# Due Date: February 16th, 2019

### Instructions

- For all questions, show your work!
- Use a document preparation system such as LaTeX.
- Submit your answers electronically via the course studium page, and via Gradescope.

Question 1. Using the following definition of the derivative and the definition of the Heaviside step function :

$$\frac{d}{dx}f(x) = \lim_{\epsilon \to 0} \frac{f(x+\epsilon) - f(x)}{\epsilon} \qquad H(x) = \begin{cases} 1 & \text{if } x > 0\\ \frac{1}{2} & \text{if } x = 0\\ 0 & \text{if } x < 0 \end{cases}$$

- 1. Show that the derivative of the rectified linear unit  $g(x) = \max\{0, x\}$ , wherever it exists, is equal to the Heaviside step function.
- 2. Give two alternative definitions of g(x) using H(x).
- 3. Show that H(x) can be well approximated by the sigmoid function  $\sigma(x) = \frac{1}{1 + e^{-kx}}$  asymptotically (i.e for large k), where k is a parameter.
- \*4. Although the Heaviside step function is not differentiable, we can define its **distributional derivative**. For a function F, consider the functional  $F[\phi] = \int_{\mathbb{R}} F(x)\phi(x)dx$ , where  $\phi$  is a smooth function (infinitely differentiable) with compact support  $(\phi(x) = 0$  whenever  $|x| \ge A$ , for some A > 0).

Show that whenever F is differentiable,  $F'[\phi] = -\int_{\mathbb{R}} F(x)\phi'(x)dx$ . Using this formula as a definition in the case of non-differentiable functions, show that  $H'[\phi] = \phi(0)$ . ( $\delta[\phi] \doteq \phi(0)$  is known as the Dirac delta function.)

#### Answer 1.

1. (a) if x > 0, then  $x + \epsilon > 0$  ( $\epsilon \to 0$ ), such that :

$$\frac{d}{dx}g(x) = \lim_{\epsilon \to 0} \frac{g(x+\epsilon) - g(x)}{\epsilon}$$

$$= \lim_{\epsilon \to 0} \frac{\max\{0, x+\epsilon\} - \max\{0, x\}}{\epsilon}$$

$$= \lim_{\epsilon \to 0} \frac{x+\epsilon - x}{\epsilon}$$

$$= \lim_{\epsilon \to 0} \frac{\epsilon}{\epsilon}$$

$$= \lim_{\epsilon \to 0} 1$$

$$= 1$$

$$H(x) = 1$$

(b) if x < 0, then  $x + \epsilon < 0 (\epsilon \to 0)$ , such that :

$$\frac{d}{dx}g(x) = \lim_{\epsilon \to 0} \frac{g(x+\epsilon) - g(x)}{\epsilon}$$

$$= \lim_{\epsilon \to 0} \frac{\max\{0, x+\epsilon\} - \max\{0, x\}}{\epsilon}$$

$$= \lim_{\epsilon \to 0} \frac{0 - 0}{\epsilon}$$

$$= \lim_{\epsilon \to 0} \frac{0}{\epsilon}$$

$$= 0$$

$$H(x) = 0$$

(c) if x = 0, then:

$$\lim_{\epsilon \to 0^+} \frac{g(x+\epsilon) - g(x)}{\epsilon} = \lim_{\epsilon \to 0^+} \frac{\max\{0, x+\epsilon\} - \max\{0, x\}}{\epsilon} = \lim_{\epsilon \to 0^+} \frac{\epsilon - 0}{\epsilon} = 1$$

$$\lim_{\epsilon \to 0^-} \frac{g(x+\epsilon) - g(x)}{\epsilon} = \lim_{\epsilon \to 0^-} \frac{\max\{0, x+\epsilon\} - \max\{0, x\}}{\epsilon} = \lim_{\epsilon \to 0^+} \frac{0 - 0}{\epsilon} = 0$$

$$\lim_{\epsilon \to 0^+} \frac{g(x+\epsilon) - g(x)}{\epsilon} \neq \lim_{\epsilon \to 0^-} \frac{g(x+\epsilon) - g(x)}{\epsilon} \Rightarrow \lim_{\epsilon \to 0} \frac{g(x+\epsilon) - g(x)}{\epsilon} \text{ does not exist.}$$

Therefore, wherever the derivative of  $g(x) = \max\{0, x\}$  exists, g(x) = H(x).

2.

$$g(x) = \max\{0, x\} = xH(x)$$

or

$$g(x) = \max\{0, x\} = \int_{-\infty}^{x} H(x)dx$$

3.

$$\lim_{k \to \infty} \frac{1}{1 + e^{-kx}} = \lim_{k \to \infty} \frac{1}{1 + \frac{1}{e^{kx}}}$$

$$= \lim_{k \to \infty} \frac{e^{kx}}{1 + e^{kx}}$$

$$= \lim_{k \to \infty} \left(1 - \frac{1}{1 + e^{kx}}\right)$$

$$= 1 - \lim_{k \to \infty} \frac{1}{1 + e^{kx}}$$

$$= \begin{cases} 1 & \text{if } x > 0 \\ \frac{1}{2} & \text{if } x = 0 \\ 0 & \text{if } x < 0 \end{cases}$$

$$= H(x)$$

\*4. Given  $F[\phi] = \int_{\mathbb{R}} F(x)\phi(x)dx$ , where  $\phi$  is infinitely differentiable, and  $\phi(x) = 0$  whenever  $|x| \ge A$  for some A > 0. If F is differentiable :

$$\int_{\mathbb{R}} (F(x)\phi(x))'dx = F(x)\phi(x)|_{-\infty}^{+\infty}$$

$$= F(+\infty)\phi(+\infty) - F(-\infty)\phi(-\infty)$$

$$= 0 - 0$$

$$= 0$$

Meanwhile,

$$\int_{\mathbb{R}} (F(x)\phi(x))'dx = \int_{\mathbb{R}} (F'(x)\phi(x) + F(x)\phi'(x))dx$$
$$= \int_{\mathbb{R}} F'(x)\phi(x)dx + \int_{\mathbb{R}} F(x)\phi'(x)dx$$

Therefore,

$$\int_{\mathbb{R}} F'(x)\phi(x)dx = -\int_{\mathbb{R}} F(x)\phi'(x)dx$$

By the definition of  $F[\phi]$ , we have,

$$F'[\phi] = \int_{\mathbb{R}} F'(x)\phi(x)dx = -\int_{\mathbb{R}} F(x)\phi'(x)dx$$

