

# CS182: Introduction to Machine Learning

## Reference Solutions of Final Exam

June 12, 2022

### I REGRESSION AND PROBABILITY ESTIMATION [12 points]

We consider the following linear regression model in which  $y$  is the sum of a deterministic linear function of  $x$ , plus random noise  $\epsilon$ , i.e.,

$$y = wx + \epsilon, \quad (1)$$

where  $x$  is the real-valued input,  $y$  is the real-valued output, and  $w$  is a single real-valued parameter to be learned. Here  $\epsilon$  is a real-valued random variable that represents noise which follows a Gaussian distribution with mean 0 and standard deviation  $\sigma$ , that is,  $\epsilon \sim \mathcal{N}(0, \sigma^2)$ .

**Note:** the probability density function  $f(X)$  of a Gaussian distributed variable  $X \sim \mathcal{N}(\mu, \sigma^2)$  takes the form

$$f(X = x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x - \mu)^2}{2\sigma^2}\right). \quad (2)$$

1. [4 points] Write down the probability distribution of  $y$  conditioned on  $x$  and  $w$ , i.e.  $\Pr(y \mid w, x)$ .

**Solution**

$$\Pr(y \mid w, x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y - wx)^2}{2\sigma^2}\right).$$

2. [4 points] Given  $n$  *i.i.d.* training examples  $\{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$ . Let  $\mathcal{Y} = (y_1, \dots, y_n)$  and  $\mathcal{X} = (x_1, \dots, x_n)$ , please write down an expression for the conditional data likelihood:  $\Pr(\mathcal{Y} \mid \mathcal{X}, w)$

**Solution**

$$\begin{aligned} \Pr(\mathcal{Y} \mid \mathcal{X}, w) &= \prod_{i=1}^n \Pr(y_i \mid x_i, w) \\ &= \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^n \prod_{i=1}^n \exp\left(-\frac{(y_i - wx_i)^2}{2\sigma^2}\right) \\ &= \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^n \exp\left(-\frac{\sum_{i=1}^n (y_i - wx_i)^2}{2\sigma^2}\right). \end{aligned}$$

3. [4 points] Suppose a Laplace prior over  $w$  with  $\mu = 0$  and  $b$  (i.e.,  $w \sim \text{Laplace}(0, b)$ ). Now you need to use MAP(maximum a posterior probability) to estimate  $w$  from the training data. Please show that finding the MAP estimate  $w^*$  is equivalent to solving the following optimization problem

$$w^* = \underset{w}{\operatorname{argmin}} \frac{1}{2} \sum_{i=1}^n (y_i - wx_i)^2 + c|w|. \quad (3)$$

Express the regularization parameter  $c$  in terms of  $\sigma$  and  $b$ .

**Hint:** the probability density function  $f(X)$  of a Laplace distributed variable  $X \sim \text{Laplace}(\mu, b)$  takes the form

$$f(X = x) = \frac{1}{2b} \exp\left(-\frac{|x - \mu|}{b}\right). \quad (4)$$

### Solution

$$\begin{aligned}\Pr(w \mid \mathcal{Y}, \mathcal{X}) &\propto \Pr(\mathcal{Y} \mid \mathcal{X}, w) \Pr(w) \\ &\propto \exp\left(-\frac{\sum_{i=1}^n (y_i - wx_i)^2}{2\sigma^2}\right) \exp\left(-\frac{|w|}{b}\right) \\ w^* &= \operatorname{argmin}_w -\ln \Pr(w \mid \mathcal{Y}, \mathcal{X}) \\ &= \operatorname{argmin}_w \frac{\sum_{i=1}^n (y_i - wx_i)^2}{2\sigma^2} + \frac{|w|}{b} \\ &= \operatorname{argmin}_w \frac{1}{2} \sum_{i=1}^n (y_i - wx_i)^2 + \frac{\sigma^2}{b} |w|.\end{aligned}$$

We can find that  $c = \frac{\sigma^2}{b}$ .

