Machine Learning Exercise Sheet 06

Optimization

Exercise sheets consist of two parts: In-class exercises and homework. The in-class exercises will be solved and discussed during the tutorial. The homework is for you to solve at home and further engage with the lecture content. There is no grade bonus and you do not have to upload any solutions. Note that the order of some exercises might have changed compared to last year's recordings.

In-class Exercises

Problem 1: Prove or disprove whether the following functions $f : D \to \mathbb{R}$ are convex

a) $D = (1, \infty)$ and $f(x) = \log(x) - x^3$,

b) $D = \mathbb{R}^+$ and $f(x) = -\min(\log(3x+1), -x^4 - 3x^2 + 8x - 42)$,

c) $D = (-10, 10) \times (-10, 10)$ and $f(x, y) = y \cdot x^3 - y \cdot x^2 + y^2 + y + 4$.

a) The second derivative of f is $\frac{d^2 f(x)}{dx^2} = \frac{d}{dx}\left(\frac{1}{x} - 3x^2\right) = -\frac{1}{x^2} - 6x$, which is negative on the given set D and therefore f is not convex.

b) Transform min to max

$$-\min\{\log(3x+1), -x^4 - 3x^2 + 8x - 42\} = \max\{-\log(3x+1), x^4 + 3x^2 - 8x + 42\}\,.$$

$\max(g_1(x), g_2(x))$ is convex if both g_1 and g_2 are convex on $D = \mathbb{R}^+$ (see Exercise Sheet 6, Problem 1c). $g_1(x) = -\log(3x+1)$ is convex since the second derivative is positive on $\mathbb{R}^+$:

$$\frac{d^2}{dx^2}\left(-\log(3x+1)\right) = \frac{d}{dx}\left(-\frac{3}{3x+1}\right) = \frac{9}{(3x+1)^2} > 0$$

$g_2(x) = x^4 + 3x^2 - 8x + 42$ is also convex:

$$\frac{d^2}{dx^2}\left(x^4 + 3x^2 - 8x + 42\right) = \frac{d}{dx}\left(4x^3 + 6x - 8\right) = 12x^2 + 6 > 0$$

Thus f is convex.

c) For the function $f(x, y)$ to be convex (on D) it has to hold for all $x_1, x_2, y \in D$ and $\lambda \in (0, 1)$ that

$$\lambda f(x_1, y) + (1-\lambda) f(x_2, y) \geq f(\lambda x_1 + (1-\lambda)x_2, y)\,.$$

It does not hold in our case, consider $y = 1, x_1 = -4, x_2 = 0$ and $\lambda = 0.5$:

$$0.5 f(-4, 1) + 0.5 f(0, 1) = 0.5 \cdot (-74) + 0.5 \cdot 6 = -34$$
$$f\big(0.5 \cdot (-4) + 0.5 \cdot 0, 0.5 \cdot 1 + 0.5 \cdot 1\big) = f(-2, 1) = -6 \;\; > -34$$

Thus $f(x, y)$ is not convex.

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Thus $f(x, y)$ is not convex.

Problem 2: Prove that the following function (the loss function of logistic regression) $f : \mathbb{R}^d \to \mathbb{R}$ is convex:

$$f(\boldsymbol{w}) = -\ln p(\boldsymbol{y} \mid \boldsymbol{w}, \boldsymbol{X}) = -\sum_{i=1}^{N} \big(y_i \ln \sigma(\boldsymbol{w}^T \boldsymbol{x}_i) + (1 - y_i) \ln(1 - \sigma(\boldsymbol{w}^T \boldsymbol{x}_i))\big) \ .$$

First, let's simplify the above expression. For this we will need the following two facts

$$\sigma(z) = \frac{1}{1+e^{-z}} = \frac{e^z}{1+e^z} \qquad \text{and} \qquad 1 - \sigma(z) = \sigma(-z) = \frac{1}{1+e^z},$$

which implies that

$$\ln \sigma(z) = \ln\left(\frac{e^z}{1+e^z}\right) = z - \ln(1+e^z) \qquad \text{and} \qquad \ln(1-\sigma(z)) = -\ln(1+e^z).$$