Let  $\epsilon > 0$ ,

$$H'[\phi] = -\int_{\mathbb{R}} H(x)\phi'(x)dx$$

$$= -\lim_{\epsilon \to 0} \left( \int_{-\infty}^{-\epsilon} H(x)\phi'(x)dx + \int_{-\epsilon}^{\epsilon} H(x)\phi'(x)dx + \int_{\epsilon}^{+\infty} H(x)\phi'(x)dx \right)$$

$$= -\left( \lim_{\epsilon \to 0} \int_{-\infty}^{-\epsilon} H(x)d\phi(x) + \lim_{\epsilon \to 0} \int_{-\epsilon}^{\epsilon} H(x)d\phi(x) + \lim_{\epsilon \to 0} \int_{\epsilon}^{+\infty} H(x)d\phi(x) \right)$$

$$= -\left( \lim_{\epsilon \to 0} \int_{-\infty}^{-\epsilon} 0d\phi(x) + \frac{1}{2}\lim_{\epsilon \to 0} (\phi(\epsilon) - \phi(-\epsilon)) + \lim_{\epsilon \to 0} \int_{\epsilon}^{+\infty} 1d\phi(x) \right)$$

$$= -\left( 0 + \frac{1}{2}(\phi(0) - \phi(0)) + (\phi(\infty) - \phi(0)) \right)$$

$$= \phi(0)$$

Question 2. Let x be an n-dimentional vector. Recall the softmax function :  $S: \mathbf{x} \in \mathbb{R}^n \mapsto S(\mathbf{x}) \in \mathbb{R}^n$  such that  $S(\mathbf{x})_i = \frac{e^{\mathbf{x}_i}}{\sum_j e^{\mathbf{x}_j}}$ ; the diagonal function :  $\operatorname{diag}(\mathbf{x})_{ij} = \mathbf{x}_i$  if i = j and  $\operatorname{diag}(\mathbf{x})_{ij} = 0$  if  $i \neq j$ ; and the Kronecker delta function :  $\delta_{ij} = 1$  if i = j and  $\delta_{ij} = 0$  if  $i \neq j$ .

- 1. Show that the derivative of the softmax function is  $\frac{dS(\boldsymbol{x})_i}{d\boldsymbol{x}_j} = S(\boldsymbol{x})_i (\delta_{ij} S(\boldsymbol{x})_j)$ .
- 2. Express the Jacobian matrix  $\frac{\partial S(x)}{\partial x}$  using matrix-vector notation. Use diag(·).

- 3. Compute the Jacobian of the sigmoid function  $\sigma(\mathbf{x}) = 1/(1 + e^{-\mathbf{x}})$ .
- 4. Let  $\boldsymbol{y}$  and  $\boldsymbol{x}$  be n-dimensional vectors related by  $\boldsymbol{y} = f(\boldsymbol{x})$ , L be an unspecified differentiable loss function. According to the chain rule of calculus,  $\nabla_{\boldsymbol{x}} L = (\frac{\partial \boldsymbol{y}}{\partial \boldsymbol{x}})^{\top} \nabla_{\boldsymbol{y}} L$ , which takes up  $\mathcal{O}(n^2)$  computational time in general. Show that if  $f(\boldsymbol{x}) = \sigma(\boldsymbol{x})$  or  $f(\boldsymbol{x}) = S(\boldsymbol{x})$ , the above matrix-vector multiplication can be simplified to a  $\mathcal{O}(n)$  operation.

#### Answer 2.

1.

$$\frac{dS(\boldsymbol{x})_{i}}{d\boldsymbol{x}_{j}} = \frac{d\frac{e^{\boldsymbol{x}_{i}}}{\sum_{j}e^{\boldsymbol{x}_{j}}}}{d\boldsymbol{x}_{j}}$$

$$= \begin{cases}
\frac{e^{\boldsymbol{x}_{i}} \sum_{j}e^{\boldsymbol{x}_{j}}-e^{\boldsymbol{x}_{i}}e^{\boldsymbol{x}_{i}}}{(\sum_{j}e^{\boldsymbol{x}_{j}})^{2}} & \text{if } i = j, \left( \text{ recall } : \frac{d\frac{f}{g}}{x} = \frac{df}{x}g - \frac{dg}{x}f}{g^{2}} \right) \\
e^{\boldsymbol{x}_{i}} \frac{-e^{\boldsymbol{x}_{j}}}{(\sum_{j}e^{\boldsymbol{x}_{j}})^{2}} & \text{if } i \neq j, \left( \text{ recall } : \frac{d\frac{c}{f}}{x} = -c\frac{df}{x} \right)
\end{cases}$$

$$= \begin{cases}
S(\boldsymbol{x})_{i} - S(\boldsymbol{x})_{i}^{2} & \text{if } i = j \\
-S(\boldsymbol{x})_{i}S(\boldsymbol{x})_{j} & \text{if } i \neq j
\end{cases}$$

$$= \begin{cases}
S(\boldsymbol{x})_{i}(1 - S(\boldsymbol{x})_{j}) & \text{if } i = j \\
S(\boldsymbol{x})_{i}(0 - S(\boldsymbol{x})_{j}) & \text{if } i \neq j
\end{cases}$$

$$= S(\boldsymbol{x})_{i}(\delta_{ij} - S(\boldsymbol{x})_{j})$$

2. For this question, Jacobian matrix  $\frac{\partial S(x)}{\partial x}$  is a  $n \times n$  matrix, where the *i*th row, *j*th column element :

$$\frac{\partial S(\boldsymbol{x})}{\partial \boldsymbol{x}}_{i,j} = \frac{dS(\boldsymbol{x})_i}{d\boldsymbol{x}_j}$$

$$= S(\boldsymbol{x})_i (\delta_{ij} - S(\boldsymbol{x})_j)$$

$$= \delta_{ij} S(\boldsymbol{x})_i - S(\boldsymbol{x})_i S(\boldsymbol{x})_j$$

$$= \operatorname{diag}(S(\boldsymbol{x}))_{ij} - S(\boldsymbol{x})_i S(\boldsymbol{x})_j$$

