Convexity, Subgradients and SVM

Optimization for Machine Learning — Homework #1

Monday 8th May, 2023

The theory part can be handed-in physically during the exercise session, or digitally if typeset on Moodle. The programming part has to be sent on Moodle. Group work is allowed (2-3 people), but submissions are personal.

Part I: Theory

12+2 points

I.1. Convexity

Exercise I.1 (2+1 points). Let $f: \mathbb{R}^d \to \mathbb{R}$ and $g: \mathbb{R}^d \to \mathbb{R}$ be two convex functions. Show that f+g is convex.

Bonus: Show that $x \mapsto \max(f(x), g(x))$ is convex.

Answer I.1. Let $f: \mathbb{R}^d \to \mathbb{R}$ and $g: \mathbb{R}^d \to \mathbb{R}$ be two convex functions. The domain of the function h := f + g is \mathbb{R}^d , which is convex. Then, let $\lambda \in [0, 1]$, $(x, y) \in \mathbb{R}^d \times \mathbb{R}^d$, and evaluate

$$\begin{split} h(\lambda x + (1-\lambda)y) &= f(\lambda x + (1-\lambda)y) + g(\lambda x + (1-\lambda)y) \\ &\leqslant \lambda f(x) + (1-\lambda)f(y) + \lambda g(x) + (1-\lambda)g(y) \quad \text{since } f \text{ and } g \text{ are convex} \\ &\leqslant \lambda (f(x) + g(x)) + (1-\lambda)(f(y) + g(y)) \\ &\leqslant \lambda h(x) + (1-\lambda)h(y), \end{split}$$

and h = f + g is convex.

Bonus: Now, let $h: x \mapsto \max(f(x), g(x))$. The domain of h is convex. For $\lambda \in [0, 1]$ and $(x, y) \in \mathbb{R}^d \times \mathbb{R}^d$, evaluate

$$\begin{split} h(\lambda x + (1-\lambda)y) &= \max \left\{ f(\lambda x + (1-\lambda)y), g(\lambda x + (1-\lambda)y) \right\} \\ &\leqslant \max \left\{ \lambda f(x) + (1-\lambda)f(y), \lambda g(x) + (1-\lambda)g(y) \right\} \qquad f, g \text{ convex} \\ &\leqslant \max \left\{ \lambda f(x), \lambda g(x) \right\} + \max \left\{ (1-\lambda)f(y), (1-\lambda)g(y) \right\} \end{split}$$

(since $\max(a+b,c+d)\leqslant \max(a,c)+\max(b,d)$ for all $(a,b,c,d)\in\mathbb{R}^4$)

$$\leq \lambda \max \left\{ f(x), g(x) \right\} + (1 - \lambda) \max \left\{ f(y), g(y) \right\} \qquad \max(ca, cb) = c \max(a, b) \text{ for } c \geqslant 0$$

$$\leq \lambda h(x) + (1 - \lambda) h(y).$$

Exercise I.2 (2+1 points). Let $f: \mathbb{R}^n \to \mathbb{R}^m$ be a linear function (i.e. f(x) = Ax, for $A \in \mathbb{R}^{m \times n}$) and $g: \mathbb{R}^m \to \mathbb{R}$ be convex functions. Show that $g \circ f: \mathbb{R}^n \to \mathbb{R}$ is convex.

Bonus: What about if f is affine, i.e. f(x) = Ax + b, with $b \in \mathbb{R}^m$?

Answer I.2. The domain of $g \circ f$ is convex (\mathbb{R}^n) . Let $\lambda \in [0,1]$, and $(x,y) \in \mathbb{R}^n \times \mathbb{R}^n$. Evaluate

$$g \circ f(\lambda x + (1 - \lambda)y) = g(A(\lambda x + (1 - \lambda)y)) = g(\lambda Ax + (1 - \lambda)Ay)$$

$$\leqslant \lambda g(Ax) + (1 - \lambda)g(Ay) \quad (g \text{ is convex})$$

$$\leqslant \lambda (g \circ f)(x) + (1 - \lambda)(g \circ f)(y),$$

and $g \circ f$ is convex.

