Exercise #9

March 14, 2023

Problem 1.

In this exercise, we study the Gauß–Newton method for solving the least-squares problem corresponding to the (overdetermined and inconsistent) system of equations

$$\begin{aligned} x + y &= 1, \\ x - y &= 0, \\ xy &= 2. \end{aligned}$$

To that end, we define

$$\begin{aligned} r_1(x,y) &:= x + y - 1, \\ r_2(x,y) &:= x - y, \\ r_3(x,y) &:= xy - 2, \end{aligned}$$

and

$$f(x,y) := \frac{1}{2}\sum_{j=1}^{3} r_j(x,y)^2.$$

We denote moreover by $J = J(x,y)$ the Jacobian of r.

a) Show that the function f is non-convex, but that it has a unique minimiser (x^*, y^*).

b) Show that the matrix $J^T J$ required in the Gauß–Newton method is positive definite for all x, y.

c) Perform one step of the Gauß–Newton method (without line search) for the solution of this least-squares problem. Use the initial value $(x_0, y_0) = (0,0)$.

Solution.

a) The gradient and Hessian of f equal

$$\nabla f(x,y) = J^\top r = \begin{bmatrix} 1 & 1 & y \\ 1 & -1 & x \end{bmatrix} \begin{bmatrix} x + y - 1 \\ x - y \\ xy - 2 \end{bmatrix} = \begin{bmatrix} 2(x-y) + xy^2 - 1 \\ 2(y-x) + yx^2 - 1 \end{bmatrix}$$

and

$$\begin{aligned} \nabla^2 f(x,y) &= J^\top J + r_1 \nabla^2 r_1 + r_2 \nabla^2 r_2 + r_3 \nabla^2 r_3 \\ &= \begin{bmatrix} 2 + y^2 & xy \\ xy & 2 + x^2 \end{bmatrix} + 0 + 0 + r_3 \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \\ &= \begin{bmatrix} 2 + y^2 & 2(xy-1) \\ 2(xy-1) & 2 + x^2 \end{bmatrix}. \end{aligned}$$

Since, for example, $\nabla^2 f(-1,1)$ has eigenvalues -1 and 7, it follows that f is non-convex. However, f does have a unique minimiser: it is smooth and coercive, and thus we infer that there is a global minimiser, which must also be a stationary point. Coercivity can be seen this way:

$$2f(x,y) \geq r_1^2(x,y) + r_2^2(x,y) = (x+y-1)^2 + (x-y)^2 = (x-1)^2 + (y-1)^2 - 1 + x^2 + y^2 \geq x^2 + y^2 - 1.$$

Now $f \mapsto +\infty$ when $\|(x,y)\| \mapsto \infty$. The stationary point for f must satisfy the equations

$$xy(x+y) = 2 \qquad \text{and} \qquad xy(x-y) = 4(x-y),$$

which can be seen by adding and subtracting the equations in the system $\nabla f = 0$. If $x \neq y$, then $xy = 4$ from the second equation, so that $y = \frac{1}{2} - x$ from the first. But as $4 = xy = x(\frac{1}{2} - x)$ has complex solutions in x, we reject this case. Therefore $x = y$, which gives solutions $x = y = 1$ from the first equation. Thus the function has only one stationary point, and since the minimum exists and must satisfy the optimality conditions, this is the point of global minimum.

b) Remember first that any matrix of the form $J^\top J$ is symmetric positive semi-definite (SPSD), which follows from

$$v^\top (J^\top J) v = (Jv)^\top (Jv) = \|Jv\|^2 \geq 0.$$

Moreover, SPSD matrices are characterised by having nonnegative eigenvalues, while a matrix is symmetric positive definite (SPD) if and onlfy if it has strictly positive eigenvalues.

Computing $\det J^\top J = 2(x^2 + y^2 + 2) > 0$, we see that $J^\top J$ is invertible. In particular, all eigenvalues are nonzero, and hence, strictly positive (being nonnegative). Therefore, $J^\top J$ is positive definite.

c) With $(x_0, y_0) = (0,0)$, we have

$$J^\top J = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} \quad \text{and} \quad J^\top r = \begin{bmatrix} -1 \\ -1 \end{bmatrix}.$$

Solving the linear system $J^\top J p = -J^\top r$ gives $p = (1/2, 1/2)$, so that

$$(x_1, y_1) = (x_0, y_0) + p = (1/2, 1/2).$$

Problem 2.

Let

$$f(x) = x_1^4 + 2x_2^4 + x_1 x_2 + x_1 - x_2 + 2.$$

Starting at the point $x_0 = (0,0)$ compute explicitly one step for the trust region method with the model function $m(p) = f(x_0) + g^T p + \frac{1}{2} p^T B p$, where $g = \nabla f(x_0)$, $B = \nabla^2 f(x_0)$, and the trust region radius $\Delta = 1$.