By default,  $S(\mathbf{x})$  is a column vector; therefore,

$$\frac{\partial S(\boldsymbol{x})}{\partial \boldsymbol{x}} = \operatorname{diag}(S(\boldsymbol{x})) - S(\boldsymbol{x})S(\boldsymbol{x})^{\top}$$

3.

$$\frac{\partial \sigma(\boldsymbol{x})}{\partial \boldsymbol{x}}_{i,j} = \frac{d\sigma(\boldsymbol{x})_i}{d\boldsymbol{x}_j} 
= \frac{d\sigma(\boldsymbol{x}_i)}{d\boldsymbol{x}_j} 
= \begin{cases} \sigma(\boldsymbol{x}_i)(1 - \sigma(\boldsymbol{x}_i)), & \text{if } i = j, \text{ recall } : \sigma'(x) = \sigma(x)(1 - \sigma(x)) \\ 0, & \text{if } i \neq j \end{cases} 
= \begin{cases} \sigma(\boldsymbol{x})_i(1 - \sigma(\boldsymbol{x})_i), & \text{if } i = j \\ 0, & \text{if } i \neq j \end{cases}$$

Therefore,

$$\frac{\partial \sigma(\boldsymbol{x})}{\partial \boldsymbol{x}} = \operatorname{diag}(\sigma(\boldsymbol{x})(1 - \sigma(\boldsymbol{x})))$$

Justification of  $\sigma'(x) = \sigma(x)(1 - \sigma(x))$ :

$$\sigma'(x) = \frac{d\sigma(x)}{dx}$$

$$= \frac{d\frac{1}{1+e^{-x}}}{dx}$$

$$= -(\frac{1}{1+e^{-x}})^2 \frac{d(1+e^{-x})}{dx}$$

$$= \frac{1}{(1+e^{-x})^2} e^{-x}$$

$$= \frac{1}{1+e^{-x}} \frac{e^{-x}}{1+e^{-x}}$$

$$= \frac{1}{1+e^{-x}} \frac{1+e^{-x}-1}{1+e^{-x}}$$

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

$$= \sigma(x)(1-\sigma(x))$$

- 4. Denote:  $\odot$  represents element-wise matrix(or column vector) multiplication, and  $\langle a, b \rangle$  represents the inner-product of two column vectors(or matrices).
  - 1). For the case  $\mathbf{y} = f(\mathbf{x}) = \sigma(\mathbf{x})$ ,

$$\nabla_{\boldsymbol{x}} L = (\frac{\partial \boldsymbol{y}}{\partial \boldsymbol{x}})^{\top} \nabla_{\boldsymbol{y}} L = (\frac{\partial \sigma(\boldsymbol{x})}{\partial \boldsymbol{x}})^{\top} \nabla_{\boldsymbol{y}} L$$
$$= \left( \operatorname{diag} \left( \sigma(\boldsymbol{x}) (1 - \sigma(\boldsymbol{x})) \right) \right)^{\top} \nabla_{\boldsymbol{y}} L$$
$$= \operatorname{diag} \left( \sigma(\boldsymbol{x}) (1 - \sigma(\boldsymbol{x})) \right) \nabla_{\boldsymbol{y}} L$$
$$= \sigma(\boldsymbol{x}) \odot (1 - \sigma(\boldsymbol{x})) \odot \nabla_{\boldsymbol{y}} L$$

which means, the computation of  $\nabla_x L$  can be decomposed to one vector minus calculation, and three element-wise vector multiplications. All these calculations can be done in  $\mathcal{O}(n)$  time complexity; therefore, the whole time complexity is  $\mathcal{O}(4n+C) = \mathcal{O}(n)$ .

2). For the case  $\mathbf{y} = f(\mathbf{x}) = S(\mathbf{x})$ ,

$$\nabla_{\boldsymbol{x}} L = (\frac{\partial \boldsymbol{y}}{\partial \boldsymbol{x}})^{\top} \nabla_{\boldsymbol{y}} L = (\frac{\partial S(\boldsymbol{x})}{\partial \boldsymbol{x}})^{\top} \nabla_{\boldsymbol{y}} L$$

$$= (\operatorname{diag}(S(\boldsymbol{x})) - S(\boldsymbol{x}) S(\boldsymbol{x})^{\top})^{\top} \nabla_{\boldsymbol{y}} L$$

$$= (\operatorname{diag}(S(\boldsymbol{x})) - S(\boldsymbol{x}) S(\boldsymbol{x})^{\top}) \nabla_{\boldsymbol{y}} L$$

$$= \operatorname{diag}(S(\boldsymbol{x})) \nabla_{\boldsymbol{y}} L - S(\boldsymbol{x}) S(\boldsymbol{x})^{\top} \nabla_{\boldsymbol{y}} L$$

$$= S(\boldsymbol{x}) \odot \nabla_{\boldsymbol{y}} L - S(\boldsymbol{x}) \langle (S(\boldsymbol{x})^{\top}, \nabla_{\boldsymbol{y}} L) \rangle$$

which means, the computation of  $\nabla_x L$  can be decomposed to one inner-product, one matrix and scalar multiplication, one element-wise vector multiplication, and a vector minor operation.

All of this calculations can be done with the time complexity of  $\mathcal{O}(n)$ , Therefore, the whole calculation has the the complexity of  $\mathcal{O}(4n+C) = \mathcal{O}(n)$ .

Question 3. Recall the definition of the softmax function :  $S(\mathbf{x})_i = e^{\mathbf{x}_i} / \sum_j e^{\mathbf{x}_j}$ .

- 1. Show that softmax is translation-invariant, that is: S(x+c) = S(x), where c is a scalar constant.
- 2. Show that softmax is not invariant under scalar multiplication. Let  $S_c(\mathbf{x}) = S(c\mathbf{x})$  where  $c \geq 0$ . What are the effects of taking c to be 0 and arbitrarily large?
- 3. Let  $\boldsymbol{x}$  be a 2-dimentional vector. One can represent a 2-class categorical probability using softmax  $S(\boldsymbol{x})$ . Show that  $S(\boldsymbol{x})$  can be reparameterized using sigmoid function, i.e.  $S(\boldsymbol{x}) = [\sigma(z), 1 \sigma(z)]^{\top}$  where z is a scalar function of  $\boldsymbol{x}$ .
- 4. Let  $\boldsymbol{x}$  be a K-dimentional vector  $(K \geq 2)$ . Show that  $S(\boldsymbol{x})$  can be represented using K-1 parameters, i.e.  $S(\boldsymbol{x}) = S([0, y_1, y_2, ..., y_{K-1}]^{\top})$  where  $y_i$  is a scalar function of  $\boldsymbol{x}$  for  $i \in \{1, ..., K-1\}$ .

