CPSC 483/583: Deep Learning on Graph-structured Data **Fall 2023**

Homework 1

Due 11:59pm ET Friday September 15, 2023

This problem set should be completed individually.

General Instructions

These questions require thought, but do not require long answers. Please be as concise as possible. You are allowed to take a maximum of 1 late period (see the course website or slides about the definition of a late period).

Submission instructions: You should submit your answers in a PDF file. LaTeX is highly preferred due to the need of formatting equations.

Submitting answers: Prepare answers to your homework in a single PDF file. Make sure that the answer to each sub-question is on a *separate page*. The number of the question should be at the top of each page.

Honor Code: When submitting the assignment, you agree to adhere to the Yale Honor Code. Please read carefully to understand what it entails!

Homework survey: After submitting your homework, please fill out the Homework 1 Feedback Form. 0.5% overall extra credit will be given if you take time to reflect on the nature of the problems and possibly provide feedbacks for the benefit of future offering of this course, by filling in the form for each written and coding assignment.

Symbol-wise: we use lowercase bold like $\mathbf{x}$ *to indicate a vector and uppercase bold like* $\mathbf{W}$ *to indicate a matrix. Others are scalars. Dimensions will be explicitly clarified if needed.*

1 Sigmoid and Softmax Function

Sigmoid function is used in the logistic regression to predict the label $l \in \{0, 1\}$ given a sample $\mathbf{x} \in \mathbb{R}^d$. The sigmoid function is defined as follows, which maps value in $\mathbb{R}$ to a number in $(0, 1)$.

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

Then the probabilities that label l equals to 0 or 1 are

$$P(l = 1|\mathbf{x}) = \frac{1}{1 + e^{-\mathbf{w}^\top \mathbf{x}}} = \sigma(\mathbf{w}^\top \mathbf{x}) \quad \text{and} \quad P(l = 0|\mathbf{x}) = 1 - P(l = 1|\mathbf{x}),$$

where $\mathbf{w} \in \mathbb{R}^d$ is the vector of weights. Softmax function is a generalization of logistic regression to multiple classes, i.e., $l \in \{0, 1, \cdots, K - 1\}$, where K denotes the number of classes. For a vector $\mathbf{z} \in \mathbb{R}^K$, softmax function normalizes it into a probability distribution by

$$Softmax(\mathbf{z})_i = \frac{e^{z_i}}{\sum_{j=0}^{K-1} e^{z_j}} \text{ for } i = 0, 1, \cdots, K - 1 \text{ where } \mathbf{z} = (z_0, z_1, \cdots, z_{K-1}) \in \mathbb{R}^K.$$

For an input vector $\mathbf{x} \in \mathbb{R}^d$, Softmax estimates the probability of each label using a weight matrix $\mathbf{W} \in \mathbb{R}^{K \times d}$ by

$$Softmax(\mathbf{W}\mathbf{x}) = \begin{bmatrix} P(l = 0|\mathbf{x}, \mathbf{w}_0) \\ P(l = 1|\mathbf{x}, \mathbf{w}_1) \\ \cdots \\ P(l = K - 1|\mathbf{x}, \mathbf{w}_{K-1}) \end{bmatrix} = \frac{1}{\sum_{i=0}^{K-1} e^{\mathbf{w}_i^\top \mathbf{x}}} \begin{bmatrix} e^{\mathbf{w}_0^\top \mathbf{x}} \\ e^{\mathbf{w}_1^\top \mathbf{x}} \\ \cdots \\ e^{\mathbf{w}_{K-1}^\top \mathbf{x}} \end{bmatrix}.$$

The matrix $\mathbf{W}$ is formed by the weight vectors as $\mathbf{W} = [\mathbf{w}_0, \mathbf{w}_1, \cdots, \mathbf{w}_{K-1}]^\top$. It is easy to verify that the sum of all elements in the output of Softmax function is 1.

