Homework 6 Fall 2024

04650 Mathematical Foundations of Machine Learning (CMU-Africa)

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- **Collaboration policy:** You can discuss HW problems with other students, but the work you submit must be written in your own words and not copied from anywhere else. However, do write down (at the top of the first page of your HW solutions) the names of all the people with whom you discussed this HW assignment. We strongly encourage you to type your solution using LaTeX, but this is not required

- **Submitting your work:** Assignment will be submitted using Gradescope. You will submit a single PDF containing your solutions.

- **Getting Help**: Please use office hours and Piazza to ask any questions related to this assigments.

- **Refrain from using ChatGPT**: These problems are easy and can be easiliy solved with the use of generative AI's like ChatGPT. However, you will not learn by using these tools. Not learning will impact your performance in other courses which require this knowledge like introduction to deep learning and introduction to machine learning for engineers. Ask questions on Piazza about anything you don't understand, the TA's and instructors will respond to you as fast as possible. Moreover, you will not have access to internet during the exam.

Learning Objectives

- Probability: Learn how to model problems using a probability distribution. Learn about the entropy of a distribution, cross entropy of two distributions, and the KL divergence between two distributions.

1. Entropy of a Bernoulli Random Variable [10 points]

Consider a random variable X that follows a Bernoulli distribution $B(1, p)$ with $0 < p < 1$. We define the entropy of X as

$$H(p) = \mathbb{E}[-\log(p(X))].$$

(You will need to read a little bit about entropy or consult a TA during office hours.)

(a) Derive the second derivative $H''(p)$ of $H(p)$. If $H''(p) \leq 0$, $H(p)$ is called concave. Is $H(p)$ a concave function of p? (5 points)

(b) Find the value of $p \in (0, 1)$ that maximizes $H(p)$. (5 points)

2. Binary Classification with Logistic Regression [70 points]

Consider a binary classification problem where $y \in \{0, 1\}$ and $\mathbf{x} \in \mathbb{R}^2$. Our goal is to model $p(y = 1 \mid \mathbf{x})$. We decide to use a Bernoulli distribution parameterized by the random vector $\mathbf{w} \in \mathbb{R}^2$, such that:

$$p_{\text{model}}(y = 1 \mid \mathbf{x}; \mathbf{w}) = \sigma(\mathbf{w}^\top \mathbf{x}),$$

$$p_{\text{model}}(y = 0 \mid \mathbf{x}; \mathbf{w}) = 1 - \sigma(\mathbf{w}^\top \mathbf{x}),$$

where $\sigma(z) = \frac{1}{1+e^{-z}}$ is the sigmoid function.

(a) Show that

$$p_{\text{model}}(y \mid \mathbf{x}; \mathbf{w}) = \big(\sigma(\mathbf{w}^\top \mathbf{x})\big)^y \big(1 - \sigma(\mathbf{w}^\top \mathbf{x})\big)^{1-y}.$$

(5 points)

(b) Table 1 contains 10 samples, $(\mathbf{x}, y)$, obtained from the data-generating distribution p_{data}. The KL divergence between p_{data} and p_{model} is given as:

$$D_{\text{KL}}(p_{\text{data}} \,||\, p_{\text{model}}) = \mathbb{E}_{\mathbf{x}, y \sim p_{\text{data}}} \big[\log p_{\text{data}}(y \mid \mathbf{x}) - \log p_{\text{model}}(y \mid \mathbf{x})\big].$$

The cross entropy of p_{data} and p_{model} is:

$$-\mathbb{E}_{\mathbf{x}, y \sim p_{\text{data}}} \big[\log p_{\text{model}}(y \mid \mathbf{x})\big].$$

Given empirical data as in Table 1, show that the cross entropy satisfies the expression:

$$-\mathbb{E}_{\mathbf{x}, y \sim p_{\text{data}}} \big[\log p_{\text{model}}(y \mid \mathbf{x})\big] = -\frac{1}{N} \sum_{i=1}^{N} \big[y_i \log\big(\sigma(\mathbf{w}^\top \mathbf{x_i})\big) + (1 - y_i) \log\big(1 - \sigma(\mathbf{w}^\top \mathbf{x_i})\big)\big].$$

(5 points)

Sample	**x**	**y**
1	$[-1, 4]$	1
2	$[-3, 2]$	0
3	$[-2, 1]$	0
4	$[1, 2]$	1
5	$[2, 1]$	1
6	$[-1, 1]$	0
7	$[-2, -2]$	0
8	$[1, -2]$	0
9	$[3, -1]$	1
10	$[2, 0]$	1

Table 1: Samples $(\mathbf{x}, y)$ obtained from the data-generating distribution p_{data}.

