THE HONG KONG UNIVERSITY OF SCIENCE & TECHNOLOGY
Machine Learning
Homework 1 Solutions

Due Date: See course webpage.

Your answers should be typed, not handwritten. You can submit a Word file or a pdf file. Submissions are to be made via Canvas. Note that penalty applies if your similarity score exceeds 40. To minimize your similarity score, don't copy the questions.

Question 1: Suppose a dataset $\mathcal{D} = \{\mathbf{x}_i\}_{i=1}^N$ is generated from some unknown distribution $p(\mathbf{x})$ and we learn from $\mathcal{D}$ a distribution $q_\theta(\mathbf{x})$ with parameters θ. What is the KL divergence $KL(p||q_\theta)$ of q_θ from p? What is the cross entropy $H(p, q_\theta)$ between p and q_θ? How are they related?

What is the log-likelihood of $l(\theta|\mathcal{D})$? How is maximizing $l(\theta|\mathcal{D})$ related to minimizing the cross entropy and the KL divergence ?

Solution:

$$
\begin{aligned}
KL(p||q_\theta) &= E_p[\log p(\mathbf{x})] - E_p[\log q_\theta(\mathbf{x})] \\
H(p, q_\theta) &= -E_p[\log q_\theta(\mathbf{x})] \\
KL(p||q_\theta) &= H(p, q_\theta) - H(p), \text{ where } H(p) = -E_p[\log p(\mathbf{x})] \text{ is the entropy of } p. \\
l(\theta|\mathcal{D}) &= \sum_{i=1}^N \log q_\theta(\mathbf{x}_i).
\end{aligned}
$$

$l(\theta|\mathcal{D})$ can be viewed as an approximation of $-NH(p, q_\theta)$. Hence, maximizing the log-likelihood $l(\theta|\mathcal{D})$ amounts to minimizing the cross entropy $H(p, q_\theta)$. It also amounts to minimizing the KL divergence $KL(p||q_\theta)$ as the entropy term $H(p)$ in the third equation above does not depend on θ.

Question 2 Consider carrying out linear regression on the following dataset. Manually compute the ordinary least squares solution.

x_1	0	0	1	1	1
x_2	1	1	1	0	0
y	0	1	2	3	4

Solution: The design matrix and the label vector $\mathbf{y}$ are:

$$
\begin{aligned}
\mathbf{X}^\top &= \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 \end{bmatrix} \\
\mathbf{y}^\top &= \begin{bmatrix} 0 & 1 & 2 & 3 & 4 \end{bmatrix}
\end{aligned}
$$

We have

$$
\begin{aligned}
\mathbf{X}^\top\mathbf{X} &= \begin{bmatrix} 5 & 3 & 3 \\ 3 & 3 & 1 \\ 3 & 1 & 3 \end{bmatrix} \\
(\mathbf{X}^\top\mathbf{X})^{-1} &= \begin{bmatrix} 2 & -1.5 & -1.5 \\ -1.5 & 1.5 & 1 \\ -1.5 & 1 & 1.5 \end{bmatrix} \\
(\mathbf{X}^\top\mathbf{y})^\top &= \begin{bmatrix} 10 & 3 & 9 \end{bmatrix}
\end{aligned}
$$

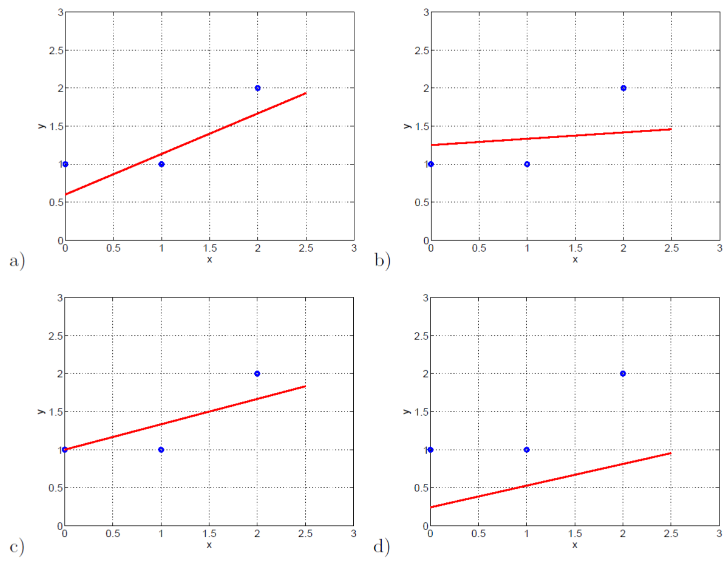
Therefore,

$$\begin{bmatrix} w_0 \\ w_1 \\ w_2 \end{bmatrix} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y} = \begin{bmatrix} 2 \\ 1.5 \\ \text{-1.5} \end{bmatrix}$$

