

Assignment 2 & 3

Paul Thillen et Louis-Philippe Noël
IFT3395/6390 - Machine learning

November 27, 2017

1 Theoretical part A

1.1

To show:

$$\text{sigmoid}(x) = \frac{1}{2}(\tanh(\frac{x}{2}) + 1)$$

Which is equivalent to showing:

$$\tanh(x) = 2 \cdot \text{sigmoid}(2x) - 1$$

We have:

$$\begin{aligned}\tanh(x) &= \frac{e^x - e^{-x}}{e^x + e^{-x}} = \frac{e^x - \frac{1}{e^x}}{e^x + \frac{1}{e^x}} = \frac{\frac{e^{2x}-1}{e^x}}{\frac{e^{2x}+1}{e^x}} \\ &= \frac{e^{2x} - 1}{e^{2x} + 1}\end{aligned}$$

and:

$$\begin{aligned}\text{sigmoid}(x) &= \frac{1}{1 + e^{-x}} = \frac{1}{1 + \frac{1}{e^x}} = \frac{1}{\frac{e^x+1}{e^x}} \\ &= \frac{e^x}{e^x + 1}\end{aligned}$$

consequently:

$$\begin{aligned}2 \cdot \text{sigmoid}(2x) - 1 &= 2 \cdot \frac{e^{2x}}{e^{2x} + 1} - 1 \\ &= \frac{2 \cdot e^{2x}}{e^{2x} + 1} - \frac{e^{2x} + 1}{e^{2x} + 1} \\ &= \frac{e^{2x} - 1}{e^{2x} + 1} = \tanh(x)\end{aligned}$$

1.2

To show:

$$\ln(\text{sigmoid}(x)) = -\text{softplus}(-x)$$

We have:

$$\ln(\text{sigmoid}(x)) = \ln\left(\frac{1}{1 + e^{-x}}\right) = -\ln(1 + e^{-x}) = -\text{softplus}(-x)$$

1.3

To show:

$$\text{sigmoid}'(x) = \text{sigmoid}(x) \cdot (1 - \text{sigmoid}(x))$$

We have:

$$\begin{aligned}\text{sigmoid}'(x) &= \left(\frac{e^x}{1 + e^x}\right)' \\ &= \frac{e^x(1 + e^x) - e^x \cdot e^x}{(1 + e^x)^2} \\ &= \frac{e^x}{1 + e^x} \left(1 - \frac{e^x}{1 + e^x}\right) \\ &= \text{sigmoid}(x) \cdot (1 - \text{sigmoid}(x))\end{aligned}$$

1.4

To show:

$$\tanh'(x) = 1 - \tanh^2(x)$$

We have:

$$\begin{aligned}\tanh'(x) &= \left(\frac{e^x - e^{-x}}{e^x + e^{-x}}\right)' \\ &= \frac{(e^x + e^{-x})^2 - (e^x - e^{-x})^2}{(e^x + e^{-x})^2} \\ &= 1 - \frac{(e^x - e^{-x})^2}{(e^x + e^{-x})^2} \\ &= 1 - \tanh^2(x)\end{aligned}$$

1.5 Write sign using only indicator functions

$$\text{sgn}(x) = \mathbb{1}_{\mathbb{R}_+}(x) - \mathbb{1}_{\mathbb{R}_-}(x)$$

1.6 Derivative of abs

$$abs(x) = \begin{cases} x, & \text{if } x > 0 \\ 0, & \text{if } x = 0 \\ -x, & \text{if } x < 0 \end{cases}$$

$$abs'(x) = \begin{cases} 1, & \text{if } x > 0 \\ 0, & \text{if } x = 0 \\ -1, & \text{if } x < 0 \end{cases}$$

1.7 Derivative of rect

$$rect(x) = \begin{cases} x, & \text{if } x > 0 \\ 0, & \text{else} \end{cases} = \mathbb{1}_{\{x>0\}}(x) \cdot x$$

$$rect'(x) = \mathbb{1}_{\{x>0\}}(x)$$

1.8 L2 gradient

$$\frac{\partial ||x||_2^2}{\partial x} = \begin{pmatrix} \frac{\partial}{\partial x_1} ||x||_2^2 \\ \dots \\ \frac{\partial}{\partial x_d} ||x||_2^2 \end{pmatrix} = \begin{pmatrix} 2x_1 \\ \dots \\ 2x_d \end{pmatrix}$$

