2021 - 2022

Homework 1

Deep Learning

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Question 1

Exercise 1

$$\frac{\delta\sigma}{\delta z}$$
$$= \frac{\delta}{\delta z}\frac{1}{(1+e^{-z})}$$
$$= \frac{\delta}{\delta z}(1+e^{-z})^{-1}$$
$$= (-1) * (1+e^{-z})^{-2} * \frac{\delta}{\delta z}(1+e^{-z})$$
$$= \frac{1}{(1+e^{-z})^2} * (e^{-z})$$
$$= \frac{1+e^{-z}-1}{(1+e^{-z})^2}$$
$$= \frac{1}{1+e^{-z}} - \frac{1}{(1+e^{-z})^2}$$
$$= \sigma(z) - \sigma^2(z)$$
$$= \sigma(z)(1-\sigma(z))$$

, as we want to show.

Exercise 2

$$L^{'}(z;y=+1) = \frac{d}{dz} - log[\sigma(z)]$$
$$= (-1) * \frac{\sigma^{'}(z)}{\sigma(z)}$$
$$= (-1) * \frac{\sigma(z) * (1-\sigma(z))}{\sigma(z)}$$
$$= (-1) * (1-\sigma(z))$$
$$= \sigma(z) - 1$$

$$L^{''}(z;y=+1) = \frac{d}{dz}(\sigma(z)-1)$$
$$= \sigma(z) * (1-\sigma(z)) > 0, \forall z.$$

Now, let's derivate the binary logistic loss with respect to z to prove that it is convex as a function of z:

$$L^{'}(z;y) =$$
$$\frac{d}{dz}[-\frac{1+y}{2}log(\sigma(z)) - \frac{1-y}{2}log(1-\sigma(z))]$$
$$\frac{1+y}{2}(\sigma(z)-1) + \frac{1-y}{2} * \frac{\sigma(z)(1-\sigma(z))}{1-\sigma(z)}$$
$$\frac{1+y}{2}(\sigma(z)-1) + \frac{1-y}{2}\sigma(z)$$

$$L^{''}(z;y) =$$
$$= \frac{1+y}{2}\sigma(z)(1-\sigma(z)) + \frac{1-y}{2}\sigma(z)(1-\sigma(z))$$
$$= \sigma(z)(1-\sigma(z)) * \frac{1+y+1-y}{2}$$
$$= \sigma(z)(1-\sigma(z)) \geq 0, \forall z.$$

Since the second order derivative of the loss with respect to z is $\geq 0, \forall z$, then the loss is convex as a function of z, as we wanted to show.

Exercise 3

So, what we need to calculate, to compute the Jacobian matrix is $\frac{\partial[softmax(z)]_i}{\partial z_j}$.

If $j = i$:

$$\frac{\partial[softmax(z)]_i}{\partial z_j} = \frac{\partial[softmax(z)]_j}{\partial z_j} =$$
$$\frac{\partial}{\partial z_j}\frac{e^{z_j}}{\sum_{k=1}^{K} e^{z_k}} = \frac{e^{z_j}(\sum_{k=1}^{K} e^{z_k}) - e^{z_j}e^{z_j}}{(\sum_{k=1}^{K} e^{z_k})^2} =$$
$$\frac{e^{z_j}}{\sum_{k=1}^{K} e^{z_k}}\frac{(\sum_{k=1}^{K} e^{z_k}) - e^{z_j}}{\sum_{k=1}^{K} e^{z_k}} =$$
$$s_j(1-s_j)$$

If $j \neq i$:

$$\frac{\partial[softmax(z)]_i}{\partial z_j}$$
$$= \frac{\partial}{\partial z_j}\frac{e^{z_i}}{\sum_{k=1}^{K} e^{z_k}} = \frac{0 - e^{z_i}e^{z_j}}{(\sum_{k=1}^{K} e^{z_k})^2} =$$
$$- \frac{e^{z_i}}{\sum_{k=1}^{K} e^{z_k}}\frac{e^{z_j}}{\sum_{k=1}^{K} e^{z_k}} = -s_i * s_j$$

Where $s_k = softmax(z)_k$.

$$\begin{bmatrix} s_0(1-s_0) & -s_1s_0 & \dots & -s_js_0 \\ -s_0s_1 & \ddots & -s_js_i & \vdots \\ \vdots & -s_js_i & s_j(1-s_j) & \vdots \\ -s_0s_i & \vdots & \ddots & \ddots \end{bmatrix}_{(K,K)}$$

Exercise 4

In the last exercise we calculated the Jacobian matrix for the softmax transformation on point z. Computing the gradient for the logistic loss, $L(z; y = a) = -log[softmax(z)]_a$ is straightforward.