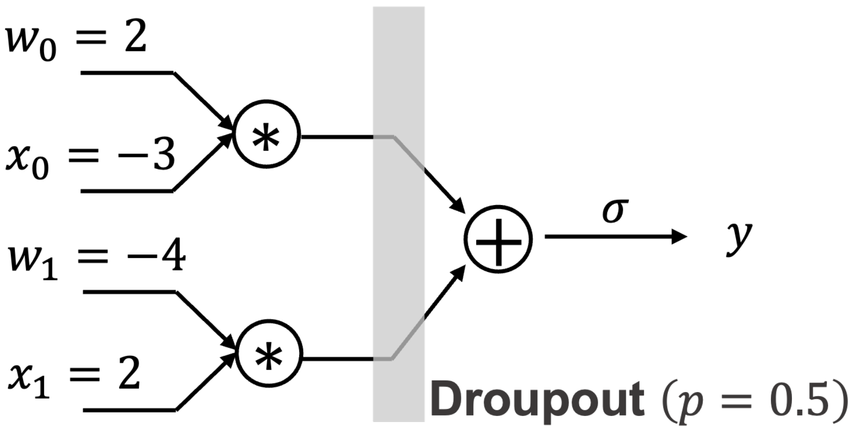
1. Assuming $t = \sigma(s)$, calculate the gradient of Sigmoid function with respect to s and rewrite the gradient as a function of t (i.e., there is no s in the gradient expression).

2. Prove that Softmax function is invariant to a weight shift. Let $\mathbf{W}' = [\mathbf{w}_0 - \mathbf{c}, \mathbf{w}_1 - \mathbf{c}, \cdots, \mathbf{w}_{K-1} - \mathbf{c}]^\top$, where $\mathbf{c}$ is a constant vector that we subtract from each elements in $\mathbf{W}$. Weight-shift invariance implies that $Softmax(\mathbf{W}'\mathbf{x}) = Softmax(\mathbf{W}\mathbf{x})$. (Hint: $e^{x-c} = e^x \cdot e^{-c}$)

3. Prove that when $K = 2$, Softmax-based logistic regression is equivalent to Sigmoid-based logistic regression. (Hint: use the weight-shift invariance property of Softmax function to prove the probabilities of label 0 and 1 estimated by Sigmoid and Softmax are equivalent.)

2 Back-Propagation

1. Let's perform back-propagation through a neural network with a sigmoid activation σ. Specifically, we insert a dropout layer before the activation. The computation graph is visualized



below. Therefore, the output $y = \sigma(\delta_0 w_0 x_0 + \delta_1 w_1 x_1)$, where $\delta_0, \delta_1 \sim$ Bernoulli(0.5). Calculate the expectation of gradients with respect to the input and parameters, i.e., $\mathbb{E}(\frac{\partial y}{\partial w_0})$, $\mathbb{E}(\frac{\partial y}{\partial x_0})$, $\mathbb{E}(\frac{\partial y}{\partial w_1})$, $\mathbb{E}(\frac{\partial y}{\partial x_1})$.

2. In a fully connected layer, let $\mathbf{y} = \mathbf{W}\mathbf{x}$, where $\mathbf{x} \in \mathbb{R}^{d_k}$ denotes the input, $\mathbf{W} \in \mathbb{R}^{d_{k+1} \times d_k}$ is the weight matrix corresponding to this fully connected layer and $\mathbf{y} \in \mathbb{R}^{d_{k+1}}$ denotes the output. $\mathcal{L}(\mathbf{y}) \in \mathbb{R}$ is the loss function. Prove that the gradient back-propagation is also in the form of a fully connected layer, where the gradient of $\mathcal{L}$ with respect to $\mathbf{y}$ is the input and the gradient of $\mathcal{L}$ with respect to $\mathbf{x}$ is the output. What is the relationship between the weight matrix of this fully connected layer and $\mathbf{W}$? (Hint: prove that $\frac{\partial \mathcal{L}}{\partial \mathbf{x}} = \tilde{\mathbf{W}} \frac{\partial \mathcal{L}}{\partial \mathbf{y}}$ with a certain weight matrix $\tilde{\mathbf{W}}$ and figure out the relationship between $\tilde{\mathbf{W}}$ and $\mathbf{W}$)

3. We have a two-layer neural network as follows,

$$f(\mathbf{x}) = \sigma(\sigma(\mathbf{x} \cdot \mathbf{W}^{(1)}) \cdot \mathbf{W}^{(2)}),$$

where σ is the sigmoid function, $\mathbf{x} \in \mathbb{R}^{d_1}$ is the input, $\mathbf{W}^{(1)} \in \mathbb{R}^{d_1 \times d_2}$ and $\mathbf{W}^{(2)} \in \mathbb{R}^{d_2 \times 1}$ are weight matrices of the first and second layer, respectively. Show the gradient of the two-layer neural network's output $f(\mathbf{x})$ with respect to parameter $\mathbf{W}^{(2)}$.

★**Additional question for students enrolled in 583** (optional for 483):

Calculate the gradients of the output $f(\mathbf{x})$ with respect to parameter $\mathbf{W}^{(1)}$ (Hint: use the chain rule and results in Q2.2).