## Regular Discussion 12 Solutions

## 1 Optimization

2023

We would like to classify some data. We have N samples, where each sample consists of a feature vector  $\mathbf{x} = [x_1, \cdots, x_k]^T$  and a label  $y \in \{0, 1\}$ .

Logistic regression produces predictions as follows:

$$P(Y = 1 \mid X) = h(\mathbf{x}) = s\left(\sum_{i} w_{i}x_{i}\right) = \frac{1}{1 + \exp(-(\sum_{i} w_{i}x_{i}))}$$
$$s(\gamma) = \frac{1}{1 + \exp(-\gamma)}$$

where  $s(\gamma)$  is the logistic function,  $\exp x = e^x$ , and  $\mathbf{w} = [w_1, \cdots, w_k]^T$  are the learned weights.

Let's find the weights  $w_j$  for logistic regression using stochastic gradient descent. We would like to minimize the following loss function (called the cross-entropy loss) for each sample:

$$L = -[y \ln h(\mathbf{x}) + (1 - y) \ln(1 - h(\mathbf{x}))]$$

(a) Show that  $s'(\gamma) = s(\gamma)(1 - s(\gamma))$ 

$$s(\gamma) = (1 + \exp(-\gamma))^{-1}$$
$$s'(\gamma) = -(1 + \exp(-\gamma))^{-2}(-\exp(-\gamma))$$
$$s'(\gamma) = \frac{1}{1 + \exp(-\gamma)} \cdot \frac{\exp(-\gamma)}{1 + \exp(-\gamma)}$$
$$s'(\gamma) = s(\gamma)(1 - s(\gamma))$$

(b) Find  $\frac{dL}{dw_j}$ . Use the fact from the previous part.

Use chain rule:

$$\frac{dL}{dw_j} = -\left[\frac{y}{h(\mathbf{x})}s'(\sum_i w_i x_i)x_j - \frac{1-y}{1-h(\mathbf{x})}s'(\sum_i w_i x_i)x_j\right]$$

Use fact from previous part:

$$\frac{dL}{dw_j} = -\left[\frac{y}{h(\mathbf{x})}h(\mathbf{x})(1-h(\mathbf{x}))x_j - \frac{1-y}{1-h(\mathbf{x})}h(\mathbf{x})(1-h(\mathbf{x}))x_j\right]$$

Simplify:

$$\frac{dL}{dw_j} = -\left[y(1-h(\mathbf{x}))x_j - (1-y)h(\mathbf{x})x_j\right]$$
$$= -x_j\left[y - yh(\mathbf{x}) - h(\mathbf{x}) + yh(\mathbf{x})\right]$$
$$= -x_j\left(y - h(\mathbf{x})\right)$$

(c) Now, find a simple expression for  $\nabla_{\mathbf{w}} L = [\frac{dL}{dw_1}, \frac{dL}{dw_2}, ..., \frac{dL}{dw_k}]^T$ 

$$\nabla_{\mathbf{w}} L = [-x_1(y - h(\mathbf{x})), -x_2(y - h(\mathbf{x})), ..., -x_k(y - h(\mathbf{x}))]^T$$
$$= -[x_1, x_2, ...x_k]^T(y - h(\mathbf{x}))$$
$$= -\mathbf{x}(y - h(\mathbf{x}))$$

(d) Write the stochastic gradient descent update for w. Our step size is  $\eta$ .

$$\mathbf{w} \leftarrow \mathbf{w} + \eta \mathbf{x} (y - h(\mathbf{x}))$$

## 2 Neural Network Representations

You are given a number of functions (a-h) of a single variable, x, which are graphed below. The computation graphs on the following pages will start off simple and get more complex, building up to neural networks. For each computation graph, indicate which of the functions below they are able to represent.



1. Consider the following computation graph, computing a linear transformation with scalar input x, weight w, and output o, such that o = wx. Which of the functions can be represented by this graph? For the options which can, write out the appropriate value of w.



This graph can only represent (a), with w = 2. Since there is no bias term, the line must pass through the origin.

