Unit 3
Support Vector Machine (SVM)

Topics to be covered...

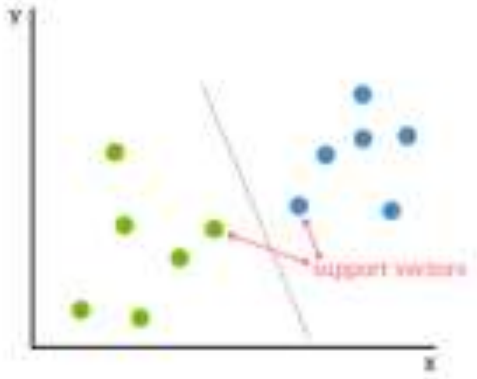
- Introduction to SVM
- Concept of maximum margin hyperplane
- Linear SVM
  - Calculation of MMH
  - Learning a linear SVM
  - Classifying a test sample using linear SVM
  - Classifying multi-class data
- Non-linear SVM
- Concept of non-linear data
- Soft-margin SVM
- Kernel Trick

Introduction

- A classification that has received considerable attention is support vector machine and popularly abbreviated as SVM.
- This technique has its roots in statistical learning theory (Vlamidir Vapnik, 1992).
- As a task of classification, it searches for optimal hyperplane(i.e., decision boundary, see Fig. 1 in the next slide) separating the tuples of one class from another.
- SVM works well with higher dimensional data and thus avoids dimensionality problem.
- Although the SVM based classification (i.e., **training** time) is extremely slow, the result, is however highly accurate. Further, testing an unknown data is very fast.
- SVM is less prone to **over fitting** than other methods. It also facilitates compact model for classification.

OBJECTIVES

- **Support vector machines (SVM)** are supervised learning models with associated learning algorithms that analyze data used for classification and regression analysis.
- It is a **machine learning** approach.
- They analyze the large amount of data to identify patterns from them.
- SVMs are based on the idea of finding a hyperplane that best divides a dataset into two classes, as shown in the image below.



Support Vectors

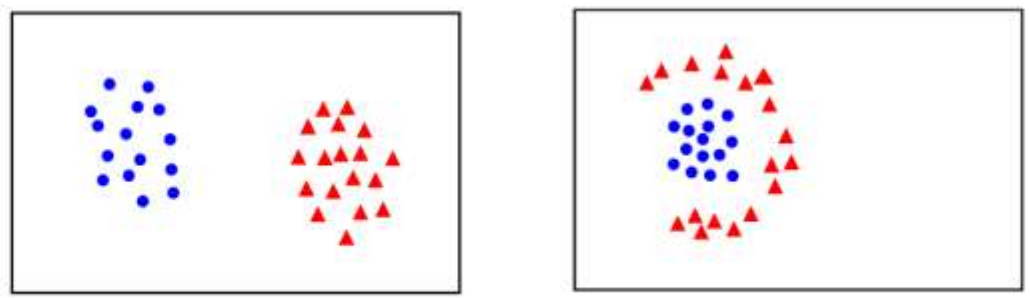
- Support Vectors are simply the co-ordinates of individual observation. Support Vector Machine is a frontier which best segregates the two classes (hyper-plane/ line).
- Support vectors are the data points that lie closest to the decision surface (or hyperplane)
- They are the data points most difficult to classify
- They have direct bearing on the optimum location of the decision surface
- We can show that the optimal hyperplane stems from the function class with the lowest “capacity” (VC dimension).
- Support vectors are the data points nearest to the hyperplane, the points of a data set that, if removed, would alter the position of the dividing hyperplane. Because of this, they can be considered the critical elements of a data set.

Binary Classification

Given training data $(\mathbf{x}_i, y_i)$ for $i = 1 \ldots N$, with $\mathbf{x}_i \in \mathbb{R}^d$ and $y_i \in \{-1, 1\}$, learn a classifier $f(\mathbf{x})$ such that

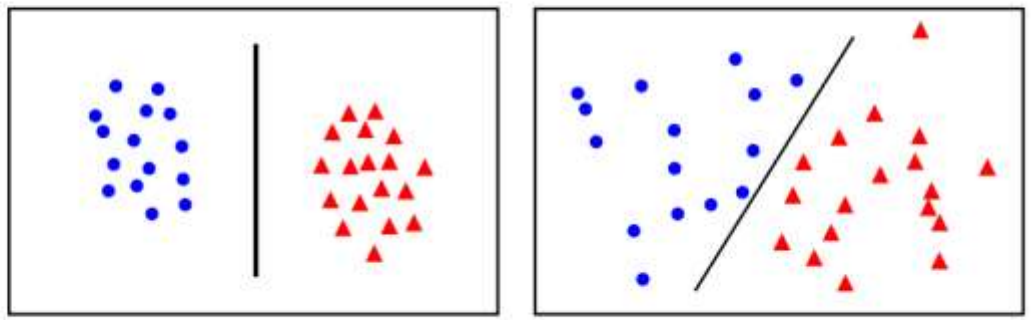
$$f(\mathbf{x}_i) \begin{cases} \geq 0 & y_i = +1 \\ < 0 & y_i = -1 \end{cases}$$

i.e. $y_i f(\mathbf{x}_i) > 0$ for a correct classification.