Remember that:

$$-\frac{dlog(u)}{du} = -\frac{u^{'}}{u}$$

This way, we now have that:

With $L : \mathbb{R}^N \to \mathbb{R}$

$$\nabla L(z; y = a) = \begin{bmatrix} \frac{\partial L_{(y=a)}}{\partial z_0} \\ \cdots \\ \frac{\partial L_{(y=a)}}{\partial z_i} \\ \cdots \\ \frac{\partial L_{(y=a)}}{\partial z_N} \end{bmatrix}_{(N,1)} \text{, where } \frac{\partial L_{(y=a)}}{\partial z_i} = softmax_i(z(x)) - 1_{(y=i)}$$

The basis to construct the Hessian matrix is this derivative: $\frac{\partial^2 L}{\partial z_i \partial z_j}$. And we also know that $\nabla^2 L(z; y = a)$ is a matrix of dimensions (N, N), where $y \in \{1, ..., N\}$ and $z \in \mathbb{R}^N$. This way, we need to calculate the *basis* derivative for the following *cases* (covering the entire Hessian matrix positions):

1) $i \neq j = a$; **2)** $j \neq i = a$; **3)** $i \neq j \neq a$; **4)** $i = j = a$; **5)** $i = j \neq a$;

For space and display motives, we are going to replace $softmax_i(z(x)) \to s_i$.

- For **1** we have $\to \frac{\partial}{\partial z_i \partial z_{j=a}} L(z; y = a) = \frac{\partial}{\partial z_a} - log(s_a) = \frac{\partial}{\partial z_i}(s_a - 1) = -s_i s_a \leq 0, \forall z.$
- For **2** we have almost the same as in **1** $\to -s_j s_a \leq 0, \forall z.$
- For **3** we have $\to \frac{\partial}{\partial z_i \partial z_j} - log(s_a) = \frac{\partial}{\partial z_i} s_j = -s_i s_j \leq 0, \forall z.$
- For **4** we have $\to \frac{\partial}{\partial z_i \partial z_j} - log(s_a) = \frac{\partial}{\partial z_a^2} - log(s_a) = \frac{\partial}{\partial z_a}(s_a - 1) = s_a(1 - s_a) \geq 0 \text{ ,} \forall z.$
- For **5** we have $\to \frac{\partial}{\partial z_i^2} - log(s_a) = \frac{\partial}{\partial z_i} s_i = s_i(1 - s_i), \geq 0 \ \forall z.$

(Note that since $s_i \in [0, 1]$ it is trivial to show that $-s_i s_j \leq 0, \forall (i, j)$ and that $s_i(a - s_i) \leq 0, \forall i$)

With these results there's something we already know: we have a positive (non negative) diagonal, since the diagonal elements are always ≥ 0 (given by cases **4** and **5**). We also know that a symmetric matrix is the one where $a_{ij} = a_{ji}$ [2]. Such characteristic can be observed by using cases **1**, **2** and **3**.

With these two characteristic, we have a very curious matrix: one with a diagonal ≥ 0, and all other elements ≤ 0. With this, there is a rule we can use to prove that the Hessian is positive semidefinite and, therefore, that the loss $L(z; y = a)$ is convex with respect to z.

Let's understand how: we have that our matrix is **1)** a square one, and also that **2)** $|H_{ii}| \geq \sum_{j \neq i} |H_{ij}| \ \forall$i. This is a **diagonally dominant matrix** [3]. The second property is easily shown since every element in the diagonal is ≥ 0, and that every other element is ≤ 0.

Moreover, by definition, a **symmetric diagonally dominant real** matrix with **nonegative diagonal** entries is **positive semidefinite**. Therefore, since it is positive semidefinite we've proven that the loss function is convex with respect to z.