The final regression equation is:

$$y = 2 + 1.5x_1 - 1.5x_2$$

Question 3 The following figures show linear regression results on a dataset of only three data points (marked blue).



The results were obtained using following regularization schemes:

1. $\frac{1}{3}\sum_{i=1}^{3}(y_i - w_0 - w_1 x_i)^2 + \lambda w_1^2$ where $\lambda = 1$.
2. $\frac{1}{3}\sum_{i=1}^{3}(y_i - w_0 - w_1 x_i)^2 + \lambda w_1^2$ where $\lambda = 10$.
3. $\frac{1}{3}\sum_{i=1}^{3}(y_i - w_0 - w_1 x_i)^2 + \lambda(w_0^2 + w_1^2)$ where $\lambda = 1$.
4. $\frac{1}{3}\sum_{i=1}^{3}(y_i - w_0 - w_1 x_i)^2 + \lambda(w_0^2 + w_1^2)$ where $\lambda = 10$.

Match the regularization schemes with the regress results. Briefly explain your answers.

Solution: The first two objective functions regularize only w_1. The results are shown in c) and b) respectively. The line in b) has a flat slope because a large regularization constant (10) is used.

The last two objective functions regularize both w_0 and w_1. The results are shown in a) and d) respectively. The intercepts are lower than in the other two cases.

Question 4 Consider applying logistic regression to the following dataset:

x_1	0	0	1	1
x_2	0	1	0	1
y	0	0	0	1

The target is to learn a model of the form $p(y = 1|\mathbf{x}, \mathbf{w}) = \sigma(w_0 + w_1 x_1 + w_2 x_2)$.

Suppose $w_0 = -2$, $w_1 = 1$ and $w_2 = 1$ initially and $\alpha = 0.1$. Manually run the batch gradient descent algorithm for one iteration. Give the weights and training error (i.e., fraction of misclassified examples) after the iteration.

Solution: $\mathbf{w}^\top\mathbf{x}_1 = -2$, $\sigma(\mathbf{w}^\top\mathbf{x}_1) = 0.12$; $\mathbf{w}^\top\mathbf{x}_2 = -1$, $\sigma(\mathbf{w}^\top\mathbf{x}_2) = 0.27$; $\mathbf{w}^\top\mathbf{x}_3 = -1$, $\sigma(\mathbf{w}^\top\mathbf{x}_3) = 0.27$; $\mathbf{w}^\top\mathbf{x}_4 = 0$, $\sigma(\mathbf{w}^\top\mathbf{x}_4) = 0.5$.

$$
\begin{aligned}
w_0 &= -2 + 0.1 \times \frac{1}{4} \times ([0-0.12]\times 1 + [0-0.27]\times 1 + [0-0.27]\times 1 + [1-0.5]\times 1) = -2.004 \\
w_1 &= 1 + 0.1 \times \frac{1}{4} \times ([0-0.12]\times 0 + [0-0.27]\times 0 + [0-0.27]\times 1 + [1-0.5]\times 1) = 1.00575 \\
w_2 &= 1 + 0.1 \times \frac{1}{4} \times ([0-0.12]\times 0 + [0-0.27]\times 1 + [0-0.27]\times 0 + [1-0.5]\times 1) = 1.00575
\end{aligned}
$$

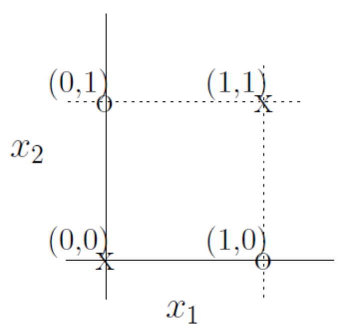
With the new parameters, we have $\mathbf{w}^\top\mathbf{x}_1 = -2.004 < 0$, and hence $\mathbf{x}_1$ is classified into class 0; $\mathbf{w}^\top\mathbf{x}_2 = -2.004 + 1.00575 < 0$, and hence $\mathbf{x}_2$ is classified into class 0; $\mathbf{w}^\top\mathbf{x}_3 = -2.004 + 1.00575 < 0$, and hence $\mathbf{x}_3$ is classified into class 0; $\mathbf{w}^\top\mathbf{x}_4 = -2.004 + 1.00575 + 1.00575 > 0$, and hence $\mathbf{x}_4$ is classified into class 1. The training error is 0.