## Answer 3.

1. Recall :  $(x + c)_i = x_i + c$ .

$$S(\boldsymbol{x} + c)_{i} = \frac{e^{(\boldsymbol{x}_{i} + c)}}{\sum_{j} e^{(\boldsymbol{x}_{j} + c)}}$$

$$= \frac{e^{\boldsymbol{x}_{i}} e^{c}}{\sum_{j} (e^{\boldsymbol{x}_{j}} e^{c})}$$

$$= \frac{e^{\boldsymbol{x}_{i}} e^{c}}{e^{c} \sum_{j} e^{\boldsymbol{x}_{j}}}$$

$$= \frac{e^{\boldsymbol{x}_{i}}}{\sum_{j} e^{\boldsymbol{x}_{j}}}$$

$$= S(\boldsymbol{x})_{i}$$

which means that each element in vectors  $S(\boldsymbol{x}+c)$  is equal to the element in  $S(\boldsymbol{x})$  with the same index. That is to say, the two vectors are same :

$$S(\boldsymbol{x}+c) = S(\boldsymbol{x})$$

2. Recall :  $(c\mathbf{x})_i = c\mathbf{x}_i$ .

To prove  $S(\mathbf{x})$  is not invariant under scalar multiplication, we only need to provide an example where  $S(c\mathbf{x}) \neq S(\mathbf{x})$ , with  $c \geq 0$ .

Consider a 2- dimensional vector  $\mathbf{x} = [0, \ln 3]^T$ , and c = 2,  $S(c\mathbf{x}) = S([0, 2 \ln 3]^T) = [0.1, 0.9]^T$ , whereas  $S(\mathbf{x}) = S([0, \ln 3]^T) = [0.25, 0.75]^T$ . Therefore:

$$S(c\boldsymbol{x}) \neq S(\boldsymbol{x})$$

That  $S(\mathbf{x})$  is not invariant under scalar multiplication with  $c \geq 0$  doesn't means  $S(c\mathbf{x})$  has no chance to be equal to  $S(\mathbf{x})$ . If elements in a *n*-dimensional vector  $\mathbf{x}$  are all equal, then:  $S(c\mathbf{x}) = S(\mathbf{x})$ , and

$$S(c\boldsymbol{x})_i = S(\boldsymbol{x})_i = \frac{1}{n}$$

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When 
$$c = 0$$
,  $e^{cx_i} = e^{x_i} = e^0 = 1$ ,

$$S(c\boldsymbol{x})_i = \frac{1}{\sum_{1}^{n} 1} = \frac{1}{n}$$

meaning that all element of  $S(c\mathbf{x})$  are equal. If the element value of  $S(c\mathbf{x})$  reflects the probability of several events, then it means all events have the same probability.

Now let's consider the situation when c is arbitrarily large and not all elements of  $\boldsymbol{x}$  are equal. Suppose the n-dimensional vector  $\boldsymbol{x}$  has  $k(0 \le k \le n-1)$  largest elements with the maximal values are all  $x^*$  and their indices forming a collection  $\mathcal{K}$ :

$$x^* = \boldsymbol{x}_{k,k\in\mathcal{K}} = max\{\boldsymbol{x}_i, \ 0 \le i \le n-1\}$$

then,

$$\lim_{c \to \infty} S(c\boldsymbol{x})_i = \lim_{c \to +\infty} \frac{e^{c\boldsymbol{x}_i}}{\sum_j e^{c\boldsymbol{x}_j}}$$

$$= \lim_{c \to +\infty} \frac{e^{c\boldsymbol{x}_i}/e^{c\boldsymbol{x}^*}}{\left(\sum_j e^{c\boldsymbol{x}_j}\right)/e^{c\boldsymbol{x}^*}}$$

$$= \lim_{c \to +\infty} \frac{e^{c(\boldsymbol{x}_i - \boldsymbol{x}^*)}}{\sum_j e^{c(\boldsymbol{x}_j - \boldsymbol{x}^*)}}$$

$$= \begin{cases} \frac{1}{k} & \text{if } i \in \mathcal{K} \\ 0 & \text{if } i \notin \mathcal{K} \end{cases}$$

To conclude, if c = 0, all elements of  $S(c\mathbf{x})_i$  are equal; if c is arbitrarily large, only the largest element(s) has(or equally share) the value 1, other elements have the value 0.

3. If x is a 2-dimensional vector, let scalar:

$$S(\mathbf{x})_0 = \frac{e^{\mathbf{x}_0}}{e^{\mathbf{x}_0} + e^{\mathbf{x}_1}} = \frac{1}{1 + e^{-(\mathbf{x}_0 - \mathbf{x}_1)}} = \sigma(\mathbf{x}_0 - \mathbf{x}_1) = \sigma(z)$$

$$S(\mathbf{x})_1 = \frac{e^{\mathbf{x}_1}}{e^{\mathbf{x}_0} + e^{\mathbf{x}_1}} = 1 - \frac{e^{\mathbf{x}_0}}{e^{\mathbf{x}_0} + e^{\mathbf{x}_1}} = 1 - S(\mathbf{x})_0 = 1 - \sigma(z)$$

 $z = f(\boldsymbol{x}) = \boldsymbol{x}_0 - \boldsymbol{x}_1$ 

Therefore,

$$S(\boldsymbol{x}) = [S(\boldsymbol{x})_0, S(\boldsymbol{x})_1]^T = [\sigma(z), 1 - \sigma(z)]^T$$

