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 $f\colon \mathbb{R}^d \to \mathbb{R}$ and $g\colon \mathbb{R}^d \to \mathbb{R}$ 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 $f\colon \mathbb{R}^d \to \mathbb{R}$ and $g\colon \mathbb{R}^d \to \mathbb{R}$ 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

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

and $h = f+g$ is convex.

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

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

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

$$\begin{aligned} &\leqslant \lambda \max\left\{ f(x), g(x) \right\} + (1-\lambda) \max\left\{ f(y), g(y) \right\} \qquad \max(ca, cb) = c \max(a,b) \text{ for } c \geqslant 0 \\ &\leqslant \lambda h(x) + (1-\lambda) h(y). \end{aligned}$$

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

$$\begin{aligned} g \circ f(\lambda x + (1-\lambda)y) = g(A(\lambda x + (1-\lambda)y)) &= g(\lambda Ax + (1-\lambda)Ay) \\ &\leqslant \lambda g(Ax) + (1-\lambda)g(Ay) \quad (g \text{ is convex}) \\ &\leqslant \lambda(g\circ f)(x) + (1-\lambda)(g\circ f)(y), \end{aligned}$$

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 $\widetilde{f}\colon \widetilde{x} \mapsto \widetilde{A}\widetilde{x}$ is linear, and $g \circ \widetilde{f} \circ (x \mapsto \widetilde{x}) = g \circ f$ 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 $b \in \mathbb{R}$,

$$\begin{array}{rccl} f & : & \mathbb{R}^d \times \mathbb{R}^p & \longrightarrow & \mathbb{R} \\ & & (x,w) & \longmapsto & \langle w, \phi(x)\rangle + b \end{array}$$

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 product rule for gradients (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 $\lambda \geqslant 0$, let $E(w) = E_{\mathrm{s}}(w) + \lambda\|w\|_1$, 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 $\nabla E_{\mathrm{s}}(w)$)? (*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 $\lambda \geqslant 0$, 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

$$\partial E(w) = \{\nabla E_{\mathrm{s}}(w)\} + \partial(w \mapsto \lambda\|w\|_1)(w)$$

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#2 I.2, $\partial|w| = \begin{cases} \{-1\} & \text{if } w < 0, \\ [-1, 1] & \text{if } w = 0, . \\ \{1\} & \text{if } w > 0 \end{cases}$
- 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

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

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

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

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

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

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

To conclude,

$$\begin{aligned} \partial E(w) &= \{\nabla E_{\mathrm{s}}(w)\} + \lambda \partial \|w\|_1 \\ &= \left\{ \nabla E_{\mathrm{w}}(w) + g \in \mathbb{R}^p \mid \forall i \in [p],\ g_i \in \begin{cases} \{-\lambda\} & \text{if } w_i < 0, \\ [-\lambda, \lambda] & \text{if } w_i = 0, \\ \{\lambda\} & \text{if } w_i > 0 \end{cases} \right\} \end{aligned}$$

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 / 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

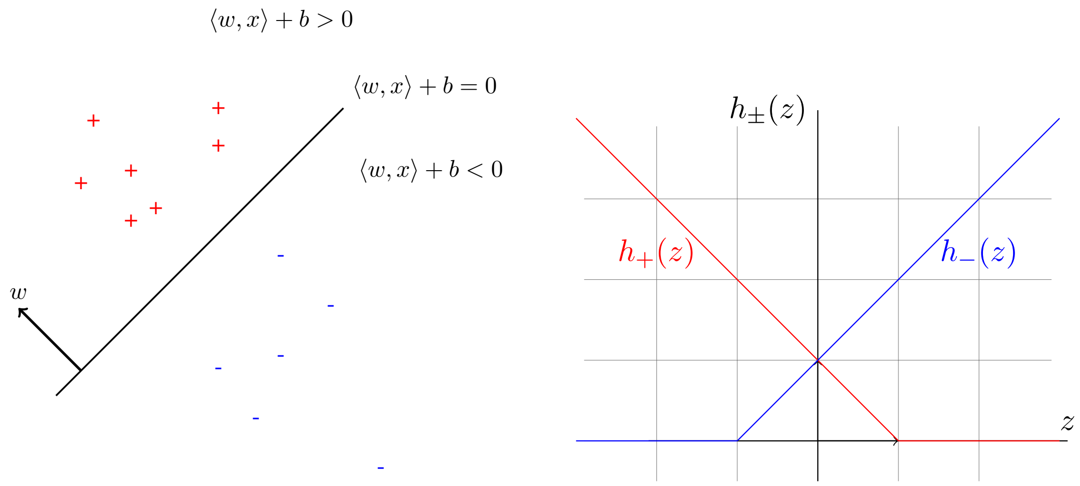
$$y(x; w, b) = \langle w, x \rangle + b. \tag{1}$$

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.



