NUS | Computing

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Computer Science

T08 – 30 Oct 2024

Week 11

CS2109s Makeup Wed 1-2pm, 7-8pm

Content I

Section 1: **Backpropagation**

Question [G]

$$f^{[1]} = W^{[1]^T} X, \quad \hat{Y} = g^{[1]}(f^{[1]}), \quad \mathcal{E} = -\frac{1}{n}\sum_{i=0}^{n-1}\Big\{[Y_{0i} \cdot log(\hat{Y}_{0i})] + [(1 - Y_{0i}) log(1 - \hat{Y}_{0i})]\Big\}$$

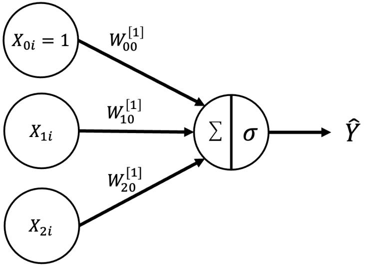


Figure 1: Simple Neural Network

Question [G]

When $n = 1$:

a. $\frac{\partial \mathcal{E}}{\partial \hat{Y}} = \left[-\frac{Y_{00}}{\hat{Y}_{00}} + \frac{1-Y_{00}}{1-\hat{Y}_{00}} \right]$ (Given)

b. $\frac{\partial \mathcal{E}}{\partial f^{[1]}} = \hat{Y} - Y$

c. $\frac{\partial \mathcal{E}}{\partial W_{20}^{[1]}} = \left(\frac{\partial \mathcal{E}}{\partial f^{[1]}} \right)_{00} X_{20}$

Recap

- What is back propagation?
- How to perform forward propagation?
- How to perform back propagation?

Answer b

Since $n = 1$, $\frac{\partial \mathcal{E}}{\partial f^{[1]}} = \frac{\partial \mathcal{E}}{\partial f_{00}^{[1]}} = \frac{\partial \mathcal{E}}{\partial \hat{Y}_{00}} \frac{\partial \hat{Y}_{00}}{\partial f_{00}^{[1]}}$ (chain rule)

Since $\hat{Y}_{00} = \sigma(f_{00}^{[1]}) \implies \frac{\partial \hat{Y}_{00}}{\partial f_{00}^{[1]}} = \sigma(f_{00}^{[1]})\Big(1 - \sigma(f_{00}^{[1]})\Big) = \hat{Y}_{00}(1 - \hat{Y}_{00})$

From (i), $\frac{\partial \mathcal{E}}{\partial \hat{Y}_{00}} = \Big[- \frac{Y_{00}}{\hat{Y}_{00}} + \frac{1 - Y_{00}}{1 - \hat{Y}_{00}} \Big]$

$$
\begin{aligned}
\frac{\partial \mathcal{E}}{\partial f^{[1]}} &= \Big[\frac{\partial \mathcal{E}}{\partial \hat{Y}_{00}} \frac{\partial \hat{Y}_{00}}{\partial f_{00}^{[1]}} \Big] \\
&= \Big[- \frac{Y_{00}}{\hat{Y}_{00}} + \frac{1 - Y_{00}}{1 - \hat{Y}_{00}} \Big] \Big[\hat{Y}_{00}(1 - \hat{Y}_{00}) \Big] \\
&= \Big[- Y_{00}(1 - \hat{Y}_{00}) + (1 - Y_{00})\hat{Y}_{00} \Big] \\
&= \Big[\hat{Y}_{00} - Y_{00} \Big] \\
&= \hat{Y} - Y.
\end{aligned}
$$

Answer c

Since $n = 1$, $\frac{\partial \mathcal{E}}{\partial W_{20}^{[1]}} = \frac{\partial \mathcal{E}}{\partial f_{00}^{[1]}} \frac{\partial f_{00}^{[1]}}{\partial W_{20}^{[1]}}$ (chain rule)

