption.
Since $\mathrm{d}^{2} / \mathrm{d}^{2} f(x+\alpha p)=p^{\mathrm{T}} Q p>0$ the linesearch problem is strictly convex, and therefore $\alpha_{x, p}$ is the unique global minimum.
c) Recall the strong Wolfe conditions:

$$
\begin{aligned}
f(x+\alpha p) & \leq f(x)+c_{1} \alpha \nabla f(x)^{T} p, \\
\left|\nabla f(x+\alpha p)^{T} p\right| & \leq c_{2}\left|\nabla f(x)^{T} p\right| .
\end{aligned}
$$

Let $x, p \in \mathbb{R}^{d}$, and $\alpha_{x, p}$ be as in the previous question. Show that the step length $\alpha_{x, p}$ satisfies the strong Wolfe conditions if and only if $c_{1} \leq 1 / 2$.

Solution: Clearly the strong curvature condition is satisfied because $\nabla f(x+$ $\left.\alpha_{x, p} p\right)^{\mathrm{T}} p=\mathrm{d} / \mathrm{d} \alpha f\left(x+\alpha_{x, p} p\right)=0$, thus the "new" slope is 0 and must be smaller than or equal in magnitude than the slope we have started with.
We check the sufficient decrease condition now:

$$
f\left(x+\alpha_{x, p} p\right)-f(x)=\frac{1}{2} \alpha_{x, p}^{2} p^{\mathrm{T}} Q p+\alpha_{x, p} p^{\mathrm{T}}(Q x-b)=-\frac{1}{2} \frac{\left[p^{\mathrm{T}}(Q x-b)\right]^{2}}{p^{\mathrm{T}} Q p}<0
$$

while

$$
c_{1} \alpha_{x, p} \nabla f(x)^{\mathrm{T}} p=-c_{1} \frac{\left[p^{\mathrm{T}}(Q x-b)\right]^{2}}{p^{\mathrm{T}} Q p}
$$

Thus the sufficient decrease condition is equivalent to the inequality $c_{1} \leq 1 / 2$.

2 Assume that $f: \mathbb{R}^{d} \rightarrow \mathbb{R}$ is a strongly convex function, meaning that there exists $c>0$ such that the function $x \mapsto f(x)-\frac{c}{2}\|x\|^{2}$ is convex.
a) Consider the Newton method with line search, the so-called damped Newton method

$$
x_{k+1}=x_{k}+\alpha_{k} p_{k} \quad \text { with } \quad p_{k}=-\nabla^{2} f\left(x_{k}\right)^{-1} \nabla f\left(x_{k}\right)
$$

where the step length parameter $\alpha_{k}$ is chosen according to backtracking Armijo line search with parameters $\bar{\alpha}>0,0<c_{1}<1$, and $0<\rho<1$.
Show that $p_{k}$ is a descent direction in each step, and that the sequence $x_{k}$ converges to the unique minimizer $x^{*}$ of $f$.
Hint: Use Theorem 1 in the note "Convergence of descent methods with backtracking (Armijo) linesearch..." by Anton Evgrafov.
We will now show that this method is invariant under affine transformations:
Assume that $B \in \mathbb{R}^{d \times d}$ is a non-singular matrix (not necessarily orthogonal) and that $c \in \mathbb{R}^{d}$. Define the function

$$
g(x):=f(B x+c)
$$

b) Find expressions for $\nabla g(x)$ and $\nabla^{2} g(x)$ in terms of $f, B$, and $c$.

Solution: For clarity, we set $y:=B x+c$, so that $g(x)=f(y(x))$. We present two ways of solving this problem. The first method is the explicit method,

$$
\begin{aligned}
\frac{\partial g}{\partial x_{i}}(x) & =\sum_{k=1}^{n} \frac{\partial f}{\partial y_{k}}(B x+c) \frac{\partial y_{k}}{\partial x_{i}}=\sum_{k=1}^{n} \frac{\partial f}{\partial y_{k}}(B x+c) B_{k i} \\
\frac{\partial^{2} g}{\partial x_{i} \partial x_{j}}(x) & =\frac{\partial}{\partial x_{j}} \sum_{k=1}^{n} \frac{\partial f}{\partial y_{k}}(B x+c) B_{k i}=\sum_{k=1}^{n} \sum_{\ell=1}^{n} \frac{\partial^{2} f}{\partial y_{k} \partial y_{\ell}}(B x+c) B_{k i} B_{\ell j},
\end{aligned}
$$

and therefore

$$
\begin{aligned}
\nabla g(x) & =B^{\mathrm{T}} \nabla f(B x+c) \\
\nabla^{2} g(x) & =B^{\mathrm{T}} \nabla^{2} f(B x+c) B
\end{aligned}
$$