(c) Minimizing the cross entropy of p_{data} and p_{model} implies that p_{model} will approximate the data-generating distribution. We define the loss function of our model as:

$$L(\mathbf{w}) = -\frac{1}{N}\sum_{i=1}^{N}\big[y_i \log\big(\sigma(\mathbf{w}^\top \mathbf{x_i})\big) + (1-y_i)\log\big(1-\sigma(\mathbf{w}^\top \mathbf{x_i})\big)\big].$$

Obtain an expression for the gradient of $L(\mathbf{w})$ with respect to $\mathbf{w}$, and show that $L(\mathbf{w})$ is a convex function. (10 points)

(d) The gradient expression obtained above can be seen as the empirical mean of the gradient for each sample i. $\nabla L(w) = \frac{1}{N}\sum_{i=1}^{N}\nabla L_i(w)$. Given that the gradient for each sample is independent and identically distributed with variance σ_g^2, Show that the standard error of the gradient given n samples from the data-generating distribution is

$$SE = \frac{\sigma_g}{\sqrt{n}}$$

Explain why a better estimate of the gradient is obtained by increasing the number of samples.

(5 points)

(e) Stochastic gradient descent (SGD) with a minibatch computes the gradient using only a subset of the total samples when performing parameter updates. The minibatch size, m, is always less than the total number of samples, N. Given that an epoch of updates involves using all available samples:

- Perform SGD updates for 1 epoch while reporting the values of the loss and the parameters after each update in the format shown in Table 2.
- Use a learning rate of 0.1 and a minibatch size of 2.
- start with $\mathbf{w} = [0, 0]$

The SGD update is given as:

$$w \leftarrow w - \alpha \nabla L(\mathbf{w})$$

Note: You must show all your workings to get full points. (20 points)

(f) Perform the calculations in (e) above using SGD with momentum. The momentum update is given as:

$$\mathbf{v} \leftarrow \beta \mathbf{v} - \alpha \nabla L(\mathbf{w}),$$

$$\mathbf{w} \leftarrow \mathbf{w} + \mathbf{v},$$

where $\beta = 0.9$ is the momentum parameter. Report the values of the loss, parameters, and velocity after each update in the format shown in Table 3. **Note: You must show all your workings to get full points.** (20 points)

(g) Compare the results obtained in (e) and (f) above, and discuss your observations. (5 points)

Update Step	**Minibatch**	**Loss $L(\mathbf{w})$**	**Parameters w**
1	$\{1, 2\}$	0.543	$[0.1, -0.2]$
2	$\{3, 4\}$	0.523	$[0.12, -0.18]$
3	$\{5, 6\}$	0.508	$[0.15, -0.15]$
4	$\{7, 8\}$	0.492	$[0.18, -0.12]$
5	$\{9, 10\}$	0.475	$[0.2, -0.1]$

Table 2: Progress of SGD over one epoch.

Note: The values for the loss and parameters in the Table 1 & 2 are just placeholders. Replace them with what you obtain from your calculations.

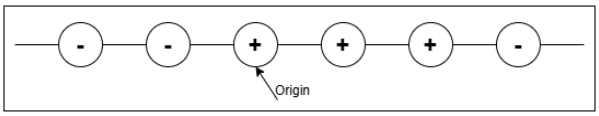
Update Step	**Minibatch**	**Loss $L(\mathbf{w})$**	**Parameters w**	**Velocity v (Momentum)**
1	$\{1, 2\}$	0.543	$[0.1, -0.2]$	$[0.0, 0.0]$
2	$\{3, 4\}$	0.523	$[0.12, -0.18]$	$[0.02, -0.02]$
3	$\{5, 6\}$	0.508	$[0.15, -0.15]$	$[0.03, 0.03]$
4	$\{7, 8\}$	0.492	$[0.18, -0.12]$	$[0.04, -0.03]$
5	$\{9, 10\}$	0.475	$[0.2, -0.1]$	$[0.05, 0.02]$

Table 3: Progress of SGD with Momentum over one epoch.

3. Feature Mapping and Linear Separability [20 points]

Using the following dataset in 1-D space, which consists of:

Positive data points: $\{0, 1, 2\}$, Negative data points: $\{-2, -1, 3\}$.



(a) Find a feature map $\phi : \mathbb{R}^1 \to \mathbb{R}^2$ that maps the data in the original 1-D input space x to a 2-D feature space $\phi(x) = (y_1, y_2)$ so that the data becomes linearly separable. Plot the dataset after mapping in the 2-D space. (8 points)

(b) Write down the equation for the separating hyperplane, $w_0 + w_1 y_1 + w_2 y_2 = 0$, given by a hard-margin linear SVM in the 2-D feature space. Draw this hyperplane on your plot and mark the corresponding support vector(s). (12 points)