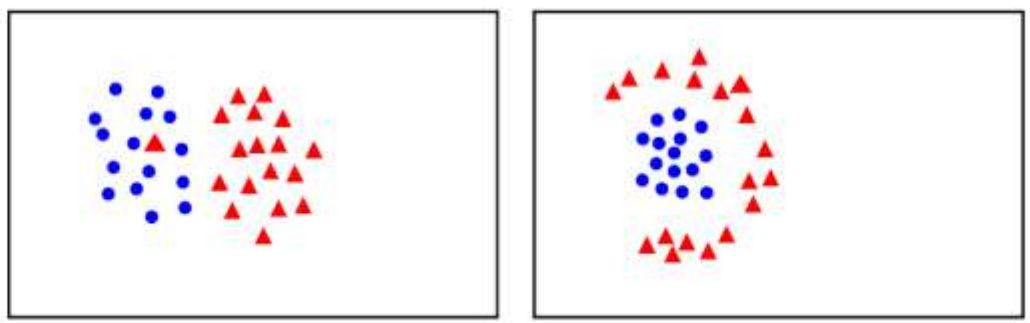


Linear separability

linearly separable



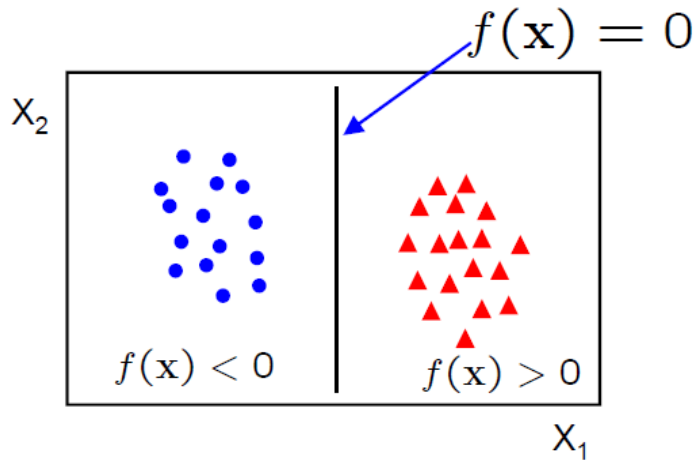
not linearly separable



Linear classifiers

A linear classifier has the form

$$f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b$$

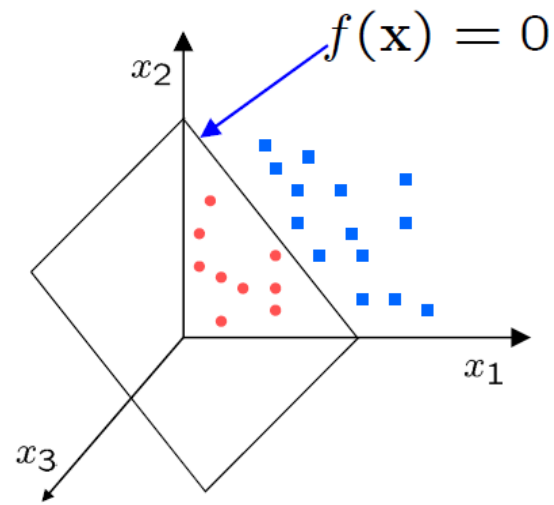


- in 2D the discriminant is a line
- $\mathbf{w}$ is the normal to the line, and b the bias
- $\mathbf{w}$ is known as the weight vector

Linear classifiers

A linear classifier has the form

$$f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b$$



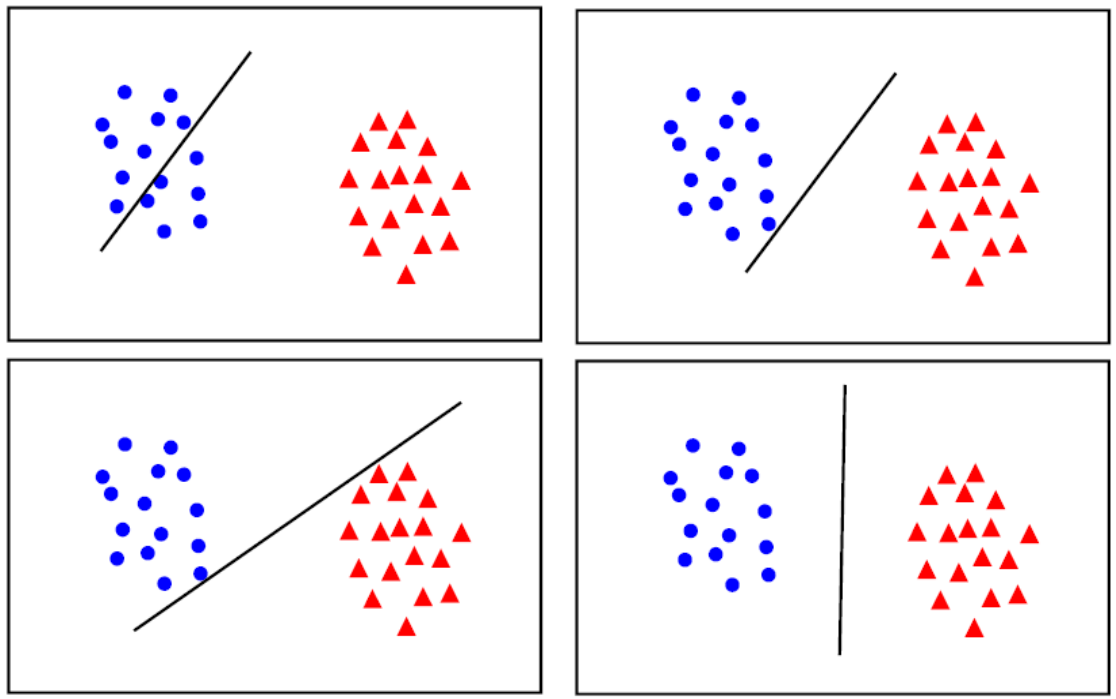
- in 3D the discriminant is a plane, and in nD it is a hyperplane

For a K-NN classifier it was necessary to `carry' the training data

For a linear classifier, the training data is used to learn **w** and then discarded

