This week's homework Homework 2 is due no later than **Monday 16.10.2023 23:55**.

Problem 4.1: Necessary Conditions for Least Squares

Consider the following unconstrained optimization problem P:

$$(P) \ : \ \text{min.} \ \ ||Ax - b||_2^2 \tag{1}$$

where A is a matrix in $\mathbb{R}^{m\times n}$ and b is a vector in $\mathbb{R}^m$. This problem is typically called a *least-squares* problem when using the Euclidean norm, and it has several applications in regression analysis, optimal control, parameter estimation, data fitting, etc.

An extension of the problem P involves minimizing $||x||_2^2$ on top of the original objective. To solve this problem, we can use *regularization* which is a common scalarization technique to find solutions to bi-criterion problems. We will consider the following *regularized* least-squares problem

$$(RP) \ : \ \text{min.} \ \ ||Ax - b||_2^2 + \delta||x||_2^2 \tag{2}$$

where the penalty term $\delta > 0$ controls the trade-off between the two objectives.

(a) Give brief interpretations of the problems (1) and (2).

(b) Find solutions for the problems (1) and (2) by writing the first-order necessary optimality conditions. Justify why these conditions are also sufficient.

Solution.

(a) In problem (1), we seek a vector $y = Ax$ in the subspace spanned by the column vectors of A that is closest to the vector b. If b is in the column space of A, we need to solve the system $Ax = b$. If b is not in the column space of A, we seek a solution to the system $Ax = y$, where y is the projection of b onto the subspace spanned by the column vectors $A_1, \dots, A_n$ of A. We assume that b is not in the column space of A, since otherwise the problem reduces to solving the system $Ax = b$.

In problem (2), we seek a vector x that has a small squared norm $||x||_2^2$ and also makes the squared residual norm $||Ax - b||_2^2$ as small as possible. The penalty term $\delta > 0$ determines how much importance we put on minimizing the value of $||x||_2^2$ vs. the value of $||Ax - b||_2^2$.

(b) Let us denote the objective function in problem (2) as $f(x)$:

$$\begin{aligned} f(x) &= ||Ax - b||_2^2 \\ &= (Ax - b)^\top (Ax - b) \\ &= (x^\top A^\top - b^\top)(Ax - b) \\ &= x^\top A^\top Ax - x^\top A^\top b - b^\top Ax + b^\top b \end{aligned}$$

The first-order necessary optimality condition for problem (1) is $\nabla f(x) = 0$. We get

$$\begin{aligned} \nabla f(x) &= \nabla(x^\top A^\top Ax) + \nabla(-x^\top A^\top b) + \nabla(-b^\top Ax) + \nabla(b^\top b) \\ &= (A^\top A + A^\top A)x + (-A^\top b) + (-A^\top b). \\ &= 2A^\top Ax - 2A^\top b = 0 \end{aligned}$$

from which we finally get the necessary optimality condition

$$A^\top Ax = A^\top b \tag{3}$$

The condition (3) is also sufficient, because $f(x) = ||Ax - b||_2^2$ is a convex function. We can also verify this by looking at the Hessian

$$\nabla^2 f(x) = 2A^\top A$$

which is positive semidefinite for all $x \in \mathbb{R}^n$ because

$$x^\top A^\top Ax = (Ax)^\top (Ax) = ||Ax||_2^2 \geq 0$$

This is a necessary and sufficient condition for the convexity of $f(x)$ (and also the second-order necessary condition). Assuming that columns of A are linearly independent, the unique optimal solution from (3) is

$$x = (A^\top A)^{-1} A^\top b$$

Let us denote the objective function in problem (2) as $g(x)$. We get

$$\begin{aligned} g(x) &= ||Ax - b||_2^2 + \delta ||x||_2^2 \\ &= (Ax - b)^\top (Ax - b) + \delta x^\top x \\ &= (x^\top A^\top - b^\top)(Ax - b)\} + \delta x^\top x \\ &= x^\top A^\top Ax - x^\top A^\top b - b^\top Ax + b^\top b + \delta x^\top x \end{aligned}$$