Plugging this into the definition of the loss function we obtain

$$\begin{aligned} f(\boldsymbol{w}) &= -\sum_{i=1}^{N} \big(y_i \ln \sigma(\boldsymbol{w}^T \boldsymbol{x}_i) + (1 - y_i) \ln(1 - \sigma(\boldsymbol{w}^T \boldsymbol{x}_i))\big) \\ &= -\sum_{i=1}^{N} \left(y_i \left(\boldsymbol{w}^T \boldsymbol{x}_i - \ln(1 + e^{\boldsymbol{w}^T \boldsymbol{x}_i})\right) - (1 - y_i) \ln(1 + e^{\boldsymbol{w}^T \boldsymbol{x}_i}))\right) \\ &= \sum_{i=1}^{N} \left(-y_i(\boldsymbol{w}^T \boldsymbol{x}_i) + \ln(1 + e^{\boldsymbol{w}^T \boldsymbol{x}_i})\right) \end{aligned}$$

We know that $\boldsymbol{w}^T \boldsymbol{x}_i$ is a convex (and concave) function of $\boldsymbol{w}$. Therefore, the first term $-y_i(\boldsymbol{w}^T \boldsymbol{x}_i)$ is also convex.

Now, if we show that $\ln(1+e^z)$ is a <u>nondecreasing</u> and <u>convex</u> function of z on $\mathbb{R}$, we will be able to use the convexity preserving operations to prove that $f(\boldsymbol{w})$ is convex.

The first derivative of $\ln(1+e^z)$ is

$$\frac{d}{dz} \ln(1+e^z) = \frac{e^z}{1+e^z} = \sigma(z),$$

which is positive for all $z \in \mathbb{R}$, which means that $\ln(1+e^z)$ is an nondecreasing function.

The second derivative is

$$\frac{d^2}{dz^2} \ln(1+e^z) = \frac{d}{dz}\sigma(z) = \sigma(z)\sigma(-z),$$

which is also positive for all $z \in \mathbb{R}$, which means that $\ln(1+e^z)$ is a convex function.

Using the following two facts

1. Sum of convex functions is convex
2. Composition of a convex function with a convex nondecreasing function is convex

we can verify that $f(\boldsymbol{w})$ is indeed convex in $\boldsymbol{w}$ on $\mathbb{R}^d$.

Problem 3: Prove that for differentiable convex functions each local minimum is a global minimum. More specifically, given a differentiable convex function $f : \mathbb{R}^d \to \mathbb{R}$, prove that

a) if $\boldsymbol{x}^*$ is a local minimum, then $\boldsymbol{\nabla} f(\boldsymbol{x}^*) = \mathbf{0}$.

b) if $\boldsymbol{\nabla} f(\boldsymbol{x}^*) = \mathbf{0}$, then $\boldsymbol{x}^*$ is a global minimum.

We will show that if the gradient at some point $\boldsymbol{x}^*$ is not equal to zero, then this point cannot be a local optimum — we could simply follow the direction of the negative gradient and end up in a point with a lower value of the function.

More formally, suppose $\nabla f(\boldsymbol{x}^*) \neq \mathbf{0}$ for some $\boldsymbol{x}^*$. Then by Taylor's theorem for a sufficiently small $\varepsilon > 0$ we get

$$\begin{aligned} f(\boldsymbol{x}^* - \varepsilon \boldsymbol{\nabla} f(\boldsymbol{x}^*)) &= f(\boldsymbol{x}^*) - (\varepsilon \boldsymbol{\nabla} f(\boldsymbol{x}^*))^T \boldsymbol{\nabla} f(\boldsymbol{x}^*) + O(\varepsilon^2 \|\boldsymbol{\nabla}^2 f(\boldsymbol{x}^*)\|_2^2) \\ &= f(\boldsymbol{x}^*) - \varepsilon ||\boldsymbol{\nabla} f(\boldsymbol{x}^*)||_2^2 + O(\varepsilon^2 \|\boldsymbol{\nabla} f(\boldsymbol{x}^*)\|_2^2) \\ &< f(\boldsymbol{x}^*) \end{aligned}$$

Which means that $\boldsymbol{x}^*$ is not a local optimum. Therefore, the gradient must be equal to zero for any local optimum $\boldsymbol{x}^*$.

We will prove (b) using the first-order criterion for convexity:

$$f(\boldsymbol{y}) \geq f(\boldsymbol{x}) + (\boldsymbol{y} - \boldsymbol{x})^T \boldsymbol{\nabla} f(\boldsymbol{x}).$$

If we plug in $\boldsymbol{x}^*$ and use the fact that $\boldsymbol{\nabla} f(\boldsymbol{x}^*) = 0$ we get: $f(\boldsymbol{y}) \geq f(\boldsymbol{x}^*)$ for all $\boldsymbol{y}$, meaning $\boldsymbol{x}^*$ is a global minimum.

