MATH3431 Machine Learning and Neural Networks III — Epiphany term 2025

Homework 4: Artificial Neural Networks

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Instructions: For Formative assessment, submit the solutions to all the parts of the Exercise.

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 $\mathcal{P} = \left\{p \in (0,1)^q : \sum_{j=1}^q p_j = 1\right\}$. 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

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

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

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

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

(a) It is

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}a_k}\sigma_2(a_j) &= \frac{\mathrm{d}}{\mathrm{d}a_k}\frac{\exp(a_j)}{\sum_{j'}\exp(a_{j'})} \\
&= \begin{cases} \frac{\mathrm{d}}{\mathrm{d}a_k}\frac{\exp(a_j)}{\sum_{j'}\exp(a_{j'})} & j = k \\ \frac{\mathrm{d}}{\mathrm{d}a_k}\frac{\exp(a_j)}{\sum_{j'}\exp(a_{j'})} & j \neq k \end{cases} \\
&= \begin{cases} \frac{\exp(a_j)\sum_{j'}\exp(a_{j'}) - \exp(a_j)}{\left(\sum_{j'}\exp(a_{j'})\right)^2}\exp(a_k) & j = k \\ \frac{1}{\left(\sum_{j'}\exp(a_{j'})\right)^2}\exp(a_k) & j \neq k \end{cases} \\
&= \begin{cases} \left(1 - \frac{\exp(a_j)}{\sum_{j'}\exp(a_{j'})}\right)\frac{\exp(a_j)}{\sum_{j'}\exp(a_{j'})} & j = k \\ \frac{1}{\sum_{j'}\exp(a_{j'})}\frac{\exp(a_k)}{\sum_{j'}\exp(a_{j'})} & j \neq k \end{cases} \\
&= \begin{cases} \sigma_2(a_j)(1 - \sigma_2(a_j)) & j = k \\ -\sigma_2(a_j)\sigma_2(a_k) & j \neq k \end{cases} \\
&= \sigma_2(a_j)(1(j = k) - \sigma_2(a_k))
\end{aligned}
$$

(b) It is

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

and

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

and

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

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:

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

Output:

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