These calculations at 'index' level can be messy and exhaustive; there are alternative methods of solving this problem, but perhaps the easiest is to simply memorize two basic chain-rules for $\nabla$ and $\nabla^{2}$. For any (smooth) maps $h: \mathbb{R}^{d} \rightarrow \mathbb{R}$ and $H: \mathbb{R}^{d} \rightarrow \mathbb{R}^{d}$, the composition $h \circ H$ satifies

1. $\nabla(h(H))=\left(J_{H}\right)^{\mathrm{T}} \nabla h(H)$,
2. $\nabla^{2}(h(H))=\left(J_{H}\right)^{\mathrm{T}} \nabla^{2} h(H) J_{H}$,
where $J_{H}$ is the Jacobian of $H$. With these in mind, the results follows immediately as $J_{y}=B$.
c) Let $x \in \mathbb{R}^{d}$ and denote by $x_{1}$ the result of one Newton step starting at $x$ for the minimisation of $g$ with (Armijo) backtracking line search with parameters $0<c_{1}<1$ and $0<\rho<1$.
Moreover, let $y=B x+c$ and denote by $y_{1}$ the result of one Newton step starting at $y$ for the minimisation of $f$ with (Armijo) backtracking line search with the same parameters $0<c_{1}<1$ and $0<\rho<1$.
Show that

$$
y_{1}=B x_{1}+c .
$$

Solution: By Newtons method we have $p_{0}=-\left[\nabla^{2} g\left(x_{0}\right)\right]^{-1} \nabla g\left(x_{0}\right)$, and so $x_{1}=x_{0}+\alpha_{0} p_{0}$, where $\alpha_{0}=\rho^{k_{0}}$ and $k_{0} \in\{0,1,2, \ldots\}$ is the smallest nonnegative integer where Armijo's condition is satisfied:

$$
g\left(x_{0}+\alpha_{0} p_{0}\right) \leq g\left(x_{0}\right)+c_{1} \alpha_{0} p_{0}^{\mathrm{T}} \nabla g\left(x_{0}\right)
$$

Turning to the minimization of $f$ with respect to $y$, we similarly obtain $\tilde{p}_{0}=$ $-\left[\nabla^{2} f\left(y_{0}\right)\right]^{-1} \nabla g\left(y_{0}\right)$ and $y_{1}=y_{0}+\tilde{\alpha}_{0} \tilde{p}_{0}$, where $\tilde{\alpha}_{0}=\rho^{\tilde{k}_{0}}$ and $\tilde{k}_{0}$ is the smallest non-negative integer where Armijo's condition is satisfied:

$$
f\left(y_{0}+\tilde{\alpha}_{0} \tilde{p}_{0}\right) \leq f\left(y_{0}\right)+c_{1} \tilde{\alpha}_{0} \tilde{p}_{0}^{\mathrm{T}} \nabla f\left(y_{0}\right) .
$$

Our task is to prove that $y_{1}=B x_{1}+c$, given that $y_{0}=B x_{0}+c$. We start by showing that $B p_{0}=\tilde{p}_{0}$. Indeed,

$$
\begin{aligned}
B p_{0} & =-B\left[\nabla^{2} g\left(x_{0}\right)\right]^{-1} \nabla g\left(x_{0}\right) \\
& =-B\left[B^{\mathrm{T}} \nabla^{2} f\left(B x_{0}+c\right) B\right]^{-1} B^{\mathrm{T}} \nabla f\left(B x_{0}+c\right) \\
& =-\left[\nabla^{2} f\left(y_{0}\right)\right]^{-1} \nabla f\left(y_{0}\right) \\
& =\tilde{p}_{0} .
\end{aligned}
$$

This further implies that all $\alpha \in \mathbb{R}$ satisfies the two equations

$$
\begin{aligned}
g\left(x_{0}+\alpha p_{0}\right) & =f\left(y_{0}+\alpha \tilde{p}_{0}\right) \\
g\left(x_{0}\right)+c_{1} \alpha_{0} p_{0}^{\mathrm{T}} \nabla g\left(x_{0}\right) & =f\left(y_{0}\right)+c_{1} \tilde{\alpha}_{0} \tilde{p}_{0}^{\mathrm{T}} \nabla f\left(y_{0}\right) .
\end{aligned}
$$

As a result, Armijo's condition is satisfied in the $(g, x)$-regime exactly when it is satisfied in the $(f, y)$-regime, that is, $k_{0}=\tilde{k}_{0}$ and consequently $\alpha_{0}=\tilde{\alpha}_{0}$. We arrive at the desired conclusion

$$
\begin{aligned}
y_{1} & =y_{0}+\tilde{\alpha}_{0} \tilde{p}_{0} \\
& =\left(B x_{0}+c\right)+\alpha_{0} B p_{0} \\
& =B\left(x_{0}+\alpha_{0} p_{0}\right)+c \\
& =B x_{1}+c .
\end{aligned}
$$

3 Consider the function

$$
f(x, y)=2 x^{2}+y^{2}-2 x y+2 x^{3}+x^{4} .
$$

a) Compute all stationary points of $f$ and find all global or local minimisers of $f$.