$f_{00}^{[1]} = W^{[1]^T} X = \sum_{i=0}^{2} (W^{[1]^T})_{0i} X_{i0} = \sum_{i=0}^{2} W_{i0}^{[1]} X_{i0} \implies \frac{\partial f_{00}^{[1]}}{\partial W_{20}^{[1]}} = X_{20}$

$$
\begin{aligned}
\frac{\partial \mathcal{E}}{\partial W_{20}^{[1]}} &= \frac{\partial \mathcal{E}}{\partial f_{00}^{[1]}} \frac{\partial f_{00}^{[1]}}{\partial W_{20}^{[1]}} \\
&= \frac{\partial \mathcal{E}}{\partial f_{00}^{[1]}} X_{20} \\
&= \left(\frac{\partial \mathcal{E}}{\partial f^{[1]}} \right)_{00} X_{20}
\end{aligned}
$$

Note: $\frac{\partial \mathcal{E}}{\partial \hat{Y}}$, and $\frac{\partial \mathcal{E}}{\partial f^{[1]}}$ are matrices since $\mathcal{E}$ is a scalar, but $\widehat{Y}$ and $f^{[1]}$ are matrices. However, $\frac{\partial \mathcal{E}}{\partial W_{20}^{[1]}}$ is a scalar since $W_{20}^{[1]}$ is a scalar.

Question 2-4 [G]

2. Derive an expression for $\frac{\partial \mathcal{E}}{\partial W^{[1]}}$, how does back propagation work?
3. Let us consider a general case where $n \in \mathbb{N}$, find $\frac{\partial \mathcal{E}}{\partial f^{[1]}}$.
4. Why do the hyper-parameters α and β? How to set their values?

$$\mathcal{E} = -\frac{1}{n}\sum_{i=0}^{n-1}\left\{\alpha[Y_{0i} \cdot log(\hat{Y}_{0i})] + \beta[(1 - Y_{0i}) \cdot log(1 - \hat{Y}_{0i})]\right\}$$

Answer 2

From (1c), the general form is $\frac{\partial \mathcal{E}}{\partial W_{i0}^{[1]}} = \left(\frac{\partial \mathcal{E}}{\partial f^{[1]}}\right)_{00} X_{i0}$

$$\frac{\partial \mathcal{E}}{\partial W^{[1]}} = \left[\frac{\partial \mathcal{E}}{\partial W_{00}^{[1]}}, \frac{\partial \mathcal{E}}{\partial W_{10}^{[1]}}, \frac{\partial \mathcal{E}}{\partial W_{20}^{[1]}}\right]^T = \left(\frac{\partial \mathcal{E}}{\partial f^{[1]}}\right)_{00} [X_{00}, X_{10}, X_{20}]^T = \left(\frac{\partial \mathcal{E}}{\partial f^{[1]}}\right)_{00} X$$
$$= \left(\hat{Y} - Y\right)_{00} X = \left(g^{[1]}(f^{[1]}) - Y\right)_{00} X = \left(g^{[1]}({W^{[1]}}^T X) - Y\right)_{00} X$$

Intuition behind back propagation $W^{[1]} = W^{[1]} - \alpha \frac{\partial \mathcal{E}}{\partial W^{[1]}}$:

- Change in first layer weighted sum $f^{[1]}$
- Change in predicted value $\hat{Y}$
- Change of loss $\mathcal{E}$
- Decrease the loss by changing the weights

Directly proportional to input X

Answer 3

From (1), $\frac{\partial \mathcal{E}}{\partial f^{[1]}_{0i}} = \left[\frac{\partial \mathcal{E}}{\partial \hat{Y}_{0i}} \frac{\partial \hat{Y}_{0i}}{\partial f^{[1]}_{0i}}\right]$

$$\frac{\partial \mathcal{E}}{\partial \hat{Y}} = \left[\frac{\partial \mathcal{E}}{\partial \hat{Y}_{00}}, \frac{\partial \mathcal{E}}{\partial \hat{Y}_{01}}, \cdots, \frac{\partial \mathcal{E}}{\partial \hat{Y}_{0n}}\right] = \left[\cdots, \frac{1}{n}\Big(-\frac{Y_{0i}}{\hat{Y}_{0i}} + \frac{1 - Y_{0i}}{1 - \hat{Y}_{0i}}\Big), \cdots\right]$$

$$\frac{\partial \hat{Y}_{0i}}{\partial f^{[1]}_{0i}} = \sigma(f^{[1]}_{0i})\Big(1 - \sigma(f^{[1]}_{0i})\Big) = \hat{Y}_{0i}(1 - \hat{Y}_{0i})$$

$$\begin{aligned}
\frac{\partial \mathcal{E}}{\partial f^{[1]}} &= \left[\frac{\partial \mathcal{E}}{\partial f^{[1]}_{00}}, \frac{\partial \mathcal{E}}{\partial f^{[1]}_{01}}, \cdots, \frac{\partial \mathcal{E}}{\partial f^{[1]}_{0n}}\right] \\
&= \frac{1}{n}\Big[(\hat{Y}_{00} - Y_{00}), (\hat{Y}_{01} - Y_{01}), \ldots, (\hat{Y}_{0n} - Y_{0n})\Big] \\
&= \frac{1}{n}(\hat{Y} - Y)
\end{aligned}$$

