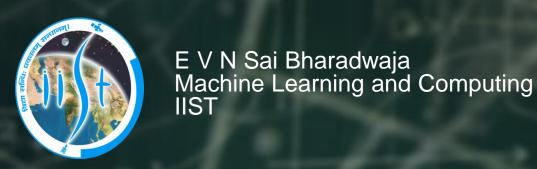
Mathematical Programming Applications in Machine Learning



Q. What is the goal of any Machine Learning algorithm?

- Training Data
- Testing Data

Three basic basic problems that are often Studied in Machine Learning are:

- Regression
- Classification
- Clustering

There are so many approaches to solve above problem

 But Mathematical Programming has now become very popular in Machine Learning Community and Mathematical Programming Community

Q. What is the Advantage of Studying Mathematical Programming?

- Most of the Machine Learning Models result into Linear Programming, Quadratic Programming, Convex Programming.
- But Mathematical Programming has
 - Theoretical results (KKT conditions and Duality Theory)
 - Efficient algorithms

Machine Learning Techniques

- Supervised Learning (Ex : Classification and Regression)
- Unsupervised Learning (Ex : Clustering)

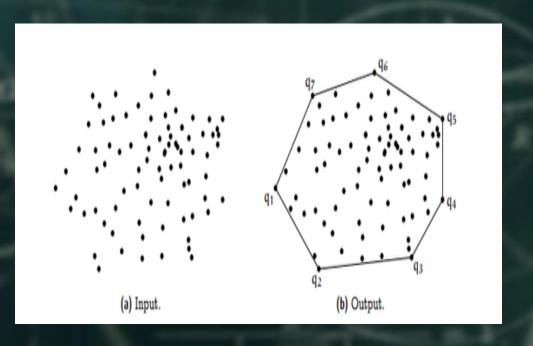
Binary (Two-Class) Pattern Classification Problems

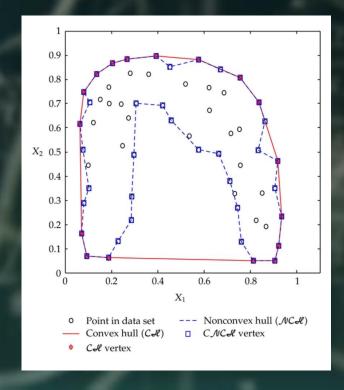
- X ∈ R^n
- m patterns ∈ Class +1
- k patterns ∈ Class -1



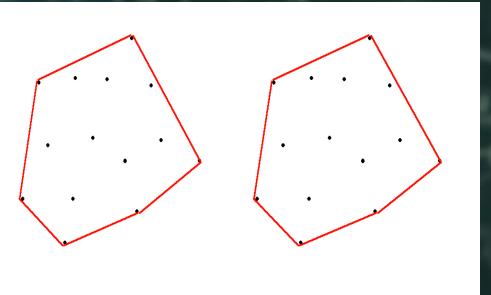
Convex Hull:

The Convex hull of a set of points X in euclidean space is the smallest convex set containing X.

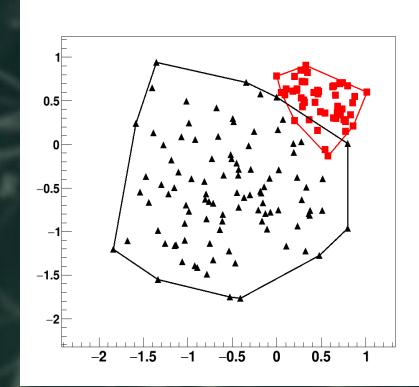




Disjoint Convex hulls Or Linearly Separable



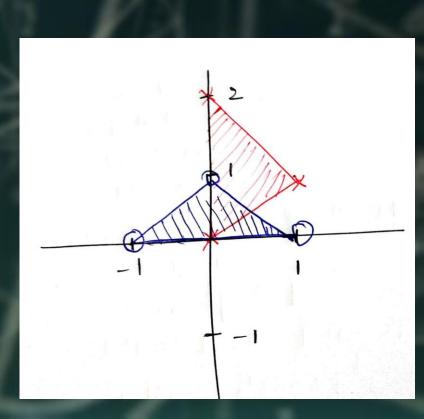
Joint Convex hulls Or Linearly non Separable



