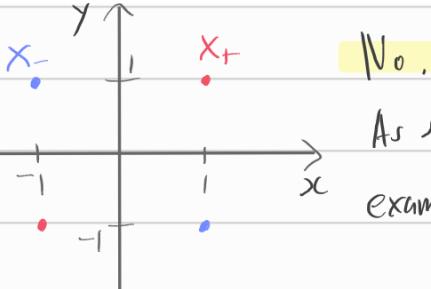


## 1.1 SVM (20 points)

2-D

Suppose that training examples are points in 2-D space. The positive examples are  $X_+ = \{(1, 1), (-1, -1)\}$ . The negative examples are  $X_- = \{(1, -1), (-1, 1)\}$ .

(a) [4 pts] Are the positive examples linearly separable from the negative examples? (i.e. can you draw a line to separate the positive examples from negative examples)?



No.  
As seen in the left graph, a single line cannot separate positive examples from the negative examples. Linear boundary fails.

(b) [8 pts] Consider the feature transformation  $\phi(x) = [1, x, y, xy]^T$ , where  $x$  and  $y$  are the first and second coordinates of an example. Write down the transformed coordinates of  $X_+$  and  $X_-$  (i.e.  $\phi(X_+)$  and  $\phi(X_-)$  for all four examples).

$$\begin{aligned} \text{For } (x, y) \in X_+, \phi((1, 1)) &= [1, 1, 1, 1]^T & \text{For } (x, y) \in X_-, \phi((1, -1)) &= [1, 1, -1, -1]^T \\ \phi((-1, -1)) &= [1, -1, -1, 1]^T & \phi((-1, 1)) &= [1, -1, 1, -1]^T \\ \therefore \phi(X_+) &= \{(1, 1, 1, 1), (1, -1, -1, 1)\}, \quad \phi(X_-) &= \{(1, 1, -1, -1), (1, -1, 1, -1)\} \end{aligned}$$

(c) [8 pts] Consider the prediction function  $y(x) = w^T \phi(x)$ . Give the coefficient  $w$  of a maximum-margin decision surface separating the positive from the negative examples.

(hint:  $w$  is  $[4 \times 1]$  vector, whose elements are only 0 or 1).

$$\begin{aligned} \text{Let } w &= [w_1, w_2, w_3, w_4]^T, \quad w_i = 0 \text{ or } 1 \\ \rightarrow \min_w \|w\|^2 \text{ s.t. } y_i(w^T \phi(x_i)) &\geq 1 \quad \text{for } i=1, 2, 3, 4 \end{aligned}$$

To express this problem as a maximization problem (dual form):

$$\rightarrow \max_{\alpha} \sum_{i=1}^4 \alpha_i - \frac{1}{2} \sum_{i=1}^4 \sum_{j=1}^4 \alpha_i \alpha_j y_i y_j \phi(x_i)^T \phi(x_j) \quad \text{s.t. } 0 \leq \alpha_i \leq C \text{ for all } i \text{ and } \sum_{i=1}^4 \alpha_i y_i = 0$$

$$\rightarrow \max_{\alpha} \sum_{i=1}^4 \alpha_i - \frac{1}{2} (4\alpha_1\alpha_1 + 4\alpha_2\alpha_2 + 4\alpha_3\alpha_3 + 4\alpha_4\alpha_4)$$

$$\rightarrow \max_{\alpha} \alpha_1(1-2\alpha_1) + \alpha_2(1-2\alpha_2) + \alpha_3(1-2\alpha_3) + \alpha_4(1-2\alpha_4)$$

$$\text{Since constraint: } \sum_{i=1}^4 \alpha_i y_i = \alpha_1 - \alpha_2 - \alpha_3 + \alpha_4 = 0$$

$$\rightarrow \alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = \frac{1}{4}$$

$$\begin{aligned} w &= \sum_{i=1}^4 \alpha_i y_i \phi(x_i) = \frac{1}{4} \cdot 1 \cdot [1, 1, 1, 1]^T + \frac{1}{4} \cdot 1 \cdot [1, -1, -1, 1]^T + \frac{1}{4} \cdot (-1) \cdot [1, 1, -1, -1]^T + \frac{1}{4} \cdot (-1) \cdot [1, -1, 1, -1]^T \\ &= [0, 0, 0, 1]^T \end{aligned}$$

## 1.2 K-means (20 points)

(a) [4 pts] Mahalanobis measure is one of many distance measure used for  $k$ -means. Given the below definition, describe the shape of the covariance matrix corresponding to  $\sigma_i$  and explain why Mahalanobis measure is also called scaled euclidean measure in this case.

$$d(x, c) = \sqrt{\sum_{i=1} (x_i - c_i)^2 / s_i^2} \quad \dots \textcircled{1}$$

As Mahalanobis measure is a measure of the distance between a point  $P$  and a distribution  $D$ , it takes into account the correlation between data. The formal definition of the Mahalanobis distance is as follows:  $d(x, c) = \sqrt{(x - c)^T C^{-1} (x - c)}$ ,  $C$  is the covariance matrix  $\dots \textcircled{2}$