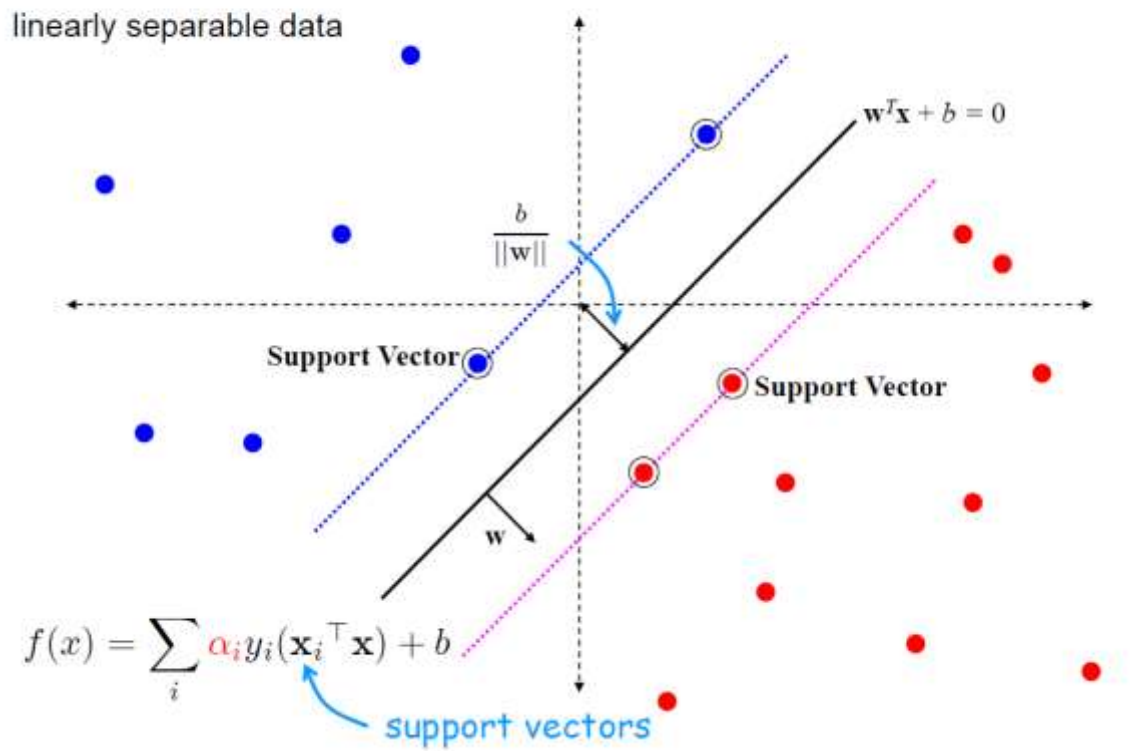
Only **w** is needed for classifying new data

What is the best w?



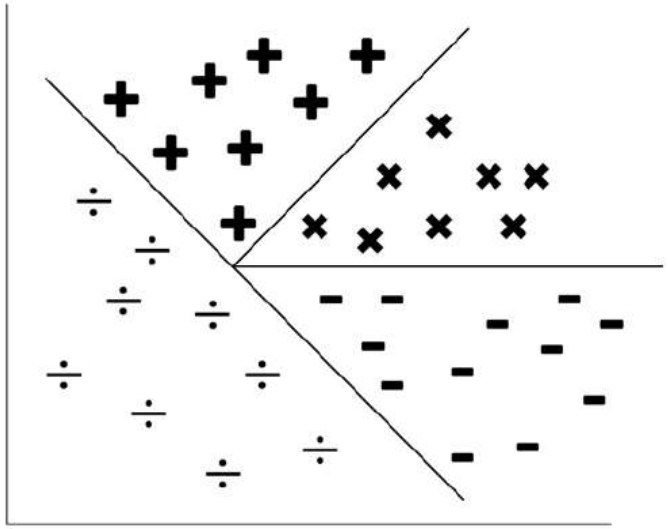
- maximum margin solution: most stable under perturbations of the inputs

Support Vector Machine



Introduction

Figure 1: Decision boundary in SVM.



Introduction

In this Unit 3, we shall discuss the following.

- Maximum margin hyperplane : a key concept in SVM.
- Linear SVM : a classification technique when training data are linearly separable.
- Non-linear SVM : a classification technique when training data are linearly non-separable.

Maximum Margin Hyperplane

- In our subsequent discussion, we shall assume a simplistic situation that given a training data

  D ={t1,t2,....tn) with a set of n samples (tuples), which belong to two classes either + or - and

  each tuple is describe

Figure 2: A 2D data linearly seperable by hyperplanes

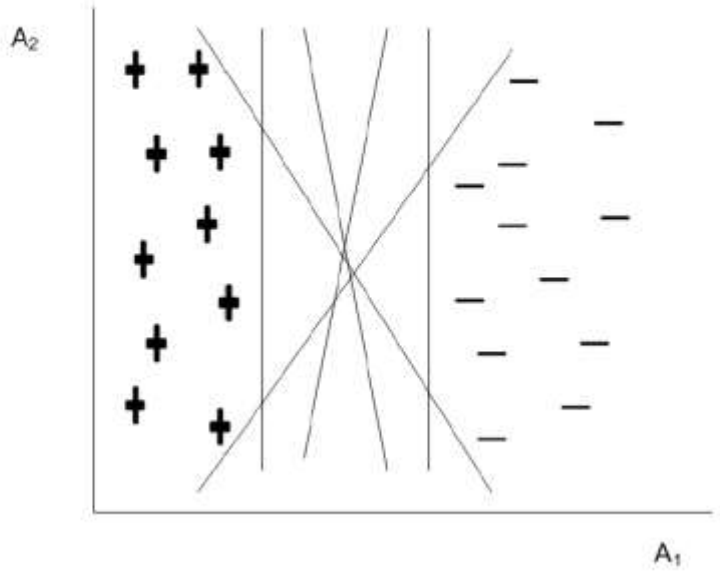
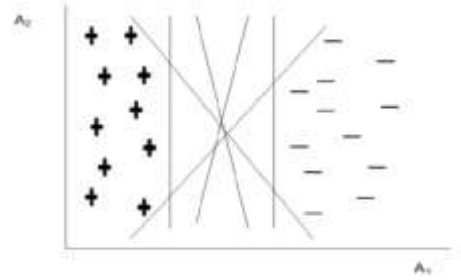


Figure 2: A 2D data linearly seperable by hyperplanes



Maximum Margin Hyperplane contd...