The first-order necessary optimality condition for problem (2) is $\nabla g(x) = 0$. We get

$$\begin{aligned} \nabla g(x) &= \nabla(x^\top A^\top Ax) + \nabla(-x^\top A^\top b) + \nabla(-b^\top Ax) + \nabla(b^\top b) + \delta \nabla(x^\top x) \\ &= (A^\top A + A^\top A)x + (-A^\top b) + (-A^\top b) + \delta(1+1)x \\ &= 2A^\top Ax - 2A^\top b + 2\delta x = 0 \end{aligned}$$

from which we get the necessary optimality condition

$$(A^\top A + \delta I)x = A^\top b \tag{4}$$

The condition (4) is also sufficient because $g(x) = ||Ax - b||_2^2 + ||x||_2^2$ is a convex function. We can also verify this by looking at the Hessian

$$\nabla^2 g(x) = 2A^\top A + 2\delta I$$

which is positive definite for all $x \in \mathbb{R}^n$ since $\delta > 0$ and

$$x^\top A^\top Ax = (Ax)^\top (Ax) = ||Ax||_2^2 \geq 0.$$

$\nabla^2 g(x) > 0$ for all $x \in \mathbb{R}^n$ is a necessary and sufficient condition for $g(x)$ to be strictly convex. Thus, the unique optimal solution from (4) is

$$x = (A^\top A + \delta I)^{-1} A^\top b$$

Problem 4.2: Optimality of Points in a Convex Problem

Consider the following convex optimization problem P:

$$\begin{aligned} (P): \ \ & \text{min. } (x_1 - 3)^2 + (x_2 - 2)^2 && (5) \\ \text{subject to: } & x_1^2 + x_2^2 \leq 5 && (6) \\ & x_1 + x_2 \leq 3 && (7) \\ & x_1 \geq 0 && (8) \\ & x_2 \geq 0 && (9) \end{aligned}$$

Let S denote the feasible set defined by the constraints (6) – (9), and let $f : \mathbb{R}^2 \to \mathbb{R}$ with $f(x) = (x_1 - 3)^2 + (x_2 - 2)^2$ denote the objective function (5). Notice that both S and f are convex. Recall the following optimality condition for convex optimization problems presented in Lecture 4 (Corollary 4):

Let $S \subseteq \mathbb{R}^n$ be a convex set and $f : S \to \mathbb{R}$ a differentiable convex function on S. Then $\overline{x} \in S$ is optimal if and only if

$$\nabla f(\overline{x})^\top (x - \overline{x}) \geq 0, \text{ for all } x \in S \tag{10}$$

Using the condition (10), examine graphically if the following points are optimal for problem P:

(a) $\overline{x}_1 = (1, 2)$

(b) $\overline{x}_2 = (2, 1)$

Solution.

(a) The point $\overline{x}_1 = (1, 2)$ is not optimal because, for example,

$$\nabla f(\overline{x}_1)^\top (\overline{x}_2 - \overline{x}_1) = (-4, 0) \cdot ((2, 1) - (1, 2))^\top = (-4, 0) \cdot (1, -1)^\top = -4 < 0$$

(b) The point $\overline{x}_2 = (2, 1)$ is optimal as can be seen from Figure 1.