1.9 L1 gradient

$$\frac{\partial ||x||_1}{\partial x} = \begin{pmatrix} \frac{\partial}{\partial x_1} ||x||_1 \\ \dots \\ \frac{\partial}{\partial x_d} ||x||_1 \end{pmatrix} = \begin{pmatrix} abs'(x_1) \\ \dots \\ abs'(x_d) \end{pmatrix}$$

2 Theoretical part B

2.1

Dimensions of $W^{(1)}$ and $b^{(1)}$:

$$\begin{aligned} dim(W^{(1)}) &= d_h \times d \\ dim(b^{(1)}) &= d_h \end{aligned}$$

Preactivation vector of neurons of the hidden layer h^a where $w_j^{(1)}$ is the j -th row of $W^{(1)}$.

$$h^a = W^{(1)} \cdot x + b^{(1)}$$

$$h_j^a = w_j^{(1)} \cdot x + b_j^{(1)}$$

Output vector of the hidden layer h^s :

$$h^s = \text{rect}(h^a)$$

$$h_k^s = \max(0, h_k^a)$$

2.2

Dimensions of $W^{(2)}$ and $b^{(2)}$:

$$\dim(W^{(2)}) = m \times d_h$$

$$\dim(b^{(2)}) = m$$

Preactivation vector of neurons of the output layer o^a where $w_j^{(2)}$ is the j -th row of $W^{(2)}$.

$$o^a = W^{(2)} \cdot h^s + b^{(2)}$$

$$o_j^a = w_j^{(2)} \cdot h^s + b_j^{(2)}$$

2.3

Output vector of the output layer o^s :

$$o^s = \text{softmax}(o^a)$$

$$o_k^s = \frac{e^{o_k^a}}{\sum_{i=1}^m e^{o_i^a}}$$

Since exponentials are always positive and both denominator and numerator are exponentials or sum of exponentials, o_k^s has to be positive too.

If we sum over all k for o_k^s , we receive:

$$\sum_{j=1}^m \frac{e^{o_j^a}}{\sum_{i=1}^m e^{o_i^a}} = \frac{\sum_{j=1}^m e^{o_j^a}}{\sum_{i=1}^m e^{o_i^a}} = \frac{\sum_{i=1}^m e^{o_i^a}}{\sum_{i=1}^m e^{o_i^a}} = 1$$

These two properties are important because o^s is a probability distribution for each possible class.

2.4

Loss function given a probability $o_y^s(x)$ for a single input vector x to be of class y :

$$\begin{aligned}
L(x, y) &= -\log(o_y^s(x)) \\
&= -\log\left(\frac{e^{o_y^a}}{\sum_{i=1}^m e^{o_i^a}}\right) \\
&= -\log(e^{o_y^a}) + \log\left(\sum_{i=1}^m e^{o_i^a}\right) \\
&= -o_y^a + \log\left(\sum_{i=1}^m e^{o_i^a}\right)
\end{aligned}$$

2.5

What is \hat{R} ? For a loss function L and training data D :

$$\hat{R}(L, D) = \frac{1}{|D|} \sum_d L(x^{(d)}, y^{(d)})$$

What is θ ?

$$\theta = \{W^{(1)}, b^{(1)}, W^{(2)}, b^{(2)}\}$$

How many scalar parameters n_θ are there?

$$\begin{aligned}
n_\theta &= |W^{(1)}| + |b^{(1)}| + |W^{(2)}| + |b^{(2)}| \\
&= d \cdot d_h + d_h + d_h \cdot m + m \\
&= (d_h + 1)d + (m + 1)d_h
\end{aligned}$$

Optimization problem:

$$\operatorname{argmin}_\theta \hat{R}(L, D) = \operatorname{argmin}_\theta \sum_d L(x^{(d)}, y^{(d)})$$