- Figure 2 shows a plot of data in 2-D. Another simplistic assumption here is that the data is linearly separable, that is, we can find a hyperplane (in this case, it is a straight line) such that all +'s reside on one side whereas all -'s reside on other side of the hyperplane.
- From Fig. 2, it can be seen that there are an infinite number of separating lines that can be drawn. Therefore, the following two questions arise:

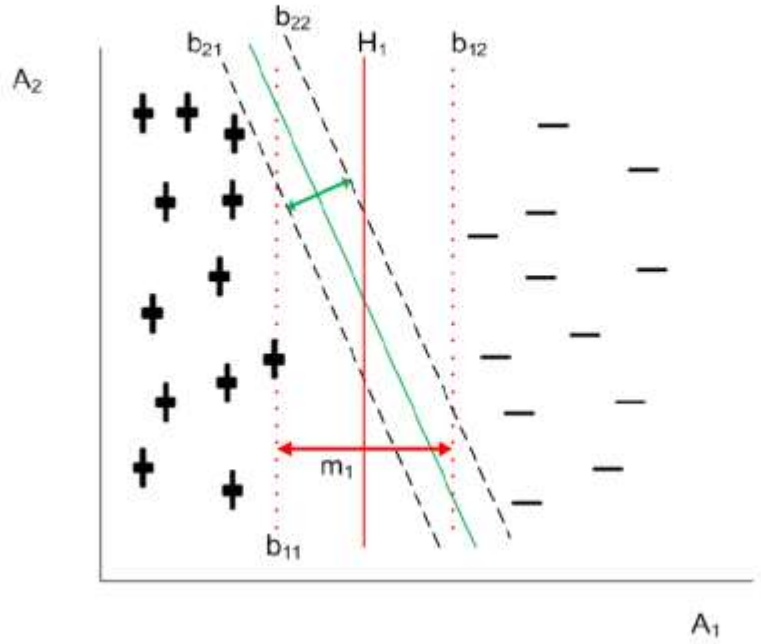
1. Whether all hyperplanes are equivalent so far the classification of data is concerned?
2. If not, which hyperplane is the best?

- We may note that so far the classification error is concerned (with training data), all of them are with zero error.
- However, there is no guarantee that all hyperplanes perform equally well on unseen (i.e., test) data.

Maximum Margin Hyperplane contd...

- Thus, for a good classifier it must choose one of the infinite number of hyperplanes, so that it performs better not only on training data but as well as test data.
- To illustrate how the different choices of hyperplane influence the classification error, consider any arbitrary two hyperplanes H1 and H2 as shown in Fig. 3.

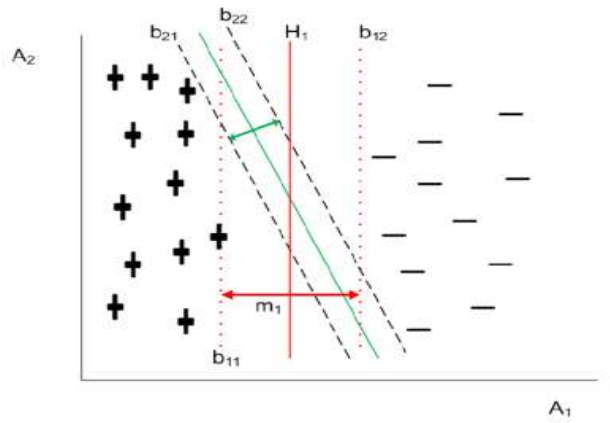
Figure 3: Hyperplanes with decision boundaries and their margins.



Maximum Margin Hyperplane contd...

- In Fig. 3, two hyperplanes H1 and H2 have their own boundaries called decision boundaries(denoted as b11 and b12 for H1 and b21 and b22 for H2).
- A decision boundary is a boundary which is parallel to hyperplane and touches the closest class in one side of the hyperplane.
- The distance between the two decision boundaries of a hyperplane is called the margin. So, if data is classified using Hyperplane H1, then it is with larger margin then using Hyperplane H2.
- The margin of hyperplane implies the error in classifier. In other words, the larger the margin, lower is the classification error.

Figure 3: Hyperplanes with decision boundaries and their margins.

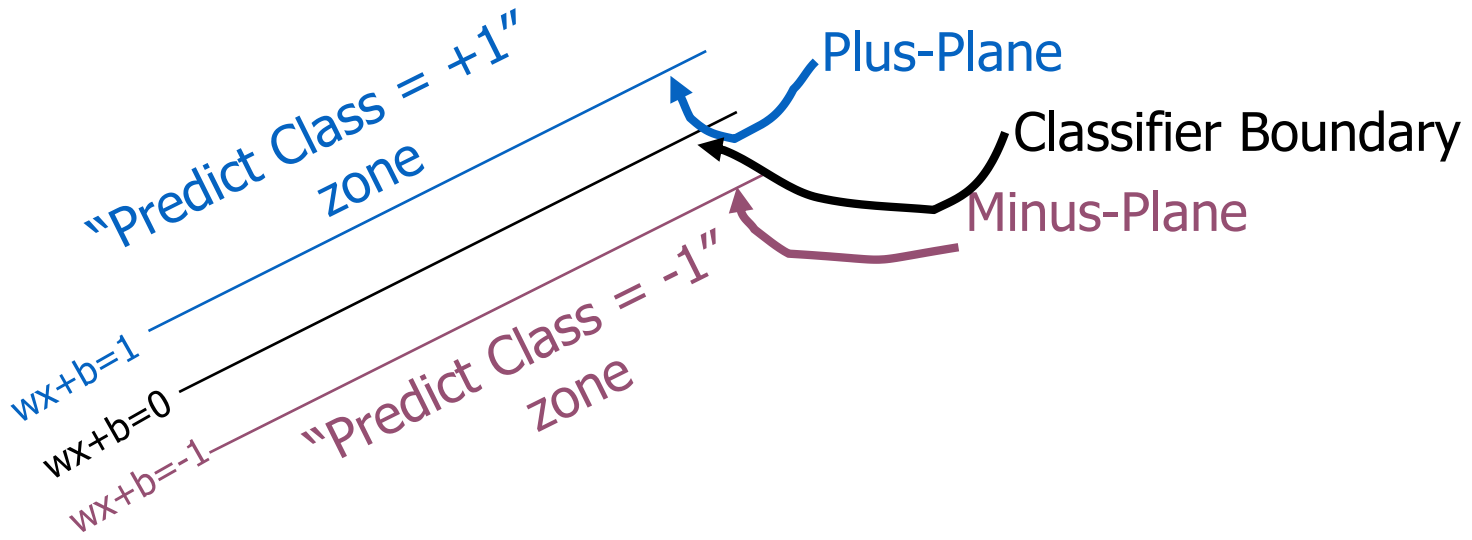


Maximum Margin Hyperplane contd...