4. If x is a K-dimensional vector, let constant  $c = -x_0$ , and :

$$y_i = x_i - x_0$$
, where  $1 \le i \le K - 1$ 

As function  $S(\mathbf{x})$  is translation-invariant, that is  $S(\mathbf{x} + c) = S(\mathbf{x})$ , we have :

$$S(\mathbf{x}) = S(\mathbf{x} + c)$$

$$= S(\mathbf{x} - \mathbf{x}_0)$$

$$= S([\mathbf{x}_0 - \mathbf{x}_0, \mathbf{x}_1 - \mathbf{x}_0, \cdots, \mathbf{x}_{K-1} - \mathbf{x}_0)]^T)$$

$$= S([0, y_1, y_2, \cdots, y_{K-1})]^T)$$

**Question 4.** Consider a 2-layer neural network  $y: \mathbb{R}^D \to \mathbb{R}^K$  of the form :

$$y(x,\Theta,\sigma)_k = \sum_{j=1}^{M} \omega_{kj}^{(2)} \sigma \left( \sum_{i=1}^{D} \omega_{ji}^{(1)} x_i + \omega_{j0}^{(1)} \right) + \omega_{k0}^{(2)}$$

for  $1 \leq k \leq K$ , with parameters  $\Theta = (\omega^{(1)}, \omega^{(2)})$  and logistic sigmoid activation function  $\sigma$ . Show that there exists an equivalent network of the same form, with parameters  $\Theta' = (\tilde{\omega}^{(1)}, \tilde{\omega}^{(2)})$  and tanh activation function, such that  $y(x, \Theta', \tanh) = y(x, \Theta, \sigma)$  for all  $x \in \mathbb{R}^D$ , and express  $\Theta'$  as a function of  $\Theta$ .

**Answer 4.** First, we show that  $\sigma(x)$  is a function of  $\tanh(x)$ 

$$\sigma(\mathbf{x}) = \frac{1}{1 + e^{-\mathbf{x}}}$$

$$= \frac{1}{1 + e^{-\frac{1}{2}\mathbf{x} - \frac{1}{2}\mathbf{x}}}$$

$$= \frac{1}{1 + \frac{e^{-\frac{1}{2}\mathbf{x}}}{e^{\frac{1}{2}\mathbf{x}}}}$$

$$= \frac{e^{\frac{1}{2}\mathbf{x}}}{e^{\frac{1}{2}\mathbf{x}}}$$

$$= \frac{e^{\frac{1}{2}\mathbf{x}}}{e^{\frac{1}{2}\mathbf{x}}}$$

$$= \frac{1}{2} \left( \frac{2 e^{\frac{1}{2}\mathbf{x}}}{e^{\frac{1}{2}\mathbf{x}} + e^{-\frac{1}{2}\mathbf{x}}} \right)$$

$$= \frac{1}{2} \left( \frac{e^{\frac{1}{2}\mathbf{x}} - e^{-\frac{1}{2}\mathbf{x}}}{e^{\frac{1}{2}\mathbf{x}} + e^{-\frac{1}{2}\mathbf{x}}} + 1 \right)$$

$$= \frac{1}{2} \left( \tanh(\frac{1}{2}\mathbf{x}) + 1 \right)$$

Then, for the 2-layer neural network  $y: \mathbb{R}^D \to \mathbb{R}^K$ :

$$y(x, \Theta, \sigma)_{k} = \sum_{j=1}^{M} \omega_{kj}^{(2)} \sigma \left( \sum_{i=1}^{D} \omega_{ji}^{(1)} x_{i} + \omega_{j0}^{(1)} \right) + \omega_{k0}^{(2)}$$

$$= \sum_{j=1}^{M} \omega_{kj}^{(2)} \frac{1}{2} \left( \tanh \left( \frac{1}{2} \left( \sum_{i=1}^{D} \omega_{ji}^{(1)} x_{i} + \omega_{j0}^{(1)} \right) \right) + 1 \right) + \omega_{k0}^{(2)}$$

$$= \sum_{j=1}^{M} \frac{1}{2} \omega_{kj}^{(2)} \tanh \left( \sum_{i=1}^{D} \frac{1}{2} \omega_{ji}^{(1)} x_{i} + \frac{1}{2} \omega_{j0}^{(1)} \right) + \left( \sum_{j=1}^{M} \frac{1}{2} \omega_{kj}^{(2)} + \omega_{k0}^{(2)} \right)$$

As  $\Theta' = (\tilde{\omega}^{(1)}, \tilde{\omega}^{(2)})$  and  $\Theta = (\omega^{(1)}, \omega^{(2)})$ , let :

$$\tilde{\omega}^{(1)} = \frac{1}{2}\omega^{(1)}$$

and for  $1 \le k \le K$ ,

$$\tilde{\omega}_{kj}^{(2)} = \begin{cases} \frac{1}{2} \omega_{kj}^{(2)} & \text{if } 1 \le j \le M \\ \omega_{kj}^{(2)} + \sum_{i=1}^{M} \frac{1}{2} \omega_{ki}^{(2)} & \text{if } j = 0 \end{cases}$$

$$y(x, \Theta, \sigma)_k = \sum_{j=1}^{M} \tilde{\omega}_{kj}^{(2)} \tanh\left(\sum_{i=1}^{D} \tilde{\omega}_{ji}^{(1)} x_i + \tilde{\omega}_{j0}^{(1)}\right) + \tilde{\omega}_{k0}^{(2)}$$
$$= y(x, \Theta', \tanh)_k$$

Question 5. Given  $N \in \mathbb{Z}^+$ , we want to show that for any  $f : \mathbb{R}^n \to \mathbb{R}^m$  and any sample set  $\mathcal{S} \subset \mathbb{R}^n$  of size N, there is a set of parameters for a two-layer network such that the output  $y(\boldsymbol{x})$  matches  $f(\boldsymbol{x})$  for all  $\boldsymbol{x} \in \mathcal{S}$ . That is, we want to interpolate f with g on any finite set of samples  $\mathcal{S}$ .

- 1. Write the generic form of the function  $y: \mathbb{R}^n \to \mathbb{R}^m$  defined by a 2-layer network with N-1 hidden units, with linear output and activation function  $\phi$ , in terms of its weights and biases  $(\boldsymbol{W}^{(1)}, \boldsymbol{b}^{(1)})$  and  $(\boldsymbol{W}^{(2)}, \boldsymbol{b}^{(2)})$ .
- 2. In what follows, we will restrict  $\mathbf{W}^{(1)}$  to be  $\mathbf{W}^{(1)} = [\mathbf{w}, \cdots, \mathbf{w}]^{\top}$  for some  $\mathbf{w} \in \mathbb{R}^n$  (so the rows of  $\mathbf{W}^{(1)}$  are all the same). Show that the interpolation problem on the sample set  $\mathcal{S} = \{\mathbf{x}^{(1)}, \cdots \mathbf{x}^{(N)}\} \subset \mathbb{R}^n$  can be reduced to solving a matrix equation :  $\mathbf{M}\tilde{\mathbf{W}}^{(2)} = \mathbf{F}$ , where  $\tilde{\mathbf{W}}^{(2)}$  and  $\mathbf{F}$  are both  $N \times m$ , given by

$$\tilde{m{W}}^{(2)} = [m{W}^{(2)}, m{b}^{(2)}]^{ op}$$
  $m{F} = [f(m{x}^{(1)}), \cdots, f(m{x}^{(N)})]^{ op}$ 

Express the  $N \times N$  matrix  $\boldsymbol{M}$  in terms of  $\boldsymbol{w}$ ,  $\boldsymbol{b}^{(1)}$ ,  $\phi$  and  $\boldsymbol{x}^{(i)}$ .