We must find  $C^{-1}$  that satisfies  $\textcircled{2} = \textcircled{1}$ . This equation can be expressed by matrices:

$$\sqrt{\begin{bmatrix} x_1 - c_1 & x_2 - c_2 & \dots & x_n - c_n \end{bmatrix} C^{-1} \begin{bmatrix} x_1 - c_1 \\ x_2 - c_2 \\ \vdots \\ x_n - c_n \end{bmatrix}} = \sqrt{\sum_{i=1} (x_i - c_i)^2 / s_i^2}$$

Therefore,  $C^{-1}$  should be  $\begin{bmatrix} 1/s_1^2 & 0 & \dots & 0 \\ 0 & 1/s_2^2 & & \vdots \\ \vdots & & \ddots & 0 \\ 0 & \dots & 0 & 1/s_n^2 \end{bmatrix}$

$$(C^{-1})^{-1} = C = \begin{bmatrix} s_1^2 & 0 & \dots & 0 \\ 0 & s_2^2 & & \vdots \\ \vdots & & \ddots & 0 \\ 0 & \dots & 0 & s_n^2 \end{bmatrix} \leftarrow \text{covariances are all } 0 \text{s}$$

$\therefore$  The covariance matrix is a diagonal matrix with  $s_i$  as the diagonal elements, i.e.,  $C = \{s_1^2, \dots, s_n^2\}$

The Euclidean distance is defined as follows:  $d(x, c) = \sqrt{\sum_{i=1} (x_i - c_i)^2}$

In the formal Euclidean distance, since distance between every data are added, the distance value can be flawed due to different scales and correlation between data. Now

$x$  can be standardized into  $z = \frac{x - c}{s}$ , where  $c$  is the vector of mean values.

Thus, the scaled Euclidean measure formula becomes  $d(x, c) = \sqrt{\sum_{i=1} \frac{(x_i - c_i)^2}{s_i^2}}$ , which is equal to the given Mahalanobis formula.

(b) [8 pts] Given a dataset  $\mathcal{X} = \{0, 2, 4, 6, 18, 20\}$ , initialize the  $k$ -means clustering algorithm with 2 cluster centers  $c_1 = 3$  and  $c_2 = 4$ . What are the values of  $c_1$  and  $c_2$  after the first iteration of  $k$ -means? Also report the values after the second iteration.

As the dataset is one-dimensional, we use the Euclidean as the distance measure.  
 $d(p, q) = |p - q|$

$X$	0	2	4	6	18	20	after first iteration:
distance from $c_1 = 3$	3	1	1	3	15	17	$\Rightarrow \frac{0+2}{2} = 1 \quad \therefore c_1 = 1$
distance from $c_2 = 4$	4	2	0	2	14	16	$\frac{4+6+18+20}{4} = 12 \quad c_2 = 12$
			↓				
distance from $c_1 = 1$	1	1	3	5	17	19	after second iteration:
distance from $c_2 = 12$	12	10	8	6	6	8	$\frac{0+2+9+6}{4} = 3 \quad \therefore c_1 = 3$ $\frac{18+20}{2} = 19 \quad c_2 = 19$

(c) [8 pts] Given the same dataset as in (b), perform greedy initialization to get the initial  $k = 3$  centers. Start with  $c_1 = 4$ . Below is the greedy initialization process.

1. Choose  $c_1$
2. Choose the next center  $c_i$  to be  $\operatorname{argmax}_{x \in \mathcal{X}} \{D(x)\}$
3. Repeat step 2 until  $k$  centers are chosen  
where at any given time, with the current set of cluster centers  $\mathcal{C}$ ,

$$D(x) = \min_{c \in \mathcal{C}} \|x - c\|_2 \quad \mathcal{X} = \{0, 2, 4, 6, 18, 20\}$$

$i=1 : C_1 = 4$	$x$	0	2	4	6	18	20	
$C = \{4\}$	$D(x)_1$	4	2	0	2	14	16	$\Rightarrow c_2 = 20$
$i=2 : C = \{4, 20\}$	$D(x)_2$	$<^4_{20}$	$<^2_{18}$	$<^0_{16}$	$<^2_{14}$	$<^{14}_{2}$	$<^{16}_{0}$	$\Rightarrow c_3 = 0$
								$\therefore C = \{0, 4, 20\}$

cf) In a more mathematical way, let the step of iteration be  $i$ .

$$i=0 : C_1 = 4 \quad (k=1)$$

$i=1 : \text{Choose the next center } C_2 \text{ to be } \operatorname{argmax}_{x \in \mathcal{X}} \{D(x)\}$

$$D(0)=4, D(2)=2, D(4)=0, D(6)=2, D(18)=14, D(20)=16 \\ \therefore C_2 = 20 \quad (k=2)$$

$i=2 : \text{Choose the next center } C_3 \text{ to be } \operatorname{argmax}_{x \in \mathcal{X}} \{D(x)\}$

$$D(0)=\min(10-4, 10-20) = \min(4, 20) = 4$$

$$D(2)=\min(12-4, 12-20) = \min(2, 18) = 2$$

$$D(4)=\min(14-4, 14-20) = \min(0, 16) = 0$$

$$D(18) = \min(|18-4|, |18-20|) = \min(14, 2) = 2$$

$$D(20) = \min(|20-4|, |20-20|) = \min(16, 0) = 0$$

$$\therefore C_3 = 0 \quad (k=3)$$

Now that  $k=3$ ,  $C = \{C_1, C_2, C_3\} = \{0, 4, 20\}$