Q. $A = \{ (-1,0),(0,1),(1,0) \}$, $B = \{ (0,0),(1,1),(0,2) \}$ Are A and B linearly Separable ? Ans:

- Convex Hulls are NOT Disjoint Hence given Problem is NOT Linearly Separable.
- But Finding convex hulls is not an easy task

So we make use of Linear Programming to decide whether the problem is Linearly Separable or not



Solving the above problem using Linear Programming

$$X = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1n} \\ x_{21} & x_{22} & \cdots & x_{2n} \\ x_{N1} & x_{NL} & \cdots & x_{Nn} \end{bmatrix}$$

$$x_{N1} \times x_{NL} - \cdots \times x_{Nn}$$

$$x_{Nn} \times x_{Nn} \times x_{Nn} \times x_{Nn} \times x_{Nn}$$

$$x_{Nn} \times x_{Nn} \times x_{Nn} \times x_{Nn} \times x_{Nn}$$

$$x_{Nn} \times x_{Nn} \times x_{Nn}$$

Error Minimizing Linear Programming Problem

For a Real number
$$a_{+} = \max(a_{1}o)$$
.

For $x \in \mathbb{R}^{n}$ $x_{+} = \left\{ \left(x_{+} \right), \left(x_{+} \right)_{2} \cdots \left(x_{+} \right)_{n} \right\} \in \mathbb{R}^{n}$.

The continuation problem.

Min $\frac{1}{m} \left\| \left(-Aw + eb + e \right)_{+} \right\|_{1}$ $\left(w_{1}b \right)$ $+ \frac{1}{k} \left\| \left(Bw - eb + e \right)_{+} \right\|_{1}$

If A and B are Linearly Separable then Error is zero and Optimal value for the Optimization problem is zero and the converse is also True.

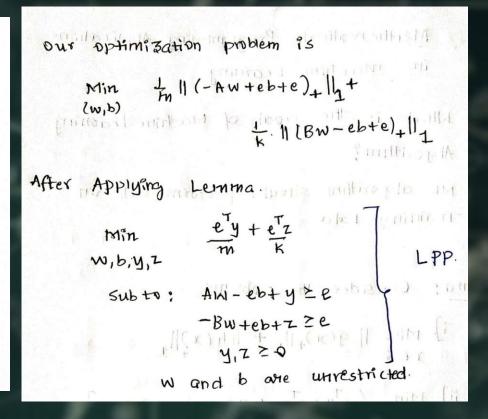
Converse Statement:

If Optimal Value for the optimization problem is zero then A and B are Linearly Separable otherwise NOT Linearly Separable

Lemma: Transforms into LPP

```
Lemma: Consider the problems
      i) Min 11 9(x)+11+ 11+(x)11,
     ii) Mîn { ety+etz : yzg(x), y 20 ]
xes { zzh(x), zzo]
 where SCRM, g: S-RM, h: S-RK
 yerm and zerk.
- Then both problem [i] and [ii]
   have identical solution sets.
```

Applying Lemma to our Optimization Problem



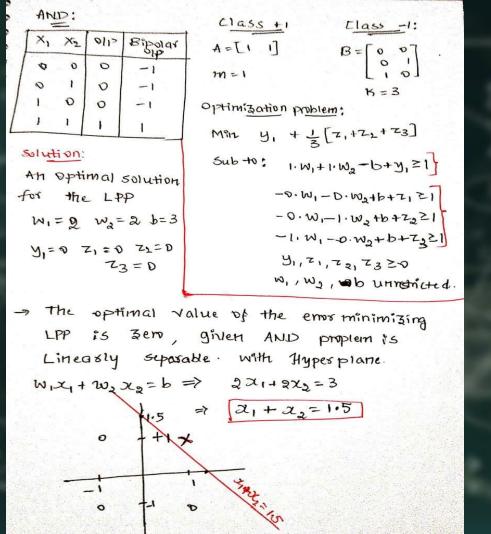
LPP can be Efficiently Solved by using Simplex Algorithm.

