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 Gradescope.*

Question 1 (4-4-4-2)**.** 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 ϕ is a smooth function (infinitely differentiable) with compact support ($\phi(x) = 0$ whenever $|x| \geq A$, 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. Write your answer here.

Question 2 (5-8-5-5)**.** Let x be an n-dimensional vector. Recall the softmax function : $S : \boldsymbol{x} \in \mathbb{R}^n \mapsto S(\boldsymbol{x}) \in \mathbb{R}^n$ such that $S(\boldsymbol{x})_i = \frac{e^{\boldsymbol{x}_i}}{\sum_j e^{\boldsymbol{x}_j}}$; the diagonal function : $\text{diag}(\boldsymbol{x})_{ij} = \boldsymbol{x}_i$ if $i = j$ and $\text{diag}(\boldsymbol{x})_{ij} = 0$ 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 $\frac{\partial S(\boldsymbol{x})}{\partial \boldsymbol{x}}$ using matrix-vector notation. Use $\text{diag}(\cdot)$.
3. Compute the Jacobian of the sigmoid function $\sigma(\boldsymbol{x}) = 1/(1 + e^{-\boldsymbol{x}})$.
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. Write your answer here.

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

1. Show that softmax is translation-invariant, that is : $S(\boldsymbol{x}+c) = S(\boldsymbol{x})$, where c is a scalar constant.

2. Show that softmax is not invariant under scalar multiplication. Let $S_c(\boldsymbol{x}) = S(c\boldsymbol{x})$ 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. Write your answer here.

Question 4 (15)**.** 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 σ. 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 Θ' as a function of Θ.

Answer 4. Write your answer here.

Question 5 (2-2-2-2)**.** 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 y 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 ϕ, 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 $\boldsymbol{W}^{(1)}$ to be $\boldsymbol{W}^{(1)} = [\boldsymbol{w}, \cdots, \boldsymbol{w}]^T$ for some $\boldsymbol{w} \in \mathbb{R}^n$ (so the rows of $\boldsymbol{W}^{(1)}$ are all the same). Show that the interpolation problem on the sample set $\mathcal{S} = \{\boldsymbol{x}^{(1)}, \cdots \boldsymbol{x}^{(N)}\} \subset \mathbb{R}^n$ can be reduced to solving a matrix equation : $\boldsymbol{M}\tilde{\boldsymbol{W}}^{(2)} = \boldsymbol{F}$, where $\tilde{\boldsymbol{W}}^{(2)}$ and $\boldsymbol{F}$ are both $N \times m$, given by

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

Express the $N \times N$ matrix $\boldsymbol{M}$ in terms of $\boldsymbol{w}$, $\boldsymbol{b}^{(1)}$, ϕ 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 ϵ 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 ϕ 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. Write your answer here.

Question 6 (6)**.** Compute the *full*, *valid*, and *same* convolution (with kernel flipping) for the following 1D matrices : $\begin{bmatrix}1,2,3,4\end{bmatrix} * \begin{bmatrix}1,0,2\end{bmatrix}$

Answer 6. Write your answer here.

Question 7 (5-5)**.** Consider a convolutional neural network. Assume the input is a colorful image of size 256×256 in the RGB representation. The first layer convolves 64 8×8 kernels with the input, using a stride of 2 and no padding. The second layer downsamples the output of the first layer with a 5×5 non-overlapping max pooling. The third layer convolves 128 4×4 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. Write your answer here.

Question 8 (4-4-4)**.** 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. Write your answer here.