Bonus: If f is affine on \mathbb{R}^n , i.e. f(x) = Ax + b with $A \in \mathbb{R}^{m \times n}$ and $b \in \mathbb{R}^m$, a common trick is to express f as a linear function on \mathbb{R}^{n+1} , by setting $\widetilde{x} = \begin{pmatrix} x \\ 1 \end{pmatrix} \in \mathbb{R}^{n+1}$ and $\widetilde{A} = \begin{pmatrix} A & b \end{pmatrix} \in \mathbb{R}^{m \times (n+1)}$. One checks that $\widetilde{A}\widetilde{x} = Ax + b$, and that for $\lambda \in [0,1]$, if $x_{\lambda} = \lambda x_1 + (1-\lambda)x_0$, then $\widetilde{x}_{\lambda} = \lambda \widetilde{x}_1 + (1-\lambda)\widetilde{x}_0$. Therefore, the function $\widetilde{f} \colon x \mapsto \widetilde{A}\widetilde{x}$ is linear, and $g \circ \widetilde{f} = g \circ f$ is convex.

I.2. (Sub-) Gradients

It is assumed known that, if E_1 and E_2 are two convex functions,

$$\partial(E_1 + E_2)(w) = \partial E_1(w) + \partial E_2(w) = \{g_1 + g_2 \mid g_1 \in \partial E_1(w), g_2 \in \partial E_2(w)\}\$$

Exercise I.3 (2 points). Let $\phi \colon \mathbb{R}^d \to \mathbb{R}^p$ be a differentiable basis function. Define the model $f \colon \mathbb{R}^d \times \mathbb{R}^p \to \mathbb{R}$ as, for $b \in \mathbb{R}$,

$$f: \mathbb{R}^d \times \mathbb{R}^p \longrightarrow \mathbb{R}$$

 $(x, w) \longmapsto \langle w, \phi(x) \rangle + b$

- 1. What is $\nabla_w f(x, w)$?
- 2. What is $\nabla_x f(x, w)$?

Answer I.3. 1. One computes, for $(x, w) \in \mathbb{R}^d \times \mathbb{R}^p$, $\nabla_w f(x, w) = \phi(x)$.

2. The function $\phi \colon \mathbb{R}^d \to \mathbb{R}^p$ is differentiable, let $J_{\phi}(x) \in \mathbb{R}^{p \times d}$ be its Jacobian at $x \in \mathbb{R}^d$. With the chain-rule for products (cf Ex Sheet#1), one computes for $(x, w) \in \mathbb{R}^d \times \mathbb{R}^p$, $\nabla_x f(x, w) = J_{\phi}(x)^{\top} w$

Exercise I.4 (2 points). For $\lambda \ge 0$, let $E(w) = E_s(w) + \lambda ||w||_1$, where E_s is assumed to be convex and everywhere differentiable, and

$$||w||_1 := \sum_{i=1}^p |w_i|$$

is the 1-norm of w.

- 1. Is E convex?
- 2. Where is $w \mapsto ||w||_1$ (not) differentiable?
- 3. What is $\partial E(w)$ (as a function of $\nabla E_s(w)$)? (Hint: see what happens for p=1,2 first.)

Answer I.4. 1. E is convex, as the sum of two convex functions in w: E_s and $w \mapsto \lambda ||w||_1$ (for $\lambda \ge 0$, λf is convex if f is).

The function $w \mapsto ||w||_1$ is convex as a sum of convex functions on the coordinates w_i $(t \mapsto |t|)$ is convex since $\forall t \in \mathbb{R}$, $|t| = \max(-t, t)$, and $t \mapsto \max(f(t), g(t))$ is convex when f and g are, see Ex I.1).

- 2. The function $\mathbb{R} \ni t \mapsto |t|$ is differentiable on $(-\infty,0) \cup (0,+\infty)$, but not on 0. Therefore, $\mathbb{R}^p \ni w \mapsto ||w||_1$ is differentiable at $w \in \mathbb{R}^p$ if and only if $\forall i \in [p], \ w_i \neq 0$.
- 3. $w \mapsto E(w)$ is convex but not differentiable everywhere (since $w \mapsto ||w||_1$ is not differentiable everywhere). Since E_s is differentiable, we always have

$$\partial E(w) = \{\nabla E_{s}(w)\} + \partial(w \mapsto \lambda ||w||_{1})(w)$$

We are looking for $\partial(w\mapsto \lambda \|w\|_1)(w)=\lambda \partial \|w\|_1$. We can see what happens for p=1,2.