- Intuitively, the classifier that contains hyperplane with a small margin are more susceptible to model over fitting and tend to classify with weak confidence on unseen data.
- Thus during the training or learning phase, the approach would be to search for the hyperplane with maximum margin.
- Such a hyperplane is called **maximum margin hyperplane** and abbreviated as MMH.
- We may note the shortest distance from a hyperplane to one of its decision boundary is equal to the shortest distance from the hyperplane to the decision boundary at its other side.
- Alternatively, hyperplane is at the middle of its decision boundaries

Linear SVM

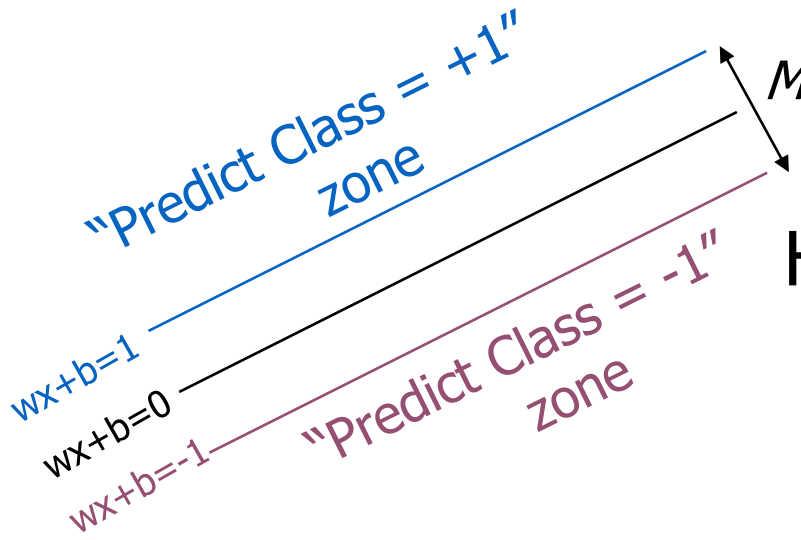
Specifying a line and margin



- Plus-plane = $\{ \boldsymbol{x} : \boldsymbol{w} \cdot \boldsymbol{x} + b = +1 \}$
- Minus-plane = $\{ \boldsymbol{x} : \boldsymbol{w} \cdot \boldsymbol{x} + b = -1 \}$

Classify as..	+1	if	$\boldsymbol{w} \cdot \boldsymbol{x} + b >= 1$
	-1	if	$\boldsymbol{w} \cdot \boldsymbol{x} + b <= -1$
	Universe explodes	if	$-1 < \boldsymbol{w} \cdot \boldsymbol{x} + b < 1$

Computing the margin width

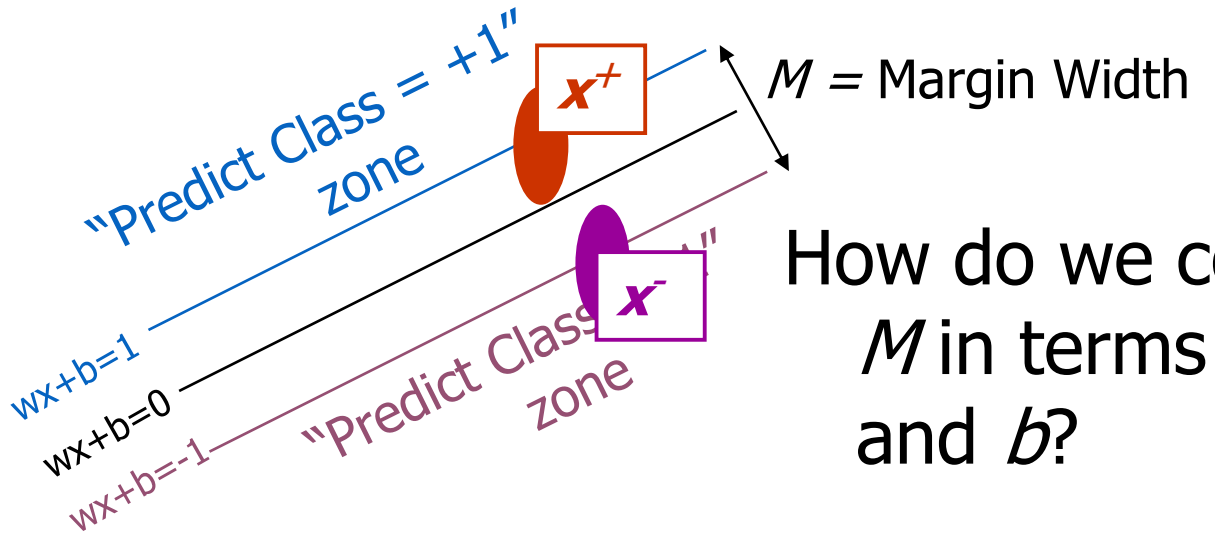


How do we compute *M* in terms of ***w*** and *b*?

- Plus-plane = $\{ \boldsymbol{x} : \boldsymbol{w} \cdot \boldsymbol{x} + b = +1 \}$
- Minus-plane = $\{ \boldsymbol{x} : \boldsymbol{w} \cdot \boldsymbol{x} + b = -1 \}$

Claim: The vector **w** is perpendicular to the Plus Plane. Why?

