

Homework 2: Artificial Neural Networks

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 Instructions: For Formative assessment, submit the solutions all of the problems

Exercise 1. (★) 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 $h_w = (h_{w,1}, \dots, h_{w,q})^\top$, 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 $k = 1, \dots, q$, with activation functions softmax function

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

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

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

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

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

- (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 $i = 1, \dots, d$

Compute:

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

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

(2) 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:

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

Output:

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