Solution: We have

$$
\nabla f=\left[4 x-2 y+6 x^{2}+4 x^{3}, 2 y-2 x\right]^{\mathrm{T}}
$$

and

$$
\nabla^{2} f=\left[\begin{array}{rr}
4+12 x+12 x^{2} & -2 \\
-2 & 2
\end{array}\right]
$$

Hence, stationary points satisfy $y=x$ by the first component of $\nabla f$, while the second component yields that $0=2 x\left(1+3 x+2 x^{2}\right)=x(x+1)(2 x+1)$. Thus critical points of $f$ are $(0,0),\left(-\frac{1}{2},-\frac{1}{2}\right)$, and $(-1,-1)$. Now,
$\nabla^{2} f(0,0)=\left[\begin{array}{rr}4 & -2 \\ -2 & 2\end{array}\right]=\nabla^{2} f(-1,-1) \quad$ and $\quad \nabla^{2} f\left(-\frac{1}{2},-\frac{1}{2}\right)=\left[\begin{array}{rr}1 & -2 \\ -2 & 2\end{array}\right]$
has eigenvalues $3 \pm \sqrt{5}>0$ and $(3 \pm \sqrt{17}) / 2$ (one positive, and one negative), respectively. We conclude that $(0,0)$, and $(-1,-1)$ are strict local minima, while $\left(-\frac{1}{2},-\frac{1}{2}\right)$ is a saddle point. Moreover, since $\nabla^{2} f$ remains SPD both for $x>0$ and $x<-1$ (the value of $y$ is irrelevant), it follows that $(0,0)$ and $(-1,-1)$ are the only candidates for global minima. Evaluating $f(0,0)=0=f(-1,-1)$, shows that both are global minimisers of $f$.
b) Consider the gradient descent method with backtracking for the minimisation of $f$. Use the parameters $\rho=1 / 2$ and $c_{1}=1 / 4$. Perform one step with starting value $\left(x_{0}, y_{0}\right)=(-1,0)$. Does the method converge to a minimiser of $f$ ?

Solution: Gradient descent method gives $\left(x_{k+1}, y_{k+1}\right)=\left(x_{k}, y_{k}\right)+p_{k}$, with $p_{k}=-\nabla f_{k}$. Starting with preliminary step length $\alpha, \rho=1 / 2$, and $c_{1}=1 / 4$, we accept a new step provided

$$
f\left(\left(x_{0}, y_{0}\right)+\alpha p_{0}\right) \leq f\left(x_{0}, y_{0}\right)+c \alpha \nabla f\left(x_{0}, y_{0}\right)^{\mathrm{T}} p_{0}=1-2 \alpha
$$

using that $p_{0}=-\nabla f\left(x_{0}, y_{0}\right)=(2,-2)$.
Beginning with $\alpha=1$, we reject the first try since $f\left(\left(x_{0}, y_{0}\right)+\alpha p_{0}\right)=13>-1$. Reducing to $\alpha \mapsto \rho \alpha=1 / 2$, still gives rejection, but $\alpha=1 / 4$ succeeds, because $f\left(\left(x_{0}, y_{0}\right)+\alpha p_{0}\right)=1 / 16 \leq 1 / 2$. Hence, we put $\left(x_{1}, y_{1}\right)=\left(-\frac{1}{2},-\frac{1}{2}\right)$, and proceed with a new round. However, $\left(x_{1}, y_{1}\right)$ is a critical (saddle) point for $f$, so the gradient method stops here, thereby failing to converge to a minimiser.
c) Consider Newton's method with backtracking for the minimisation of $f$. Use the parameters $\rho=1 / 2$ and $c_{1}=1 / 4$. Perform one step with starting value $\left(x_{0}, y_{0}\right)=(-1,0)$. Does the method converge to a minimiser of $f$ ?

Solution: Similarly as in the previous exercise, the backtracking acceptance criterion for Newton's method reads

$$
f\left(\left(x_{0}, y_{0}\right)+\alpha p_{0}\right) \leq f\left(x_{0}, y_{0}\right)+c \alpha \nabla f\left(x_{0}, y_{0}\right)^{\mathrm{T}} p_{0}=1-\frac{1}{2} \alpha,
$$

since $p_{0}=-\nabla^{2} f\left(x_{0}, y_{0}\right)^{-1} \nabla f\left(x_{0}, y_{0}\right)=(0,-1)$ and $c_{1}=1 / 4$. Starting with $\alpha=1$, we have $f\left(\left(x_{0}, y_{0}\right)+\alpha p_{0}\right)=0 \leq 1 / 2$, so the step is accepted. We then put $\left(x_{1}, y_{1}\right)=\left(x_{0}, y_{0}\right)+p_{0}=(-1,-1)$. This point is a global minimiser, the conclusion being that Newton's method converged in one step.