## II LINEAR CLASSIFICATION [12 points]

Let  $X$  be a  $d$ -dimensional binary vector, drawn from one of two classes:  $P$  or  $Q$ . Assume each element  $X_i$  in  $X$  is an independent Bernoulli random variable with parameter  $p_i$  when  $X$  drawn from class  $P$  (similarly, with parameter  $q_i$  for class  $Q$ ). That is

$$\begin{aligned} X_i|Y = P &\sim \text{Bernoulli}(p_i), & 1 \leq i \leq d, \\ X_i|Y = Q &\sim \text{Bernoulli}(q_i), & 1 \leq i \leq d. \end{aligned}$$

Note: for this problem, the values of  $p_i$  and  $q_i$ , along with priors  $\Pr(Y = P) = \pi_p$  and  $\Pr(Y = Q) = \pi_q$ , are known.

1. [3 points] Given a vector  $x \in \{0, 1\}^d$ , compute the probabilities  $\Pr(X = x|Y = P)$  and  $\Pr(X = x|Y = Q)$  in terms of class parameters  $p_i$  and  $q_i$ . Your answer must be a single expression for each probability.

**Solution**

$$\begin{aligned} \Pr(X = x|Y = P) &= \prod_{i=1}^d p_i^{x_i} (1 - p_i)^{1-x_i}, \\ \Pr(X = x|Y = Q) &= \prod_{i=1}^d q_i^{x_i} (1 - q_i)^{1-x_i}. \end{aligned}$$

2. [4 points] Please write down the equation which holds if and only if  $x$  is at the decision boundary of the Bayes' optimal classifier.

**Solution**

$$\begin{aligned} \Pr(Y = P|X = x) &= \frac{\Pr(X = x|Y = P) \Pr(Y = P)}{\Pr(X = x)}, \\ \Pr(Y = Q|X = x) &= \frac{\Pr(X = x|Y = Q) \Pr(Y = Q)}{\Pr(X = x)}, \end{aligned}$$

Therefore, the equation of decision boundary is

$$\pi_p \Pr(X = x|Y = P) = \pi_q \Pr(X = x|Y = Q).$$

3. [5 points] The decision boundary derived above is actually linear in  $x$ , which can be expressed as:

$$\{x \in \{0, 1\}^d | w^T x + b = 0\},$$

for some vector  $w$  and scalar  $b$ . Please find expressions for  $w$  and  $b$  in terms of priors ( $\pi_p$  and  $\pi_q$ ) and class parameters ( $p_i$  and  $q_i$ ).

**Solution**

$$\begin{aligned} \Pr(Y = P) \Pr(X = x|Y = P) &= \Pr(Y = Q) \Pr(X = x|Y = Q) \\ \pi_p \prod_{i=1}^d p_i^{x_i} (1 - p_i)^{1-x_i} &= \pi_q \prod_{i=1}^d q_i^{x_i} (1 - q_i)^{1-x_i} \\ \ln(\pi_p) + \sum_{i=1}^d [x_i \ln(p_i) + (1 - x_i) \ln(1 - p_i)] &= \ln(\pi_q) + \sum_{i=1}^d [x_i \ln(q_i) + (1 - x_i) \ln(1 - q_i)] \end{aligned}$$

where we can get:

$$\sum_{i=1}^d \left[ \ln \frac{p_i}{q_i} - \ln \frac{1-p_i}{1-q_i} \right] x_i + \ln \frac{\pi_p}{\pi_q} + \sum_{i=1}^d \ln \frac{1-p_i}{1-q_i} = 0.$$

Therefore,

$$w_i = \ln \frac{p_i}{q_i} - \ln \frac{1-p_i}{1-q_i}$$
$$b = \ln \frac{\pi_p}{\pi_q} + \sum_{i=1}^d \ln \frac{1-p_i}{1-q_i}.$$

### III GRAPHICAL MODEL [12 points]

We have a Bayesian network shown below, in which  $X_1, X_2, \dots, X_8$  are eight boolean random variables. Please answer the following questions.

**Note:** correct answers without proof will get 0 point.

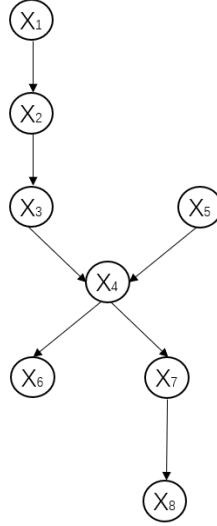


Figure 1: The Bayesian network with eight variables.