Solution.

We invoke Theorem 4.1 in Nocedal & Wright, which says that p_0 is a global minimizser to the trust-region subproblem

$$\min_{\|p\| \leq \Delta} m(p),$$

with $\Delta = 1$, if and only if there exists a $\lambda \geq 0$ such that

$$(B + \lambda \,\mathrm{Id}) p_0 = -g, \tag{1}$$
$$\lambda(\Delta - \|p_0\|) = 0, \text{ and} \tag{2}$$
$$B + \lambda \,\mathrm{Id} \quad \text{is positive semi-definite.} \tag{3}$$

Routine calculations yield that

$$g = \nabla f(x_0) = \begin{bmatrix} 1 \\ -1 \end{bmatrix}, \qquad \text{and} \qquad B = \nabla^2 f(x_0) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

Since B has eigenvalues ± 1, we must have $\lambda \geq 1$ in order to guarantee the positive semi-definiteness of the matrix $B + \lambda\,\mathrm{Id}$. As a result, from complementarity condition (2) we must have $\|p_0\| = 1$, so p_0 lies on the trust-region boundary.

The solution of (1) equals

$$p_0 = \frac{1}{1-\lambda} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

provided $\lambda \neq 1$ (there is no solution for $\lambda = 1$), and from the conditions $\|p_0\| = 1$ and $\lambda > 1$, we thus end up with

$$\lambda = 1 + \sqrt{2}, \qquad \text{and} \qquad p_0 = \frac{1}{\sqrt{2}} \begin{bmatrix} -1 \\ 1 \end{bmatrix}.$$

The next step is therefore $x_1 = x_0 + p_0 = p_0$.

Problem 3. (Problem 4.1 in N&W)

Let

$$f(x) = 10(x_2 - x_1^2)^2 + (1 - x_1)^2.$$

At $x = (0, -1)$ draw the contour lines of the quadratic model

$$\min_p m(p) = f(x) + \langle \nabla f(x), p \rangle + \frac{1}{2}\langle p, Bp \rangle \qquad \text{subject to } \|p\| \leq \Delta, \tag{4}$$

assuming that B is the Hessian of f. Draw the family of solutions of (4) as the trust region radius varies from $\Delta = 0$ to $\Delta = 2$. Repeat this at $x = (0, 0.5)$.

Solution.

The gradient and Hessian of the objective function $f(x) = 10(x_2 - x_1^2)^2 + (1 - x_1)^2$ are

$$\nabla f(x) = \begin{pmatrix} -40(x_2 - x_1^2)x_1 - 2(1 - x_1) \\ 20(x_2 - x_1^2), \end{pmatrix}$$

$$\text{and } \nabla^2 f(x) = \begin{pmatrix} 40(3x_1^2 - x_2) + 2 & -40x_1 \\ -40x_1 & 20 \end{pmatrix}, \text{ respectively.}$$

We see that f has only one minimum, that is $x^* = (1, 1)^T$. For $x_k = (0, -1)^T$, we have that

$$f_k = 11, \nabla f_k = \begin{pmatrix} -2 \\ -20 \end{pmatrix} \text{ and } \nabla^2 f_k = \begin{pmatrix} 42 & 0 \\ 0 & 20 \end{pmatrix}.$$

Hence,

$$m_k(p) = f_k + \nabla f_k^T p + \frac{1}{2} p^T \nabla^2 f_k p = 11 - 2p_1 - 20p_2 + 21p_1^2 + 10p_2^2,$$

is a strictly convex quadratic function with minimizer $p_k^B = -\nabla^2 f_k^{-1} \nabla f_k = (\frac{1}{21}, 1)^T$. We can rewrite $m_k(p)$ to

$$m_k(p) = 21(p_1 - \frac{1}{21})^2 + 10(p_2 - 1)^2 + \frac{20}{21}.$$

Thus the contours of $m_k(p)$ are ellipses. We can get the solution of

$$\min_{\|p\| \leq \Delta} m_k(p) \tag{5}$$

as

$$\begin{cases} \|P\| = \Delta, & \|p_k^B\| > \Delta, \\ p = p_k^B, & \text{otherwise.} \end{cases}$$

For $x_k = (0, 0.5)^T$, we have that

$$f_k = \frac{7}{2}, \; \nabla f_k = \begin{pmatrix} -2 \\ 10 \end{pmatrix}, \; \nabla^2 f_k = \begin{pmatrix} -18 & 0 \\ 0 & 20 \end{pmatrix}.$$

Hence,

$$m_k(p) = \frac{7}{2} - 2p_1 + 10p_2 - 9p_1^2 + 10p_2^2 = -9(p_1 + \frac{1}{9})^2 + 10(p_2 + \frac{1}{2})^2 + \frac{10}{9}$$

has no global maximum or minimum, but a saddle point at $(-\frac{1}{9}, -\frac{1}{2})^T$. Since we have no minimum in the interior of the trust-region, the minimizer p_k of (5) will also here satisfy $\|p_k\| = \Delta$. Observe that the contours of $m_k(p)$ will be hyperbolas. Contour plots of $m_k(x)$, the family of solutions of (5) for $\Delta \in (0, 2]$ and trust region radii for the two different x_k are shown in Figure 1.