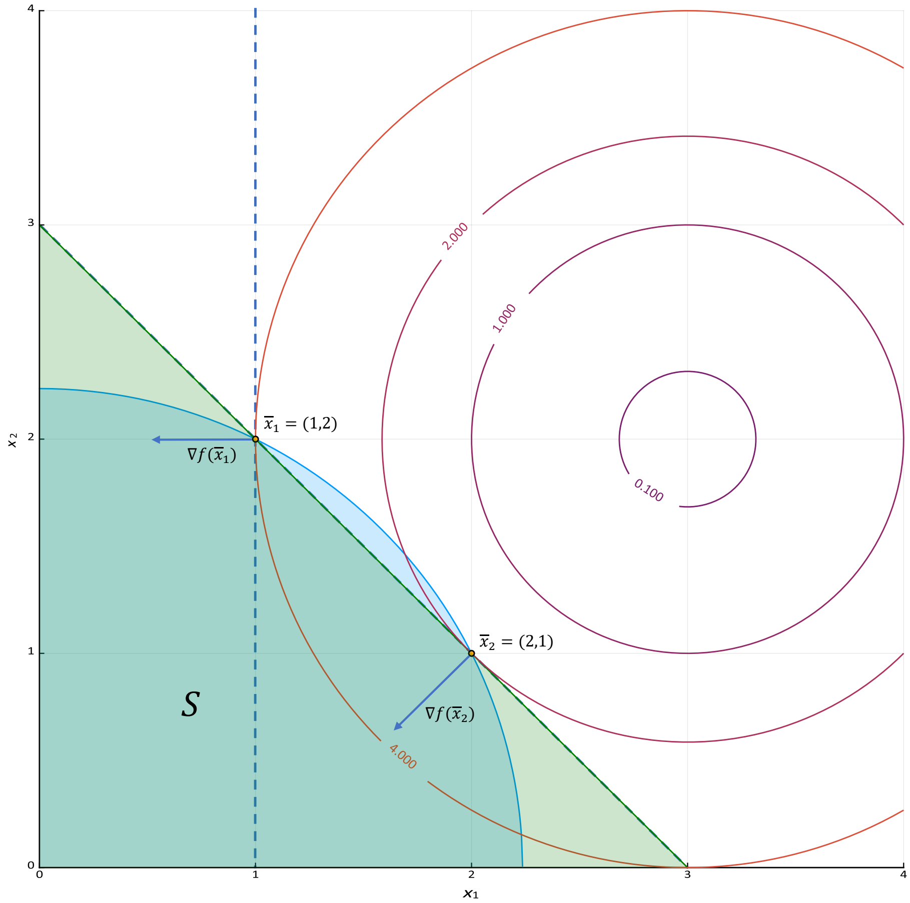

Figure 1: Description of problem P

Problem 4.3: Optimal Point of a Nonsmooth Convex Problem

Consider the following nonsmooth optimization problem P:

$$(P): \text{ min. } f(x) = \begin{cases} -\frac{3}{2}x + 6, & \text{if } 0 < x \leq 2 \\ -\frac{1}{2}x + 4, & \text{if } 2 \leq x \leq 4 \\ \frac{1}{4}x + 1 & \text{if } 4 \leq x \leq 8 \\ x - 5 & \text{if } x \geq 8 \end{cases} \tag{11}$$

$$\text{subject to: } x \in \mathbb{R}^+. \tag{12}$$

Let S denote the feasible set defined by the constraint (12), and let $f : \mathbb{R}^+ \to \mathbb{R}$ with $f(x)$ denote the objective function (11). Notice that both S and f are convex.

Characterize the subdifferential sets of f at points $\overline{x}_1 = 2$, $\overline{x}_2 = 4$, and $\overline{x}_3 = 8$. Use Corollary 3 from Lecture 4 to show that $\overline{x}_2 = 4$ is the unique optimal solution to the problem P. Corollary 3 states that a point $\overline{x} \in S$ is an optimal solution to P if and only if $0 \in \partial f(\overline{x})$, that is, f has a subgradient $\xi = 0$ at $\overline{x}$ that belongs to the subdifferential set $\partial f(\overline{x})$.

Solution.

