

Exercise sheet

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Part 1. Stochastic learning

Exercise 1. (★) Let $f : \mathbb{R}^d \rightarrow \mathbb{R}$ such that $f(w) = g(\langle w, x \rangle + y)$ for 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 $\alpha \in [0, 1]$. It is

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

Exercise 2. (★) 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. (★) 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 $(\beta \|x\|^2)$ -smooth.

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

$$f(v) = g(\langle w, x \rangle + y)$$

$$\leq g(\langle w, x \rangle + y) + g'(\langle w, x \rangle + y) \langle v - w, x \rangle + \frac{\beta}{2} (\langle v - w, x \rangle)^2 \quad (g \text{ is smooth})$$

$$\leq g(\langle w, x \rangle + y) + g'(\langle w, x \rangle + y) \langle v - w, x \rangle + \frac{\beta}{2} (\|v - w\| \|x\|)^2 \quad (\text{Cauchy-Schwarz inequality})$$

$$= f(w) + \langle \nabla f(w), v - w \rangle + \frac{\beta \|x\|^2}{2} \|v - w\|^2$$

Exercise 4. (★) Show that $f : S \rightarrow \mathbb{R}$ 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. \Rightarrow Let $f : S \rightarrow \mathbb{R}$ 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 $\|v\| \leq \rho$.

\Leftarrow 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

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

- 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 swapped in (1) as they both are any values in S .

Exercise 5. (★) Let $g_1(w), \dots, g_r(w)$ 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 $\nabla g_k(w) \in \partial f(w)$

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

Exercise 6. (★) Consider the binary classification problem with inputs $x \in \mathcal{X}$ where $\mathcal{X} := \{x \in \mathbb{R}^d : \|x\|_2 \leq L\}$ for some given value $L > 0$, target $y \in \mathcal{Y}$ where $\mathcal{Y} := \{-1, +1\}$, and prediction rule $h_w : \mathbb{R}^d \rightarrow \{-1, +1\}$ with

$$\begin{aligned} (2) \quad h_w(x) &= \text{sign}(w^\top x) \\ (3) \quad &= \text{sign}\left(\sum_{j=1}^d w_j x_j\right) \end{aligned}$$

Let the hypothesis class of prediction rules be

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

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 $y = \text{sign}(w^\top x) \in \mathcal{Y} := \{\pm 1\}$.

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

$$(4) \quad \ell(w, z = (x, y)) = \max(0, 1 - yw^\top x) + \lambda \|w\|_2^2$$

for some given value $\lambda > 0$.

Assume there is available a dataset of examples $S_n = \{z_i = (x_i, y_i) ; i = 1, \dots, n\}$ 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 $f : \mathbb{R} \rightarrow \mathbb{R}_+$ 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 $\mathcal{X} := \{x \in \mathbb{R}^d : \|x\|_2 \leq L\}$.

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 $1 - yw_2^\top x \leq 1 - yw_1^\top x$, and then take cases $1 - yw_2^\top x > \text{or} < 0$ and $1 - yw_1^\top x > \text{or} < 0$ to deal with the max.

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

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

is $v \in \partial_w \ell(w, z = (x, y))$, aka a sub-gradient of $\ell(w, z = (x, y))$ 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

$$(5) \quad w^* = \arg \min_{w: h_w \in \mathcal{H}} (\mathbb{E}_{z \sim g} (\ell(w, z = (x, y))))$$

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 $\{w^{(t)}\}$ 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 $(x, y) \in \{x \in \mathbb{R}^d : \|x'\|_2 \leq R\} \times \{-1, 1\}$.

Assume $w_1, w_2 \in \mathbb{R}^d$. Let $\ell_i = \max\{0, 1 - yx^\top w_i\}$, 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

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

(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

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

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 $\nabla_w \ell(w, z = (x, y)) = \nabla_w (0 + \lambda \sum_{j=1}^d w_j^2) = 2\lambda w$;
as

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

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

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

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

$$\begin{aligned} \forall u, \quad f(u) &\geq \cancel{f(w)}^0 + \langle u - w, v \rangle \\ \max(0, 1 - yu^\top x) &\geq 0 + (u - w)^\top 0 \end{aligned}$$

So

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

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 $t = 1, 2, 3, \dots$ iterate:

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

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

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

- Terminate if a termination criterion is satisfied

(5)

- 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.R
- The figures are presented below

