Homework 6 - Mathetmatical Foundations of Machine Learning Engineers

kipngeno koech - bkoech

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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)

The probability mass function of a Bernoulli random variable is given by:

$$p(x) = \begin{cases} p & \text{if } x = 1, \\ 1-p & \text{if } x = 0. \end{cases}$$

The expected value is given by:

$$\mathbb{E}[X] = \sum_{x \in \{0,1\}} x \cdot p(x).$$

so the entropy of X is:

$$H(p) = -\sum_{x \in \{0,1\}} p(x) \log(p(x)).$$

this is equivalent to:

$$H(p) = -p \log(p) - (1-p) \log(1-p).$$

The first derivative of $H(p)$ with respect to p is:

$$H'(p) = -\log(p) - 1 + \log(1-p).$$

The second derivative of $H(p)$ with respect to p is:

$$H''(p) = -\frac{1}{p} - \frac{1}{1-p}.$$

The second derivative is always negative for $0 < p < 1$, so $H(p)$ is a concave function of p.
This means that the entropy of a Bernoulli random variable is a concave function of the probability p.

(b) Find the value of $p \in (0, 1)$ that maximizes $H(p)$. (5 points) To maximize $H(p)$, we set the first derivative to zero:

$$H'(p) = -\log(p) - 1 + \log(1-p) = 0.$$

$$\log(1-p) - \log(p) = 1.$$

$$\log\left(\frac{1-p}{p}\right) = 1.$$

$$1 - p = p$$

$$p = \frac{1}{2}.$$

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:

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

(5 points)

Sample	$\mathbf{x}$	**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:

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

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** $\mathbf{w}$
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.

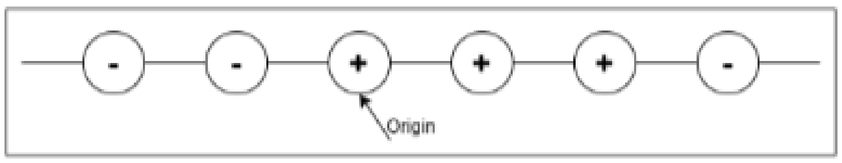
Update Step	Minibatch	Loss $L(\mathbf{w})$	Parameters $\mathbf{w}$	Velocity $\mathbf{v}$ (Momentum)
1	$\{1,2\}$	0.543	$[0.1, -0.2]$	$[0.0, 0.0]$
2	$\{3,4\}$	0.523	$[0.12, -0.18]$	$[0.02, -0.02]$
3	$\{5,6\}$	0.508	$[0.15, -0.15]$	$[0.03, 0.03]$
4	$\{7,8\}$	0.492	$[0.18, -0.12]$	$[0.04, -0.03]$
5	$\{9,10\}$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

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



(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)

we are given the following dataset in 1-D space:

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

to transform the data into a linearly separable form, we can use the kernel function: polynomial kernel of degree 2:

$$\phi(x) = (y_1, y_2) = (x, x^2).$$

to transform the Positive data points:
the first positive data point is 0:

$$\phi(0) = (0, 0^2) = \mathbf{(0,\ 0)}$$

the second positive data point is 1:

$$\phi(1) = (1, 1^2) = \mathbf{(1,\ 1)}$$

the third positive data point is 2:

$$\phi(2) = (2, 2^2) = \mathbf{(2,\ 4)}$$

to transform the Negative data points:
the first negative data point is -2:

$$\phi(-2) = (-2, (-2)^2) = \mathbf{(\text{-}2,\ 4)}$$

the second negative data point is -1:

$$\phi(-1) = (-1, (-1)^2) = \mathbf{(\text{-}1,\ 1)}$$

the third negative data point is 3:

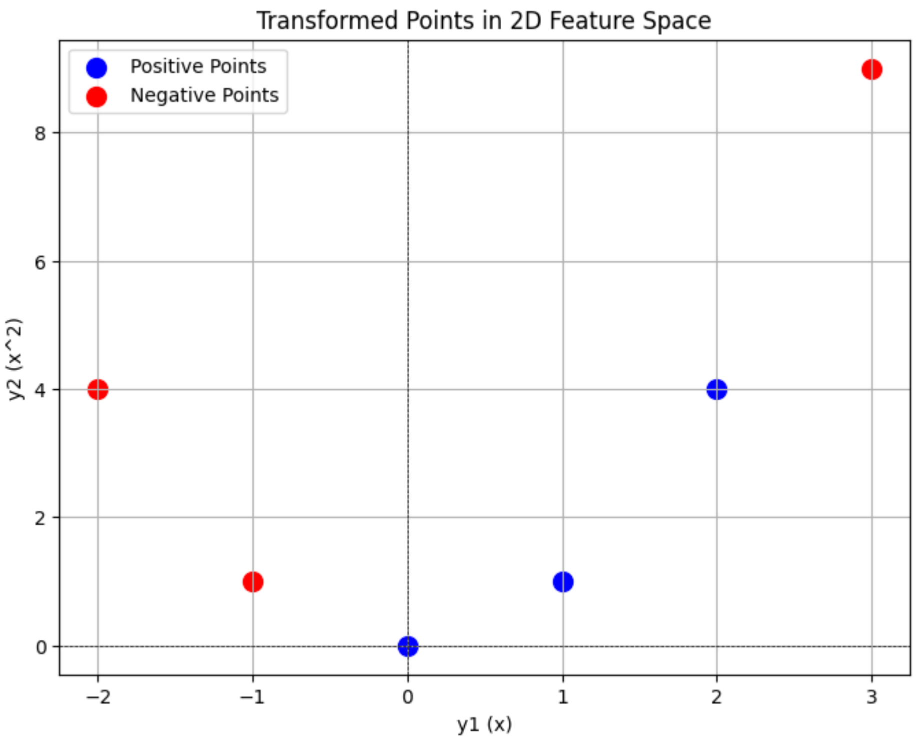
$$\phi(3) = (3, 3^2) = \mathbf{(3,\ 9)}$$

the transformed dataset in 2-D space is:

$$\text{Positive data points: } \{(0,0), (1,1), (2,4)\}, \quad \text{Negative data points: } \{(-2,4), (-1,1), (3,9)\}.$$

the plot of the dataset after mapping in the 2-D space is shown below: **Note:** the figure might have floated to a different page.

(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)


Transformed Points in 2D Feature Space
Positive Points
Negative Points
y2 (x^2)
y1 (x)
0
2
4
6
8
−2
−1
0
1
2
3