MATH3431 Machine Learning and Neural Networks III — Epiphany term 2023

Exercise sheet

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Part 1. Stochastic learning

Exercise 1. ($\star$)Let $f:\mathbb{R}^d\rightarrow\mathbb{R}$ such that $f(w)=g(<w,x>+y)$ or some $x\in\mathbb{R}^d$, $y\in\mathbb{R}$. Show that: If g is convex function then $f$is convex function.

Solution. Let $u,v\in\mathbb{R}^d$ and $a\in[0,1]$. It is

$$\begin{aligned}
f(\alpha u+(1-\alpha)v) =& g(<\alpha u+(1-\alpha)v,x>+y)\\
=& g(<\alpha u,x>+<(1-\alpha)v,x>+y)\\
=& g(\alpha(<u,x>+y)+(1-\alpha)(<v,x>+y)) \qquad y=\alpha y+(1-\alpha)y\\
\leq& \alpha g(<u,x>+y)+(1-\alpha)g(<v,x>+y) \qquad (g\text{ is convex})\\
=& \alpha f(u)+(1-\alpha)f(v)
\end{aligned}$$

Exercise 2. ($\star$)Let functions g_1 be ρ_1-Lipschitz and g_2 be ρ_2-Lipschitz. Then, show that, f with $f(x)=g_1(g_2(x))$ is $\rho_1\rho_2$-Lipschitz.

Solution.

$$\begin{aligned}
|f(w_1)-f(w_2)| =& |g_1(g_2(w_1))-g_1(g_2(w_2))|\\
\leq& \rho_1|g_2(w_1)-g_2(w_2)|\\
\leq& \rho_1\rho_2|w_1-w_2|
\end{aligned}$$

Exercise 3. ($\star$)Let $f:\mathbb{R}^d\rightarrow\mathbb{R}$ with $f(w)=g(\langle w,x\rangle+y)$ $x\in\mathbb{R}^d$ and $y\in\mathbb{R}$. Let $g:\mathbb{R}\rightarrow\mathbb{R}$ be a β-smooth function. Then show that f is a $\left(\beta\|x\|^2\right)$-smooth.

Hint:: You may use Cauchy-Schwarz inequality $\langle y,x\rangle\leq\|y\|\|x\|$

$$
\begin{aligned}
f(v) =& g(\langle w, x\rangle + y) \\
\leq & g(\langle w, x\rangle + y) + g'(\langle w, x\rangle + y)\langle v - w, x\rangle + \frac{\beta}{2}(\langle v - w, x\rangle)^2 && (g \text{ is smooth}) \\
\leq & g(\langle w, x\rangle + y) + g'(\langle w, x\rangle + y)\langle v - w, x\rangle + \frac{\beta}{2}(\|v - w\| \|x\|)^2 && (\text{Cauchy-Schwatz inequality}) \\
=& f(w) + \langle \nabla f(w), v - w\rangle + \frac{\beta \|x\|^2}{2}\|v - w\|^2
\end{aligned}
$$

Exercise 4. ($\star$)Show that $f : S \to \mathbb{R}$ is ρ-Lipschitz over an open convex set S if and only if for all $w \in S$ and $v \in \partial f(w)$ it is $\|v\| \leq \rho$.

Hint:: You may use Cauchy-Schwarz inequality $\langle y, x\rangle \leq \|y\| \|x\|$

Solution. $\Longrightarrow$ Let $f : S \to \mathbb{R}$ be ρ-Lipschitz over convex set S, $w \in S$ and $v \in \partial f(w)$.

- Since S is open we get that there exist $\epsilon > 0$ such as $u := w + \epsilon \frac{v}{\|v\|}$ where $u \in S$. So $\langle u - w, v\rangle = \epsilon \|v\|$ and $\|u - w\| = \epsilon$.
- From the subgradient definition we get

$$f(u) - f(w) \geq \langle u - w, v\rangle = \epsilon \|v\|$$

- From the Lipschitzness of $f(\cdot)$ we get

$$f(u) - f(w) \geq \rho \|u - w\| = \rho\epsilon$$

Therefore $\|v\| \leq \rho$.

$\Longleftarrow$ It is for all $w \in S$ and $v \in \partial f(w)$ it is $\|v\| \leq \rho$.

- For any $u \in S$, it is

$$
\begin{aligned}
f(w) - f(u) \leq & \langle v, w - u\rangle && (\text{ because } v \in \partial f(w) \text{ }) \\
\leq & \|v\| \|w - u\| && \text{by Cauchy-Schwarz inequality} \\
\leq & \rho \|w - u\| && \text{because } \|v\| \leq \rho
\end{aligned}
\tag{1}
$$

- Similarly it results $u, w \in S$

$$f(w) - f(u) \leq \langle v, u - w\rangle \|v\| \leq \|v\| \|u - w\| \leq \rho \|u - w\|$$

from (1) because w, u can be swaped in (1) as they both are any values in S.

Exercise 5. ($\star$)Let $g_1(w), ..., g_r(w)$ be r convex functions, and let $f(\cdot) = \max_{\forall j}(g_j(\cdot))$. Show that for some w it is $\nabla g_k(w) \in \partial f(w)$ where $k = \arg\max_j(g_j(w))$ is the index of function $g_j(\cdot)$ presenting the greatest value at w.

Solution. Since g_k is convex, for all u

$$g_k(u) \geq g_k(w) + \langle u - w, \nabla g_k(w) \rangle$$

However $f(u) = \max_{\forall j}(g_j(u)) \geq g_k(u)$ for any j, and $f(w) = g_k(w)$ at w. Then

$$\begin{aligned} f(u) \geq & g_k(u) \\ \geq & g_k(w) + \langle u - w, \nabla g_k(w) \rangle \\ = & f(w) + \langle u - w, \nabla g_k(w) \rangle \end{aligned}$$

Then by the definition of the sub-gradient $\nabla g_k(w) \in \partial f(w)$

Exercise 6. $(\star)$Consider the regression learning problem $(\mathcal{H}, \mathcal{Z}, \ell)$ with predictor rule $h(x) = \langle w, x \rangle$ labeled by some unknown parameter $w \in \mathcal{W}$, loss function $\ell(w, (x, y)) = (\langle w, x \rangle - y)^2$, feature $x \in \mathcal{X}$, and target $y \in \mathbb{R}$. Let $\mathcal{W} = \mathcal{X} = \left\{\omega \in \mathbb{R}^d : |\omega| \leq \rho\right\}$ for some $\rho > 0$.