- \*3. Proof with Relu activation. Assume  $\boldsymbol{x}^{(i)}$  are all distinct. Choose  $\boldsymbol{w}$  such that  $\boldsymbol{w}^{\top}\boldsymbol{x}^{(i)}$  are also all distinct (Try to prove the existence of such a  $\boldsymbol{w}$ , although this is not required for the assignment See Assignment 0). Set  $\boldsymbol{b}_{j}^{(1)} = -\boldsymbol{w}^{\top}\boldsymbol{x}^{(j)} + \epsilon$ , where  $\epsilon > 0$ . Find a value of  $\epsilon$  such that  $\boldsymbol{M}$  is triangular with non-zero diagonal elements. Conclude. (Hint: assume an ordering of  $\boldsymbol{w}^{\top}\boldsymbol{x}^{(i)}$ .)
- \*4. Proof with sigmoid-like activations. Assume  $\phi$  is continuous, bounded,  $\phi(-\infty) = 0$  and  $\phi(0) > 0$ . Decompose  $\boldsymbol{w}$  as  $\boldsymbol{w} = \lambda \boldsymbol{u}$ . Set  $\boldsymbol{b}_j^{(1)} = -\lambda \boldsymbol{u}^{\top} \boldsymbol{x}^{(j)}$ . Fixing  $\boldsymbol{u}$ , show that  $\lim_{\lambda \to +\infty} \boldsymbol{M}$  is triangular with non-zero diagonal elements. Conclude. (Note that doing so preserves the distinctness of  $\boldsymbol{w}^{\top} \boldsymbol{x}^{(i)}$ .)

#### Answer 5.

1. for  $0 \le k \le m - 1$ ,

$$y(\boldsymbol{x})_k = \sum_{j=0}^{N-1} \boldsymbol{W}_{kj}^{(2)} \ \phi\left(\sum_{i=0}^{n-1} \boldsymbol{W}_{ji}^{(1)} \boldsymbol{x}_i + \boldsymbol{b}_j^{(1)}\right) + \boldsymbol{b}_k^2$$

or the matrix form:

$$y(x) = W^{(2)}\phi(W^{(1)}x + b^{(1)}) + b^{(2)}$$

2. Consider the interpolation problem on the sample set  $S = \{x^{(1)}, \dots x^{(N)}\} \subset \mathbb{R}^n$  with N samples, let:

$$m{X} = [m{x}^{(1)}, m{x}^{(2)}, \cdots, m{x}^{(N)}]^{ op}$$

and

$$Y = [y(x^{(1)}), y(x^{(2)}), \cdots, y(x^{(N)})]^{\top}$$

That  $y(\boldsymbol{x})$  matches  $f(\boldsymbol{x})$  for all  $\boldsymbol{x} \in \mathcal{S}$  means:

$$Y = [f(x^{(1)}), f(x^{(2)}), \cdots, f(x^{(N)})]^{\top} = F$$

$$\begin{aligned} \boldsymbol{F} &= \phi \left( \boldsymbol{X} (\boldsymbol{W}^{(1)})^\top + [\boldsymbol{b}^{(1)}, \cdots, \boldsymbol{b}^{(1)}]^\top \right) (\boldsymbol{W}^{(2)})^\top + [\boldsymbol{b}^{(2)}, \cdots, \boldsymbol{b}^{(2)}]^\top \\ &= [\phi([\boldsymbol{X}, 1] \cdot [\boldsymbol{W}^{(1)}, \boldsymbol{b}^{(1)}]^\top), 1] \cdot [\boldsymbol{W}^{(2)}, \boldsymbol{b}^{(2)}]^\top \end{aligned}$$

As  $\tilde{\boldsymbol{W}}^{(2)} = [\boldsymbol{W}^{(2)}, \boldsymbol{b}^{(2)}]^{\top}$  and  $\boldsymbol{W}^{(1)} = [\boldsymbol{w}, \cdots, \boldsymbol{w}]^{\top}, \ \boldsymbol{w} \in \mathbb{R}^{n}$ , Let:

$$\boldsymbol{M} = \left[\phi([\boldsymbol{X},1] \cdot [\boldsymbol{W}^{(1)}, \boldsymbol{b}^{(1)}]^{\top}), 1\right]$$

Which means for  $0 \le i, j \le N-1$ :

$$\boldsymbol{M}_{ij} = \begin{cases} \phi(\boldsymbol{w}^{\top} \boldsymbol{x}^{(i)} + \boldsymbol{b}_{j}^{(1)}) & \text{for } 0 \leq j < N - 1\\ 1 & \text{for } j = N - 1 \end{cases}$$

Obviously, M is  $N \times N$ . So we have :

$$oldsymbol{F} = oldsymbol{M} ilde{oldsymbol{W}}^{(2)}$$

\*3. As  $\boldsymbol{x}^{(i)}$  are distinct, and  $\boldsymbol{w}^{\top}\boldsymbol{x}^{(i)} \in \mathbb{R}$  are also distinct, we can permutate  $\boldsymbol{x}^{(i)}$  by sorting  $\boldsymbol{w}^{\top}\boldsymbol{x}^{(i)}$ , such that for all  $0 \leq j < i \leq N-1$ :

$$oldsymbol{w}^{ op} oldsymbol{x}^{(j)} > oldsymbol{w}^{ op} oldsymbol{x}^{(i)}$$

Let  $\boldsymbol{b}_{j}^{(1)} = -\boldsymbol{w}^{\top} \boldsymbol{x}^{(j)} + \epsilon$ , where  $\epsilon > 0$ , we have :

$$\boldsymbol{M}_{ij} = \begin{cases} \phi(\boldsymbol{w}^{\top} \boldsymbol{x}^{(i)} - \boldsymbol{w}^{\top} \boldsymbol{x}^{(j)} + \epsilon) & \text{for } 0 \leq j < N - 1\\ 1 & \text{for } j = N - 1 \end{cases}$$