Homework

1 Convexity of functions

Problem 4: Assume that $f : \mathbb{R} \to \mathbb{R}$ and $g : \mathbb{R} \to \mathbb{R}$ are convex functions. Prove or disprove the following statements:

a) The function $h(x) = g(f(x))$ is convex.

b) The function $h(x) = g(f(x))$ is convex if g is non-decreasing.

Note: For this exercise you are not allowed to use the convexity preserving operations from the lecture.

a) Statement is false. Proof by counterexample: Suppose $f(x) = x^2$ and $g(z) = -x$. Since the function $h(x) = g(f(x)) = -x^2$ is twice differentiable, we can inspect its second derivative:

$$\frac{d^2}{dx^2}h(x) = -1.$$

Since the second derivative is negative for all x, we conclude that the function h is not convex.

(Note: It would actually be sufficient to show that the second derivative is negative for a single value of x)

b) Statement is true. Suppose $x_0, x_1 \in \mathbb{R}$ and $\lambda \in (0, 1)$. We will use a shorthand notation $x_\lambda = \lambda x_1 + (1 - \lambda)x_0$.

We will prove the convexity of h using the definition of convexity and the properties of f and g:

$$\begin{aligned}
&f \text{ convex} && \Rightarrow && f(x_\lambda) \leq \lambda f(x_1) + (1-\lambda) f(x_0) && \\
&g \text{ non-decresing} && \Rightarrow && g(f(x_\lambda)) \leq g(\lambda f(x_1) + (1-\lambda) f(x_0)) && (1)\\
&g \text{ convex} && \Rightarrow && g(\lambda f(x_1) + (1-\lambda) f(x_0)) \leq \lambda g(f(x_1)) + (1-\lambda) g(f(x_0)) && (2)\\
&(1) \text{ and } (2) && \Rightarrow && g(f(x_\lambda)) \leq \lambda g(f(x_1)) + (1-\lambda) g(f(x_0)) && \\
& && \Leftrightarrow && h(x_\lambda) \leq \lambda h(x_1) + (1-\lambda) h(x_0). &&
\end{aligned}$$

Therefore h is convex.

2 Optimization / Gradient descent

Problem 5: You are given the following objective function $f : \mathbb{R}^2 \to \mathbb{R}$

$$f(x_1, x_2) = 0.5x_1^2 + x_2^2 + 2x_1 + x_2 + \cos(\sin(\sqrt{\pi})).$$

a) Compute the minimizer $\boldsymbol{x}^*$ of f analytically.

As f is a sum of convex functions, it is convex. To find the global minimizer, we compute the gradient and set it to zero

$$\nabla f(x_1, x_2) = \begin{pmatrix} x_1 + 2 \\ 2x_2 + 1 \end{pmatrix} \stackrel{!}{=} \begin{pmatrix} 0 \\ 0 \end{pmatrix} \Rightarrow \begin{pmatrix} x_1^* \\ x_2^* \end{pmatrix} = \begin{pmatrix} -2 \\ -\frac{1}{2} \end{pmatrix}.$$

b) Perform 2 steps of gradient descent on f starting from the point $\boldsymbol{x}^{(0)} = (0, 0)$ with a constant learning rate $\tau = 1$.

We already know how to compute the gradient from a).

first step $$\begin{pmatrix} x_1^{(1)} \\ x_2^{(1)} \end{pmatrix} = \begin{pmatrix} x_1^{(0)} \\ x_2^{(0)} \end{pmatrix} - \tau \begin{pmatrix} x_1^{(0)} + 2 \\ 2x_2^{(0)} + 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} - 1 \begin{pmatrix} 0 + 2 \\ 0 + 1 \end{pmatrix} = \begin{pmatrix} -2 \\ -1 \end{pmatrix}$$

second step $$\begin{pmatrix} x_1^{(2)} \\ x_2^{(2)} \end{pmatrix} = \begin{pmatrix} x_1^{(1)} \\ x_2^{(1)} \end{pmatrix} - \tau \begin{pmatrix} x_1^{(1)} + 2 \\ 2x_2^{(1)} + 1 \end{pmatrix} = \begin{pmatrix} -2 \\ -1 \end{pmatrix} - 1 \begin{pmatrix} -2 + 2 \\ -2 + 1 \end{pmatrix} = \begin{pmatrix} -2 \\ 0 \end{pmatrix}$$

c) Will the gradient descent procedure from Problem b) ever converge to the true minimizer $\boldsymbol{x}^*$? Why or why not? If the answer is no, how can we fix it?