- For p=1, from Ex Sheet#1, $\partial |w|=\begin{cases} \{-1\} & \text{if } w<0,\\ [-1,1] & \text{if } w=0,.\\ \{1\} & \text{if } w>0 \end{cases}$
- For p=2, $\partial \|w\|_1=\partial \left(|w_1|+|w_2|\right)=\partial \left((w_1,w_2)\mapsto |w_1|\right)(w)+\partial \left((w_1,w_2)\mapsto |w_2|\right)(w)$. The subdifferential $\partial \left((w_1,w_2)\mapsto |w_1|\right)(w)\subset \mathbb{R}^2$ can be written

$$\partial ((w_1, w_2) \mapsto |w_1|) (w) = \left\{ \begin{pmatrix} g_1 \\ 0 \end{pmatrix} \mid g_1 \in \begin{cases} \{-1\} & \text{if } w_1 < 0, \\ [-1, 1] & \text{if } w_1 = 0, \\ \{1\} & \text{if } w_1 > 0 \end{cases} \right\}.$$

Likewise, the subdifferential $\partial \left((w_1, w_2) \mapsto |w_2| \right) (w) \subset \mathbb{R}^2$ can be written

$$\partial \left((w_1, w_2) \mapsto |w_2| \right) (w) = \left\{ \begin{pmatrix} 0 \\ g_2 \end{pmatrix} \mid g_2 \in \begin{cases} \{-1\} & \text{if } w_2 < 0, \\ [-1, 1] & \text{if } w_2 = 0, \\ \{1\} & \text{if } w_2 > 0 \end{cases} \right\}.$$

$$\text{Therefore, } \partial \left(\left(w_1, w_2 \right) \mapsto \left\| w \right\|_1 \right) \left(w_1, w_2 \right) = \left\{ \begin{pmatrix} g_1 \\ g_2 \end{pmatrix} \mid \forall i \in \{1, 2\}, \ g_i \in \left\{ \begin{aligned} \{-1\} & \text{if } w_i < 0, \\ [-1, 1] & \text{if } w_i = 0, \\ \{1\} & \text{if } w_i > 0 \end{aligned} \right\}$$

This carries out to any dimension p, so that, for $w \in \mathbb{R}^p$,

$$\partial (w \mapsto ||w||_1) (w) = \left\{ g \in \mathbb{R}^p \mid \forall i \in [p], g_i \in \begin{cases} \{-1\} & \text{if } w_i < 0, \\ [-1, 1] & \text{if } w_i = 0, \\ \{1\} & \text{if } w_i > 0 \end{cases} \right\}$$

To conclude,

$$\partial E(w) = \{ \nabla E_{\mathbf{s}}(w) \} + \lambda \partial \|w\|_{1}$$

$$= \left\{ \nabla E_{\mathbf{w}}(w) + g \in \mathbb{R}^{p} \mid \forall i \in [p], g_{i} \in \begin{cases} \{-\lambda\} & \text{if } w_{i} < 0, \\ [-\lambda, \lambda] & \text{if } w_{i} = 0, \\ \{\lambda\} & \text{if } w_{i} > 0 \end{cases} \right\}$$

I.3. Support Vector Machines

Exercise I.5 (4 points). The Support Vector Machines (SVM) algorithm solves a binary classification task. Given N couples samples I targets $\{x_i, t_i\}_{i \in [N]}$, with $x_i \in \mathbb{R}^d$ and $t_i \in \{-1, 1\}$ for each $i \in [N] := \{1, \ldots, N\}$, the goal is to classify the samples, i.e. find the regions where the positive (resp. negative) samples lie. We will do that by finding a **hyperplane that separates** (or **splits**) the dataset, with positive samples on one side of the hyperplane and the negative on the other. We assume that **such an hyperplane exists** (the samples are said to be *linearly separable*). One can picture the case for d = 2 or d = 3, where points are clustered in two groups and can be separated by a straight line (d = 2) or a plane (d = 3), see Figure 1a.

