



MFML Team



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#### Q4 Answer the following questions with justifications.

The figure below shows 4 points, representing some data in  $\mathbb{R}^2$ 

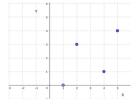


Figure 1. PCA

(A) Find the principal components for the given points.

NOTE: use

$$cov(X) = \frac{1}{N}(X - \mu)^{T}(X - \mu)$$

(5 marks)

- $\mbox{\bf (B)}$  Find the components of the four points along their first principal component.
  - (2 marks)
- (C) What is the percentage variance captured by the first principal component?

(1 mark)

(D) If the points are rotated anticlockwise by 90 degrees, what will the components (of the rotated points) along their first principal component be? (2 marks)



The figure below shows 4 points, representing some data in  $\mathbb{R}^2$ 

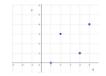


Figure 1. PCA

(A) The four points are (2, 3), (4, 1), (5, 4) and (1, 0) This data X is represented as:

$$\mathbf{X} = \begin{bmatrix} 2 & 4 & 5 & 1 \\ 3 & 1 & 4 & 0 \end{bmatrix}$$
  
 $\mu = \begin{bmatrix} 12/4 \\ 8/4 \end{bmatrix} = \begin{bmatrix} 3 \\ 2 \end{bmatrix}$ 

(1 mark)

$$\mathbf{X} - \mu = \begin{bmatrix} -1 & 1 & 2 & -2 \\ 1 & -1 & 2 & -2 \end{bmatrix}$$

$$\mathbf{cov}(\mathbf{X}) = \frac{1}{4} \begin{bmatrix} -1 & 1 & 2 & -2 \\ 1 & -1 & 2 & -2 \end{bmatrix} \begin{bmatrix} -1 & 1 \\ 1 & -1 \\ 2 & 2 \\ -2 & -2 \end{bmatrix} = \frac{1}{4} \begin{bmatrix} 10 & 6 \\ 6 & 10 \end{bmatrix}$$

(2 marks)

To find eigen values and eigen vectors:  
eigen values:  

$$\lambda^2 - 5\lambda + 4 = 0 \implies \lambda = 4.1$$

 $\lambda^2 - 5\lambda + 4 = 0 \implies \lambda$ 

$$\lambda = 4 \implies v_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$
  
 $\lambda = 1 \implies v_2 = \begin{bmatrix} -1 \\ 1 \end{bmatrix}$ 

Principal component directions:  $\lceil 1/\sqrt{2} \rceil$ 

$$\begin{bmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$$

(B) The components along first PC are:

$$\begin{split} \vec{x}_1 &= x_1^T * e_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 2 & 3 \end{bmatrix} * \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \frac{5}{\sqrt{2}} \\ \vec{x}_2 &= \frac{5}{\sqrt{2}} \\ \vec{x}_3 &= \frac{9}{\sqrt{2}} \\ \vec{x}_4 &= \frac{1}{\sqrt{6}} \end{split}$$

(2 marks)

(2 marks)

(C) Percentage variance captured by first component =  $\frac{4}{4+1} = 0.8$  (i.e., 80%) (1 mark)

(D) Rotating all the points by same angle does not affect the components along the principal component. It will be smae as the answer in part (R) (2 mark)

### Agenda



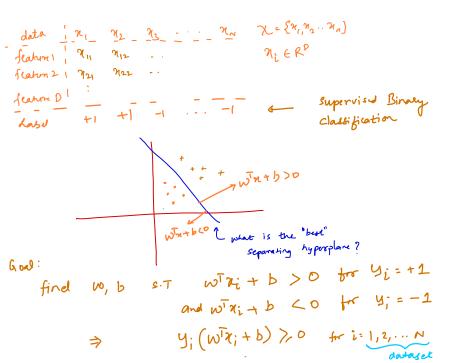
# Mathematical preliminaries for Support Vector Machines Profession of plane of sym Constrained optimization and Lagrange multipliers.