Computing the margin width

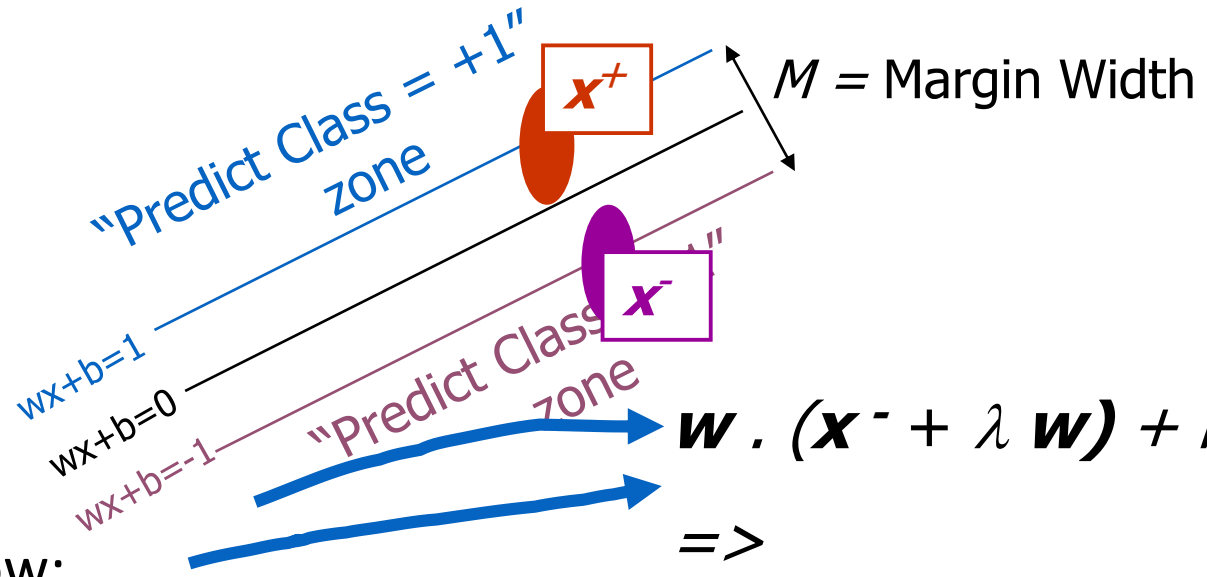


How do we compute *M* in terms of ***w*** and *b*?

- Plus-plane = $\{ \boldsymbol{x} : \boldsymbol{w} \cdot \boldsymbol{x} + b = +1 \}$
- Minus-plane = $\{ \boldsymbol{x} : \boldsymbol{w} \cdot \boldsymbol{x} + b = -1 \}$
- The vector **w** is perpendicular to the Plus Plane
- Let $\boldsymbol{x}^-$ be any point on the minus plane
- Let $\boldsymbol{x}^+$ be the closest plus-plane-point to $\boldsymbol{x}^-$.

Any location in R^m: not necessarily a datapoint

Computing the margin width



What we know:

- $\boldsymbol{w} \cdot \boldsymbol{x}^+ + b = +1$
- $\boldsymbol{w} \cdot \boldsymbol{x}^- + b = -1$
- $\boldsymbol{x}^+ = \boldsymbol{x}^- + \lambda \boldsymbol{w}$
- $|\boldsymbol{x}^+ - \boldsymbol{x}^-| = M$

It's now easy to get M in terms of $\boldsymbol{w}$ and b

$\boldsymbol{w} \cdot (\boldsymbol{x}^- + \lambda \boldsymbol{w}) + b = 1$

$\Rightarrow$

$\boldsymbol{w} \cdot \boldsymbol{x}^- + b + \lambda \boldsymbol{w} \cdot \boldsymbol{w} = 1$

$\Rightarrow$

$-1 + \lambda \boldsymbol{w} \cdot \boldsymbol{w} = 1$

$\Rightarrow$

$$\lambda = \frac{2}{\mathbf{w} \cdot \mathbf{w}}$$

Linear SVM

- A SVM which is used to classify data which are linearly separable is called linear SVM.
- In other words, a linear SVM searches for a hyperplane with the maximum margin.
- This is why a linear SVM is often termed as a **maximal margin classifier** (MMC).

Finding MMH for a Linear SVM

- In the following, we shall discuss the mathematics to find the MMH given a training set.
- In our discussion, we shall consider a binary classification problem consisting of n training data.
- Each tuple is denoted by (Xi ,Yi) where Xi = (xi1,xi2.....xim) corresponds to the attribute set for the ith tuple (data in m-dimensional space) and Yi [+,-] denotes its class label.
- Note that choice of which class should be labeled as + or – is arbitrary. Thus, given f(Xi ;Yi)i=1, we are to obtain a hyperplane which separates all Xi into two sides of it (of course with maximum gap).
- Before, going to a general equation of a plane in n-dimension, let us consider first, a hyperplane in 2-D plane.

Equation of a hyperplane in 2-D

- Let us consider a 2-D training tuple with attributes A1 and A2 as X =(x1,x2), where x1 and x2 are values of attributes A1 and A2, respectively for X.
- Equation of a plane in 2-D space can be written as

  w0 + w1x1 + w2x2 = 0 [e.g., ax + by + c = 0]

- where w0, w1, and w2 are some constants defining the slope and intercept of the line.
- Any point lying above such a hyperplane satisfies

  w0 + w1x1 + w2x2 > 0 ---------- (1)
- Similarly, any point lying below the hyperplane satisfies

  w0 + w1x1 + w2x2 < 0 ---------- (2)
- An SVM hyperplane is an n-dimensional generalization of a straight line in 2-D.
- It can be visualized as a plane surface in 3-D, but it is not easy to visualize when dimensionality is greater than 3!

Equation of a hyperplane

- In fact, Euclidean equation of a hyperplane in Rm is

  $w1x1 + w2x2 + \ldots\ldots + wmxm = b$ ----------(3)

- where wi ’s are the real numbers and b is a real constant (called the intercept, which can be positive or negative).
- In matrix form, a hyperplane thus can be represented as

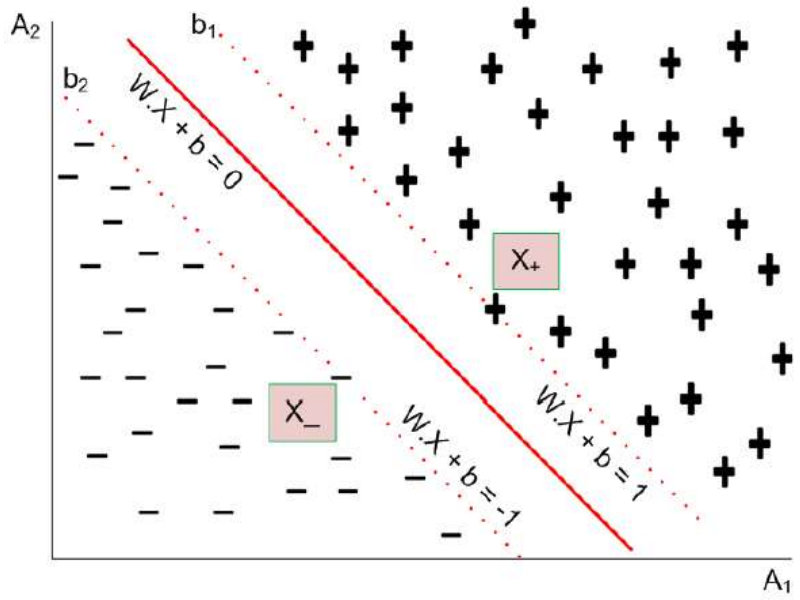
  $W.X + b = 0$ ----------(4)

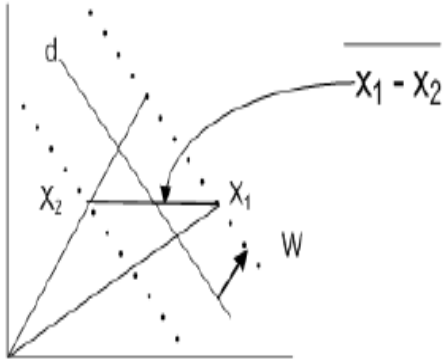
- where W =[w1,w2.....wm] and X = [x1,x2.....xm] and b is a real constant.
- Here, W and b are parameters of the classifier model to be evaluated given a training set D.