(1) Show that the resulting learning problem is Convex-Lipschitz-Bounded learning problem.
(2) Specify the parameters of Lipschitnzess.

Solution. According to the definitions given in the lecture:

- Convex-Lipschitz-Bounded Learning Problem $(\mathcal{H}, \mathcal{Z}, \ell)$ with parameters ρ, and B, is called the learning problem whose the hypothesis class $\mathcal{H}$ is a convex set, for all $w \in \mathcal{H}$ it is $\|w\| \leq B$, and the loss function $\ell(\cdot, z)$ is convex and ρ-Lipschitz function for all $z \in \mathcal{Z}$.

I have:

Convexity: The function $g : \mathbb{R} \to \mathbb{R}$, defined by $g(a) = a^2$ is convex convex. Eg. $\frac{\mathrm{d}^2}{\mathrm{d}a^2} g(a) = 1 \geq 0$ is non-negative. The convexity of $\ell(w, z = (x, y))$ for all z follows as a composition of g with a linear function.

Lipschitzness: The function $g(a) = a^2$ is 1-Lipschitz since It is

$$|g(a_2) - g(a_1)| = \left|a_2^2 - a_1^2\right| = |(a_2 + a_1)(a_2 - a_1)| \leq 2\rho(a_2 - a_1) = 2\rho|a_2 - a_1|$$

Hence because $|x| \leq \rho$, $g(a)$ is $2\rho^2$-Lipschitz as a composition.

Boundness: The norm of each hypothesis w is bounded by ρ according to the assumptions.

Therefore,

(1) the learning problem under consideration is a Convex-Lipschitz-Bounded learning problem.
(2) the parameter of Lipschitzness is $2\rho^2$.

The following is given as a homework (Formative assessment 1)

Exercise 7. $(\star)$Consider the binary classification problem with inputs $x \in \mathcal{X}$ where $\mathcal{X} := \left\{x \in \mathbb{R}^d : \|x\|_2 \leq L\right\}$ for some given value $L > 0$, target $y \in \mathcal{Y}$ where $\mathcal{Y} := \{-1, +1\}$, and prediction rule $h_w : \mathbb{R}^d \to$

$\{-1,+1\}$ with

$$h_w(x) = \text{sign}\left(w^\top x\right) \tag{2}$$

$$= \text{sign}\left(\sum_{j=1}^{d} w_j x_j\right) \tag{3}$$

Let the hypothesis class of prediction rules be

$$\mathcal{H} = \left\{x \to w^\top x : \forall w \in \mathbb{R}^d\right\}$$

In other words, the hypothesis $h_w \in \mathcal{H}$ is parametrized by $w \in \mathbb{R}^d$ it receives an input vector $x \in \mathcal{X} := \mathbb{R}^d$ and it returns the label $y = \text{sign}\left(w^\top x\right) \in \mathcal{Y} := \{\pm 1\}$.

Consider a loss function $\ell : \mathbb{R}^d \to \mathbb{R}_+$ with

$$\ell\left(w, z = (x, y)\right) = \max\left(0, 1 - y w^\top x\right) + \lambda \|w\|_2^2 \tag{4}$$

for some given value $\lambda > 0$.

Assume there is available a dataset of examples $S_n = \{z_i = (x_i, y_i)\,;\, i = 1, ..., n\}$ of size n.

Do the following tasks.

Hint-1:: We denote

$$\text{sign}(\xi) = \begin{cases} -1, & \text{if}\, \xi < 0 \\ +1, & \text{if}\, \xi > 0 \end{cases}$$

Hint-2:: The notation ± 1 means either -1 or $+1$.

HInt-3:: We define $\mathbb{R}_+ := (0, +\infty)$

Hint-4:: We denote $\|x\|_2 := \sqrt{\sum_{\forall j} (x_j)^2}$ the Euclidean distance.

(1) Show that the function $f : \mathbb{R} \to \mathbb{R}_+$ with $f(x) = \max(0, 1 - x)$ is convex in $\mathbb{R}$; and show that the loss (4) is convex.

Hint:: You may use Example 13 from Handout 1.

(2) Show that the loss $\ell(w, z)$ for $\lambda = 0$ (4) is L-Lipschitz (with respect to w) when $x \in \mathcal{X}$ where $\mathcal{X} := \left\{x \in \mathbb{R}^d : \|x\|_2 \le L\right\}$.

Hint:: You may use the definition of Lipschitz function. Without loss of generality, you can consider any $w_1 \in \mathbb{R}^d$ and $w_2 \in \mathbb{R}^d$ such that $1 - y w_2^\top x \le 1 - y w_1^\top x$, and then take cases $1 - y w_2^\top x$ $>$ or $<$ 0 and $1 - y w_1^\top x$ $>$ or $<$ 0 to deal with the max.

(3) Construct the set of sub-gradients $\partial f(x)$ for $x \in \mathbb{R}$ of the function $f : \mathbb{R} \to \mathbb{R}_+$ with $f(x) = \max(0, 1 - x)$. Show that the vector v with

$$v = \begin{cases} 2\lambda w, & y w^\top x > 1 \\ 2\lambda w, & y w^\top x = 1 \\ -yx + 2\lambda w, & y w^\top x < 1 \end{cases}$$

is $v \in \partial_w \ell\left(w, z = (x, y)\right)$, aka a sub-gradient of $\ell\left(w, z = (x, y)\right)$ at w, for any $w \in \mathbb{R}^d$.