2.6

Batch gradient descent equation:

$$\theta \leftarrow \theta - \eta \frac{d\hat{R}}{d\theta}$$

2.7

To show:

$$\nabla L(o^a) = o^s - \text{onehot}_m(y) \tag{1}$$

We have:

$$\nabla L(o^a) = \begin{pmatrix} \dots \\ \frac{d}{do_k^a} - o_y^a + \log(\sum_{i=1}^m e^{o_i^a}) \\ \dots \end{pmatrix}$$

with

$$\begin{aligned} \frac{d}{do_k^a} - o_y^a + \log(\sum_{i=1}^m e^{o_i^a}) &= \begin{cases} -1 + \frac{e^{o_k^a}}{\sum_{i=1}^m e^{o_i^a}}, & \text{if } y = k \\ 0 + \frac{e^{o_k^a}}{\sum_{i=1}^m e^{o_i^a}}, & \text{if } y \neq k \end{cases} \\ &= \begin{cases} -1 + \text{softmax}(o_k^a), & \text{if } y = k \\ \text{softmax}(o_k^a), & \text{if } y \neq k \end{cases} \end{aligned}$$

so

$$\nabla L(o^a) = o^s - \text{onehot}_m(y)$$

2.8

```
onehot = np.zeros(m)
onehot[y-1] = 1
grad_oa = os - onehot
```

2.9

To compute: $\nabla L(W^{(2)}), \nabla L(b^{(2)})$. We know $\frac{d}{do_k^a} L$ and we have with W_k being the k -th line of W :

$$\begin{aligned} \frac{d}{dW_k^{(2)}} L &= \frac{d}{do_k^a} L \frac{d}{dW_k^{(2)}} o_k^a \\ \frac{d}{db_k^{(2)}} L &= \frac{d}{do_k^a} L \frac{d}{db_k^{(2)}} o_k^a \end{aligned}$$

We have to compute:

$$\begin{aligned} \frac{d}{dW_k^{(2)}} o_k^a &= \frac{d}{dW_k^{(2)}} (W_k^{(2)} \cdot h^S + b^{(2)}) = h^S \\ \frac{d}{db_k^{(2)}} o_k^a &= \frac{d}{dW_k^{(2)}} (W_k^{(2)} \cdot h^S + b^{(2)}) = 1 \end{aligned}$$

Finally, we have:

$$\begin{aligned}\frac{d}{dW_k^{(2)}}L &= (o_k^s - \text{onehot}_m(y)) \cdot h^S \\ \frac{d}{db_k^{(2)}}L &= o_k^s - \text{onehot}_m(y)\end{aligned}$$

2.10

In matrix form, we can write:

$$\begin{aligned}\nabla L(W^{(2)}) &= \nabla L(o^a) \cdot (h^S)^T \in m \times d_h \\ \nabla L(b^{(2)}) &= \nabla L(o^a) \in m \times 1\end{aligned}$$

Dimensions:

$$\begin{aligned}\nabla L(o^a) &\in 1 \times m \\ h^S &\in 1 \times d_h \\ (h^S)^T &\in d_h \times 1\end{aligned}$$

In Python:

```
grad_b2 = grad_oa
grad_W2 = numpy.dot(grad_oa , numpy.transpose(h_s))
```

2.11

To compute:

$$\frac{d}{dh_j^s}L = \sum_{k=1}^m \frac{dL}{do_k^a} \frac{d}{dh_j^s} o_k^a$$

The only unknown is $\frac{d}{dh_j^s} o_k^a$. We have:

$$\frac{d}{dh_j^s} o_k^a = \frac{d}{dh_j^s} (W_k^{(2)} \cdot h^S + b^{(2)}) = w_{k,j}^{(2)}$$

$w_{k,j}$ being the j -th column of the k -th line of W . With the sum, we have:

$$\frac{d}{dh_j^s}L = \sum_{k=1}^m \frac{dL}{do_k^a} \frac{do_k^a}{dh_j^s} = \sum_{k=1}^m \frac{dL}{do_k^a} w_{k,j}^{(2)} = (W_{\bullet,j}^{(2)})^T \frac{dL}{do^a}$$

2.12

In matrix form, we can write :

$$\nabla L(h^s) = (W^{(2)})^T \nabla L(o^a) \in d_h \times 1$$

Dimensions :

$$\begin{aligned} \dim((W^{(2)})^T) &= d_h \times m \\ \dim(\nabla L(o^a)) &= m \times 1 \end{aligned}$$