1. [3 points] Now we have known probabilities for some random variables. For  $X_1$ , we have  $\Pr(x_1) = 0.7$ . For  $X_2$ , we have  $\Pr(x_2|x_1) = 0.6$  and  $\Pr(x_2|\neg x_1) = 0.3$ . For  $X_3$ , we have  $\Pr(x_3|x_2) = 0.4$  and  $\Pr(x_3|\neg x_2) = 0.8$ . Apply the method of inference to calculate marginal probability  $\Pr(\neg x_3)$ .

**Note:** please round your results to 3 decimal places.

#### Solution

$$\begin{aligned}
 \Pr(\neg x_3) &= \sum_{x_1, x_2} \Pr(x_1, x_2, \neg x_3) \\
 &= \Pr(x_1) \Pr(x_2|x_1) \Pr(\neg x_3|x_2) + \Pr(x_1) \Pr(\neg x_2|x_1) \Pr(\neg x_3|\neg x_2) \\
 &\quad + \Pr(\neg x_1) \Pr(x_2|\neg x_1) \Pr(\neg x_3|x_2) + \Pr(\neg x_1) \Pr(\neg x_2|\neg x_1) \Pr(\neg x_3|\neg x_2) \\
 &= 0.7 \times 0.6 \times 0.6 + 0.7 \times 0.4 \times 0.2 + 0.3 \times 0.3 \times 0.6 + 0.3 \times 0.7 \times 0.2 \\
 &= 0.404.
 \end{aligned}$$

2. [3 points] Using the same probabilities for  $X_1, X_2, X_3$  in III.1, and apply the method of inference to calculate conditional probability  $\Pr(\neg x_2|\neg x_3)$ .

**Note:** please round your results to 3 decimal places.

#### Solution

$$\begin{aligned}
 \Pr(\neg x_2, \neg x_3) &= \sum_{x_1} \Pr(x_1, \neg x_2, \neg x_3) \\
 &= \Pr(x_1) \Pr(\neg x_2|x_1) \Pr(\neg x_3|\neg x_2) + \Pr(\neg x_1) \Pr(\neg x_2|\neg x_1) \Pr(\neg x_3|\neg x_2) \\
 &= 0.7 \times 0.4 \times 0.2 + 0.3 \times 0.7 \times 0.2 \\
 &= 0.098.
 \end{aligned}$$

$$\text{So } \Pr(\neg x_2|\neg x_3) = \frac{\Pr(\neg x_2, \neg x_3)}{\Pr(\neg x_3)} = 0.243.$$

3. [3 points] Prove that  $X_1 \perp\!\!\!\perp X_3 | X_2$  without using D-separation.

**Solution**

$$\Pr(X_1, X_3 | X_2) = \frac{\Pr(X_1, X_2, X_3)}{\Pr(X_2)} = \frac{\Pr(X_1, X_2) \Pr(X_3 | X_2)}{\Pr(X_2)} = \Pr(X_1 | X_2) \Pr(X_3 | X_2).$$

4. [3 points] Discuss whether the statement,  $X_1 \perp\!\!\!\perp X_5 | X_6$ , is true or not, and explain the reason based on D-separation.

**Solution**

The statement is false.

Given  $X_6$ , the path through  $X_1$  to  $X_5$  is open.

## IV EXPECTATION-MAXIMIZATION [10 points]

Given a Bayesian network with four discrete variables  $\{A, B, C, D\}$ , where  $\{A, C, D\}$  are boolean variables and  $B \in \{0, 1, 2\}$ . Suppose that  $\{A, C, D\}$  are observed variables and  $\{B\}$  is a latent variable. Now we implement EM algorithm for this model. Suppose there are  $K$  observations in total.  $(\{a_k, c_k, d_k\}_{k=1}^K)$ .

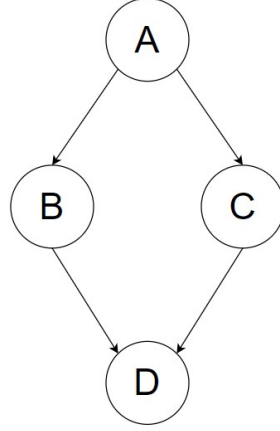


Figure 2: The Bayesian network with four discrete variables  $\{A, B, C, D\}$ .