(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

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

which has the effect of pushing the product $t_i y_i$ 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 $(-\infty, -1)$ 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 $y \in \mathbb{R}$,

$$\begin{aligned} & h_-(y) \geqslant h_-(-1) + g \cdot (y - (-1)) \\ \iff \quad & \max(0, 1+y) \geqslant g \cdot (y+1) \end{aligned} \tag{3}$$

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

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 $\widetilde{w}$
$$\begin{aligned} E(w, b) = E(\widetilde{w}) &= \sum_{i\in\mathcal{I}_+} h_+(y_i) + \sum_{i\in\mathcal{I}_-} h_-(y_i) \\ &= \sum_{i\in\mathcal{I}_+} h_+(A_i\widetilde{w}) + \sum_{i\in\mathcal{I}_-} h_-(A_i\widetilde{w}) \end{aligned}$$
We can apply the formula for the subdifferential chain rule. For $(w, b) \in \mathbb{R}^d \times \mathbb{R}$,
$$\begin{aligned} \partial E(\widetilde{w}) &= \sum_{i\in\mathcal{I}_+} \partial(h_+ \circ A_i)(\widetilde{w}) + \sum_{i\in\mathcal{I}_-} \partial(h_- \circ A_i)(\widetilde{w}) \\ &= \sum_{i\in\mathcal{I}_+} A_i^\top \partial h_+(A_i\widetilde{w}) + \sum_{i\in\mathcal{I}_-} A_i^\top \partial h_-(A_i\widetilde{w}) \\ &= \sum_{i\in\mathcal{I}_+} \begin{pmatrix} x_i \\ 1 \end{pmatrix} \partial h_+(y_i) + \sum_{i\in\mathcal{I}_-} \begin{pmatrix} x_i \\ 1 \end{pmatrix} \partial h_-(y_i), \end{aligned} \tag{4}$$
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
   $$\widetilde{w}^{(k+1)} = \widetilde{w}^{(k)} - \eta \cdot \mathrm{sg}^{(k)},$$
   where $\mathrm{sg}^{(k)} \in \mathbb{R}^{d+1}$ is a subgradient at time k, computed as $\mathrm{sg}^{(k)} \in \partial E(\widetilde{w}^{(k)})$. From (4), we see that $\mathrm{sg}^{(k)} = \sum_{i\in[N]} \mathrm{sg}_i^{(k)}$ is a sum of contributions over all samples $i \in [N]$ (each $\mathrm{sg}_i^{(k)} \in \mathbb{R}^{d+1}$). More explicitly:

   For all $i \in \mathcal{I}_+$, compute $y_i^{(k)} = \langle w^{(k)}, x_i\rangle + b^{(k)}$. The contribution $\mathrm{sg}_i^{(k)}$ depends on t_i and $y_i^{(k)}$:
      i. If $i \in \mathcal{I}_+$ (i.e. $t_i = +1$), then
      $$\mathrm{sg}_i^{(k)} = \alpha_i \cdot \begin{pmatrix} x_i \\ 1 \end{pmatrix},\ \alpha_i \in \begin{cases} \{-1\} & \text{if } y_i^{(k)} < 1, \\ [-1, 0] & \text{if } y_i^{(k)} = 1, \\ \{0\} & \text{if } y_i^{(k)} > 1. \end{cases} \tag{5}$$

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

$$\mathrm{sg}_i^{(k)} = \alpha_i \cdot \begin{pmatrix} x_i \\ 1 \end{pmatrix}, \; \alpha_i \in \begin{cases} \{0\} & \text{if } y_i^{(k)} < -1, \\ [0,1] & \text{if } y_i^{(k)} = -1, \\ \{1\} & \text{if } y_i^{(k)} > -1. \end{cases} \tag{6}$$

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

The energy is not ensured to decrease at each step. One clever way around it is to record the current minimizer and output it.

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