Exercise 5

On the last exercise we've proven that the **multinomial logistic loss** is convex with respect to **z**. As such, if we now have that $z = W\phi(x) + b$, since we have, using the **hint** that the composition of an affine map (in this case $z = W\phi(x) + b$), with a convex function (**the multinomial logistic loss, as we have shown**), then using the hint, this composition:

$((L(z; y = j) \circ (W\phi(x) + b))(x)$, **is also convex**.

What this says is that, since $z = W\phi(x) + b$ is a linear transformation of both $W\phi(x)$ and b, then the function is convex to both parameters on their own, **just as we want to show**.

In case z is not a linear function, then the multinomial logistic loss may not be convex with respect to its parameters. Since we prove the convex property to z, we can only generalize it to linear transformations of itself (as we have just did). If the transformation is not linear (or a composition of an affine map), then we need to test each case on its own to see if it may be convex (in the case we can even compute its properties).

A pragmatic explanation is that if this was true, then the gold objective of Artificial Intelligence would be within our reach, since we could compute any problem where we have a defined loss, and get a viable model. Obviously, we aren't there yet.

Question 2

Exercise 1

Even though the second part of this solution, using matrices and vectors, works just as well, for the case where the output is scalar, and w is a vector, we have:

$$1)\frac{\delta L}{\delta b} = \frac{\delta}{\delta b}\frac{1}{2}\sum_{i=1}^{N}((\sum_j w_j x_j^i) + b - y^i)^2 =$$

$$= \sum_{i=1}^{N}((\sum_j w_j x_j^i) + b - y^i))$$

$$2)\frac{\delta^2 L}{\delta b^2} = \sum_{i=1}^{N}(0 + \frac{\delta}{\delta b}b + 0) = \sum_{i=1}^{N} 1 \geq 0$$

$$3)\frac{\delta L}{\delta w_j} = \frac{\delta}{\delta w_j}\frac{1}{2}\sum_{i=1}^{N}((\sum_{j'} w_{j'} x_{j'}^i) + b - y^i)^2$$

$$= \sum_{i=1}^{N} x_j^i((\sum_{j'} w_{j'} x_{j'}^i) + b - y^i)$$

$$4)\frac{\delta^2 L}{\delta w_j^2} = \frac{\delta}{\delta w_j}\frac{1}{2}\sum_{i=1}^{N} x_j^i * \left[(\sum_k w_k x_k^i) + b - y^i\right]$$

$$= \frac{1}{2}\sum_{i=1}^{N} x_j^i * \left[(x_j^i) + 0 + 0\right] = \frac{1}{2}\sum_{i=1}^{N}(x_j^i)^2 \geq 0$$

Since both **2)** and **4)** are $\geq$0, then L is convex with respect to (W, b).

More generally, if we want to use matrix and vector notation, we have:

With $z = \mathbf{W}^\intercal\phi(x) + b$, let's include a constant feature to get rid of the explicit b. This way we have that $b = W_0$, where W_0 is the constant column added to W. Therefore, we have $z = \mathbf{W}^\intercal\phi(x) = Wx$, where, by abuse of notation we are using $\phi(x) = x$.

Thus we have that squared error $= \frac{1}{2}||Y - Wx||^2$

$$L(z; y) = \frac{1}{2}(z - y)^\intercal(z - y) =$$
$$\frac{1}{2}(Wx - y)^\intercal(Wx - y) =$$
$$\frac{1}{2}(x^\intercal W^\intercal - y^\intercal)(Wx - y) =$$
$$\frac{1}{2}(x^\intercal W^\intercal Wx - x^\intercal W^\intercal y - y^\intercal Wx + y^\intercal y)$$

Now, calculating its first derivative with respect to w we have:

$$\frac{\delta L(z; y)}{\delta W} =$$
$$\frac{1}{2}\frac{\delta}{\delta W}(x^\intercal W^\intercal Wx - x^\intercal W^\intercal y - y^\intercal Wx + y^\intercal y) =$$
$$\frac{1}{2}(2Wxx^\intercal - yx^\intercal - yx^\intercal + 0) =$$
$$\frac{1}{2}(2Wxx^\intercal - 2yx^\intercal) =$$
$$Wxx^\intercal - yx^\intercal = (Wx - y)x^\intercal$$

If we now calculate the second derivative, we have:

$$\frac{\delta}{\delta W}[Wxx^\intercal - yx^\intercal] =$$
$$(xx^\intercal)^\intercal - 0 =$$
$$x^\intercal x$$