Hence we can find whether A and B are Linearly separable or Not

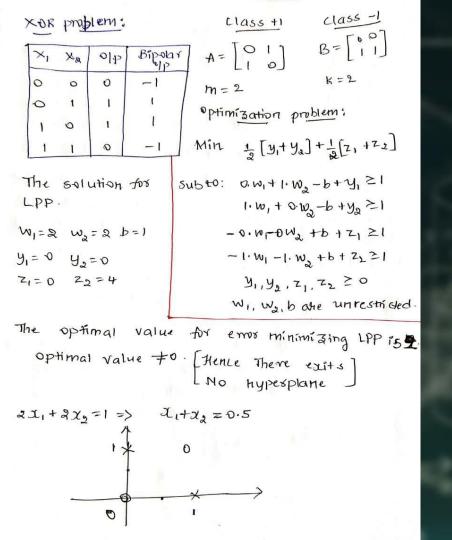
Conclusion:

- A and B are linearly separable iff optimal value for the error minimizing LPP is ZERO. Hence there exists a Hyperplane w.T *x = b which is Linear Separator
- A and B are NOT linearly separable then optimal value for the error minimizing LPP is NOT ZERO. Hence there exists NO Hyperplane w.T *x = b which is Linear Separator

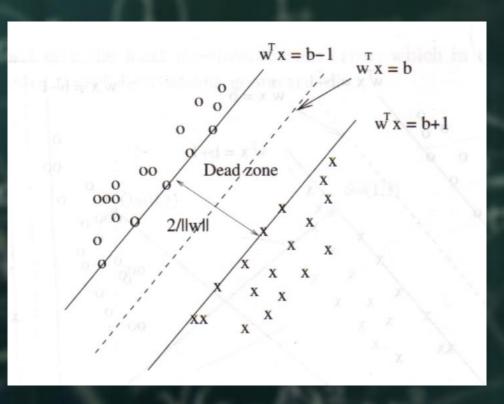
Q. Write error minimizing LPP for AND problem and check if the given Problem is Linearly Separable?

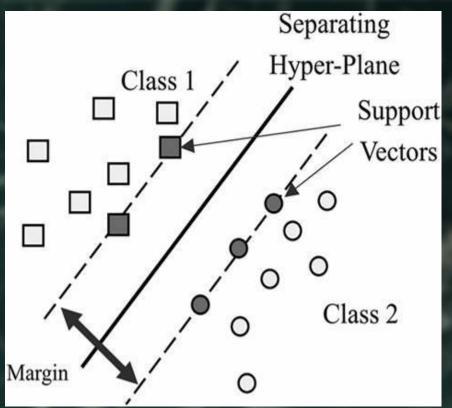


Q. Write error minimizing LPP for XOR problem and check if the given Problem is Linearly Separable?



- If A and B are linearly separable then there exists infinitely many hyperplanes
- So how should we choose a Hyperplane?
- Is there any optimal Hyperplane?