Answer 4

Weighted Error:

$$\mathcal{E} = -\frac{1}{n}\sum_{i=0}^{n-1}\left\{\alpha[Y_{0i} \cdot log(\hat{Y}_{0i})] + \beta[(1 - Y_{0i}) \cdot log(1 - \hat{Y}_{0i})]\right\}$$

Apply a weight to how much each class contributes to the loss function:

- Error due to Cultiva A ($p_A = 100/1100$): $Y_{0i} \cdot log(\hat{Y}_{0i})$
- Error due to Cultiva B ($p_B = 1000/1100$): $(1 - Y_{0i}) \cdot log(1 - \hat{Y}_{0i})$

Since we have unbalanced dataset, we can weight using the ratio $\frac{\alpha}{\beta} = \frac{1/100}{1/1000}$:

- $\alpha = 1/100$
- $\beta = 1/1000$

We punish the model more heavily if it misclassifies A, so the model won't be biased towards predicting all samples as B.

Section 2: **Backpropagation for a Deep(er) Network**

When $n = 1$, compute $\frac{\partial \mathcal{E}}{\partial W_{11}^{[1]}}$, where
$f^{[1]} = {W^{[1]}}^T X, \quad a^{[1]} = g^{[1]}(f^{[1]}), \quad f^{[2]} = {W^{[2]}}^T a^{[1]}, \quad \hat{Y} = g^{[2]}(f^{[2]}), \quad g^{[1]}(s) = ReLU(s), \quad g^{[2]}(s) = \sigma(s) = \frac{1}{1+e^{-s}}, \quad W^{[1]} \in \mathbb{R}^{3\times 2}, \quad W^{[2]} \in \mathbb{R}^{2\times 1}$.

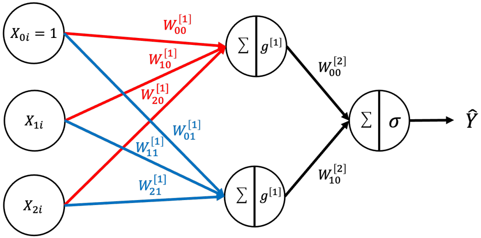


Figure 2: Complex NN

[@] Is ReLU continous/discontinuous, not/differentiable; Can we use discontinuous activation functions?

Question 1

When $n = 1$, compute $\frac{\partial \mathcal{E}}{\partial W^{[1]}_{11}}$, where
$f^{[1]} = {W^{[1]}}^T X$, $a^{[1]} = g^{[1]}(f^{[1]})$, $f^{[2]} = {W^{[2]}}^T a^{[1]}$, $\hat{Y} = g^{[2]}(f^{[2]})$, $g^{[1]}(s) = ReLU(s)$, $g^{[2]}(s) = \sigma(s) = \frac{1}{1+e^{-s}}$, $W^{[1]} \in \mathbb{R}^{3\times 2}$, $W^{[2]} \in \mathbb{R}^{2\times 1}$.

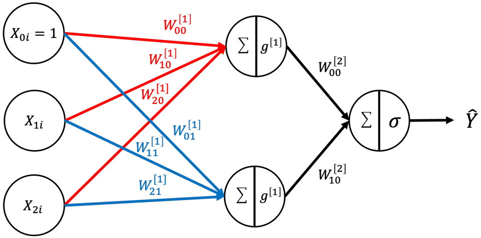


Figure 2: Complex NN

[@] Is ReLU continous/discontinuous, not/differentiable; Can we use discontinuous activation functions? Continuous but not differentiable.