By definition [5] we now have that the second derivative, the Hessian matrix, is positive semi-definite, therefore L is convex with respect to W (also to b, since we've *added* the bias, b, implicitly to the weights matrix). (We don't present the proof at [5] because we would just reproduce a proof already available)

Exercise 2

Exercise 2a

We know that we are in an over-fitting situation when we are losing model generalization. What we see here is that until around epoch 70, the test loss decreases, as well as the training loss. Then, roughly after epoch 70, while the training loss continues to decrease, the test loss doesn't, it even increases! What this shows us, is that the model is not able anymore to correctly generalize the train data to the test data.
If the test data distributions aren't similar to the training data ones, this is expected, however, if we assume they are - and we assume it -, this clearly shows that the model is over-fitting to the training data at the expense of losing generalization and performing worse in the test data.

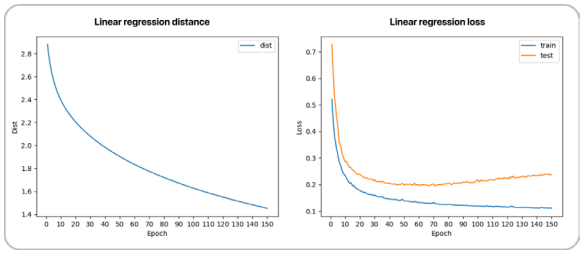

Figure 1: Left: the distance for linear regression between the analytical and non-analytical methods. Right: the loss for the linear regression for the train and test sets.

Exercise 2b

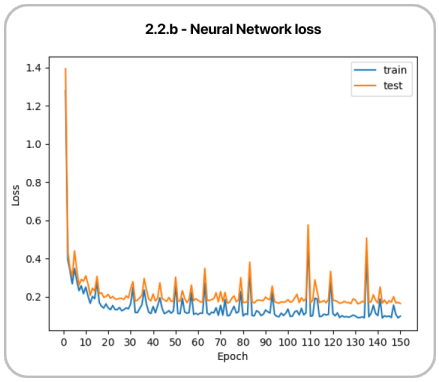

Figure 2: Loss for train and test sets for neural network.

Question 3

Exercise 1

Exercise 1a

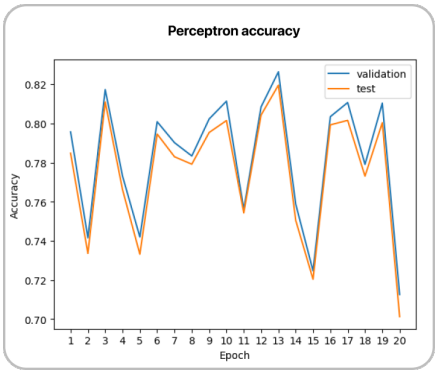

Figure 3: Accuracy for train and test sets for perceptron.

Exercise 1b

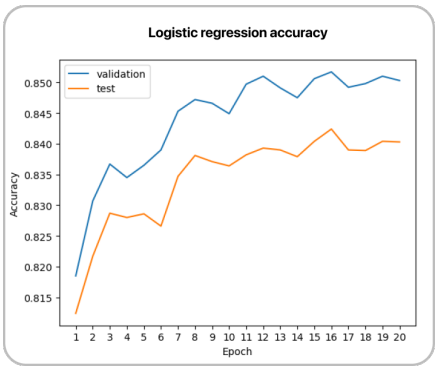

Figure 4: Accuracy for train and test sets for logistic regression.

Exercise 2

Exercise 2a

Intuitively speaking, just the fact that we have multi-layer perceptrons (meaning we have multiple parameters and 'nobs' to manipulate) gives us an explosion of combinatory possibilities and granularity to predict whatever we want. As such, we can gain much more predictive power by combining multiple perceptrons.

With one and one only perceptron we have a linear relationship between inputs and outputs, this means that if we want to solve more complex problems, where there are non-linear relationships between inputs and outputs, we need more complex models, something solved by the multi-layer perceptrons.

Moreover, non-linear activation functions imply that the model's output can't be reproduced from a linear combination of the inputs. This means that a multilayer perceptron with linear activation functions in all neurons, no matter how many layers it has, can be reduced to a two-layer input-output model

[1] since adding those layers would just give another linear function.