1. [4 points] Derive the E-step.

### Solution

In E-step, calculate  $P(B|A, C, D, \theta)$ .

$$\begin{aligned}
 P(b_k = 0|a_k, c_k, d_k, \theta) &= \frac{P(b_k = 0, a_k, c_k, d_k|\theta)}{\sum_{i=0}^2 P(b_k = i, a_k, c_k, d_k|\theta)}, \\
 P(b_k = 1|a_k, c_k, d_k, \theta) &= \frac{P(b_k = 1, a_k, c_k, d_k|\theta)}{\sum_{i=0}^2 P(b_k = i, a_k, c_k, d_k|\theta)}, \\
 P(b_k = 2|a_k, c_k, d_k, \theta) &= \frac{P(b_k = 2, a_k, c_k, d_k|\theta)}{\sum_{i=0}^2 P(b_k = i, a_k, c_k, d_k|\theta)}.
 \end{aligned}$$

2. [6 points] Derive the M-step, and update parameters for the Bayesian network

### Solution

In M-step, choose  $\theta'$  which maximize  $E_{P(B|A, C, D, \theta)} \log P(A, B, C, D|\theta')$ , where

$$\begin{aligned}
 &E_{P(B|A, C, D, \theta)} \log P(A, B, C, D|\theta') \\
 &= \sum_{k=1}^K \sum_{i=0}^2 P(b_k = i|a_k, c_k, d_k, \theta) [\log P(a_k) + \log P(b_k|a_k) + \log P(c_k|a_k) + \log P(d_k|b_k, c_k)].
 \end{aligned}$$

Parameters are updated based on:

$$\begin{aligned}
\theta_a &= \frac{\sum_{k=1}^K \delta(a_k = 1)}{K}, \\
\theta_{b|a} &= \frac{\sum_{k=1}^K P(b_k = b) \delta(a_k = a)}{\sum_{k=1}^K \delta(a_k = a)}, \\
\theta_{c|a} &= \frac{\sum_{k=1}^K \delta(a_k = a, c_k = 1)}{\sum_{k=1}^K P(a_k = a)}, \\
\theta_{d|b,c} &= \frac{\sum_{k=1}^K \delta(d_k = 1, c_k = c) P(b_k = b)}{\sum_{k=1}^K \delta(c_k = c) P(b_k = b)}.
\end{aligned}$$



## V SUPPORT VECTOR MACHINES [12 points]

Support vector machines (SVM) are supervised learning models, that directly optimize for the maximum margin separator. Fig. 3 shows an example of maximum margin separator over a dataset  $S = \{(x_i, y_i)\}_{i=1}^n$ , in which  $x_i \in \mathbb{R}^2$  and  $y_i \in \{-1, 1\}$  denote the  $i$ -th sample and the  $i$ -th label ( $\forall i$ ), respectively. For simplicity, here we assume that the dataset  $S$  has been standardized, and thus the bias can be omitted in the linear model. In Fig. 3, “+” and “-” denote the samples with labels “1” and “-1”, respectively, and  $\mathbf{w}$  is the normal vector of the maximum margin separator  $\mathbf{w}^\top x = 0$ . You need to derive the optimization problem of SVM in the linearly separable case.

**Note:** correctly giving the results without detailed derivation will get 0 point.

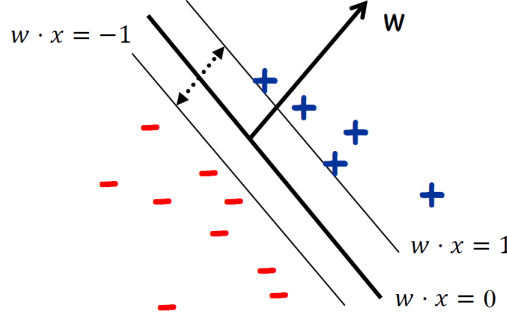


Figure 3: Maximum margin separator in the linearly separable case.

1. [5 points] Derive the constraint optimization problem of SVM in the separable case shown in Fig. 3.