A hyperplane in \mathbb{R}^d is represented with a vector $w \in \mathbb{R}^d$ and a bias $b \in \mathbb{R}$ with the equation

$$y(x; w, b) = \langle w, x \rangle + b. \tag{1}$$

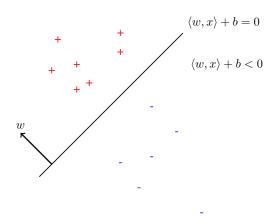
For $i \in [N]$, denote $y_i := y(x_i; w, b) = \langle w, x_i \rangle + b$. Note that y_i still depends on (w, b) even if the notation is dropped.

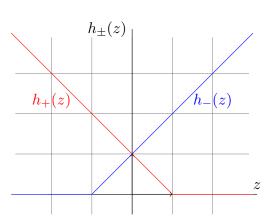
The hyperplane equation (1) splits \mathbb{R}^d into three regions:

- points x such that y(x) > 0,
- points x such that y(x) = 0 (the hyperplane itself),
- points x such that y(x) < 0.

Therefore, we would like to find an hyperplane such that the samples x_i that have a positive target $t_i = 1$ all lie on the side of the hyperplane where y(x) > 0, i.e. $t_i = 1 \implies y_i > 0$, and reciprocally all samples x_i such that $t_i = -1$ should be on the side where y(x) < 0, i.e. $t_i = -1 \implies y_i < 0$. Then, the target t_i could simply by read from y_i by looking at its sign.

 $\langle w, x \rangle + b > 0$





- (a) Possible solution found by SVM. Points with $t_i = +1$ (in red) are on the side where y(x) > 0, points with $t_i = -1$ (in blue) are on the side where y(x) < 0.
- (b) In red, the loss function for the samples that have $t_i = +1$. In blue, the loss function for the samples with $t_i = -1$.

Figure 1: SVM illustration, d = 2.

With this requirement, the product $t_i y_i$ should **always be positive**, and the loss we define is

$$\forall (w,b) \in \mathbb{R}^d \times \mathbb{R}, \quad E(w,b) = \sum_{i=1}^N \max(0, 1 - t_i y_i) = \sum_{i=1}^N \max(0, 1 - t_i (\langle w, x_i \rangle + b)), \quad (2)$$

which has the effect of pushing the product t_iy_i towards the greatest value possible, for all $i \in [N]$.

Let $\mathcal{I}_+ = \{i \in [N] \mid t_i = +1\}$ and $\mathcal{I}_- = \{i \in [N] \mid t_i = -1\}$ be the sets of the indices of the positive and negative samples. The loss can be further written as

$$\forall (w,b) \in \mathbb{R}^d \times \mathbb{R}, \quad E(w,b) = \sum_{i \in \mathcal{I}_+} \max(0,1-y_i) + \sum_{i \in \mathcal{I}_-} \max(0,1+y_i) =: \sum_{i \in \mathcal{I}_+} h_+(y_i) + \sum_{i \in \mathcal{I}_-} h_-(y_i)$$

The functions h_+ and h_- are plotted in Figure 1b.

1. Why is the loss $(w, b) \mapsto E(w, b)$ convex? (*Hint*: if f and g are convex, then $\max(f, g)$ is convex).

Recall that the function $h_+ \colon \mathbb{R} \ni z \mapsto \max(0, 1 - z)$ has the following subgradient (see Exercise Sheet #2, I.2):

$$\partial h_{+}(z) = \begin{cases} \{-1\} & \text{if } z < 1, \\ [-1, 0] & \text{if } z = 1, \\ \{0\} & \text{if } z > 1. \end{cases}$$

2. Show that the subgradient of the function $h_-: \mathbb{R} \ni z \mapsto \max(0, 1+z)$ is

$$\partial h_{-}(z) = \begin{cases} \{0\} & \text{if } z < -1, \\ [0,1] & \text{if } z = -1, \\ \{1\} & \text{if } z > -1. \end{cases}$$

- 3. Using the chain rule for the subgradients $\partial(g \circ A)(\widetilde{w}) = A^{\top} \partial g(A\widetilde{w})$, for any linear operator $A \in \mathbb{R}^{m \times p}$, and convex function $g \colon \mathbb{R}^m \to \mathbb{R}$, and $\widetilde{w} \in \mathbb{R}^p$, compute the subgradient of the loss E with respect to w and b at $(w, b) \in \mathbb{R}^d \times \mathbb{R}$.
- 4. What should be the (sub-) gradient descent algorithm to minimize E?