Ultimately, most of the real-world data has non-linear decision boundaries [4], and non-linearity is needed in activation functions for the neural networks to be able to produce exactly these non-linear decision boundaries via non-linear combinations of weights and inputs.

Exercise 2b

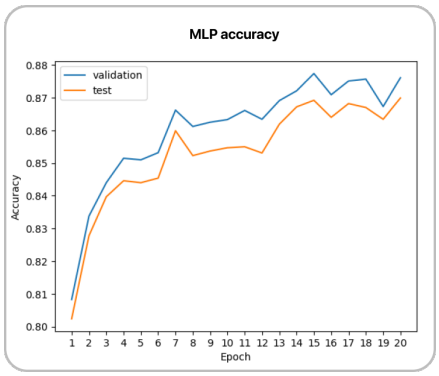

Figure 5: Accuracy for train and test sets for multi layer perceptron.

Question 4

Exercise 1

Regarding the best configuration, we found it using as learning rate the value 0.001. For it, the training loss we found 0.4398, and validation accuracy of 0.8513. For the final test accuracy the value obtained is 0.8402.

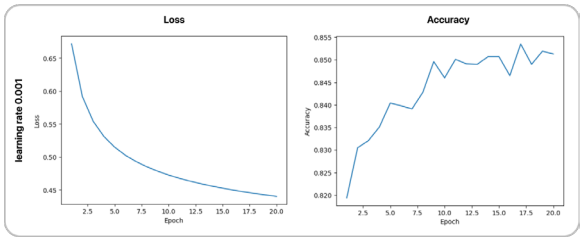

Figure 6: Plot for the best configuration, with 0.001 as the learning rate.

Exercise 2

Regarding the best configuration, we found it also using as learning rate the value 0.001. For it, the training loss we found 0.3696, and validation accuracy of 0.8871. For the final test accuracy the value obtained is 0.8774.

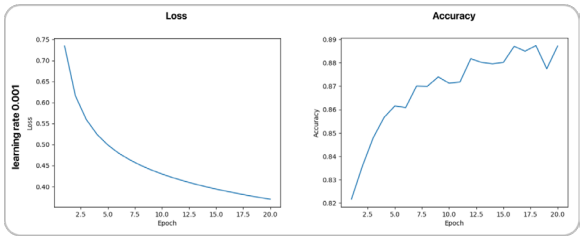

Figure 7: Plot for the best configuration, with 0.001 as the learning rate.

Exercise 3

The difference between 2 and 3 layers is more subtle! With **2** layers we got a training loss of: 0.4028, a validation accuracy of: 0.8677 and a final test accuracy of 0.8613. With **3** layers we got a training loss of: 0.4277, a validation accuracy of: 0.8688 and a final test accuracy of 0.8608.

With this, we choose the best model as the one with the highest accuracy on the test set! As such, the best model is the one with 2 layers. With the remark that for the validation set, the model with 3 layers is the one that behaves the best, and is also the one with the lowest loss, however, it didn't accomplish the best accuracy.

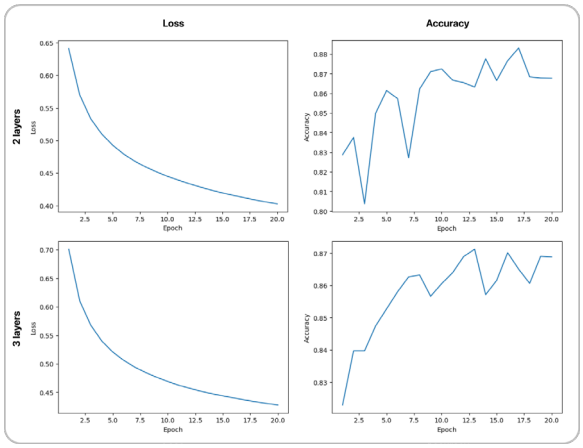

Figure 8: Plot for 2 and 3 layers.

References

[1] Multilayer perceptron. https://en.wikipedia.org/wiki/Multilayer_perceptron.

[2] Symmetric matrix. https://en.wikipedia.org/wiki/Symmetric_matrix.

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[5] Associate Professor in Algebra Enrico Gregorio. Is the product between the transpose of a matrix and itself a positive definite? https://www.quora.com/Is-A-T-A-always-positive-definite.