Question 5 Consider applying logistic regression to the following dataset:

x_1	0	0	1	1
x_2	0	1	0	1
y	1	0	0	1

1. If we use raw feature x_1 and x_2, the model is
$$p(y=1|\mathbf{x},\mathbf{w}) = \sigma(w_0 + w_1x_1 + w_2x_2).$$
What is the minimum achievable training error in this case? Give weights that achieve the minimum error.
2. Next consider using an additional feature x_1x_2 in addition to the raw feature x_1 and x_2. The model now is
$$p(y=1|\mathbf{x},\mathbf{w}) = \sigma(w_0 + w_1x1 + w_2x_2 + w_3x_1x_2).$$
What is the minimum achievable training error in this case? Give weights that achieve the minimum error.

Solution:



1. As shown above, the dataset is not linearly separable. The minimum achievable error using a linear classifier is 0.25. It is achieved by, for instance, the weights $w_0 = 0.5$, $w_1 = -1$ and $w_2 = -1$. In this case, the first three examples are classified correctly and the last example is classified incorrectly.
2. With the additional feature x_1x_2, we can correctly classify all four examples using weights $w_0 = 0.5$, $w_1 = -1$, $w_2 = -1$ and $w_3 = 2$.

Question 6 Consider the gradient vector in logistic regression $\nabla J(\mathbf{w}) = (\frac{\partial J(\mathbf{w})}{\partial w_0}, \frac{\partial J(\mathbf{w})}{\partial w_1}, \ldots, \frac{\partial J(\mathbf{w})}{\partial w_D})$ where

$$\frac{\partial J(\mathbf{w})}{\partial w_j} = -\frac{1}{N}\sum_{i=1}^{N}[y_i - \sigma(z_i)]x_{i,j}.$$

Suppose the feature x_1 is binary and, in the training set, it takes value 1 only in a small number of training examples with class label 1 (i.e., $y = 1$), and it takes value 0 in all training examples with class label 0 (i.e., $y = 0$). What will happen to the weight w_1 if we update it repeatedly using the following rule:

$$w_1 \leftarrow w_1 + \alpha \frac{1}{N} \sum_{i=1}^{N} [y_i - \sigma(\mathbf{w}^\top \mathbf{x}_i)] x_{i,1}$$

What if we use the following update rule instead:

$$w_1 \leftarrow w_1 + \alpha[-\lambda w_1 + \frac{1}{N} \sum_{i=1}^{N} [y_i - \sigma(\mathbf{w}^\top \mathbf{x}_i)] x_{i,1}],$$

where λ is the regularization constant?

Solution: Since $\sigma(\mathbf{w}^\top \mathbf{x}_i) < 1$, $\frac{1}{N} \sum_{i=1}^{N} [y_i - \sigma(\mathbf{w}^\top \mathbf{x}_i)] x_{i,1}$ is always positive. If we use the first (unregularized) update rule, the weight w_1 might increase without bound, leading to numerical instability.

If we use the second (regularized) update rule, w_1 will stop increasing when $\lambda w_1 \geq \frac{1}{N} \sum_{i=1}^{N} [y_i - \sigma(\mathbf{w}^\top \mathbf{x}_i)] x_{i,1}$. So, regularization makes logistic regression numerically stable with regard to the scenario described in this problem.

Self-Practice Questions: I will minimize the amount math derivations in class for the sake of the majority of the students. Those interested in understanding all the math can try to solve the following problems. This is for self-practice. **Do not include the answers in your submission.**

- Prove Theorem 1.1 in Lecture 01-2.
- Let $I(X;Y) = H(X) - H(X|Y)$. Prove that

$$I(X;Y) = KL(P(X,Y)||P(X)P(Y)).$$

- Derive the OLS solution for linear regression.
- Derive the gradient descent update rule for Softmax.