$\xi \in \mathbb{R}^n$ is a subgradient of the convex function $f(x)$ at a point $\overline{x} \in S$ if

$$f(x) \geq f(\overline{x}) + \xi^\top (x - \overline{x}). \tag{13}$$

One may show that the subdifferential set at $\overline{x}$ for a convex function $f(x)$ is a nonempty closed interval $[a, b]$, where a and b are one-sided limits

$$a = \lim_{x \to \overline{x}_0^-} \frac{f(x) - f(\overline{x})}{x - \overline{x}} \tag{14}$$

$$b = \lim_{x \to \overline{x}_0^+} \frac{f(x) - f(\overline{x})}{x - \overline{x}}. \tag{15}$$

We can characterize the subdifferential sets at each point $\overline{x}_1$, $\overline{x}_2$, and $\overline{x}_3$ using (14)–(15). Thus, we get the following sets:

$$\partial f(\overline{x}_1) = \{\xi \in \mathbb{R} : -\frac{3}{2} \leq \xi \leq -\frac{1}{2}\} \tag{16}$$

$$\partial f(\overline{x}_2) = \{\xi \in \mathbb{R} : -\frac{1}{2} \leq \xi \leq \frac{1}{4}\} \tag{17}$$

$$\partial f(\overline{x}_3) = \{\xi \in \mathbb{R} : \frac{1}{4} \leq \xi \leq 1\}. \tag{18}$$

Since $0 \in \partial f(\overline{x}_2)$, the point $\overline{x}_2 = 4$ must be the unique optimal solution.

The problem (11) – (12) is illustrated on Figure 2. Notice that the subgradients ξ at the points $\overline{x}_1$, $\overline{x}_2$, and $\overline{x}_3$ are the scalars corresponding to the slopes of the tangent lines (the lines that are perpendicular to the vectors $(\xi, -1)$ to the graph of the function at that points. However, to be able to represent the subgradients ξ on the figure not as scalars but vectors we can use an auxiliary variable y and generate the equivalent reformulation of (11) – (12) as follows

$$
\begin{aligned}
(P'):\ & \text{min. } y \\
\text{subject to: } & y \geq -\frac{3}{2}x + 6 \\
& y \geq -\frac{1}{2}x + 4 \\
& y \geq \frac{1}{4}x + 1 \\
& y \geq x - 5 \\
& x \in \mathbb{R}^{+} \\
& y \geq 0 \\
& y \in \mathbb{R}
\end{aligned}
$$

By doing so, we represent one-dimensional points $\overline{x}_1$, $\overline{x}_2$, and $\overline{x}_3$ as two-dimensional vectors $\begin{bmatrix}\overline{x}_1\\ \overline{y}_1\end{bmatrix} = \begin{bmatrix}2\\ 3\end{bmatrix}$, $\begin{bmatrix}\overline{x}_2\\ \overline{y}_2\end{bmatrix} = \begin{bmatrix}4\\ 2\end{bmatrix}$, and $\begin{bmatrix}\overline{x}_3\\ \overline{y}_3\end{bmatrix} = \begin{bmatrix}8\\ 3\end{bmatrix}$. And therefore, this allows to define the subdifferential sets at each point $\overline{x}_1$, $\overline{x}_2$, and $\overline{x}_3$ using (14)–(15) as follows.

$$\partial f\begin{pmatrix}\overline{x}_1\\ \overline{y}_1\end{pmatrix} = \left\{\xi \in \mathbb{R}^2 : \begin{bmatrix}-\frac{3}{2}\\ -1\end{bmatrix} \leq \xi \leq \begin{bmatrix}-\frac{1}{2}\\ -1\end{bmatrix}\right\} \tag{19}$$

$$\partial f\begin{pmatrix}\overline{x}_2\\ \overline{y}_2\end{pmatrix} = \left\{\xi \in \mathbb{R}^2 : \begin{bmatrix}-\frac{1}{2}\\ -1\end{bmatrix} \leq \xi \leq \begin{bmatrix}\frac{1}{4}\\ -1\end{bmatrix}\right\} \tag{20}$$

$$\partial f\begin{pmatrix}\overline{x}_3\\ \overline{y}_3\end{pmatrix} = \left\{\xi \in \mathbb{R}^2 : \begin{bmatrix}-\frac{1}{4}\\ -1\end{bmatrix} \leq \xi \leq \begin{bmatrix}1\\ -1\end{bmatrix}\right\} \tag{21}$$

On the Figure 2 subdifferential sets $\partial f(\overline{x})$ correspond to the "cones" between the dashed lines at each point $\begin{bmatrix}\overline{x}_1\\ \overline{y}_1\end{bmatrix}$, $\begin{bmatrix}\overline{x}_2\\ \overline{y}_2\end{bmatrix}$, and $\begin{bmatrix}\overline{x}_3\\ \overline{y}_3\end{bmatrix}$.