2.13

From theoretical part A we know that :

$$rect'(x) = \begin{cases} 1, & \text{if } x > 0 \\ 0, & \text{if } x \leq 0 \end{cases} = \mathbb{1}_{\{x>0\}}(x)$$

To compute:

$$\frac{d}{dh_j^a} L = \frac{dL}{dh_j^s} \frac{d}{dh_j^a} h_j^s$$

We know $\frac{d}{dh_j^s} L$ and we have:

$$\begin{aligned} \frac{d}{dh_j^a} h_j^s &= \frac{d}{dh_j^a} rect(h_j^a) = \begin{cases} 1, & \text{if } h_j^a > 0 \\ 0, & \text{if } h_j^a \leq 0 \end{cases} \\ &= \mathbb{1}_{\{h_j^a>0\}}(h_j^a) \end{aligned}$$

Finally, we have:

$$\frac{d}{dh_j^a} L = (W_{\bullet,j}^{(2)})^T \nabla L(o^a) \mathbb{1}_{\{h_j^a>0\}}(h_j^a)$$

2.14

In matrix form, we can write with \odot being element-wise multiplication:

$$\nabla L(h^a) = \nabla L(h^s) \odot \mathbb{1}_{\{h_j^a>0\}}(h_j^a)$$

Dimensions :

$$\begin{aligned} \dim(\nabla L(h^s)) &= d_h \times 1 \\ \dim(\mathbb{1}_{\{h_j^a>0\}}(h_j^a)) &= d_h \times 1 \end{aligned}$$

2.15

To compute: $\nabla L(W^{(1)}), \nabla L(b^{(1)})$. We know $\frac{d}{dh_j^a} L$ and we have:

$$\begin{aligned}\frac{d}{dW_j^{(1)}} L &= \frac{d}{dh_j^a} L \frac{d}{dW_j^{(1)}} h_j^a \\ \frac{d}{db_j^{(1)}} L &= \frac{d}{dh_j^a} L \frac{d}{db_j^{(1)}} h_j^a\end{aligned}$$

We have to compute:

$$\begin{aligned}\frac{d}{dW_j^{(1)}} h_j^a &= \frac{d}{dW_j^{(1)}} (W_j^{(1)} \cdot x + b^{(1)}) = x \\ \frac{d}{db_j^{(1)}} h_j^a &= \frac{d}{db^{(1)}} (W_j^{(1)} \cdot x + b^{(1)}) = 1\end{aligned}$$

Finally, we have:

$$\begin{aligned}\frac{d}{dW_j^{(1)}} L &= \frac{d}{dh_j^a} L \cdot x \\ \frac{d}{db_j^{(1)}} L &= \frac{d}{dh_j^a} L\end{aligned}$$

2.16

In matrix form, we can write :

$$\begin{aligned}\nabla L(W^{(1)}) &= \nabla L(h^a) \cdot x^T \in d^h \times d \\ \nabla L(b^{(1)}) &= \nabla L(h^a)\end{aligned}$$

Dimensions :

$$\begin{aligned}dim(\nabla L(h^a)) &= d_h \times 1 \\ dim(x) &= d \times 1\end{aligned}$$

2.17

Following the same logic than in question 2.13, we have:

$$\frac{dL}{dx} = \sum_{k=1}^{d_h} \frac{dL}{dh_k^a} \frac{dh_k^a}{dx_j} = (W_{\bullet,j}^{(1)})^T \frac{dL}{dh^a}$$

And in matrix form:

$$\nabla L(x) = (W^{(1)})^T \nabla L(h^a)$$

2.18

We have two parameters: W and b . The gradient of b is unchanged. The gradient of W will be affected by the deduction of its sign (L^1) and by the addition of two times its value (L^2) :

$$\begin{aligned}\nabla L(W^{(2)}) &= \nabla L(o^a) \cdot (h^S)^T + 2 \cdot W^{(2)} - \text{sign}(W^{(2)}) \\ \nabla L(W^{(1)}) &= \nabla L(h^a) \cdot x^T + 2 \cdot W^{(1)} - \text{sign}(W^{(1)})\end{aligned}$$