Answer I.5. 1. • The model y_i is affine in w, hence convex

- The functions h_+ and h_- are the maximum of convex (affine) functions of w, hence they are convex.
- The loss $w \mapsto E(w)$ is a sum of convex functions in w, hence is itself convex in w.
- 2. With the chain rule formula, $h_{-}(z) = h_{+}(-z)$, hence $\partial h_{-}(z) = -\partial h_{+}(-z)$ (!).

Without the chain rule formula, or to practice the definition of a subgradient, let $h_-: \mathbb{R} \ni z \mapsto \max(0, 1 + z)$. h_- is differentiable on $(-\infty, -1) \cup (-1, +\infty)$, with derivative 0 on $\{0\}$ if z < -1,

$$(-\infty, -1)$$
 and 1 on $(-1, +\infty)$, hence $\partial h_{-}(z) = \begin{cases} \{0\} & \text{if } z < -1, \\ \{1\} & \text{if } z > -1 \end{cases}$.

At z = -1, h_- is not differentiable. We argue by necessary conditions. We are looking a subgradient $g \in \mathbb{R}$, such that, for any $y \in \mathbb{R}$,

$$h_{-}(y) \geqslant h_{-}(-1) + g \cdot (y - (-1))$$

$$\iff \max(0, 1 + y) \geqslant g \cdot (y + 1)$$
(3)

- At y=-1, the condition become $0 \ge g \cdot 0$, which is true for any $g \in \mathbb{R}$ (condition is not discriminative).
- For y < -1 (i.e. y + 1 < 0), the condition becomes $0 \ge g \cdot (y + 1) \implies 0 \le g$.
- For y > -1 (i.e. y+1 > 0), the condition becomes $1+y \ge g \cdot (y+1) \implies 1 \ge g$.

Therefore, a subgradient g of h_- at z=-1 will have to be such that $g \in [0,1]$ (necessary condition).

One checks that, which such a $g \in [0, 1]$, the subgradient condition (3) is verified.

Therefore, $\partial h_{-}(-1) = [0, 1]$, and we conclude

$$\partial h_{-}(z) = \begin{cases} \{0\} & \text{if } z < -1, \\ [0, 1] & \text{if } z = -1, \\ \{1\} & \text{if } z > -1. \end{cases}$$

3. For
$$(w,b) \in \mathbb{R}^d \times \mathbb{R}$$
, let $\widetilde{w} = \begin{pmatrix} w \\ b \end{pmatrix} \in \mathbb{R}^{d+1}$, and for each sample $x_i \in \mathbb{R}^d$, $i \in [N]$, let $A_i = \begin{pmatrix} x_i^\top & 1 \end{pmatrix} \in \mathbb{R}^{1 \times (d+1)}$. Then,

$$A_i \widetilde{w} = x_i^{\top} w + b = y_i(w, b).$$

This is the usual trick to express an affine function as a linear function, with an increment in the dimension. Now, E can be expressed as a function of \widetilde{w}

$$\begin{split} E(w,b) &= E(\widetilde{w}) = \sum_{i \in \mathcal{I}_{+}} h_{+}(y_{i}) + \sum_{i \in \mathcal{I}_{-}} h_{-}(y_{i}) \\ &= \sum_{i \in \mathcal{I}_{+}} h_{+}(A_{i}\widetilde{w}) + \sum_{i \in \mathcal{I}_{-}} h_{-}(A_{i}\widetilde{w}) \end{split}$$

We can apply the formula for the subdifferential chain rule. For $(w,b) \in \mathbb{R}^d \times \mathbb{R}$,

$$\partial E(\widetilde{w}) = \sum_{i \in \mathcal{I}_{+}} \partial (h_{+} \circ A_{i})(\widetilde{w}) + \sum_{i \in \mathcal{I}_{-}} \partial (h_{-} \circ A_{i})(\widetilde{w})$$

$$= \sum_{i \in \mathcal{I}_{+}} A_{i}^{\top} \partial h_{+}(A_{i}\widetilde{w}) + \sum_{i \in \mathcal{I}_{-}} A_{i}^{\top} \partial h_{-}(A_{i}\widetilde{w})$$

$$= \sum_{i \in \mathcal{I}_{+}} \begin{pmatrix} x_{i} \\ 1 \end{pmatrix} \partial h_{+}(y_{i}) + \sum_{i \in \mathcal{I}_{-}} \begin{pmatrix} x_{i} \\ 1 \end{pmatrix} \partial h_{-}(y_{i}), \tag{4}$$

with the subgradients $\partial h_+(y_i)$ and $\partial h_-(y_i)$ derived earlier.