### Solution

Let  $r$  be the margin between  $\mathbf{w}^\top x = 0$  and  $\mathbf{w}^\top x = 1$ . Assume there are two points  $x_0 \in \mathbb{R}^2$  and  $x_1 \in \mathbb{R}^2$  on  $\mathbf{w}^\top x = 0$  and  $\mathbf{w}^\top x = 1$ , respectively, and we make  $x_1 - x_0$  paralleled with  $\mathbf{w}$ . Hence, we have the following equations:

$$\begin{cases} \mathbf{w}^\top x_1 = 1, \\ \mathbf{w}^\top x_0 = 0, \\ x_1 - x_0 = r \times \frac{\mathbf{w}}{\|\mathbf{w}\|_2}, \end{cases}$$

where  $\|\cdot\|_2$  denotes the  $\ell_2$ -norm. By multiplying  $\mathbf{w}^\top$  on both sides of the third equation, and plugging the first two equations into it, we have

$$\begin{aligned} \mathbf{w}^\top (x_1 - x_0) &= r \times \frac{\mathbf{w}^\top \mathbf{w}}{\|\mathbf{w}\|_2} \\ 1 &= r \times \|\mathbf{w}\|_2, \\ \Rightarrow r &= \frac{1}{\|\mathbf{w}\|_2}. \end{aligned}$$

In the separable case, a maximum margin separator should satisfy the following three conditions:

- maximize the margin  $r = \frac{1}{\|\mathbf{w}\|_2}$  over a dataset;
- put positive samples ( $y_i = 1$ ) on one side of the separator, i.e.,  $\mathbf{w}^\top x_i \geq 1$ ;
- put negative samples ( $y_i = -1$ ) on another side of the separator, i.e.,  $\mathbf{w}^\top x_i \leq -1$ .

Therefore, the constraint optimization problem of SVM is

$$\begin{aligned} \min_{\mathbf{w}} \quad & \|\mathbf{w}\|_2^2, \\ \text{s.t.} \quad & y_i \mathbf{w}^\top x_i \geq 1, \quad \forall i \in \{1, 2, \dots, n\}. \end{aligned}$$

2. [5 points] Derive the dual problem of the above primal problem based on K.K.T. conditions.

### Solution

We first formulate the Lagrangian function of the primal problem:

$$L(\mathbf{w}, \xi, \alpha, \lambda) = \|\mathbf{w}\|_2^2 - \sum_{i=1}^n \alpha_i (y_i \mathbf{w}^\top x_i - 1),$$

where  $\alpha_i \geq 0$  ( $\forall i$ ) is the dual variable. Because strong duality holds in the primal problem, the optimal optimization variables  $\{\mathbf{w}^*, \alpha^*\}$  should satisfy K.K.T. conditions:

- primal:  $y_i \mathbf{w}^{*\top} x_i \geq 1, \forall i$ ,
- dual:  $\alpha_i^* \geq 0, \forall i$ ,
- complementary:  $\alpha_i^* (y_i \mathbf{w}^{*\top} x_i - 1) = 0, \forall i$ ,
- stationary:  $\nabla_{\mathbf{w}^*} L = 0$ .

According to the stationary condition, we have

$$\nabla_{\mathbf{w}} L = 2\mathbf{w} - \sum_{i=1}^n \alpha_i y_i x_i = 0, \quad \Rightarrow \quad \mathbf{w} = \frac{1}{2} \sum_{i=1}^n \alpha_i y_i x_i,$$

Substituting them into the Lagrangian function yields the dual function  $g(\alpha, \lambda)$ ,

$$\begin{aligned} g(\alpha) &= \inf_{\mathbf{w}, \xi} L(\mathbf{w}, \alpha) \\ &= \frac{1}{4} \left\langle \sum_{i=1}^n \alpha_i y_i x_i, \sum_{j=1}^n \alpha_j y_j x_j \right\rangle - \sum_{i=1}^n \alpha_i \left( y_i \left\langle \frac{1}{2} \sum_{j=1}^n \alpha_j y_j x_j, x_i \right\rangle - 1 \right) \\ &= -\frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n y_i y_j \alpha_i \alpha_j \langle x_i, x_j \rangle + \sum_{i=1}^n \alpha_i. \end{aligned}$$