Finding a hyperplane

- Let us consider a two-dimensional training set consisting two classes + and - as shown in Fig. 4.
- Suppose, b1 and b2 are two decision boundaries above and below a hyperplane, respectively.
- Consider any two points X+ and X_ as shown in Fig. 4.
- For X+ located above the decision boundary, the equation can be written as
- W.X+ + b = K where K > 0 ---------- (5)

Figure 4: Computation of the MMH





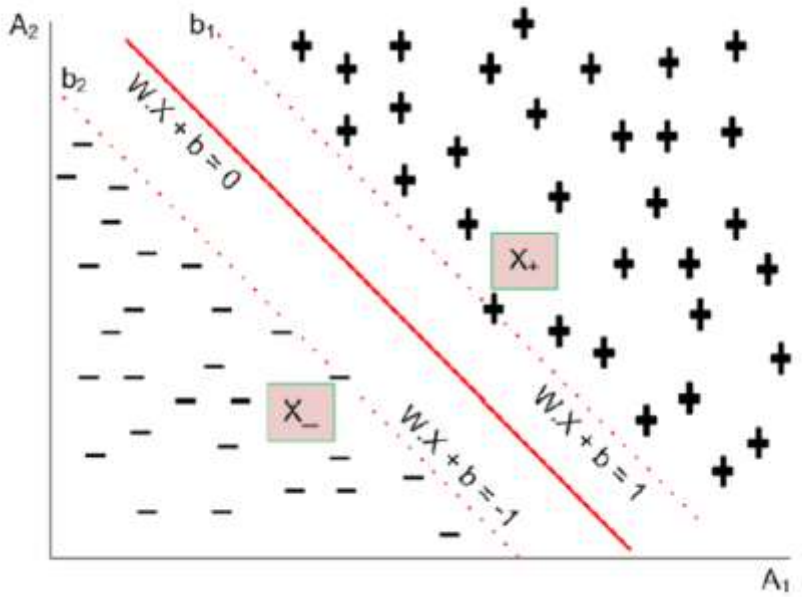
Finding a hyperplane

- Similarly, for any point X located below the decision boundary, the equation is

  W.X + b = K where K < 0 -----(6)

- Thus, if we label all +'s are as class label + and all -'s are class label -, then we can predict the class label Y for any test data X as
- Y = + if W:X + b > 0
- Y= - if W:X + b < 0

Figure 4: Computation of the MMH



Hyperplane and Classification

- Note that W.X + b = 0, the equation representing hyperplane can be interpreted as follows.
  - Here, W represents the orientation and b is the intercept of the hyperplane from the origin.
  - If both W and b are scaled (up or down) by dividing a non zero constant, we get the same hyperplane.
  - This means there can be infinite number of solutions using various scaling factors, all of them geometrical representing the same hyperplane.

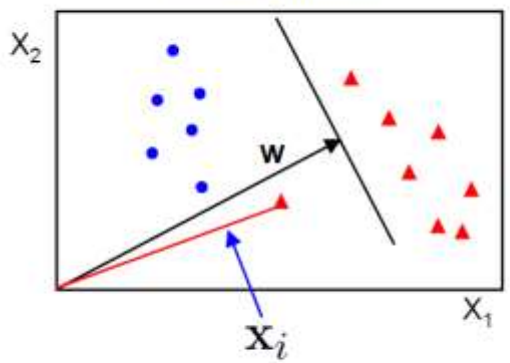
Hyperplane and Classification

- To avoid such a confusion, we can make W and b unique by adding a constraint that $W.X + b = \pm 1$ for data points on boundary of each class.
- It may be noted that $W.X + b = \pm 1$ represents two hyperplane parallel to each other.
- For clarity in notation, we write this as $W.X + b = \pm 1$.
- Having this understating, now we are in the position to calculate the margin of a hyperplane.

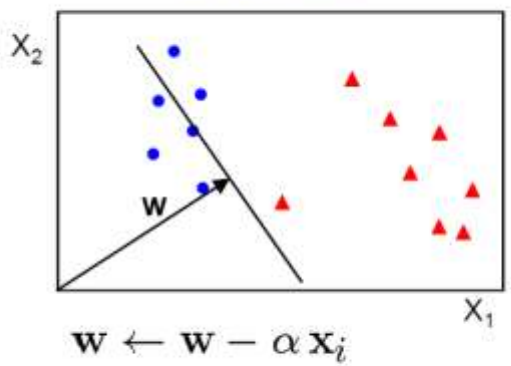
For example in 2D

- Initialize **w** = 0
- Cycle though the data points { $\mathbf{x}_i$, y_i }
  - if $\mathbf{x}_i$ is misclassified then $\mathbf{w} \leftarrow \mathbf{w} + \alpha\, \text{sign}(f(\mathbf{x}_i))\, \mathbf{x}_i$
- Until all the data is correctly classified

before update



after update



NB after convergence $\mathbf{w} = \sum_i^N \alpha_i \mathbf{x}_i$

Calculating Margin of a Hyperplane

- Suppose, x_1 and x_2 (refer Figure 3) are two points on the decision boundaries b_1 and b_2, respectively. Thus,

$$W.x_1 + b = 1 \tag{7}$$

$$W.x_2 + b = -1 \tag{8}$$

or

$$W.(x_1 - x_2) = 2 \tag{9}$$

- This represents a dot (.) product of two vectors W and x_1-x_2. Thus taking magnitude of these vectors, the equation obtained is

$$d = \frac{2}{||W||} \tag{10}$$

where $||W|| = \sqrt{w_1^2 + w_2^2 + ...w_m^2}$ in an m-dimension space.