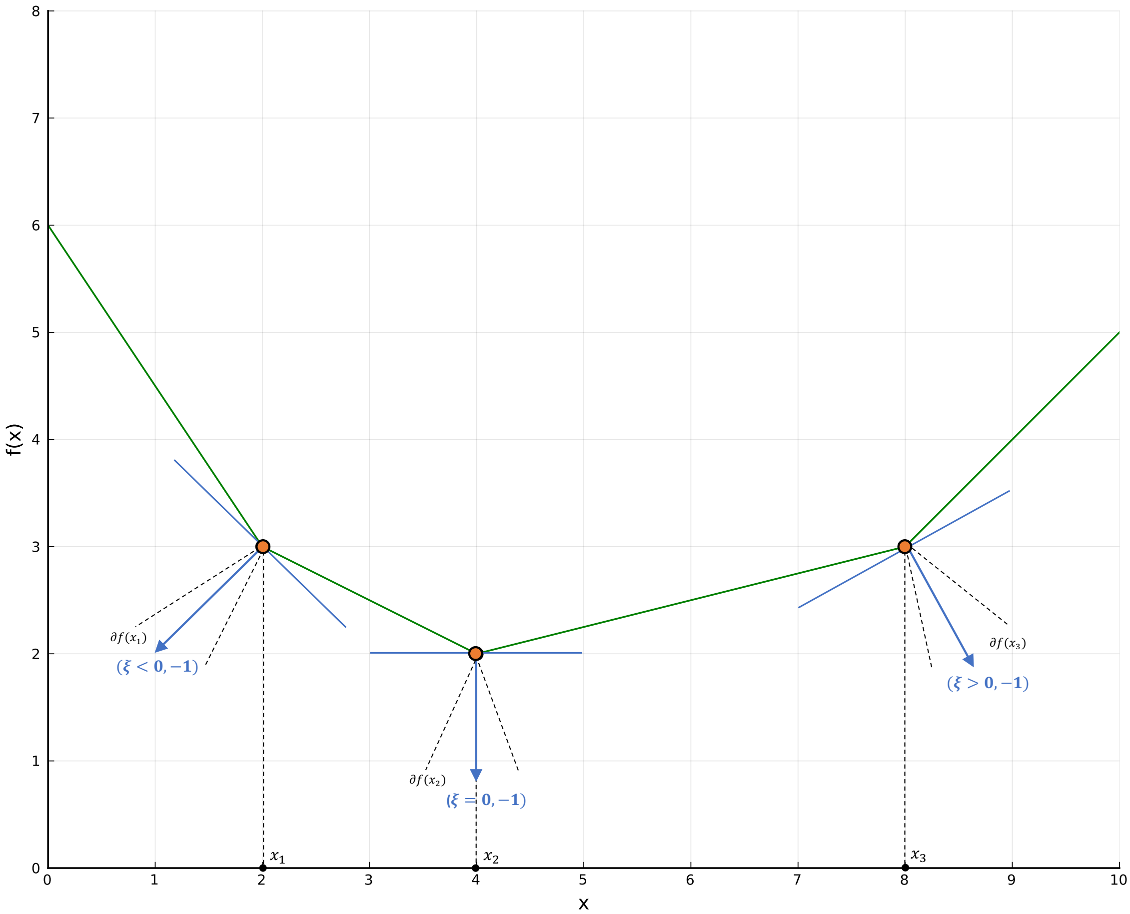

Figure 2: Description of problem P in 4.3