As  $\phi$  is Relu activation function,

$$\phi(\boldsymbol{w}^{\top}\boldsymbol{x}^{(i)} - \boldsymbol{w}^{\top}\boldsymbol{x}^{(j)} + \epsilon) = 0$$

$$\iff \boldsymbol{w}^{\top}\boldsymbol{x}^{(i)} - \boldsymbol{w}^{\top}\boldsymbol{x}^{(j)} + \epsilon \leq 0$$

$$\iff \epsilon \leq \boldsymbol{w}^{\top}\boldsymbol{x}^{(j)} - \boldsymbol{w}^{\top}\boldsymbol{x}^{(i)}$$

Let,

$$0 < \epsilon \le \min\{ \boldsymbol{w}^{\top} \boldsymbol{x}^{(j)} - \boldsymbol{w}^{\top} \boldsymbol{x}^{(i)} \mid 0 \le j < i \le N - 1 \}$$

for  $0 \le i$ ,  $j \le N - 1$ , we have :

$$\boldsymbol{M}_{ij} = \begin{cases} 0 & 0 \le j < i \le N-1 \\ \epsilon & 0 \le i = j < N-1 \\ \boldsymbol{w}^{\top} \boldsymbol{x}^{(i)} - \boldsymbol{w}^{\top} \boldsymbol{x}^{(j)} + \epsilon & 0 \le i < j < N-1 \\ 1 & j = N-1 \end{cases}$$

indicating M is a triangular matrix with non-zero diagonal elements.

This proves that, for any  $f: \mathbb{R}^n \to \mathbb{R}^m$  and any finite sample set  $\mathcal{S} \subset \mathbb{R}^n$  of size N, there always exists a set of parameters for a two-layer network with N-1 neurons in hidden layer(with  $\mathbf{W}^{(1)}$  specially chosen) and a ReLU activation function, such that the output  $y(\mathbf{x})$  matches  $f(\mathbf{x})$  for all  $\mathbf{x} \in \mathcal{S}$ .

\*4. Re-use the ordering of  $\boldsymbol{w}^{\top}\boldsymbol{x}^{(i)}$ , which for all  $0 \leq j < i \leq N-1$ :

$$\boldsymbol{w}^{\top}\boldsymbol{x}^{(j)} > \boldsymbol{w}^{\top}\boldsymbol{x}^{(i)}$$

Given,  $\boldsymbol{w} = \lambda \boldsymbol{u}, \boldsymbol{b}_{j}^{(1)} = -\lambda \boldsymbol{u}^{\top} \boldsymbol{x}^{(j)}, \phi(-\infty) = 0$  and  $\phi(0) > 0$ , for  $0 \le i, \ j \le N-1$ , we have :

$$\boldsymbol{M}_{ij} = \begin{cases} \phi \left( \lambda (\boldsymbol{u}^{\top} \boldsymbol{x}^{(i)} - \boldsymbol{u}^{\top} \boldsymbol{x}^{(j)}) \right) & \text{for } 0 \leq j < N - 1 \\ 1 & \text{for } j = N - 1 \end{cases}$$

Similarly,

$$\lim_{\lambda \to \infty} \mathbf{M} = \begin{cases} \phi(-\infty) = 0 & 0 \le j < i \le N - 1\\ \phi(0) > 0 & 0 \le i = j < N - 1\\ \phi(+\infty) > 0 & 0 \le i < j < N - 1\\ 1 & j = N - 1 \end{cases}$$

indicating it is a triangular matrix with non-zero diagonal elements.

This proves that, for any  $f: \mathbb{R}^n \to \mathbb{R}^m$  and any finite sample set  $\mathcal{S} \subset \mathbb{R}^n$  of size N, there always exists a set of parameters for a two-layer network with N-1 neurons in hidden layer and a sigmoid-like activation function, such that the output  $y(\boldsymbol{x})$  matches  $f(\boldsymbol{x})$  for all  $\boldsymbol{x} \in \mathcal{S}$ .

**Question 6.** Compute the *full*, *valid*, and *same* convolution (with kernel flipping) for the following 1D matrices: [1, 2, 3, 4] \* [1, 0, 2]

**Answer 6.** To compute the result of a convolution with **kernel flipping** for 1D matrices, we can use the following formula :

$$\boldsymbol{S}(i) = (\boldsymbol{K} * \boldsymbol{X})(i) = \sum_{n=0}^{k-1} \boldsymbol{X}(i+n) \boldsymbol{K}(k-1-n)$$

where the input X, in this question, is variant for different convolution patterns, the kernel K, in this question, is [1,0,2], and k, the size of kernel, is 3.

Let s, i, k, p, o represent the size of stride, input, kernel, zero-padding, and output size respectively, we have :

$$o = \lfloor \frac{i + 2p - k}{s} \rfloor + 1$$

For full, valid and same convolution in this question, i = 4, s = 1 and k = 3 hold.

1. for full convolution: p = k - 1 = 2, o = 6, X = [0, 0, 1, 2, 3, 4, 0, 0], and the convolution result

$$\mathbf{S} = [1, 2, 5, 8, 6, 8]$$

2. for valid convolution:  $p = 0, o = 2, \mathbf{X} = [1, 2, 3, 4]$ , and the convolution result

$$S = [5, 8]$$

3. for same convolution:  $p = 1, o = i = 4, \mathbf{X} = [0, 1, 2, 3, 4, 0]$ , and the convolution result

$$S = [2, 5, 8, 6]$$

Question 7. Consider a convolutional neural network. Assume the input is a colorful image of size  $256 \times 256$  in the RGB representation. The first layer convolves  $64.8 \times 8$  kernels with the input, using a stride of 2 and no padding. The second layer downsamples the output of the first layer with a  $5 \times 5$  non-overlapping max pooling. The third layer convolves  $128.4 \times 4$  kernels with a stride of 1 and a zero-padding of size 1 on each border.

- 1. What is the dimensionality (scalar) of the output of the last layer?
- 2. Not including the biases, how many parameters are needed for the last layer?

### Answer 7.

For question1, the dimensionality of the output of the last(third) layer is  $128 \times 24 \times 24 = 73728$ ; for question 2, 131072 parameters are need for the last layer.