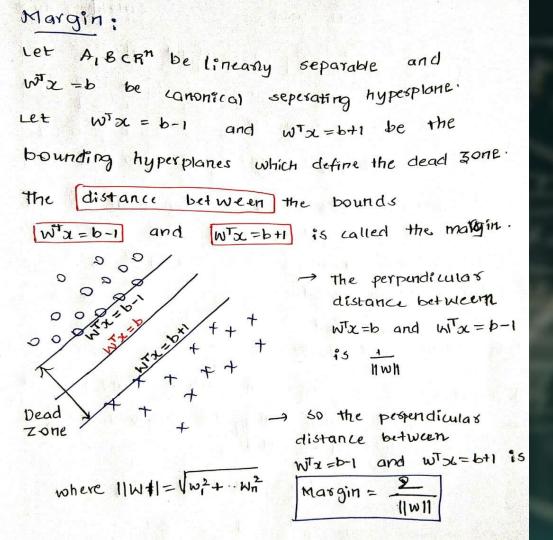


Canonical Hyperplane

Dead Zone

```
-> Canonical Hyperplane;
   Let A,BCRM be linearly separable.
  Then the seperating hyperplane w.x = b
  is called canonical hyperplane if it
  Satisfies
            AW Zeb+E
   Bw Eeb-E
-> Dead Zone:
Let A, BCRn be linearly separable and
wix=b be a canonical separating hyperplane
 Then there exists a lacross Region
If x; (b-1) < WTX < (b+1) y CR" syrrounding the
  seperating hyperplane work = b, which is
 Upid of points sets A and B.
 This Region is called Dead zone for the
 Separating Hyperplane
                    wx =b
```

Margin



[The distance of a point (x', y') to the plane ax + by = 0 is given by $\frac{|ax' + by'|}{\sqrt{a^2 + b^2}}$]

The distance of a point $x_i = (x_{i1}, x_{i2}, \dots x_{in})$ to the hyperplane $w^T x + b = 0$ is given by

$$dist(x_{i}, \tilde{f}(x)) = \frac{|w_{1}x_{i1} + w_{2}x_{i2} + \dots + w_{n}x_{in} + b|}{\sqrt{w_{1}^{2} + w_{2}^{2} + \dots + w_{n}^{2}}}$$
$$= \frac{|w^{T}x_{i} + b|}{||w||}$$

 $w^Tx + b \ge 1$ for all x in the positive class. Therefore $dist(x, \tilde{f}(x)) \ge \frac{1}{||w||}$, for all x in the positive class. The points in the positive class, that lie closest to the separating hyperplane $w^Tx + b = 0$ lies in the hyperplane

Therefore
$$d+=rac{1}{||w||}$$
.

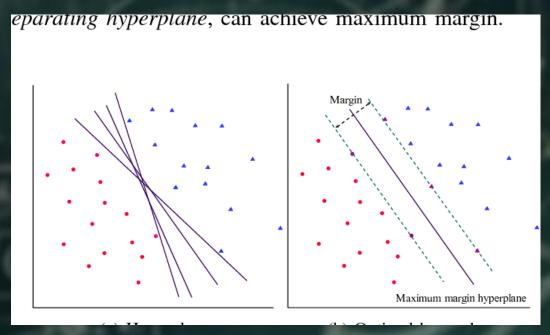
In the negative class, for all points $w^Tx + b \le -1$. Therefore $dist(x, \tilde{f}(x)) \ge \frac{1}{||w||}$ for all x in the negative class. The points in

the negative class, that lie closest to the separating hyperplane $w^Tx + b = 0$ lies in the hyperplane

$$H_2: w^Tx + b = -1$$
 Therefore $d^- = \frac{1}{||w||}$. Hence margin $\gamma = d^+ + d^- = \frac{2}{||w||}$

Optimal Separating Hyperplanes:

- Let sets A, B be linearly separable and w.T * x = b be a canonical hyperplane.
- Then w.T * x = b is called Optimal Separating Hyperplane if it's Margin is Maximum among all the Canonical Hyperplanes



- In Classification, our aim is not only to classify the available to classify the training data in accordance with the class labels
- But also to have good generalization on Unseen Data or Test Data
- The Larger the dead Zone, the smaller the misclassification Error will be.
- Therefore we would like to Maximize the dead Zone, which implies we would like to Maximize the Margin
- From the above Point of View, for the linearly Separable patterns, our aim is not only just finding the Hyperplane, But also for which the Margin is Maximum
- Ques: Will Error Minimizing LPP gives Optimal Separating Hyperplane?
- So we should construct a Optimization problem in which Objective Function should contain Margin
- This Discussion Leads us to Hard Margin Classifier and Support Vector Machines