(4) Write down the algorithm of online AdaGrad (Adaptive Stochastic Gradient Descent) with learning rate $\eta_t > 0$, batch size m, and termination criterion $t > T_{\max}$ for some $T_{\max} > 0$ in

order to discover w^* such as

$$w^* = \arg \min_{\forall w: h_w \in \mathcal{H}} \left(\mathrm{E}_{z \sim g} \left(\ell \left(w, z = (x, y) \right) \right) \right) \tag{5}$$

The formulas in your algorithm have to be tailored to 4.

(5) Use the R code given below in order to generate the dataset of observed examples $S_n = \{z_i = (x_i, y_i)\}_{i=1}^{n}$ that contains $n = 10^6$ examples with inputs x of dimension $d = 2$. Consider $\lambda = 0$. Use a seed $w^{(0)} = (0, 0)^\top$.

(a) By using appropriate values for m, η_t and $T_{\max}$, code in R the algorithm you designed in part 4, and run it.

(b) Plot the trace plots for each of the dimensions of the generated chain $\left\{w^{(t)}\right\}$ against the iteration t.

(c) Report the value of the output w^*_{adaGrad} (any type) of the algorithm as the solution to (5).

(d) To which cluster y (i.e., -1 or 1) $x_{\text{new}} = (1, 0)^\top$ belongs?

```
# R code. Run it before you run anything else
#
data_generating_model <- function(n,w) {
z <- rep( NaN, times=n*3 )
z <- matrix(z, nrow = n, ncol = 3)
z[,1] <- rep(1,times=n)
z[,2] <- runif(n, min = -10, max = 10)
p <- w[1]*z[,1] + w[2]*z[,2] p <- exp(p) / (1+exp(p))
z[,3] <- rbinom(n, size = 1, prob = p)
ind <- (z[,3]==0)
z[ind,3] <- -1
x <- z[,1:2]
y <- z[,3]
return(list(z=z, x=x, y=y))
}
n_obs <- 1000000
w_true <- c(-3,4)
set.seed(2023)
out <- data_generating_model(n = n_obs, w = w_true)
set.seed(0)
z_obs <- out$z #z=(x,y)
x <- out$x
y <- out$y
#z_obs2=z_obs
#z_obs2[z_obs[,3]==-1,3]=0
#w_true <- as.numeric(glm(z_obs2[,3]~ 1+ z_obs2[,2],family = "binomial"
)$coefficients)
```

Solution.

(1) $f_1(x) = 0$ is convex, $f_2(x) = 1 - x$ is convex, hence from the example in Handout 1, $f(x) = \max(f_1(x), f_2(x))$ is convex as well. Regarding the loss function, we just have $f_2(w) = 1 - yx^\top w$ which is convex as a composition due to linearity.

(2) Given a fixed example $(x, y) \in \left\{x \in \mathbb{R}^d : \|x'\|_2 \leq R\right\} \times \{-1, 1\}$.

Assume $w_1, w_2 \in \mathbb{R}^d$. Let $\ell_i = \max\left\{0, 1 - yx^\top w_i\right\}$, for $i = 1, 2$. It suffices to show that $|\ell_1 - \ell_2|_2 \leq R\,|w_1 - w_2|_2$. I take cases

Case-1: Assume $yx^\top w_1 \geq 1$ and $yx^\top w_2 \geq 1$ then $|\ell_1 - \ell_2|_2 = 0 \leq R\,|w_1 - w_2|_2$

Case-2: Assume that at least one of $yx^\top w_1 < 1$ or $yx^\top w_2 < 1$ but not both is true. Assume without loss of generality that $1 - yx^\top w_1 < 1 - yx^\top w_2$. Then

$$\begin{aligned}
|\ell_1 - \ell_2|_2 =& \ell_1 - \ell_2 \\
=& 1 - yx^\top w_1 - \max\left(0, 1 - yx^\top w_2\right) \\
\leq& 1 - yx^\top w_1 - \left(1 - yx^\top w_2\right) \\
=& yx^\top \left(w_2 - w_1\right) \\
\leq& y\left\|x^\top\right\|_2 \|w_1 - w_2\|_2 \quad \text{because} \quad a^\top b \leq \|a\| \, \|b\|
\end{aligned}$$

(3) It is

$$f(x) = \max(0, 1 - x) = \begin{cases} 0 & x > 1 \\ 0 & x = 1 \\ 1 - x & x < 1 \end{cases}$$

- For $x > 1$, f is differentiable so $\partial f(x) = \{f'(x)\} = \{0\}$.
- For $x < 1$, f is differentiable so $\partial f(x) = \{f'(x)\} = \{-1\}$.
- For $x = 1$, f is not differentiable. By definition I have that v is subgradient of $f(x)$ at $x = 0 \in S$ if

$$\forall u \in \mathbb{R}, \;\; f(u) \geq f(x) + \langle u - x, v \rangle$$

So, for $u \geq 1$, it is $0 \geq (u - 1)v \implies v \leq 0$, and for $u < 1$ it is $(1 - u) \geq (u - 1)v \implies v \geq -1$. Hence the common space is $v \in [0, 1]$ So $\partial f(x) = [0, 1]$. Hence,

$$\partial f(x) = \begin{cases} 0, & x > 1 \\ [-1, 0], & x = 1 \\ -1, & x < 1 \end{cases}$$

Now regarding the loss $\partial_w \ell(w, z = (x, y))$

- for $yw^\top x > 1$ it is differentiable so $\nabla_w \ell(w, z = (x, y)) = \nabla_w \left(0 + \lambda \sum_{j=1}^d w_j^2\right) = 2\lambda w$; as

$$\frac{\mathrm{d}}{\mathrm{d}w_j} \sum_{j'=1}^d w_{j'}^2 = 2\lambda w_j$$

- for $yw^\top x > 1$ it is differentiable so $\nabla_w \ell(w, z = (x, y)) = \nabla_w \left(1 - yw^\top x + \lambda \sum_{j=1}^d w_j^2\right) = yx + 2\lambda w$ as

$$\frac{\mathrm{d}}{\mathrm{d}w_j}\left(1 - yw^\top x\right) = \frac{\mathrm{d}}{\mathrm{d}w_j}\left(1 - y\sum_{j'=1}^d w_{j'} x_{j'}\right) = -yx_j$$