2. Now we introduce a bias term b into the graph, such that o = wx + b (this is known as an *affine* function). Which of the functions can be represented by this network? For the options which can, write out an appropriate value of w, b.



(a) with w = 2 and b = 0, and (b) with w = 4 and b = -5

3. We can introduce a non-linearity into the network as indicated below. We use the ReLU non-linearity, which has the form ReLU(x) = max(0, x). Now which of the functions can be represented by this neural network with weight w and bias b? For the options which can, write out an appropriate value of w, b.



With the output coming directly from the ReLU, this cannot produce any values less than zero. It can produce (c) with w = 2 and b = -5, and (d) with w = -2 and b = -5

4. Now we consider neural networks with multiple affine transformations, as indicated below. We now have two sets of weights and biases  $w_1, b_1$  and  $w_2, b_2$ . We denote the result of the first transformation h such that  $h = w_1 x + b_1$ , and  $o = w_2 h + b_2$ . Which of the functions can be represented by this network? For the options which can, write out appropriate values of  $w_1, w_2, b_1, b_2$ .



Applying multiple affine transformations (with no non-linearity in between) is not any more powerful than a single affine function:  $w_2(w_1x + b_1) + b_2 = w_2w_1x + w_2b_1 + b_2$ , so this is just a affine function with different coefficients. The functions we can represent are the same as in 1, if we choose  $w_1 = w, w_2 =$  $1, b_1 = 0, b_2 = b$ : (a) with  $w_1 = 2, w_2 = 1, b_1 = 0, b_2 = 0$ , and (b) with  $w_1 = 4, w_2 = 1, b_1 = 0, b_2 = -5$ .

5. Next we add a ReLU non-linearity to the network after the first affine transformation, creating a hidden layer. Which of the functions can be represented by this network? For the options which can, write out appropriate values of  $w_1, w_2, b_1, b_2$ .



(c), (d), and (e). The affine transformation after the ReLU is capable of stretching (or flipping) and shifting the ReLU output in the vertical dimension. The parameters to produce these are: (c) with  $w_1 = 2, b_1 = -5, w_2 = 1, b_2 = 0$ , (d) with  $w_1 = -2, b_1 = -5, w_2 = 1, b_2 = 0$ , and (e) with  $w_1 = 1, b_1 = -2, w_2 = -1, b_2 = 1$ 

6. Now we add another hidden layer to the network, as indicated below. Which of the functions can be represented by this network?



(c), (d), (e), and (f). The network can represent all the same functions as Q5 (because note that we could have  $w_2 = 1$  and  $b_2 = 0$ ). In addition it can represent (f): the first ReLU can produce the first flat segment, the affine transformation can flip and shift the resulting curve, and then the second ReLU can produce the second flat segment (with the final affine layer not doing anything). Note that (h) cannot be produced since its line has only one flat segment (and the affine layers can only scale, shift, and flip the graph in the vertical dimension; they can't rotate the graph).

7. We'd like to consider using a neural net with just one hidden layer, but have it be larger – a hidden layer of size 2. Let's first consider using just two affine functions, with no nonlinearity in between. Which of the functions can be represented by this network?



(a) and (b). With no non-linearity, this reduces to a single affine function (in the same way as Q4)

8. Now we'll add a non-linearity between the two affine layers, to produce the neural network below with a hidden layer of size 2. Which of the functions can be represented by this network?



All functions except for (g). Note that we can recreate any network from (5) by setting  $w_4$  to 0, so this allows us to produce (c), (d) and (e). To produce the rest of the functions, note that  $h'_1$  and  $h'_2$  will be two independent functions with a flat part lying on the x-axis, and a portion with positive slope. The final layer takes a weighted sum of these two functions. To produce (a) and (b), the flat portion of one ReLU should start at the point where the other ends (x = 0 for (a), or x = 1 for (b). The final layer

then vertically flips the ReLU sloping down and adds it to the one sloping up, producing a single sloped line. To produce (h), the ReLU sloping down should have its flat portion end (at x = 0 before the other's flat portion begins (at x = 3). The down-sloping one is again flipped and added to the up-sloping. To produce (f), both ReLUs should have equal slope, which will cancel to produce the first flat portion above the x-axis.