- Primal and dual problems and how their solutions are related
- Karash-Kuhn-Tucker conditions.
- Definition of Kernel Functions
- Linear Classifiers

Equation of normal to a plane Po -> a specific point on plane P -> any point on plane P-Po -> line completely on the plane n -> I' dir. to plane  $\Rightarrow$   $(P-P_0)$ .  $\hat{n}=0$ 2 - P-P. y-40 7-50 [ nx ] = 0 (x-70) nx + (y-40) ny + (x-20) n2 =0 ax + by + C2 +d=0 Plane egn: n = [a b c]intersection on 2-axis = d

Distance between two planes P1: Ax + by + C= = d, p2: an + by + c2 = d2 n= (a b c)  $\sqrt{a^2+b^2+c^2}$ 2=0 y=0 => == d1 distance between = [0 0 planes = for planes in higher dim: = d1 P1: ax + azy + azz + ..... = d2 P2: 0/2 + 0/2 + 0/3 + 0/11 distance blue planes = d2-011 - = oh- di

 $\sqrt{a_1^2 + a_2^2 + \cdots}$ 



Add a margin y; (w<sup>T</sup>x;tb) ≥ ~ Y; (wa; +b) > 1 fr i= 1,2,... N dayaset  $\Rightarrow \begin{array}{c} \alpha_{1}\alpha_{1}+\alpha_{2}\alpha_{1}+\dots=d_{1} \\ \alpha_{1}\alpha_{1}+\alpha_{2}\alpha_{1}+\dots=d_{2} \end{array}$ For the sample on boundary: WTX + b = 1 For -re sample on boundary: WTx +b = -1 Distance between these planes = (1-b)-(-1-b) = 2 JW2+W2+.. 11 W11 Goal: i=1,2,...~ 4; (wTx; +b) >, 1 Susj to: maximize 2 or min 1/11111 Subj to Y; (WTX; +b) 7,1 ; 2 1, 2, .. N

min  $\frac{1}{2} \| w \|^{2} + C \sum_{i=1}^{N} i$ ; Sug to  $y_{i} (w^{2}x_{i} + b) > 1 - 8i - 2$ 

0<8;<1 >> for its Sample, we are relaxing the constraint.

The Sample can be inside the boundary

8;>1 >> Sample is mis classified.

:, C, now acts as a regularization term.

C is large => all 8; are small (as we are minimizing (1);)

=> all samples perfectly classified -> Hard Margin

classifier.

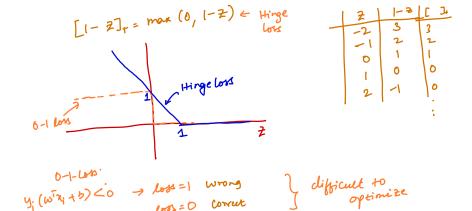
C is Small ⇒ 8°; Can be large to allow some misclassifications

→ Soft margin

classifier.

min  $\frac{1}{2} \| \mathbf{w} \|^{2} + C \sum_{i=1}^{N} \left[ 1 - y_{i} \left( \mathbf{w}^{T} a_{i} + b \right) \right]_{+}$ where [2], = max (9,2) Contet. =) [1- 4; (wx; +6)] = 1 means incorrectly classified (or inside boundary)

into picture for mis classified Samples only.



$$y_i(\omega^i x_i + b) > 0 \rightarrow loss = 0$$
 convut  
 $y_i(\omega^i x_i + b) > 0 \rightarrow loss = 0$  convut  
 $0$  So. (3) Can be thought  $0$ :

### Optimization problem



We shall work with the following optimization problem:

Together 
$$f(x)$$
 subject to 
$$g_i(x) \leq 0 \ \forall i \in [m] \quad \text{Inequality}$$
 constraint. 
$$h_j(x) = 0 \ \forall j \in [p] \quad \text{equality}$$
 constraint. 
$$\lim_{x \to \infty} \frac{1}{2} \lim_{x \to \infty} \frac{1}{x} + C \sum_{i \geq 1}^{n} \frac{1}{x^2} + C \sum_{i \geq 1}^{n} \frac{1}{x^2}$$

### Optimization problem: Lagrangian



The Lagrangian associated with this optimization problem is

$$\min f(\mathbf{x}) + \sum_{i=1}^{i=m} \lambda_i g_i(\mathbf{x}) + \sum_{j=1}^{j=p} \nu_j h_j(\mathbf{x})$$

V;

▶ The  $\lambda_i$ 's and  $\kappa$ 's are called Lagrange multipliers.

$$\mathcal{L}(x, \lambda_{i}, \nu_{j}) = f(x) + \sum_{i=1}^{\infty} \lambda_{i} g(x) + \sum_{j=1}^{\infty} \nu_{j} h_{j}(x)$$

when  $x$  is
$$f(x) = f(x)$$

Strong duality exists if: - f(x) is Convex - 9; (m) is conver - him are linear - mild Regularity Condition holds Lo one Such is Slater condition - at least one point exists in feasible region where  $g_i(x) < 0 \leftarrow Strict$ inequality & L:(x) = 0