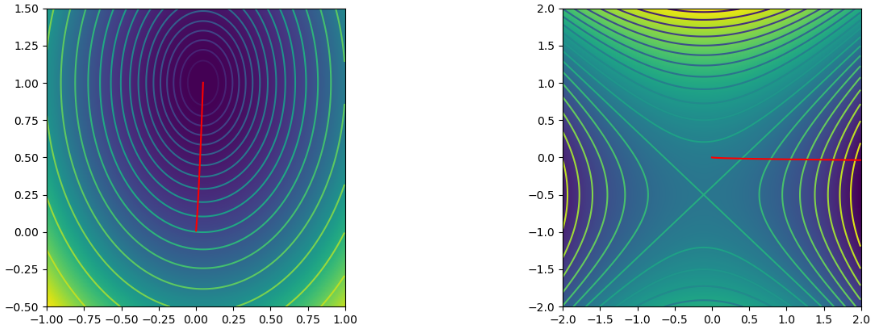

Figure 1: Contour plot of $m_k(p)$ and the family of solutions of (5)(in red)

Problem 4. (Problem 4.5 in N&W)

Let $\phi(\tau) = m_k(\tau p_k^s)$, where $p_k^s = -\frac{\Delta_k}{\|g_k\|} g_k$ and $m_k(p) = f_k + g_k^T p + \frac{1}{2} p^T B p$ with $B \in \mathbb{R}^{d \times d}$ symmetric. Show that the minimizer of $\phi(\tau)$ subject to $\|\tau p_k^s\| \le \Delta_k$ and $\tau \ge 0$ is given as

$$\begin{cases} 1, & \text{if } g_k^T B_k g_k \le 0, \\ \min(\frac{\|g_k\|^3}{\Delta_k g_k^T B_k g_k}, 1), & \text{otherwise.} \end{cases} \tag{6}$$

Solution.

With the definition of $m_k(p)$ and p_k^s, we can write

$$\begin{aligned} \phi(\tau) &= f_k + g_k^T \left(-\frac{\tau \Delta_k g_k}{\|g_k\|} \right) + \frac{1}{2} \left(-\frac{\tau \Delta_k g_k}{\|g_k\|} \right)^T B_k \left(-\frac{\tau \Delta_k g_k}{\|g_k\|} \right) \\ &= f_k - \tau \Delta_k \|g_k\| + \frac{\frac{1}{2} \tau^2 \Delta_k^2 g_k^T B_k g_k}{\|g_k\|^2}. \end{aligned}$$

Furthermore, observe that the constraint $\|\tau p_k^s\| \le \Delta_k$ is equivalent to $|\tau| \le 1$. Together with $\tau > 0$, this means that $\tau \in (0, 1]$. First, if $g_k = 0$, then $\phi(\tau)$ is a constant, so $\tau = 1$ will be a minimizer. This is in agreement with (6). Second, if

$g_k^T B_k g_k = 0$, then $\phi(\tau)$ is linear and decreasing, so the minimizer is the highest possible value, i.e., $\tau = 1$, which is also in agreement with (6). Lastly, if $g_k^T B_k g_k \neq 0$, then we have a critical point where

$$\phi'(\tau) = -\Delta_k \|g_k\| \frac{\tau \Delta_k^2 g_k^T B_k g_k}{\|g_k\|^2} = 0,$$

that is

$$\tau = \frac{\|g_k\|^3}{\Delta_k g_k^T B_k g_k}. \tag{7}$$

Now if $g_k^T B_k g_k < 0$ then this is a maximizer, and the minimizer must be at the endpoints of the interval $(0, 1]$. Since we have $\phi(0) > \phi(1)$, the minimizer must be $\tau = 1$. This is in agreement with (6). Otherwise, if $g_k^T B_k g_k > 0$ then (7) is a minimizer. If this value in bigger than 1, then ϕ is decreasing across the interval $(0, 1]$, and thus the minimizer is $\tau = 1$, as in (6). If (7) is less than 1, then (7) is the minimizer. This is captured by (6).