- for $yw^\top x = 1$, $v = 0$ satisfies the definition of the sub-gradient

$$\forall u, \quad f(u) \geq \cancelto{0}{f(w)} + \langle u - w, v \rangle$$
$$\max\left(0, 1 - yu^\top x\right) \geq 0 + (u - w)^\top 0$$

So

$$\begin{aligned}
\partial \ell (w, z = (x, y)) &= \partial \left(\max\left(0, 1 - yw^\top x\right) + \lambda \|w\|_2^2 \right) \\
&= \partial \left(\max\left(0, 1 - yw^\top x\right) \right) + \partial \left(\lambda \|w\|_2^2 \right) \\
&= \partial \left(\max\left(0, 1 - yw^\top x\right) \right) + \nabla \left(\lambda \|w\|_2^2 \right) \\
& 0 + 2\lambda w
\end{aligned}$$

but $\partial \left(\lambda \|w\|_2^2 \right) = \left\{ \nabla \left(\lambda \|w\|_2^2 \right) \right\}$ because $\lambda \|w\|_2^2$ is differentiable. Hence

$$\partial \ell (w, z = (x, y)) = 0 + 2\lambda w$$

Hence

$$v = \begin{cases} 2\lambda w, & yw^\top x > 1 \\ 2\lambda w, & yw^\top x = 1 \\ -yx + 2\lambda w, & yw^\top x < 1 \end{cases}$$

(4)

Algorithm. *For $t = 1, 2, 3, \ldots$ iterate:*

(a) *Get a random sub-sample $\left\{ \tilde{z}_i^{(t)} = \left(\tilde{x}_i^{(t)}, \tilde{y}_i^{(t)} \right); i = 1, \ldots, m \right\}$ of size m with or without replacement from the complete data-set $\mathcal{S}_n$.*

(b) *For $j = 1, \ldots, d$ (index j indicates the dimension of w) compute*

$$w_j^{(t+1)} = w_j^{(t)} - \eta_t \frac{1}{\sqrt{[G_t]_{j,j} + \epsilon}} \bar{v}_{t,j}$$

$[G_t]_{j,j} = [G_{t-1}]_{j,j} + (\bar{v}_{t,j})^2$ *where* $\bar{v}_t = \frac{1}{m} \sum_{i=1}^m \tilde{v}_{t,i}$ *and*

$$\tilde{v}_{t,i} = \begin{cases} 2\lambda w^{(t)}, & \tilde{y}_i^{(t)} \left(w^{(t)} \right)^\top \tilde{x}_i^{(t)} > 1 \\ 2\lambda w^{(t)}, & \tilde{y}_i^{(t)} \left(w^{(t)} \right)^\top \tilde{x}_i^{(t)} = 1 \\ -\frac{1}{m} \tilde{y}_i^{(t)} \tilde{x}_i^{(t)} + 2\lambda w^{(t)}, & \tilde{y}_i^{(t)} \left(w^{(t)} \right)^\top \tilde{x}_i^{(t)} < 1 \end{cases}$$

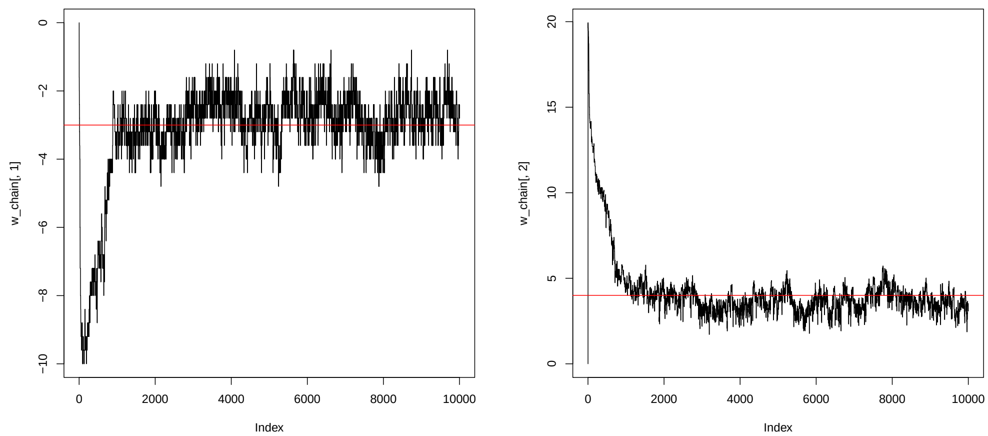
where index i indicates the sub-sample, and $\epsilon > 0$ small.

(c) *Terminate if a termination criterion is satisfied*

(5)

(a) The R code can be found in the link `https://raw.githubusercontent.com/georgios-stats/Machine_Learning_and_Neural_Networks_III_Epiphany_2023/main/Exercises/supplementary/q6_adagrad.R`

(b) The figures are presented below



(A) $w_1^{(t)}$ (B) $w_2^{(t)}$

FIGURE 1. trace plots

(c) I found $w = (-2.674615, 3.205785)$

(d) It belongs to -1

Exercise 8. ($\star$)Assume a Bayesian model

$$\begin{cases} z_i|w & \overset{\text{ind}}{\sim} f\left(z_i|w\right),\ i = 1, ..., n \\ w & \sim f\left(w\right) \end{cases}$$

and consider that our objective is the discovery of MAP estimate w^* i.e.