### Quadratic programming



#### Consider the following primal problem:

► We now consider the case of a quadratic objective function subject to affine constraints:

$$\min_{oldsymbol{x} \in \mathbb{R}^d} rac{1}{2} oldsymbol{x}^T oldsymbol{Q} oldsymbol{x} + oldsymbol{c}^T oldsymbol{x}$$
 subject to  $oldsymbol{A} oldsymbol{x} \leq oldsymbol{b}$ 

▶ Here  $\mathbf{A} \in \mathbb{R}^{m \times d}, b \in \mathbb{R}^m, c \in \mathbb{R}^d$ 

### Quadratic programming



- The Lagrangian  $\mathfrak{L}(x, \lambda)$  is given by  $\frac{1}{2}x^TQx + c^Tx + \lambda^T(Ax b)$ .
- Rearranging the above we have  $\mathfrak{L}(\mathbf{x}, \boldsymbol{\lambda}) = \frac{1}{2} \mathbf{x}^T \mathbf{Q} \mathbf{x} + (\mathbf{c} + \mathbf{A}^T \boldsymbol{\lambda})^T \mathbf{x} \boldsymbol{\lambda}^T \mathbf{b}$



▶ Taking the derivative of  $\mathfrak{L}(x, \lambda)$  and setting it equal to zero gives  $Qx + (c + A^T\lambda) = 0$ .

### Quadratic programming



#### We will now derive the dual problem

- ▶ If we take Q to be invertible, we have  $x = Q^{-1}(c + A^T \lambda)$ .
- Plugging this value of  $\mathbf{x}$  into  $\mathfrak{L}(\mathbf{x}, \lambda)$  gives us  $\mathfrak{D}(\lambda) = -\frac{1}{2}(\mathbf{c} + \mathbf{A}^T \lambda)\mathbf{Q}^{-1}(\mathbf{c} + \mathbf{A}^T \lambda) \lambda^T \mathbf{b}$ .
- This gives us the dual optimization problem:  $\max_{\boldsymbol{\lambda} \in \mathbb{R}^m} -\frac{1}{2}(\boldsymbol{c} + \boldsymbol{A}^T\boldsymbol{\lambda})\boldsymbol{Q}^{-1}(\boldsymbol{c} + \boldsymbol{A}^T\boldsymbol{\lambda}) \boldsymbol{\lambda}^T\boldsymbol{b}$  subject to  $\boldsymbol{\lambda} > \boldsymbol{0}$ .



### Summary



#### The original problem is:



$$\min_{\boldsymbol{x} \in \mathbb{R}^d} \frac{1}{2} \boldsymbol{x}^T \boldsymbol{Q} \boldsymbol{x} + \boldsymbol{c}^T \boldsymbol{x}$$
subject to  $\boldsymbol{A} \boldsymbol{x} \leq \boldsymbol{b}$ 

The dual problem is

$$\max_{\boldsymbol{\lambda} > 0} -\frac{1}{2} (\boldsymbol{c} + \boldsymbol{A}^T \boldsymbol{\lambda}) \boldsymbol{Q}^{-1} (\boldsymbol{c} + \boldsymbol{A}^T \boldsymbol{\lambda}) - \boldsymbol{\lambda}^T \boldsymbol{b}$$

### Weak duality



- Weak duality establishes an inequality connecting primal and dual problems
- Weak duality condition states that the optimal solution of the primal problem is greater than or equal to that of the dual problem.
- In the Quadratic Optimization problem discussed previously , weak duality exists

### Strong duality



- Strong duality condition states that the optimal solution of the primal problem is equal to that of the dual problem
- One can solve the dual problem to get the same solution as solving the primal problem.
- ▶ In some optimization problems, solving the dual problem may be easier.
- Question: When does strong duality hold?