Thus, the dual problem is

$$\begin{aligned} \max_{\alpha} \quad & -\frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n y_i y_j \alpha_i \alpha_j \langle x_i, x_j \rangle + \sum_{i=1}^n \alpha_i, \\ \text{s.t.} \quad & \alpha_i \geq 0, \forall i. \end{aligned}$$

3. **[2 points]** Kernel functions implicitly define some mapping function  $\phi(\cdot)$  that transforms an input instance  $x \in \mathbb{R}^d$  to a high or even infinite dimensional feature space  $Q$ , by giving the form of dot product in  $Q$ :  $k(x_i, x_j) = \phi(x_i)^\top \phi(x_j)$ . Please kernelize the dual problem, in order to learn a non-linear SVM classifier.

### Solution

Based on the dual problem, the kernelized SVM problem becomes

$$\begin{aligned} \max_{\alpha} \quad & -\frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n y_i y_j \alpha_i \alpha_j k(x_i, x_j) + \sum_{i=1}^n \alpha_i, \\ \text{s.t.} \quad & \alpha_i \geq 0, \forall i. \end{aligned}$$

## VI CLUSTERING [10 points]

Given six data points in 2D space (shown in Table 1) and two initial cluster centers  $c_1 = (0, 1), c_2 = (0, -1)$ , please answer the following questions.

$i$	$x$	$y$
1	-2	1
2	0	2
3	2	1
4	2	-1
5	0	-2
6	-2	-1

Table 1: Six input data points

1. [5 points] Please use  $k$ -means algorithm to cluster the given points into two groups.

### Solution

The first iteration is shown at Table 2.

According to the table, it is obvious that  $x_1, x_2$  and  $x_3$  should be clustered into one group and  $x_4, x_5$  and  $x_6$  should be clustered into the other group. The center points for two groups are  $c_1^{new} = (0, \frac{4}{3})$  and  $c_2^{new} = (0, -\frac{4}{3})$ .

$i$	$x$	$y$	distance to $c_1$	distance to $c_2$
1	-2	1	2	$2\sqrt{2}$
2	0	2	1	3
3	2	1	2	$2\sqrt{2}$
4	2	-1	$2\sqrt{2}$	2
5	0	-2	3	1
6	-2	-1	$2\sqrt{2}$	2

Table 2: Results of the first iteration.

2. [5 points] Please give the center points for the two groups after the algorithm converges.

### Solution

The second iteration is shown at Table 3.

We can find that the clustering result keeps the same as the first iteration so the algorithm converges. Above all,  $x_1, x_2$  and  $x_3$  should be clustered into one group with the center point  $(0, \frac{4}{3})$  and  $x_4, x_5$  and  $x_6$  should be clustered into the other group with center point  $(0, -\frac{4}{3})$ .

$i$	$x$	$y$	distance to $c_1^{new}$	distance to $c_2^{new}$
1	-2	1	$\sqrt{37}/3$	$\sqrt{85}/3$
2	0	2	$2/3$	$10/3$
3	2	1	$\sqrt{37}/3$	$\sqrt{85}/3$
4	2	-1	$\sqrt{85}/3$	$\sqrt{37}/3$
5	0	-2	$10/3$	$2/3$
6	-2	-1	$\sqrt{85}/3$	$\sqrt{37}/3$

Table 3: Results of the second iteration.

## VII DIMENSIONALITY REDUCTION [12 points]

Given three data points in 2D space:  $x_1 = \begin{bmatrix} -1 \\ 0 \end{bmatrix}$ ,  $x_2 = \begin{bmatrix} 0 \\ -1 \end{bmatrix}$ ,  $x_3 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$ , please answer the following questions:

**Note:** correct answers without detailed derivation will get 0 point.

1. [4 points] What are the first and second principal components?