In general, a CNN architecture follows the following rules:

- 1. dimensionality of input data are user-defined.
- 2. number of channels(#Channels) of a convolutional layer is free to define.
- 3. pooling downsampling operation has **no** parameters and doesn't change the number of channels.
- 4. the output size per channel of a convolutional layer o is determined by its input size per channel i, kernel size :k, number of zero-padding :p, and strides :s, of the convolutional operation :s

$$o = \lfloor \frac{i + 2p - k}{s} \rfloor + 1$$

5. not including the biases, number of parameters (#Parameters) for a convolutional layer is :

$$\#$$
Parameters = (kernel width) × (kernel height) ×  $\#$ Channels(input) ×  $\#$ Channels(output)

6. A squared kernel for a non-overlapping max polling operation means k = sBased on the above rules, we built the table describing the detail of the CNN architecture.

Table 1 – CNN architecture

Layer	Role	#Channels	Size per channel	#Parameters
Input	original data	3	(256, 256)	0
First	convolution(k=8,s=2,p=0)	64	(125,125)	$8 \times 8 \times 3 \times 64 = 12288$
Second	pooling&down sampling(s=5)	64	(25,25)	0
Third	convolution(k=4,s=1,p=1)	128	(24,24)	$4 \times 4 \times 64 \times 128 = 131072$

**Question 8.** Assume we are given data of size  $3 \times 64 \times 64$ . In what follows, provide the correct configuration of a convolutional neural network layer that satisfies the specified assumption. Answer with the window size of kernel (k), stride (s), padding (p), and dilation (d), with convention d = 1 for no dilation). Use square windows only (e.g. same k for both width and height).

- 1. The output shape of the first layer is (64, 32, 32).
  - (a) Assume k = 8 without dilation.
  - (b) Assume d = 7, and s = 2.
- 2. The output shape of the second layer is (64, 8, 8). Assume p = 0 and d = 1.
  - (a) Specify k and s for pooling with non-overlapping window.
  - (b) What is output shape if k = 8 and s = 4 instead?
- 3. The output shape of the last layer is (128, 4, 4).
  - (a) Assume we are not using padding or dilation.
  - (b) Assume d = 2, p = 2.
  - (c) Assume p = 1, d = 1.

**Answer 8.** Using square windows only, the following two formulas define the relationship of following hyper-parameters: input size(i), output size(o), kernel size(k), effective kernel size(k'), zeropaddings(p), strides(s), and dilations(d):

$$o = \lfloor \frac{i + 2p - k'}{s} \rfloor + 1$$

$$k' = k + (k-1)(d-1)$$

where  $i, o, s, k, k' \in \mathbb{N}$ , and  $p \in \mathbb{Z}^{\geq 0}$ .

All of the sub-questions can be regarded as finding the possible combinations of some hyperparameters given others. I will first show the relationship between parameters by a formula, then list all possible combinations if there are finite solutions, and some possible combinations followed by  $\cdots$  if the solution has infinity combinations, such as by infinitely and meaninglessly increasing the number of zero-padding while still fit the formula. Combination(s) marked with a '\*' indicates it is practically usable or preferred to be used in practice.

- 1. i = 64, output shape of (64, 32, 32) means o = 32.
  - (a) Given k = 8, d = 1 (without dilation):

$$k' = 8 + (8 - 1)(1 - 1) = 8$$
$$32 = \lfloor \frac{64 + 2p - 8}{s} \rfloor + 1 \Leftrightarrow \lfloor \frac{56 + 2p}{s} \rfloor = 31$$

s, p could be the following (\* indicates the preferred configuration(s) for a CNN network, applied to all the following):

i. 
$$s = 2, p = 3 *$$

ii. 
$$s = 3, p = 18$$

iii. 
$$s = 4, p = 34$$

iv. · · ·

(b) Given d = 7, s = 2, then:

$$\lfloor \frac{64 + 2p - k'}{2} \rfloor = 31$$

$$s' = k + (k - 1)(d - 1) = 7k - 4$$

$$k' = k + (k-1)(d-1) = 7k - 6$$

p, k could be the following:

i. 
$$k = 1 (k' = 1), p = 0 *$$

ii. 
$$k = 2 (k' = 8), p = 3 *$$

iii. 
$$k = 3 \ (k' = 15), p = 7 *$$

iv. 
$$k = 4 \ (k' = 22), p = 10$$

2. 
$$o = 8, i = 32, p = 0, d = 1$$

(a) For polling with non-overlapping window, it should be k = s,

$$8 = \lfloor \frac{32 - k}{k} \rfloor + 1 \Rightarrow k = 4$$

Therefore:

$$k = 4, s = 4$$

(b) if k = 8(k' = 8, as d = 1), s = 4, the output size should be:

$$o = \lfloor \frac{32 + 2 \times 0 - 8}{4} \rfloor + 1 = 7$$

Therefore, the output shape could be (64, 7, 7) if the number of channels maintains 64.

3. Given i = 8, o = 4

(a) Given p = 0, d = 1(k' = k)

$$4 = \lfloor \frac{8-k}{s} \rfloor + 1 \Rightarrow \lfloor \frac{8-k}{s} \rfloor = 3$$

Here are the following possible configurations:

i. 
$$s = 1, k = 5 *$$

ii. 
$$s = 2, k = 2 *$$

(b) Given d = 2(k' = 2k - 1), p = 2

$$4 = \lfloor \frac{8+4-(2k-1)}{s} \rfloor + 1 \Rightarrow \lfloor \frac{13-2k}{s} \rfloor = 3$$

Here are the following possible configurations :

i. 
$$k = 1(k' = 1), s = 3 *$$

ii. 
$$k = 2(k' = 3), s = 3 *$$

iii. 
$$k = 3(k' = 5), s = 2 *$$

iv. 
$$k = 5(k' = 9), s = 1 *$$

(c) Given p = 1, d = 1(k' = k)

$$4 = \lfloor \frac{8+2-k}{s} \rfloor + 1 \Rightarrow \lfloor \frac{10-k}{s} \rfloor = 3$$

Here are the following possible configurations:

i. 
$$s = 1, k = 7 *$$

ii. 
$$s = 2, k = 4 *$$

iii. 
$$s = 2, k = 3 *$$

iv. 
$$s = 3, k = 1$$
 (not often used)