- 4. The subgradient algorithm to minimize E is as follows.
 - a) Start with a zero $\widetilde{w}^{(0)}=\begin{pmatrix} w^{(0)} \\ b^{(0)} \end{pmatrix}=\mathbf{0}_{d+1}.$ Choose a learning rate $\eta>0.$
 - b) From a time step k, update the parameters to k+1 as

$$\widetilde{w}^{(k+1)} = \widetilde{w}^{(k)} - \eta \cdot \operatorname{sg}^{(k)},$$

where $\operatorname{sg}^{(k)} \in \mathbb{R}^{d+1}$ is a subgradient at time k, computed as $\operatorname{sg}^{(k)} \in \partial E(\widetilde{w}^{(k)})$. From (4), we see that $\operatorname{sg}^{(k)} = \sum_{i \in [N]} \operatorname{sg}_i^{(k)}$ is a sum of contributions over all samples $i \in [N]$ (each $\operatorname{sg}_i^{(k)} \in \mathbb{R}^{d+1}$). More explicitly:

For all $i \in \mathcal{I}_+$, compute $y_i^{(k)} = \langle w^{(k)}, x_i \rangle + b^{(k)}$. The contribution $\operatorname{sg}_i^{(k)}$ depends on t_i and $y_i^{(k)}$:

i. If $i \in \mathcal{I}_+$ (i.e. $t_i = +1$), then

$$\operatorname{sg}_{i}^{(k)} = \alpha_{i} \cdot \begin{pmatrix} x_{i} \\ 1 \end{pmatrix}, \ \alpha_{i} \in \begin{cases} \{-1\} & \text{if } y_{i}^{(k)} < 1, \\ [-1, 0] & \text{if } y_{i}^{(k)} = 1, \\ \{0\} & \text{if } y_{i}^{(k)} > 1. \end{cases}$$
 (5)

ii. If $i \in \mathcal{I}_-$ (i.e. $t_i = -1$), then

$$\operatorname{sg}_{i}^{(k)} = \alpha_{i} \cdot \begin{pmatrix} x_{i} \\ 1 \end{pmatrix}, \, \alpha_{i} \in \begin{cases} \{0\} & \text{if } y_{i}^{(k)} < -1, \\ [0, 1] & \text{if } y_{i}^{(k)} = -1, \\ \{1\} & \text{if } y_{i}^{(k)} > -1. \end{cases}$$

$$(6)$$

c) Once a convergence criterion is reached, output $\widetilde{w}^{(K)}$.

$$\textit{Remark I.3.1.} \ \ \text{Notice how } \text{sg}_i^{(k)} = t_i \alpha_i \begin{pmatrix} x_i \\ 1 \end{pmatrix}, \ \alpha_i \in \begin{cases} \{-1\} & \text{if } t_i y_i^{(k)} < 1, \\ [-1,0] & \text{if } t_i y_i^{(k)} = 1, \text{: one could} \\ \{0\} & \text{if } t_i y_i^{(k)} > 1. \end{cases}$$

have worked with the expression (2) without splitting the samples into \mathcal{I}_+ and \mathcal{I}_- , but one goal was to practice the definition of the subgradient with h_- . In addition, the expression with split \mathcal{I}_+ , \mathcal{I}_- has a more detailed interpretation.

Part II: Programming

8+2 points

Exercise II.1 (8+2 points). This exercise implements some material from Exercise I.5. The data is generated with the helper function gen_binary_data in ex02/utils.py. The dimension is set to d=2 in order to visualize the result at the end. The generation simply draws some random points on the plane, draws an hyperplane, and classify the points depending on the sign of $\langle w, x \rangle + b$. Therefore, the training data is linearly separable.

- 1. Implement the loss from (2).
- 2. Implement the (sub-) gradient algorithm derived in I.5.4
- 3. Visualize the solution found by the algorithm, as well as its convergence.
- 4. *Bonus*: What happens if the data is not linearly separable?