#### Slater's condition



- ► For a primal optimization problem we say that it obeys Slater's condition if
  - 1. the objective function  $\underline{f}$  is convex, the constraints  $\underline{g}_i$  are all convex, the contraint functions  $h_i$  are all linear
  - 2. there exists a point  $\bar{x}$  in the interior of the region, i.e  $g_i(\bar{x}) < 0$  for all  $i \in [m]$  and  $h_i(\bar{x}) = 0$  for all  $j \in [p]$ .
- **/**
- Suppose Slater's condition holds then we have strong duality.
- Strong duality condition states that the optimal solution of the primal problem is equal to that of the dual problem

### Example of Slater's condition



We will consider an optimization problem as given below

$$\min x^2 + y^2$$
  
$$\operatorname{st} x + y - 3 \le 0$$

- ► Here  $f(x,y) = x^2 + y^2$  is a convex function and g(x,y) = x + y 3 is a convex function
- ▶ We can find a point that satisfies the condition x + y 3 < 0
- Slaters condition is satisfied

when strong duality holds., (x\*, x\*, v\*) satisfy KKT by not is primal Sol. Primal is Convex & Slater's Condition is 7, or are dual set? Satisfical if primal is:

min f(n) swj to g; (n) < 0 i = 1,2,...m n; m) = 0 j=1,2,...P then K.K.T for (2", 1", U") is: 1) Prime featibility: 9; (no) < 0 h hills = 0 i= cm), i= (n)
2) Dual featibility: 1; >, 0 i= (n) 3) Complementary slacenes: 1; 9; (x\*) =0 [m] > elther ); =0 or f; (x) =0 4) Vanishing gradients (stationarity):  $\nabla d: \nabla f(x^*) + \sum_{j=1}^{n} \lambda_j^* \nabla g_j(x^*) + \sum_{j=1}^{p} v_j^* \nabla h_j(x^*) = 0$ 

#### KKT conditions



min 
$$f(\mathbf{x})$$
 st  $g_i(\mathbf{x}) \leq 0 \ \forall i \in [m], \ h_i(\mathbf{x}) = 0 \ \forall j \in [p]$ 

We say that  $\mathbf{x}^*$  and  $(\lambda^*, \nu^*) \in \mathbb{R}^m \times \mathbb{R}^p$  respect the Karash-Kuhn-Tucker conditions if:

- 1.  $g_i(\mathbf{x}^*) \leq 0 \ \forall i \in [m], \ h_i(\mathbf{x}^*) = 0 \ \forall i \in [p].$
- 2.  $\lambda_i^* \geq 0 \ \forall i \in [m]$ .
- 3.  $\lambda_i^* g_i(\mathbf{x}^*) = 0 \ \forall i \in [m].$
- 4.  $\nabla f(\mathbf{x}^*) + \sum_{i=1}^{i=m} \lambda_i^* \nabla g_i(\mathbf{x}^*) + \sum_{i=1}^{i=p} \nu_i^* \nabla h_i(\mathbf{x}^*) = 0.$

If strong duality holds then any primal optimal solution  $x^*$  and dual optimal solution  $(\lambda^*, \nu^*)$  satisfy the KKT conditions.

#### KKT condition



## We will consider an optimization problem and will write its KKT conditions

$$\min x^2 + y^2$$
  
st  $x + y - 3 \le 0$ 

► Here 
$$f(x,y) = x^2 + y^2$$
 and  $g(x,y) = x + y - 3$ 

1. 
$$x + y - 3 \le 0$$

2. 
$$\lambda \geq 0$$

3. 
$$\lambda(x + y - 3) = 0$$

**4**. 
$$\nabla f + \lambda \nabla g = \mathbf{0}$$

### Classification Problem in Machine Learning



- ► Classification of data into different classes is one of the primary problems in machine learning
- Binary classification involves classifying data into exactly 2 classes
- There exists different algorithms for binary classification
- We will discuss a model called Support Vector Machine.
- SVM is a linear classifer model for binary classification

#### Linear Classifier

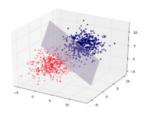


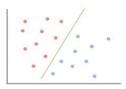
$$\mathbf{w}^T \mathbf{x} = 0$$

$$y = ax + b$$

### Hyperplane

### Line





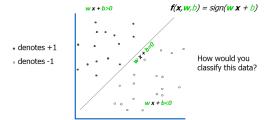
### Linear Classifier and Hyperplane



- Consider line  $w^T x + b = 0$ . Let  $x_a$  and  $x_b$  lie on this line. So  $w^T x_a + b = 0$  and  $w^T x_b + b = 0$ .
- ► This means  $w^T(x_a x_b) = 0$ .  $x_a x_b$  lies on the line and is directed from  $x_b$  to  $x_a$ .
- ▶ Hence w is orthogonal to  $x_a x_b$  and in turn, to the line.

