MATH3431 Machine Learning and Neural Networks III — Epiphany term 2023

Exercise sheet

Lecturer: Georgios P. Karagiannis — georgios.karagiannis@durham.ac.uk

Part 1. **Stochastic learning**

Exercise 1. ($\star$)Let $f : \mathbb{R}^d \to \mathbb{R}$ 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

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

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 $f : \mathbb{R}^d \to \mathbb{R}$ with $f(w) = g(\langle w, x\rangle + y)$ $x \in \mathbb{R}^d$ and $y \in \mathbb{R}$. Let $g : \mathbb{R} \to \mathbb{R}$ 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.

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. ($\star$)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

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

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

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

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

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

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

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

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 $\mathcal{X} := \left\{x \in \mathbb{R}^d : \|x\|_2 \leq L\right\}$.

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 $1 - yw_2^\top x \leq 1 - yw_1^\top x$, and then take cases $1 - yw_2^\top x >$ or < 0 and $1 - yw_1^\top x >$ 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

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

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

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

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

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

(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

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

  So, for $u \ge 1$, it is $0 \ge (u - 1)v \implies v \le 0$, and for $u < 1$ it is $(1 - u) \ge (u - 1)v \implies v \ge -1$. 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 $t = 1, 2, 3, ...$ iterate:*

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

(b) *For $j = 1, ..., d$ (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*

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

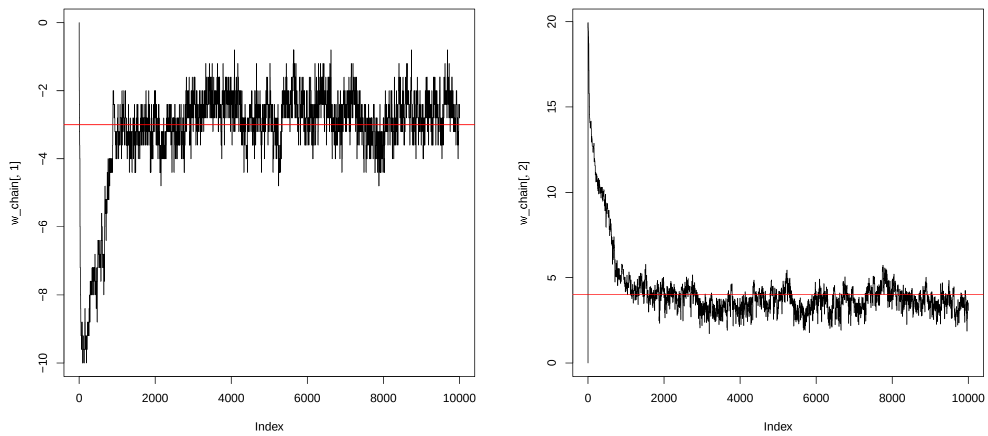
where index i indicates the sub-sample, and $\epsilon > 0$ small.

(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.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 7. ($\star$)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 8. ($\star$) 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-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

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

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

Exercise 9. ($\star$)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 $\mathcal{P} = \left\{ p \in (0,1)^q : \sum_{j=1}^{q} p_j = 1 \right\}$. We assume $h_w = (h_{w,1}, ..., h_{w,q})^\top$, and 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 $k = 1, ..., q$, with activation functions softmax function

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

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 quantities.

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

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

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

(1) It is

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

(2) 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:

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

Output:

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