Answer

Intuition: Plot the forward path and take the derivative.

$$W_{11}^{[1]} \xrightarrow{f^{[1]}={W^{[1]}}^T X} f_{10}^{[1]} \xrightarrow{a^{[1]}=g^{[1]}(f^{[1]})} a_{10}^{[1]} \xrightarrow{f^{[2]}={W^{[2]}}^T a^{[1]}} f_{00}^{[2]} \xrightarrow{\hat{Y}=g^{[2]}(f^{[2]})} \hat{Y}_{00} \to \mathcal{E}$$

$$f^{[1]} = \begin{bmatrix} W_{00}^{[1]} & W_{01}^{[1]} \\ W_{10}^{[1]} & W_{11}^{[1]} \\ W_{20}^{[1]} & W_{21}^{[1]} \end{bmatrix}^T \begin{bmatrix} X_{00} \\ X_{10} \\ X_{20} \end{bmatrix} = \begin{bmatrix} \sum_i W_{i0}^{[1]} X_{i0} \\ \sum_i W_{i1}^{[1]} X_{i0} \end{bmatrix}$$

$$f^{[2]} = \begin{bmatrix} W_{00}^{[2]} \\ W_{10}^{[2]} \end{bmatrix}^T \begin{bmatrix} a_{00}^{[1]} \\ a_{10}^{[1]} \end{bmatrix} = \begin{bmatrix} \sum_i W_{i0}^{[2]} a_{i0}^{[1]} \end{bmatrix}$$

Expand using chain rule: $\frac{\partial \mathcal{E}}{\partial W_{11}^{[1]}} = \frac{\partial \mathcal{E}}{\partial \hat{Y}_{00}} \frac{\partial \hat{Y}_{00}}{\partial f_{00}^{[2]}} \frac{\partial f_{00}^{[2]}}{\partial a_{10}^{[1]}} \frac{\partial a_{10}^{[1]}}{\partial f_{10}^{[1]}} \frac{\partial f_{10}^{[1]}}{\partial W_{11}^{[1]}}$

Find each of the terms in $\frac{\partial \mathcal{E}}{\partial W_{11}^{[1]}} = \frac{\partial \mathcal{E}}{\partial \hat{Y}_{00}} \frac{\partial \hat{Y}_{00}}{\partial f_{00}^{[2]}} \frac{\partial f_{00}^{[2]}}{\partial a_{10}^{[1]}} \frac{\partial a_{10}^{[1]}}{\partial f_{10}^{[1]}} \frac{\partial f_{10}^{[1]}}{\partial W_{11}^{[1]}}$:

- $\frac{\partial \mathcal{E}}{\partial \hat{Y}_{00}} = -\frac{\alpha Y_{00}}{\hat{Y}_{00}} + \frac{\beta(1-Y_{00})}{1-\hat{Y}_{00}}$
- $\frac{\partial \hat{Y}_{00}}{\partial f_{00}^{[2]}} = \sigma(f_{00}^{[2]})\Big(1 - \sigma(f_{00}^{[2]})\Big)$
- $\frac{\partial f_{00}^{[2]}}{\partial a_{10}^{[1]}} = W_{10}^{[2]}$
- $\frac{\partial a_{10}^{[1]}}{\partial f_{10}^{[1]}} = \begin{cases} 0, \text{if } f_{10}^{[1]} \leq 0 \\ 1, \text{otherwise} \end{cases} = \mathbb{1}_{f_{10}^{[1]}>0}$
- $\frac{\partial f_{10}^{[1]}}{\partial W_{11}^{[1]}} = X_{10}$

where $\mathbb{1}_{f_{10}^{[1]}>0}$ is an indicator function. Therefore,

$$\frac{\partial \mathcal{E}}{\partial W_{11}^{[1]}} = \Big[-\frac{\alpha Y_{00}}{\hat{Y}_{00}} + \frac{\beta(1-Y_{00})}{1-\hat{Y}_{00}} \Big] \sigma(f_{00}^{[2]})\Big(1 - \sigma(f_{00}^{[2]})\Big) W_{10}^{[2]} \mathbb{1}_{f_{10}^{[1]}>0} X_{10}$$

Section 3: **Potential Issues with Training Deep Neural Networks**

Question 1a-c [G]

Play around with the code given in the `ipynb`, layer 0 gradient is $< 10^{-40}$

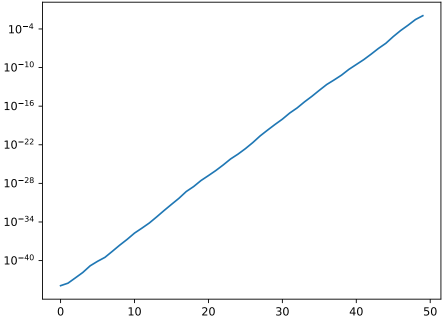


Figure 3: Layers / Max Abs Gradient, using sigmoid

1. Gradient magnitudes of the first few layers are extremely small, what's the problem?
2. Based on what we have learnt thus far, how can we mitigate this problem?
   - [@] Other sophisticated ways to resolve the issue, and why does it work?