**Solution**

$$\mathbf{X} = [x_1, x_2, x_3] = \begin{bmatrix} -1 & 0 & 1 \\ 0 & -1 & 1 \end{bmatrix}, \mathbf{X}^T = \begin{bmatrix} -1 & 0 \\ 0 & -1 \\ 1 & 1 \end{bmatrix}, \mathbf{X}\mathbf{X}^T = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$$

$$\mathbf{X}\mathbf{X}^T - \lambda\mathbf{I} = \begin{bmatrix} 2-\lambda & 1 \\ 1 & 2-\lambda \end{bmatrix}, |\mathbf{X}\mathbf{X}^T - \lambda\mathbf{I}| = (2-\lambda)^2 - 1 = 0 \Rightarrow (\lambda-3)(\lambda-1) = 0 \Rightarrow \lambda_1 = 3, \lambda_2 = 1$$

$$\text{When } \lambda = 3, \mathbf{X}\mathbf{X}^T - \lambda\mathbf{I} = \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix} \Rightarrow \begin{bmatrix} -1 & 1 \\ 0 & 0 \end{bmatrix} \Rightarrow v_1 = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}$$

$$\text{When } \lambda = 1, \mathbf{X}\mathbf{X}^T - \lambda\mathbf{I} = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \Rightarrow \begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix} \Rightarrow v_2 = \begin{bmatrix} -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}$$

So the first and second principal component directions are  $v_1 = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}$ ,  $v_2 = \begin{bmatrix} -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}$  respectively.

2. [4 points] If we project the original data points on the new coordinate system represented by the principal components, what are their coordinates?

**Solution**

Let  $z_1, z_2, z_3$  denote the points in the new coordinate system represented by the principal component directions.

$$z_1 = \begin{bmatrix} x_1^T v_1 \\ x_1^T v_2 \end{bmatrix} = \begin{bmatrix} -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}, z_2 = \begin{bmatrix} -\frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix}, z_3 = \begin{bmatrix} \sqrt{2} \\ 0 \end{bmatrix}.$$

3. [4 points] What is the variance of the data in each direction? Verify that it is equal to the total variance of the origin data.

**Solution**

Variance of the first direction:  $Var_1 = \frac{1}{3}[(-\frac{1}{\sqrt{2}})^2 + (-\frac{1}{\sqrt{2}})^2 + (\sqrt{2})^2] = 1$ .

Variance of the second direction:  $Var_2 = \frac{1}{3}[(\frac{1}{\sqrt{2}})^2 + (-\frac{1}{\sqrt{2}})^2] = \frac{1}{3}$ .

Total variance of the origin data:  $Var_{origin} = \frac{1}{3}[(-1)^2 + 1^2 + (-1)^2 + 1^2] = \frac{4}{3}$ .

It is obvious that  $Var_{origin} = Var_1 + Var_2$ .

## VIII NEURAL NETWORKS [12 points]

As shown in Fig.4, we have a feed-forward neural network with two hidden-layer nodes and one output node, and  $x_1$  and  $x_2$  are two inputs. For simplicity, the bias  $b$  is omitted here. For the following questions, assume the learning rate  $\eta$  in gradient descent is fixed by  $\eta = 0.1$ . Both hidden and output units use the same activation function  $g(\cdot)$ .

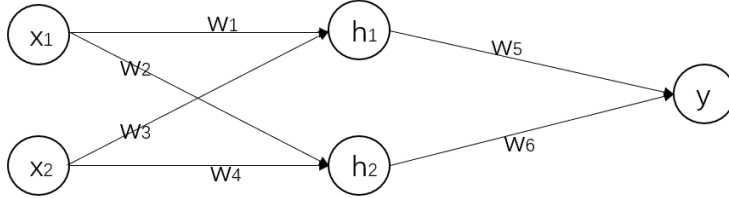


Figure 4: The Neural network with one hidden layer.

1. [4 points] Express the output  $y_{\text{output}}$  in terms of inputs  $x_1, x_2$ , weights  $w_1, w_2, w_3, w_4, w_5, w_6$  and the activation function  $g$ .

**Solution**

$$y_{\text{output}} = g(w_5 h_1 + w_6 h_2) = g(w_5 g(w_1 x_1 + w_3 x_2) + w_6 g(w_2 x_1 + w_4 x_2)).$$

2. [8 points] Assume we have one input  $\{x_1 = 1, x_2 = 1\}$  and the real target of it is  $y_{\text{target}} = 1$ . The initial value of  $w_1^{(0)}, w_2^{(0)}, w_3^{(0)}, w_4^{(0)}, w_5^{(0)}, w_6^{(0)}$  is  $1, 2, -1, \frac{1}{2}, -2, 1$ . And the loss on the given example is defined as  $L = \frac{1}{2}(y_{\text{target}} - y_{\text{output}})^2$ . Suppose that the sigmoid activation function  $g(z) = \frac{1}{1+e^{-z}}$  is used.  
**Note:** please round your results to 3 decimal places.