$$w^* = \arg\min_{\forall w \in \Theta} \left(-\log\left(L_n\left(w\right)\right) - f\left(w\right)\right) = \arg\min_{\forall w \in \Theta} \left(-\sum_{i=1}^{n} \log\left(f\left(z_i|w\right)\right) - \log\left(f\left(w\right)\right)\right)$$

by using SGD with update

$$w^{(t+1)} = w^{(t)} + \eta_t \left(\frac{n}{m} \sum_{j \in \mathcal{J}^{(t)}} \nabla_w \log\left(f\left(z_j|w^{(t)}\right)\right) + \nabla_w \log\left(f\left(w^{(t)}\right)\right)\right)$$

for some randomly selected set $\mathcal{J}^{(t)} \subseteq \{1, ..., n\}^m$ of m integers from 1 to n via simple random sampling (SRS) with replacement. Show that

$$\mathrm{E}_{\mathcal{J}^{(t)} \sim \text{simple-random-sampling}} \left(\frac{n}{m} \sum_{j \in \mathcal{J}^{(t)}} \nabla_w \log\left(f\left(z_j|w^{(t)}\right)\right)\right) = \sum_{i=1}^{n} \nabla_w \log\left(f\left(z_i|w^{(t)}\right)\right)$$

Solution. It is

$$\begin{aligned}
\mathrm{E}_{\mathcal{J}^{(t)}\sim\mathrm{SRS}}\left(\frac{n}{m}\sum_{j\in\mathcal{J}^{(t)}}\nabla_w \log\left(f\left(z_j|w^{(t)}\right)\right)\right) =& \frac{n}{m}\sum_{j\in\mathcal{J}^{(t)}}\mathrm{E}_{\mathcal{J}^{(t)}\sim\mathrm{SRS}}\left(\nabla_w \log\left(f\left(z_j|w^{(t)}\right)\right)\right)\\
=& \frac{n}{m}\sum_{j\in\mathcal{J}^{(t)}}\mathrm{E}_{\mathcal{J}^{(t)}\sim\mathrm{SRS}}\left(\nabla_w \log\left(f\left(z_j|w^{(t)}\right)\right)\right)\\
=& \frac{n}{m}\sum_{j\in\mathcal{J}^{(t)}}\frac{1}{n}\sum_{i=1}^{n}\nabla_w \log\left(f\left(z_i|w^{(t)}\right)\right)\\
=& \sum_{i=1}^{n}\nabla_w \log\left(f\left(z_i|w^{(t)}\right)\right)
\end{aligned}$$

It is $\mathrm{E}_{\mathcal{J}^{(t)}\sim\mathrm{SRS}}\left(\nabla_w \log\left(f\left(z_j|w^{(t)}\right)\right)\right) = \frac{1}{n}\sum_{i=1}^{n}\nabla_w \log\left(f\left(z_i|w^{(t)}\right)\right)$ because the expectation is under the probability I get randomly an integer and for the jth on the probability is $1/n$ due to the random scheme. Also $\left|\mathcal{J}^{(t)}\right| = m$.

Part 2. **Artificial Neural Networks**

Exercise 9. ($\star$)Consider the regression problem, with a predictive rule $h_w : \mathbb{R}^d \to \mathbb{R}$, as a classification probability , that receives values $x \in \mathbb{R}^d$ returns vales in $\mathbb{R}$. Let $h_w(x)$ be modeled as an ANN

$$h(x) = \sigma_2\left(\sum_{j=1}^{c} w_{2,1,j}\sigma_1\left(\sum_{i=1}^{d} w_{1,j,i}x_i\right)\right)$$

and let the associated activation function be

$$\sigma_2(a) = a\Phi(a)$$

where $\Phi(x) = \int_{-\infty}^{x}\phi(t)\,\mathrm{d}t$ is considered as known function, and $\phi(t) = \frac{1}{\sqrt{2\pi}}\exp\left(-\frac{1}{2}t^2\right)$ and

$$\sigma_1(a) = \exp\left(-a^2\right)$$

Consider a loss

$$\ell(w, z = (x,y)) = \frac{1}{2}\left(y - h_w(x)\right)^2$$

at w and example $z = (x, y)$, where $x \in \mathbb{R}^d$ is the input vector (features), and y is the output vector (targets) with $y \in \mathbb{R}$. Consider that d, c, and q are known integers.

(1) Perform the forward pass of the back-propagation procedure to compute the activations which may be denoted as $\{a_{t,i}\}$ and outputs which may be denoted as $\{o_{t,i}\}$ at each layer t.
(2) Perform the backward pass of the back-propagation procedure in order to compute the elements of the gradient $\nabla_w \ell(w,(x,y))$.

Solution.

(1)

Forward pass:

Set: $o_{0,i} = x_i$ for $i = 1, ..., d$

Compute:

at $t = 1$**:** for $j = 1, ...c$

comp: $\alpha_{1,j} = \sum_{i=1}^{d} w_{1,j,i} x_i$

comp: $o_{1,j} = \exp\left(-\alpha_{1,j}^2\right)$

at $t = 2$**:**

comp: $\alpha_{2,1} = \sum_{j=1}^{c} w_{2,1,j} o_{1,j}$

comp: $o_{2,1} = \alpha_{2,1} \Phi\left(\alpha_{2,1}\right)$

get: $h_1 = o_{2,1}$

(2) It is

$$\frac{\mathrm{d}}{\mathrm{d}a} \sigma_1(a) = -2a \exp\left(-a^2\right)$$

and

$$\frac{\mathrm{d}}{\mathrm{d}a} \sigma_2(a) = \Phi(a) + a\phi(a)$$

and

$$\frac{\mathrm{d}\ell_2}{\mathrm{d}\alpha_{2,1}} = \frac{\mathrm{d}\ell_2}{\mathrm{d}o_{2,1}} \frac{\mathrm{d}o_{2,1}}{\mathrm{d}\alpha_{2,1}} = \left(o_{2,1} - y_1\right)\left(\Phi\left(\alpha_{2,1}\right) + \alpha_{2,1}\phi\left(\alpha_{2,1}\right)\right)$$