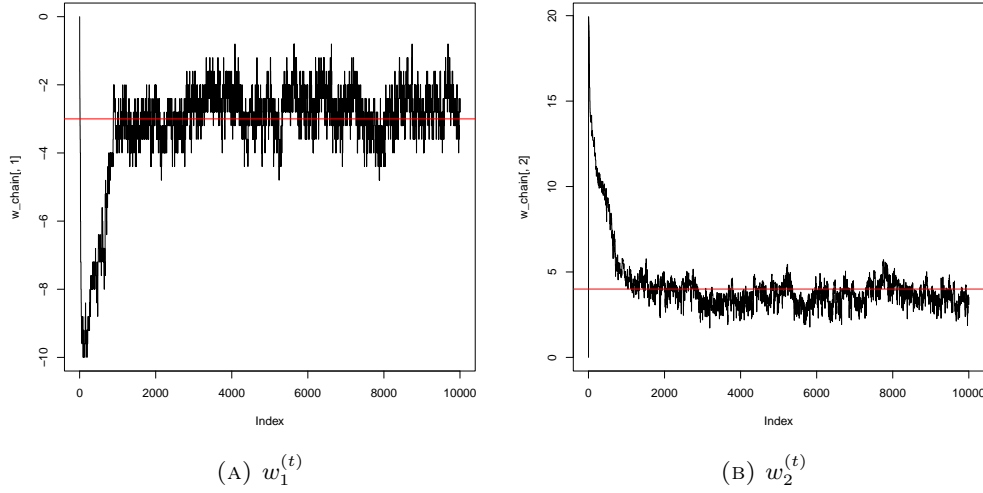


FIGURE 1. trace plots

- (c) I found $w = (-2.674615, 3.205785)$
- (d) It belongs to -1

Exercise 7. (★) Assume a Bayesian model

$$\begin{cases} z_i|w & \stackrel{\text{ind}}{\sim} f(z_i|w), \quad i = 1, \dots, n \\ w & \sim f(w) \end{cases}$$

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

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

by using SGD with update

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

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

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

Solution. It is

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

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

Part 2. Artificial Neural Networks

Exercise 8. (★) 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://www.microsoft.com/en-us/research/wp-content/uploads/2016/05/prml-web-sol-2009-09-08.pdf>
- <https://www.maths.dur.ac.uk/users/georgios.karagiannis/temp/Pattern%20recognition%20and%20machine%20learning-solutions-1.pdf>
- <https://www.maths.dur.ac.uk/users/georgios.karagiannis/temp/Pattern%20recognition%20and%20machine%20learning-solutions-2.pdf>

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

Exercise 9. (★) Consider the multi-class classification problem, with a predictive rule $h_w : \mathbb{R}^d \rightarrow \mathcal{P}$, 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 $h_w = (h_{w,1}, \dots, h_{w,q})^\top$, 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 $k = 1, \dots, q$, and let the associated activation functions be

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

(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 $y = (y_1, \dots, y_q)$ 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

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

- (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 $k = 1, \dots, q$. 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 $i = 1, \dots, d$

Compute:

at $t = 1$: for $j = 1, \dots, c$

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

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

at $t = 2$: for $k = 1, \dots, q$

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

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

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

(3) It is

$$\frac{d}{da} \sigma_1(a) = \frac{1}{1 + a^2}$$

and

$$\begin{aligned} \frac{d}{da_k} \sigma_2(a_k) &= \sigma_2(a_j) (1(j = k) - \sigma_2(a_k)) \\ &= o_j (1(j = k) - o_k) \end{aligned}$$

and

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

and

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

Backward pass:

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

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

at $t = 1$: **for** $j = 1, \dots, c$

comp:

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

Output:

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

Part 3. Support Vector Machines

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

Exercise 10. (**) 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:

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

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

$$(8) \quad \xi_i \geq 0, \quad \forall i = 1, \dots, m$$

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 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

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

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

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

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

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

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

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

$$1 - y_i (\langle w, x_i \rangle + b) - \xi_i \leq 0, \quad \forall i = 1, \dots, m \quad \text{Primal feasibility}$$

$$\xi_i \geq 0$$

(12)

$$\alpha_i \geq 0 \quad \forall i = 1, \dots, m \quad \text{Dual feasibility}$$

(13)

$$\beta_i \geq 0 \quad \forall i = 1, \dots, m$$

(14)

$$\alpha_i (1 - y_i (\langle w, x_i \rangle + b) - \xi_i) = 0, \quad \forall i = 1, \dots, m \quad \text{Complementary slackness}$$

(15)

$$\beta_i \xi_i = 0, \quad \forall i = 1, \dots, m$$

(4) It is

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

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

(17)

$$\alpha_i \in [0, C] \quad \forall i = 1, \dots, m$$

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

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

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

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

Exercise 11. (★) 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.

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://www.microsoft.com/en-us/research/wp-content/uploads/2016/05/prml-web-sol-2009-09-08.pdf>
- <https://www.maths.dur.ac.uk/users/georgios.karagiannis/temp/Pattern%20recognition%20and%20machine%20learning-solutions-1.pdf>
- <https://www.maths.dur.ac.uk/users/georgios.karagiannis/temp/Pattern%20recognition%20and%20machine%20learning-solutions-2.pdf>

Part 4. Gaussian process regression

Exercise 12. (★) 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.

available from

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

The solutions are available from

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 - <https://www.microsoft.com/en-us/research/wp-content/uploads/2016/05/prml-web-sol-2009-09-08.pdf>
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 - <https://www.maths.dur.ac.uk/users/georgios.karagiannis/temp/Pattern%20recognition%20and%20machine%20learning-solutions-1.pdf>
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