Answer 1

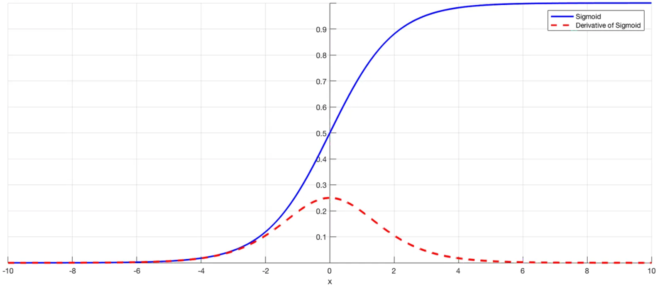


Figure 4: Sigmoid Function

Vanishing gradient problem: Earlier weights need more terms for updates.

- we need to take product of many, many derivatives
- derivatives of sigmoid is in $(0, 1/4]$
- ending up with a really small number
- causing convergence to be slow.

Answer 2

Derivative of ReLU (continuous but not differentiable at $x = 0$ – usually defined as 1):

$$\mathrm{ReLU}(x) = \max(0, x), \quad \frac{\partial \mathrm{ReLU}(x)}{\partial x} = \begin{cases} 0, \text{if } x < 0 \\ 1, \text{if } x > 0 \end{cases}$$

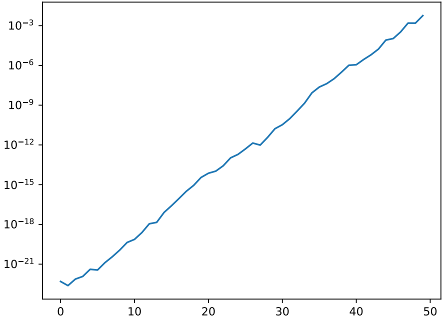
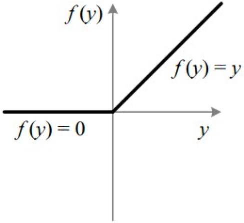


Figure 5: Layers / Max Abs Gradient, using ReLU

Section 4: **Dying ReLU Problem**

Question 1 [G]

Dying ReLU Problem - majority of the activations are 0 (meaning the underlying pre-activations are mostly negative), resulting in the network dying midway.



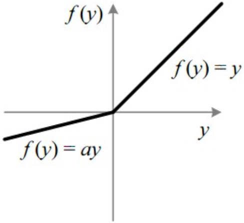


Figure 6: The Rectified Linear Unit (`ReLU`) (left) vs The Leaky Rectified Linear Unit (`Leaky ReLU`) with a as the slope when the values are negative. (right)

- How does `Leaky ReLU` fix this? What happens if we set $a = 1$ in the Leaky ReLU?

Answer

$$\mathrm{ReLU}(x) = \max(0, x), \quad \frac{\partial \mathrm{ReLU}(x)}{\partial x} = \begin{cases} 0, \text{if } x < 0 \\ 1, \text{if } x > 0 \end{cases}$$

- ReLU being stuck at 0 because the gradient is 0.
- Leaky ReLU get around this by creating small positive gradient a
- When $a = 1$, the activatation function becomes a linear function (NN loses power)[1].

[1] Last week tutorial

Bonus Qn

Investigate for exploding gradient as per the question about vanishing gradient, use the code given for tutorial as a starting point.

Tasks

1. Implement a neural network that exhibits exploding gradient.
2. Plot the magnitudes for all layers like done in vanishing gradient.
3. Analyse ways to mitigate the issue.

Attendance Taking (Makeup)

Figure 7: Attendance: https://forms.gle/FDuQWNu52zwWfGRv9

References I