Backward pass:

at $t = 2$**:**

comp: $\tilde{\delta}_{2,1} = \frac{\mathrm{d}}{\mathrm{d}\alpha_{2,1}} \ell_T = \left(o_{2,1} - y_1\right)\left(\Phi\left(\alpha_{2,1}\right) + \alpha_{2,1}\phi\left(\alpha_{2,1}\right)\right)$

at $t = 1$**:** for $j = 1, ...c$

comp:

$$\begin{aligned} \tilde{\delta}_{1,j} &= \frac{\mathrm{d}}{\mathrm{d}\xi} \sigma_1(\xi)\bigg|_{\xi=\alpha_{1,j}} w_{2,1,j} \tilde{\delta}_{2,1} \\ &= -2\alpha_{1,j} \exp\left(-\alpha_{1,j}^2\right) w_{2,1,j} \tilde{\delta}_{2,1} \end{aligned}$$

Output:

$$\frac{\mathrm{d}}{\mathrm{d}w_{1,j,i}} \ell = \tilde{\delta}_{1,j} x_i \text{ and } \frac{\mathrm{d}}{\mathrm{d}w_{2,1,j}} \ell = \tilde{\delta}_{2,1} o_{1,j}$$

Exercise 10. ($\star$) Students are encouraged to practice on the Exercises 5.1-5.28 from the textbook

- Bishop, C. M. (2006). Pattern recognition and machine learning (Vol. 4, No. 4, p. 738). New York: Springer.

available from

- https://www.microsoft.com/en-us/research/uploads/prod/2006/01/Bishop-Pattern-Recognition-and-Machine-Learning-2006.pdf

The solutions are available from

- https://blackboard.durham.ac.uk/ultra/courses/_44662_1/outline/create/document?id=_1396738_1

The following is given as a homework (Formative assessment 2)

Exercise 11. ($\star$)Consider the multi-class classification problem, with a predictive rule $h_w : \mathbb{R}^d \to \mathcal{P}$, as a classification probability i.e, $h_{w,k}(x) = \Pr(x \text{ belongs to class } k)$, that receives values $x \in \mathbb{R}^d$ returns vales in $\mathcal{P} = \left\{ p \in (0,1)^q : \sum_{j=1}^q p_j = 1 \right\}$. Let $h_w = (h_{w,1}, ..., h_{w,q})^\top$, let $h_w(x)$ be modeled as an ANN

$$h_k(x) = \sigma_2 \left(\sum_{j=1}^c w_{2,k,j} \sigma_1 \left(\sum_{i=1}^d w_{1,j,i} x_i \right) \right)$$

for $k = 1, ..., q$, and let the associated activation functions be

$$\sigma_2(a_k) = \frac{\exp(a_k)}{\sum_{k'=1}^q \exp(a_{k'})}, \text{ for } k = 1, ..., q$$

(called softmax function) and $\sigma_1(a) = \arctan(a)$. Consider a loss

$$\ell(w, z = (x, y)) = -\sum_{k=1}^q y_k \log(h_{w,k}(x))$$

at w and example $z = (x, y)$, where $x \in \mathbb{R}^d$ is the input vector (features), and $y = (y_1, ..., y_q)$ is the output vector (labels) with $y \in \{0,1\}^q$ and $\sum_{k=1}^q y_k = 1$. Consider that d, c, and q are known integers.

Hint: You may use

$$\frac{\mathrm{d}}{\mathrm{d}x} \arctan(x) = \frac{1}{1+x^2}$$

(1) Perform the forward pass of the back-propagation procedure to compute the activations which may be denoted as $\{a_{t,i}\}$ and outputs which may be denoted as $\{o_{t,i}\}$ at each layer t.

(2) Show that

$$\frac{\partial}{\partial a_k} \sigma_2(a_j) = \sigma_2(a_j)(1(j = k) - \sigma_2(a_k))$$

for $k = 1, ..., q$. Let $1(j = k) = \begin{cases} 1 & j = k \\ 0 & j \neq k \end{cases}$.

(3) Perform the backward pass of the back-propagation procedure in order to compute the elements of the gradient $\nabla_w \ell(w, (x, y))$.

Solution.

(1) Forward pass

Set: $o_{0,i} = x_i$ for $i = 1, ..., d$

Compute:

at $t = 1$**:** for $j = 1, ...c$

comp: $\alpha_{1,j} = \sum_{i=1}^d w_{1,i,j} x_i$

comp: $o_{1,j} = \arctan(\alpha_{1,j})$

at $t = 2$**:** for $k = 1, ...q$

comp: $\alpha_{2,k} = \sum_{j=1}^d w_{2,k,j} o_{2,j}$

comp: $o_{2,k} = \frac{\exp(\alpha_{2,k})}{\sum_{k'=1}^q \exp(\alpha_{2,k})}$

get: $h_k = o_{2,k}$

(2) It is

$$\frac{\mathrm{d}}{\mathrm{d}a_k}\sigma_2\left(a_j\right) = \frac{\mathrm{d}}{\mathrm{d}a_k}\frac{\exp\left(a_j\right)}{\sum_{j'}\exp\left(a_{j'}\right)} = \begin{cases}\sigma_2\left(a_j\right)\left(1-\sigma_2\left(a_j\right)\right) & j=k\\ -\sigma_2\left(a_j\right)\sigma_2\left(a_k\right) & j\neq k\end{cases}$$
$$= \sigma_2\left(a_j\right)\left(1\left(j=k\right)-\sigma_2\left(a_k\right)\right)$$

(3) It is

$$\frac{\mathrm{d}}{\mathrm{d}a}\sigma_1\left(a\right) = \frac{1}{1+a^2}$$

and

$$\frac{\mathrm{d}}{\mathrm{d}a_k}\sigma_2\left(a_k\right) = \sigma_2\left(a_j\right)\left(1\left(j=k\right)-\sigma_2\left(a_k\right)\right)$$
$$= o_j\left(1\left(j=k\right)-o_k\right)$$

and

$$\frac{\mathrm{d}\ell_2}{\mathrm{d}o_{2,j}} = -y_j\frac{1}{o_{2,j}}$$

and

$$\begin{aligned}\frac{\mathrm{d}\ell_2}{\mathrm{d}a_{2,k}} &= \sum_{j=1}^{q}\frac{\mathrm{d}\ell_2}{\mathrm{d}o_{2,j}}\frac{\mathrm{d}o_{2,j}}{\mathrm{d}o_{2,k}}\\ &= \sum_{j=1}^{q}\left(-y_j\frac{1}{o_{2,j}}o_{2,j}\left(1\left(j=k\right)-o_{2,k}\right)\right)\\ &= \sum_{j=1}^{q}\left(-y_j\left(1\left(j=k\right)-o_{2,k}\right)\right)\\ &= o_{2,k}-y_k\end{aligned}$$