Hard Margin Classifier:

For the given patterns which are Linearly separable

writting in more compact form. y; (WTx(19) -b) ≥1 + 1=1,2...P. -> Amongst all separating hyperplanes wtx=b we trave to Choose the one for which margin 2 is maximum, (of) Equivalently 1/2 is minimum. - How ever minimizing 11w11 is equivalent to minimi zing \frac{||w||^2}{2} because ||w|| is monotonically increasing for w>0 - optimization problem: Min & WTW (wip) sub to: y; [wTx (1) b) ≥1 + 1=1,2...p. - The above problem is in the form of Standard quadratic Programming Problem [OPP]. Which can be solved by Standard OPP againthm. - once optimal solution of (w, b) is known: The maximum margin classifier will be found WTX=b >> Hard Matgin classifier

Difficulties in Solving Quadratic Programming Problem

- QPP has as many constraints as the number of patterns and hence extremely hard to solve for Large Data sets
- This QPP will make use of Kernel Methods, which again is difficult to Store kernel matrices.
- In Machine Learning there are special algorithms so that Not all Constraints are included at once
 - Chunking algorithm
 - Decomposition algorithm
 - SMO algorithm (Special Case of Decomposition)
- The above Techniques are also called as Active Set or Working Set approach

 In Mathematical Programming, Standard approach to handle Large number of constraints is to examine if Dual problem can be solved efficiently

This analysis requires KKT conditions

KKT conditions

min 1/2 || w || **2 Sub : yi(<w, xi> + b) >= 1

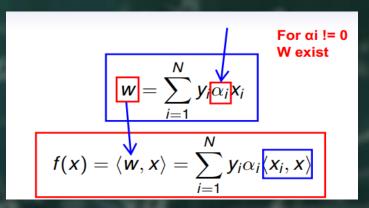
$$L(w,b,\alpha) = \frac{1}{2}\langle w,w\rangle - \sum_{i=1}^{N} \alpha_i [y_i(\langle w,x_i\rangle + b) - 1]$$

where $\alpha_i \geq 0$ are the Lagrange multipliers.

The corresponding dual is found by differentiating with respe to w and b, imposing stationarity,

$$\frac{\partial L(w,b,\alpha)}{\partial w} = w - \sum_{i=1}^{N} y_i \alpha_i x_i = 0$$

$$\frac{\partial L(w,b,\alpha)}{\partial b} = \sum_{i=1}^{N} y_i \alpha_i = 0$$



Support Vectors:

- Only Those points for which Xi is influencing Weights 'W'
- KKT multipliers (Alpha) > 0
- So vector W is know once KKT multipliers are know.

KKT Complimentary Condition

Using Karush-Kuhn-Tucker complementarity conditions,

$$\alpha_i^*[y_i(\langle w, x_i \rangle + b) - 1] = 0, i = 1, 2, \dots N$$

Therefore two cases

- $\alpha_i^* = 0$
 - $y_i(\langle w, x_i \rangle + b) 1 \geq 0$
 - x_i lies either above H_1 or on H_1 or above H_2 or on H_2
- $\Rightarrow \alpha_i^* \neq 0$
 - $y_i(\langle w, x_i \rangle + b) 1 = 0$
 - x_i lies either on H_1 or H_2

Support Vectors:

 $\alpha != 0$,

α Contributes in weight W

Hence those Xi for α ! = 0 are called Support Vectors

- The SVM algorithm clearly needs the knowledge of KKT multipliers
- Once KKT multipliers are known Support Vectors

Support Vectors:

- Only Those points for which Xi is influencing Weights 'W'
- KKT multipliers (Alpha) > 0
- So vector W is know once KKT multipliers are know.
- Hence we get to know vector (w) and b
- From the concept of Non Linear Programming Duality, KKT multipliers are nothing but Dual Variables.
- Therefore we go for Wolfe Dual of the Problem to find KKT multipliers

$$||w||^{2} = \langle w, w \rangle$$

$$= \langle \sum_{i} \alpha_{i} y_{i} x_{i}, \sum_{i} \alpha_{i} y_{i} x_{i} \rangle$$

$$||w||^{**2} = \sum_{i} \sum_{j} \alpha_{i} \alpha_{j} y_{i} y_{j} \langle x_{i}, x_{j} \rangle$$

$$\sum_{i=1}^{N} \alpha_{i}[y_{i}(\langle w, x_{i} \rangle)] = \sum_{i=1}^{N} \alpha_{i}[y_{i}(\langle \sum_{j=1}^{N} y_{j}\alpha_{j}x_{j}, x_{i} \rangle)]$$

$$= \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_{i}\alpha_{j}y_{i}y_{j}\langle x_{i}, x_{j} \rangle$$

$$L(w,b,\alpha) = \frac{1}{2}\langle w,w \rangle - \sum_{i=1}^{N} \alpha_{i}[y_{i}(\langle w,x_{i} \rangle + b) - 1]$$

$$Dual Formulation$$

$$b \sum_{i} \alpha_{i}[y_{i}(\langle w,x_{i} \rangle)] = \sum_{i=1}^{N} \alpha_{i}[y_{i}(\langle x,x_{i} \rangle)]$$

$$= \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_{i}[y_{j}(\langle x,x_{j} \rangle)]$$

$$= \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_{i}[y_{j}(\langle x,x_{j} \rangle)]$$

$$W(\alpha) = \frac{1}{2} \sum_{i,j=1}^{N} y_i y_j \alpha_i \alpha_j \langle x_i, x_j \rangle - \sum_{i,j=1}^{N} y_i y_j \alpha_i \alpha_j \langle x_i, x_j \rangle + \sum_{i=1}^{N} \alpha_i$$

$$= \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{N} y_i y_j \alpha_i \alpha_j \langle x_i, x_j \rangle$$

Wolfe Dual:

- If we clearly observe dual problem, we can notice that there is only one constraint
- The objective Function of the Dual problem is Concave
- Therefore Dual problem is Easier to Solve Than Primal problem
- Once optimal alpha is known [w] and b can be computed.
- Hence separating hyperplane with Maximum Margin can be determined

Primal Problem : Number of Constraints = Number of Data Points

Dual Problem : Number of Constraints = 1 [Easy to Solve]

Hence the dual optimisation problem is

maximise
$$W(\alpha) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{N} y_i y_j \alpha_i \alpha_j \langle x_i, x_j \rangle$$
Only One Constraint Easy to Solve

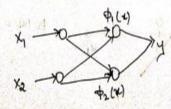
$$\frac{\partial L(w,b,\alpha)}{\partial b} = \sum_{i=1}^{N} y_i \alpha_i = 0$$

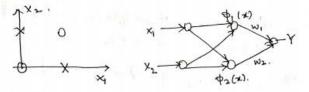
$$\alpha_i \ge 0, i = 1, 2, \dots N$$

 $L(w, \alpha, b)$ and $W(\alpha)$ arise from the same objective function but with different constraints and the solution is found by minimizing $L(w, \alpha, b)$ or by maximizing $W(\alpha)$.

1. Gaussian function
$$\phi \omega = e^{-\frac{3c^2}{2\sigma^2}}$$

3. Inverse multi quadratic on
$$\phi(x) = \frac{1}{\sqrt{x^2 + c^2}}$$
 c>0





where ci + cz are the center of the patres clusters.