By performing one more iteration of gradient descent we observe that

$$\begin{pmatrix} x_1^{(3)} \\ x_2^{(3)} \end{pmatrix} = \begin{pmatrix} x_1^{(2)} \\ x_2^{(2)} \end{pmatrix} - \tau \begin{pmatrix} x_1^{(2)} + 2 \\ 2x_2^{(2)} + 1 \end{pmatrix} = \begin{pmatrix} -2 \\ 0 \end{pmatrix} - 1 \begin{pmatrix} -2 + 2 \\ 0 + 1 \end{pmatrix} = \begin{pmatrix} -2 \\ -1 \end{pmatrix} = \begin{pmatrix} x_1^{(1)} \\ x_2^{(1)} \end{pmatrix}.$$

That is, we are stuck iterating between $\boldsymbol{x}^{(1)}$ and $\boldsymbol{x}^{(2)}$ forever. We can fix this by decreasing the learning rate (adaptive stepsize, etc.).

Problem 6: Load the notebook `exercise_06_notebook.ipynb` from Moodle. Fill in the missing code and run the notebook. Export (download) the evaluated notebook as PDF and add it to your submission.

Note: We suggest that you use Anaconda for installing Python and Jupyter, as well as for managing packages. We recommend that you use Python 3.

For more information on Jupyter notebooks, consult the Jupyter documentation. Instructions for converting the Jupyter notebooks to PDF are provided on Piazza.

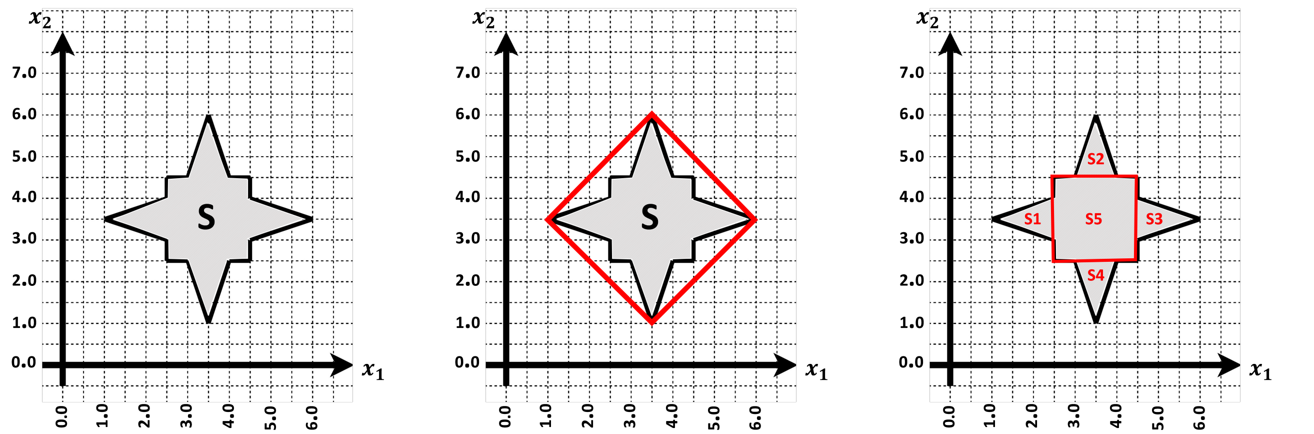
The solution notebook is uploaded to Moodle.

Problem 7: Let $f : \mathbb{R}^2 \to \mathbb{R}$ be the following convex function:

$$f(x_1, x_2) = e^{x_1+x_2} - 5 \cdot \log(x_2)$$

a) Consider the following shaded region $S \subset \mathbb{R}^2$. Is this region convex? Why?

b) Assume that we are given an algorithm $\texttt{ConvOpt}(f, D)$ that takes as input a convex function f and convex region D, and returns the <u>minimum</u> of f over D. Using the $\texttt{ConvOpt}$ algorithm, how would you find the global <u>minimum</u> of f over the shaded region S?