Backward pass:

at $t=2$**:** for $k=1,...q$

comp: $\tilde{\delta}_{2,k} = \frac{\mathrm{d}}{\mathrm{d}\alpha_{2,k}}\ell_T = o_{2,k}-y_k$

at $t=1$**:** for $j=1,...c$

comp:

$$\begin{aligned}\tilde{\delta}_{1,j} &= \left.\frac{\mathrm{d}}{\mathrm{d}\xi}\sigma_1\left(\xi\right)\right|_{\xi=\alpha_{1,j}}\sum_{k=1}^{q}w_{2,k,j}\tilde{\delta}_{2,k}\\ &= \left(\frac{1}{1+\alpha_{1,j}^2}\right)\sum_{k=1}^{q}w_{2,k,j}\tilde{\delta}_{2,k}\end{aligned}$$

Output:

$$\frac{\mathrm{d}}{\mathrm{d}w_{1,j,i}}\ell = \tilde{\delta}_{1,j}x_i \text{ and } \frac{\mathrm{d}}{\mathrm{d}w_{2,k,j}}\ell = \tilde{\delta}_{2,k}o_{1,j}$$

Part 3. **Support Vector Machines**

The following is given as a homework (Formative assessment 3)

Exercise 12. ($\star\star$) Consider a training data set $\mathcal{D} = \{z_i = (x_i, y_i)\}_{i=1}^{m}$. Consider the Soft-SVM Algorithm that requires the solution of the following quadratic minimization problem (in a slightly modified but equivalent form to what we have discussed)

Primal problem:

$$(w^*, b^*, \xi^*) = \arg\min_{(w,b,\xi)} \left(\frac{1}{2} \|w\|_2^2 + C \sum_{i=1}^{m} \xi_i \right) \tag{6}$$

$$\text{subject to: } y_i \left(\langle w, x_i \rangle + b \right) \geq 1 - \xi_i, \ \forall i = 1, ..., m \tag{7}$$

$$\xi_i \geq 0, \ \forall i = 1, ..., m \tag{8}$$

for some user-specified fixed parameter $C > 0$.

(1) Specify the Lagrangian function L associated to the above primal quadratic minimization problem, where $\{\alpha_i\}$ are the Lagrange coefficients wrt (7), and $\{\beta_i\}$ are the Lagrange coefficients wrt (8). Write down any possible restrictions on the Lagrange coefficients.

(2) Compute the dual Lagrangian function denoted as $\tilde{L}$ as a function of the Lagrange coefficients and the data points $\mathcal{D}$.

(3) Apply the Karush–Kuhn–Tucker (KKT) conditions to the above problem, and write them down.

(4) Derive and write down the dual Lagrangian quadratic maximization problem, along with the inequality and equality constraints, where you seek to find $\{\alpha_i\}$.

(5) Justify why the i-th point x_i lies on the margin boundary when $\alpha_i \in (0, C)$ (beware it is $\alpha_i \neq C$), and why the i-th point x_i lies inside the margin when $\alpha_i = C$.

(6) Given optimal values $\{\alpha_i^*\}$ for Lagrangian coefficients $\{\alpha_i\}$ as they are derived by solving the dual Lagrangian maximization problem in part 4, derive the optimal values w^* and b^* for the parameters w and b as function of the support vectors. Regarding parameter b it should be in the derived in the form

$$b^* = \frac{1}{|\mathcal{M}|} \sum_{i \in \mathcal{M}} \left(y_i - \sum_{j \in \mathcal{S}} \alpha_j^* y_j \langle x_j, x_i \rangle \right)$$

where you determine the sets $\mathcal{M}$ and $\mathcal{S}$.

(7) Report the halfspace predictive rule $h_{w,b}(x)$ of the above problem as a function of α^* and b^*.

Solution.

(1) It is

$$L(w, b, \xi, \alpha, \beta) = \frac{1}{2} \|w\|_2^2 + \sum_{i=1}^{m} C\xi_i + \sum_{i=1}^{m} \alpha_i \left(1 - y_i \left(\langle w, x_i \rangle + b\right) - \xi_i\right) - \sum_{i=1}^{m} \beta_i \xi_i \tag{9}$$

(2) Let α, β be fixed. We minimize (9) wrt w, b and we get

$$0 = \frac{\partial L}{\partial w}(w, b, \xi, \alpha, \beta) \implies w = \sum_{i=1}^{m} \alpha_i y_i x_i \tag{10}$$

$$0 = \frac{\partial L}{\partial b}(w, b, \xi, \alpha, \beta) \implies 0 = \sum_{i=1}^{m} \alpha_i y_i$$

$$0 = \frac{\partial L}{\partial \xi_i}(w, b, \xi, \alpha, \beta) \implies \alpha_i = C - \beta_i \tag{11}$$

and we substitute (10)-(11) in (9) and we get

$$\tilde{L}(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_i \alpha_j y_i y_j \langle x_j, x_i \rangle$$