- (1) [3 points] Without any optimization, calculate the output  $h_1, h_2$  and  $y_{\text{output}}$  on the given example.

**Solution**

$$\begin{aligned}
 h_1 &= g(w_1 x_1 + w_3 x_2) = g(0) = \frac{1}{2} \\
 h_2 &= g(w_2 x_1 + w_4 x_2) = g(2.5) = 0.924 \\
 y_{\text{output}} &= g(w_5 g(w_1 x_1 + w_3 x_2) + w_6 g(w_2 x_1 + w_4 x_2)) \\
 &= g(-2g(0) + g(2.5)) \\
 &= 0.481.
 \end{aligned}$$

- (2) [5 points] Compute the updated weights  $w_1^{(1)}, w_2^{(1)}, w_3^{(1)}, w_4^{(1)}, w_5^{(1)}, w_6^{(1)}$  by performing ONE step of gradient descent. Show all steps in your calculation.

**Solution**

$$\begin{aligned}
\Delta w_5 &= (0.481 - 1) \times 0.481 \times (1 - 0.481) \times 0.5 = -0.0648, \\
\Delta w_6 &= (0.481 - 1) \times 0.481 \times (1 - 0.481) \times 0.924 = -0.1198, \\
\Delta w_1 &= (0.481 - 1) \times 0.481 \times (1 - 0.481) \times (-2) \times 0.5 \times (1 - 0.5) \times 1 = 0.0648, \\
\Delta w_2 &= (0.481 - 1) \times 0.481 \times (1 - 0.481) \times (1) \times 0.924 \times (1 - 0.924) \times 1 = -0.0091, \\
\Delta w_3 &= (0.481 - 1) \times 0.481 \times (1 - 0.481) \times (-2) \times 0.5 \times (1 - 0.5) \times 1 = 0.0648, \\
\Delta w_4 &= (0.481 - 1) \times 0.481 \times (1 - 0.481) \times (1) \times 0.924 \times (1 - 0.924) \times 1 = -0.0091, \\
w_1^{(1)} &= w_1^{(0)} - 0.1 \times \Delta w_1 = 0.994, \\
w_2^{(1)} &= w_2^{(0)} - 0.1 \times \Delta w_2 = 2.001, \\
w_3^{(1)} &= w_3^{(0)} - 0.1 \times \Delta w_3 = -1.006, \\
w_4^{(1)} &= w_4^{(0)} - 0.1 \times \Delta w_4 = 0.501, \\
w_5^{(1)} &= w_5^{(0)} - 0.1 \times \Delta w_5 = -1.994, \\
w_6^{(1)} &= w_6^{(0)} - 0.1 \times \Delta w_6 = 1.012.
\end{aligned}$$

## IX CONVOLUTIONAL NEURAL NETWORKS [8 points]

Convolutional neural networks are designed to process 2D features instead of the 1D ones in multi-layer perceptron (MLP).

1. [4 points] Please calculate the feature map based on 2D convolution, if you are given the following  $5 \times 5$  image matrix in Table 4 and  $2 \times 2$  kernel matrix in Table 5. (stride = 1, no padding)

1	2	3	4	5
6	7	8	9	10
11	12	13	14	15
16	17	18	19	20
21	22	23	24	25

Table 4:  $5 \times 5$  image matrix.

1	0
0	1

Table 5:  $2 \times 2$  kernel matrix.

### Solution

The feature map is shown in Table 6.

8	10	12	14
18	20	22	24
28	30	32	34
38	40	42	44

Table 6:  $4 \times 4$ -feature maps.

2. [4 points] Based on the above result, calculate the feature maps after max-pooling and average-pooling, respectively. (both pooling with  $2 \times 2$  filters and stride = 2)

### Solution

Please refer to Tables 7 and 8.

20	24
40	44

Table 7: After max-pooling.

14	18
34	38

Table 8: After average-pooling.