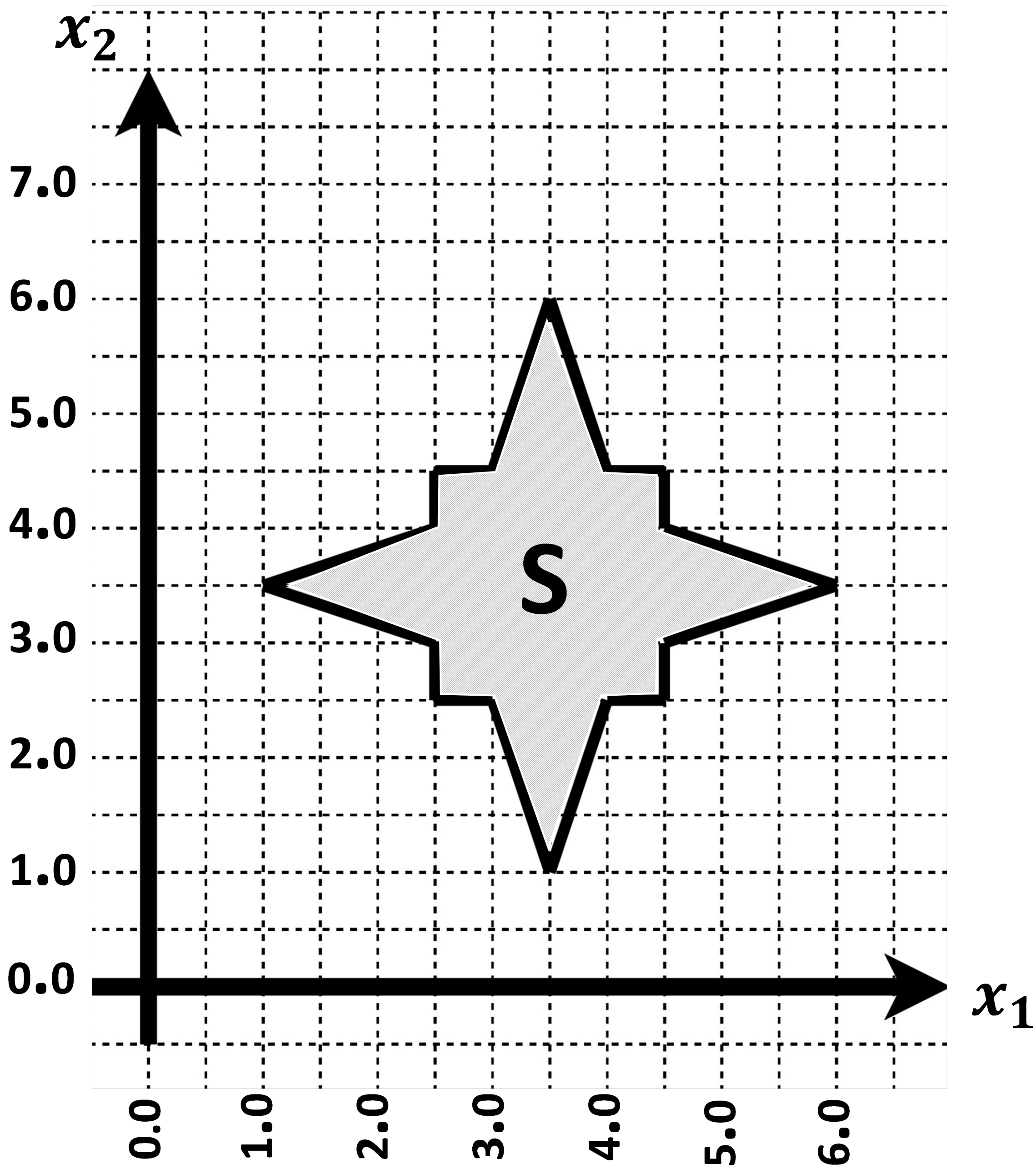
(a) initial non-convex set (b) convex hull (c) union of convex sets

a) It is not because we can choose two points in S such that the line connecting the points does not completely resides in S, for example $(1.0, 3.5)^T$ and $(3.5, 6.0)^T$ (see Figure 1b).

b) We can partition the shaded region S to the following five convex regions $S_1, \dots, S_5$ (see Figure 1c). Afterwards, we run the $\texttt{ConvOpt}$ algorithm separately for the 5 regions and obtain

$$m_i = \min_{\boldsymbol{x} \in S_i} f(\boldsymbol{x}) = \texttt{ConvOpt}(f, S_i)\,.$$

Finally, the minimum over the whole S can be computed as the smallest of these values, that is $\min_{\boldsymbol{x} \in S} f(\boldsymbol{x}) = \min(m_1, \dots, m_5)$.


x_2
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
S
x_1
0.0
1.0
2.0
3.0
4.0
5.0
6.0