Let
$$C_1 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$
 $C_2 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$ $x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$

\propto	χ_2	\$. (x)	\$2 (x)	Y These Centre's	
0	O	(·	٠١ ه	o can be found out	
0	1	0.4	0.4	in Clusturing Techniques	
١	0	0.4	0.4	1 sc-c1=[6]-[6]	
1	1	1.0	1	D MOK- 411 = 11[8]11 = 4	٥

Soft Margin Classifier:

For the given patterns which are **NOT** Linearly separable

```
→ let {(211, y;), i= 1,2. Py be a finite
 Training sample of patterns where
 xlider and y; E-{-1,13.
 - We consides the case where the patterns we
  NOT linearly separable
 - In this case Error minimizing problem will
   have a non-zero objective function value.
 -> In the optimal solution not all the errors
  Will be Zero
- Let the error variables will be denoted by
  gi (i= 1, 2 ... p).
- So our aim is to maximize margin 2 | 1 wh
 and E &; is least.
 -> : Iminimize both www and Eg;
       This will be mutt objective optimization,
  - since this is not possible, we consider
   weighted sum min wto + c. \ \frac{2}{9};
```

Optimisation Problem

$$egin{aligned} \min_{f \in \mathcal{F}, b \in \mathbb{R}} & rac{1}{2} ||f||^2 + C \sum_{i=1}^N \xi_i \ & ext{subject to} \ & y_i (& \langle f, k_{x_i}
angle + b) - 1 + \xi_i \geq 0, \ i = 1, \dots, N \ & \xi_i \geq 0. \end{aligned}$$

The objective function is quadratic and all the constrair linear

The primal Lagrangian is,

$$L(f, b, \xi, \alpha) = \frac{||f||^2}{2} + C \sum_{i=1}^{N} \xi_i - \sum_{i} \alpha_i [y_i(\langle f, k_{x_i} \rangle + b) - 1 + \xi_i] - \sum_{i} \mu_i \xi_i$$

$$\frac{\partial L}{\partial f} = f - \sum_{i=1}^{N} \alpha_i y_i k_{x_i} = 0$$

$$f = \sum_{i=1}^{N} \alpha_i y_i k_{x_i}$$

$$\frac{\partial L}{\partial b} = \sum_{i=1}^{N} \alpha_i y_i = 0$$

For i=1,2,..., N,

$$rac{\partial L(w,b,lpha)}{\partial \xi_i} = C - lpha_i - \mu_i = 0$$
 $lpha_i \geq 0$
 $\mu_i \geq 0$

The KKT complimentary conditions are,

$$lpha_i[y_i(\langle f, k_{x_i} \rangle + b) - 1 + \xi_i] = 0$$
 $\mu_i \xi_i = 0$

 $C - \alpha_i = \mu_i \geq 0$

$$0 \le \alpha_i \le C, i = 1, 2, ... N$$

Three cases

•
$$\alpha_i = 0$$
 $y_i(\langle f, k_{x_i} \rangle + b) \geq 1$

•
$$0 < \alpha_i < C$$
 $y_i(\langle f, k_{x_i} \rangle + b) = 1$

•
$$\alpha_i = C$$
 $y_i(\langle f, k_{x_i} \rangle + b) \leq 1$

Support vectors are those points for which $y_i(\langle f, k_{x_i} \rangle + b) \leq 1$.

- $y_i(\langle f, k_{x_i} \rangle + b) = 1$, k_{x_i} on H_1 or on H_2
- $0 \le y_i(\langle f, k_{x_i} \rangle + b) < 1$ Between H_1 and H or H_2 and H or on H
- $y_i(\langle f, k_{x_i} \rangle + b) < 0$ Incorrect classification

Dual Optimisation

$$\max_{\alpha} W(\alpha) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{N} y_i y_j \alpha_i \alpha_j k(x_i, x_j)$$
subject to
$$\sum_{i=1}^{N} y_i \alpha_i = 0$$

 $C \geq \alpha_i \geq 0, i = 1, 2, ... N.$

$$f = \sum_{i=1}^{sv} y_i \alpha_i^* k_{x_i}$$

where sv is the number of support vectors. Then

$$\tilde{f}(x) = \langle f, k_x \rangle + b$$

$$= \sum_{i=1}^{sv} y_i \alpha_i^* \langle k_{x_i}, k_x \rangle + b$$

$$= \sum_{i=1}^{sv} y_i \alpha_i^* k(x_i, x) + b$$