### Linear Classifer for Binary Classification

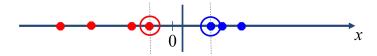




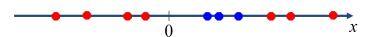
### Two examples of data



Dataset that are linearly separable with some noise



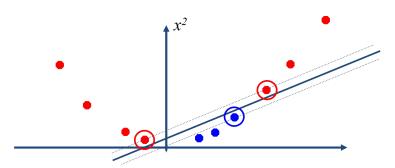
Dataset is not linearly separable



### Mapping of Data



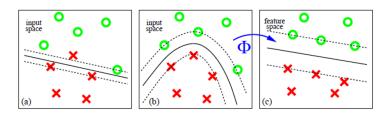
### mapping data to a higher-dimensional space:



### Mapping of Data



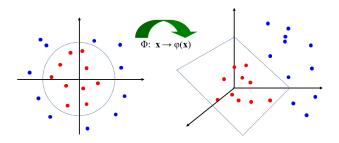
#### Find a feature space



If every data point is mapped into high-dimensional space via some transformation  $\phi: x \to \phi(x)$ 

### Feature spaces

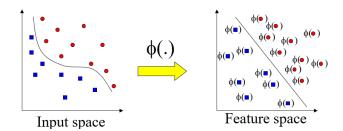




General idea: the original input space can always be mapped to some higher-dimensional feature space where the training set is separable.

### Transforming the Data





- Computation in the feature space can be costly because it is high dimensional.
- ▶ The feature space is typically infinite-dimensional.
- ▶ The kernel trick using kernel functions comes to rescue

#### Kernel Functions



Kernel is a continuous function K(x,y)Kernel takes two arguments x and yx and y could be real numbers, functions, vectors, etc K(x,y) maps x and y to a real value Kernel value is independent of the order of the arguments, i.e.,

$$K(x,y) = K(y,x)$$



#### Kernel Functions



A kernel function is some function that corresponds to an inner product in some expanded feature space.

$$K(x_i, x_j) = \phi(x_i)^T \phi(x_j)$$

- ightharpoonup Linear classifier relies on dot product between vectors  $x_i^T x_j$
- If every data point is mapped into high-dimensional space via some transformation  $\phi: x \to \phi(x)$ , the dot product becomes:  $K(x_i, x_j) = \phi(x_i)^T \phi(x_j)$
- For some functions  $K(x_i, x_j)$  checking  $K(x_i, x_j) = \phi(x_i)^T \phi(x_j)$  is difficult.
  - ► Mercer's theorem: Every positive-semidefinite symmetric function is a kernel function.



#### Kernel Functions Construction



We can construct kernels from scratch:

- For any  $\varphi:\mathcal{X}\to\mathbb{R}^m$ ,  $k(x,x')=\langle \varphi(x),\varphi(x')\rangle_{\mathbb{R}^m}$  is a kernel.
- If  $d: \mathcal{X} \times \mathcal{X} \to \mathbb{R}$  is a distance function, i.e.
  - $d(x, x') \ge 0$  for all  $x, x' \in \mathcal{X}$ ,
- $d(x,x') = 0 \quad \text{only for } x = x',$   $d(x,x') = d(x',x) \quad \text{for all } x,x' \in \mathcal{X},$   $d(x,x') \leq d(x,x'') + d(x'',x') \quad \text{for all } x,x',x'' \in \mathcal{X},$   $\text{then } k(x,x') := \exp(-d(x,x')) \text{ is a kernel.}$



#### Kernel Functions Construction

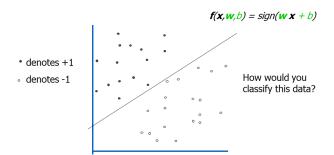


- 2) We can construct kernels from other kernels:
  - if k is a kernel and  $\alpha > 0$ , then  $\alpha k$  and  $k + \alpha$  are kernels.
  - if  $k_1, k_2$  are kernels, then  $k_1 + k_2$  and  $k_1 \cdot k_2$  are kernels.

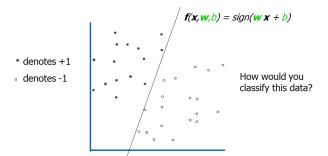
#### Examples of Kernels

Linear:  $K(x_i, x_j) = x_i^T x_j$ Polynomial of power  $p: K(x_i, x_j) = (1 + x_i^T x_j)^p$ Sigmoid:  $K(x_i, x_j) = tanh(\beta_0 x_i^T x_j + \beta_1)$ 

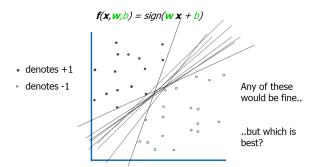












#### Linear Classifier