(3) The Karush–Kuhn–Tucker (KKT) conditions applied to the above problem are

$$0 = \nabla \frac{1}{2} \|w\|_2^2 + \nabla \sum_{i=1}^{m} C\xi_i + \nabla \sum_{i=1}^{m} \alpha_i (1 - y_i (\langle w, x_i \rangle + b) - \xi_i) - \nabla \sum_{i=1}^{m} \beta_i \xi_i \qquad \text{Stationarity}$$

$$1 - y_i (\langle w, x_i \rangle + b) - \xi_i \le 0, \;\; \forall i = 1, ..., m \qquad \text{Primal feasibility}$$

$$\xi_i \ge 0 \tag{12}$$

$$\alpha_i \ge 0 \;\; \forall i = 1, ..., m \qquad \text{Dual feasibility} \tag{13}$$

$$\beta_i \ge 0 \;\; \forall i = 1, ..., m \tag{14}$$

$$\alpha_i (1 - y_i (\langle w, x_i \rangle + b) - \xi_i) = 0, \;\; \forall i = 1, ..., m \qquad \text{Complementary slackness} \tag{15}$$

$$\beta_i \xi_i = 0, \;\; \forall i = 1, ..., m$$

(4) It is

$$\alpha^* = \arg \max_{\alpha \in \mathbb{R}^m : \alpha \ge 0} \left(\sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_i \alpha_j y_i y_j \langle x_j, x_i \rangle \right) \tag{16}$$

$$\text{subject to } \; 0 = \sum_{i=1}^{m} \alpha_i y_i$$

$$\alpha_i \in [0, C] \;\; \forall i = 1, ..., m \tag{17}$$

constrain (17) results from (11), (13), and (12).

(5)

- By (10), if $\alpha_i = 0$ then x_i does not contribute to the computation of the weights.
- By (10), if $\alpha_i \neq 0$, then x_i is a support vector and contributes.

- If $\alpha_i \in (0, C)$ (where $\alpha_i \neq C$) then (11) implies that $\beta_i > 0$. By (15) if $\beta_i > 0$ then $\xi_i = 0$. Hence, given these, from (14), it is $1 = y_i (\langle w, x_i \rangle + b)$ i.e. x_i lies on the boundary.
- If $\alpha_i = C$, then x_i lies inside the boundary.

(6) From (14), it is either $\alpha_i = 0$ or $(1 - y_i (\langle w, x_i \rangle + b) - \xi_i) = 0$. Let $\mathcal{S} = \{i : y_i (\langle w, x_i \rangle + b) = 1 - \xi_i\}$. From (10) , it is

$$w^* = \sum_{i \in \mathcal{S}} \alpha_i^* y_i x_i \tag{18}$$

Using (14) and summing up indexes in $\mathcal{M} = \{i : \alpha_i \in (0, C)\}$ for which $\xi_i = 0$ it is

$$b^* = \frac{1}{|\mathcal{M}|} \sum_{i \in \mathcal{M}} \left(y_i - \sum_{j \in \mathcal{S}} \alpha_j^* y_j \langle x_j, x_i \rangle \right)$$

(7) The formula is

$$\begin{aligned} h_{w,b}(x) &= \operatorname{sign}(\langle w^*, x \rangle + b^*) \\ &= \operatorname{sign}\left(\sum_{i=1}^{m} \alpha_i^* y_i \langle x_i, x \rangle + b^* \right) \end{aligned} \tag{19}$$

Exercise 13. ($\star\star$) Show that K with

$$K(x, y) = \frac{\sin\left(2\pi\left(N + \frac{1}{2}\right)(x - y)\right)}{\sin(\pi(x - y))}$$

is a valid kernel.

Hint-1: You may use that $\sum_{n=0}^{r} z^n = \frac{1 - z^{r+1}}{1 - z}$
Hint-2: You may use that $e^{ix} = \cos(x) + i \sin(x)$

Solution. It is

$$\begin{aligned} K(x, y) &= \frac{\sin\left(2\pi\left(N + \frac{1}{2}\right)(x - y)\right)}{\sin(\pi(x - y))} = \frac{-2i \sin\left(2\pi\left(N + \frac{1}{2}\right)(x - y)\right)}{-2i \sin(\pi(x - y))} \\ &= \frac{e^{-2\pi\left(N + \frac{1}{2}\right)i(x-y)} - e^{2\pi\left(N + \frac{1}{2}\right)i(x-y)}}{e^{-\pi i(x-y)} - e^{\pi i(x-y)}} \\ &= \frac{e^{\pi i(x-y)}}{e^{\pi i(x-y)}} \frac{e^{-2\pi\left(N + \frac{1}{2}\right)i(x-y)} - e^{2\pi\left(N + \frac{1}{2}\right)i(x-y)}}{e^{-\pi i(x-y)} - e^{\pi i(x-y)}} \\ &= e^{-2\pi i N(x-y)} \frac{1 - \left(e^{2\pi i(x-y)}\right)^{2N+1}}{1 - e^{2\pi i(x-y)}} \\ &= e^{-2\pi i N(x-y)} \sum_{n=0}^{2N} \left(e^{2\pi i(x-y)}\right)^n = \sum_{n=-N}^{N} e^{2\pi i n(x-y)} = \sum_{n=-N}^{N} e^{2\pi i n x} e^{-2\pi i n y} \\ &= \sum_{n=-N}^{N} e^{2\pi i n x} \overline{e^{2\pi i n y}} = \langle \psi(x), \psi(y) \rangle \end{aligned}$$

with $\psi(x) = \left(e^{-2\pi i N x}, e^{-2\pi i(N-1)x}, ..., 1, ..., e^{2\pi i(N-1)x}, e^{2\pi i N x}\right)^{\top}$. Based on the theorem in the Handout, the Kernel can be expressed as an inner product of a vector of bases, hence it is a valid kernel.

Note that given Hint 2 it is

$$\begin{aligned} e^{-2\pi i n y} &= \cos(-2\pi n y) + i \sin(-2\pi n y) \\ &= \cos(2\pi n y) - i \sin(2\pi n y) \\ &= \overline{\cos(2\pi n y) + i \sin(2\pi n y)} \\ &= \overline{e^{2\pi i n y}} \end{aligned}$$

Exercise 14. ($\star$) Students are encouraged to practice on the Exercises 6.1-6.19 from the textbook

- Bishop, C. M. (2006). Pattern recognition and machine learning (Vol. 4, No. 4, p. 738). New York: Springer.

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Part 4. **Gaussian process regression**

Exercise 15. ($\star$) Students are encouraged to practice on the Exercises 6.19-6.27 from the textbook

- Bishop, C. M. (2006). Pattern recognition and machine learning (Vol. 4, No. 4, p. 738). New York: Springer.

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