Calculating Margin of a Hyperplane

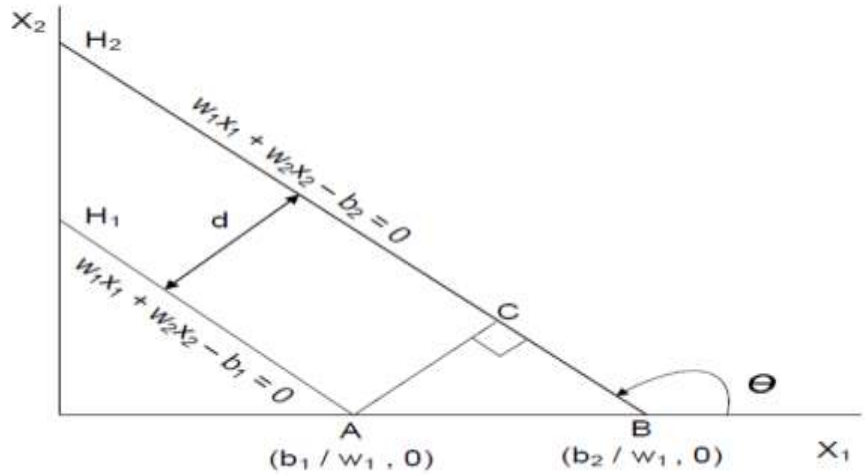
- We calculate the margin more mathematically, as in the following.
- Consider two parallel hyperplanes H1 and H2 as shown in Fig. 5. Let the equations of hyperplanes be

H1 : w1x1 + w2x2 - b1 = 0 ----------(11)

H2 : w1x1 + w2x2 - b2 = 0 ----------(12)

- To draw a perpendicular distance d between H1 and H2, we draw a right-angled triangle ABC as shown in Fig.5.

Figure 5: Detail of margin calculation.



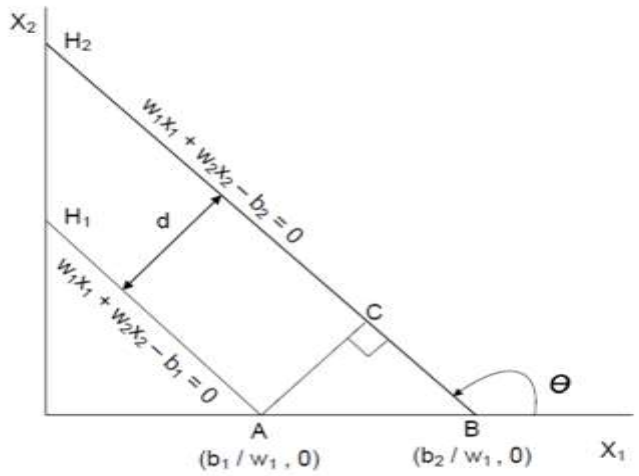
Calculating Margin of a Hyperplane

- Being parallel, the slope of H_1 (and H_2) is $tan\theta = -\frac{w_1}{w_2}$.
- In triangle ABC, AB is the hypotenuse and AC is the perpendicular distance between H_1 and H_2.
- Thus , $sin(180 - \theta) = \frac{AC}{AB}$ or $AC = AB \cdot sin\theta$.

  $AB = \frac{b_2}{w_1} - \frac{b_1}{w_1} = \frac{|b_2 - b_1|}{w_1}$, $sin\theta = \frac{w_1}{\sqrt{w_1^2 + w_2^2}}$

  (Since, $tan\theta = -\frac{w_1}{w_2}$).
- Hence, $AC = \frac{|b_2 - b_1|}{\sqrt{w_1^2 + w_2^2}}$.

Figure 5: Detail of margin calculation.



Calculating Margin of a Hyperplane

- This can be generalized to find the distance between two parallel margins of any hyperplane in n-dimensional space as

$$d = \frac{|b_2 - b_1|}{\sqrt{w_1^2 + w_2^2 + \cdots + w_n^2}} \simeq \frac{|b_2 - b_1|}{\parallel W \parallel}$$

where, $\parallel W \parallel = \sqrt{w_1^2 + w_2^2 + \cdots + w_n^2}$.

- In SVM literature, this margin is famously written as $\mu(W, b)$.

- The training phase of SVM involves estimating the parameters W and b for a hyperplane from a given training data.
- The parameters must be chosen in such a way that the following two inequalities are satisfied.

$$W.x_i + b \geq 1 \text{ if } y_i = 1 \quad \text{----------(13)}$$

$$W.x_i + b \leq 1 \text{ if } y_i = -1 \quad \text{---------- (14)}$$

- These conditions impose the requirements that all training tuples from class Y = + must be located on or above the hyperplane
- W.x + b = 1, while those instances from class Y = - must be located on or below the hyperplane W.x + b = -1 (also see Fig. 4).

Learning for a Linear SVM

- Both the inequalities can be summarized as

  $Y_i (W.x_1 + b) \geq 1$ $\quad\quad$ $i = 1, 2, \ldots\ldots\ldots n$ $\quad$ ------(15)

- Note that any tuples that lie on the hyperplanes H_1 and H_2 are called support vectors.
- Essentially, the support vectors are the most difficult tuples to classify and give the most information regarding classification.
- In the following, we discuss the approach of finding MMH and the support vectors.
- The above problem is turned out to be an optimization problem, that is, to maximize $\mu(W, b) = \frac{2}{\|w\|}$.

Searching for MMH

- Maximizing the margin is, however, equivalent to minimizing the following objective function

$$\mu^{'}(W, b) = \frac{||W||}{2} \tag{16}$$

- In nutshell, the learning task in SVM, can be formulated as the following constrained optimization problem.

$$\begin{aligned} &\textit{minimize} && \mu^{'}(W, b) \\ &\textit{subject to} && y_i(W.x_i + b) \geq 1, \quad i = 1, 2, 3.....n \end{aligned} \tag{17}$$

SVM – Optimization

- Learning the SVM can be formulated as an optimization:

$$\max_{\mathbf{w}} \frac{2}{||\mathbf{w}||} \text{ subject to } \mathbf{w}^\top \mathbf{x}_i + b \begin{array}{ll} \geq 1 & \text{if } y_i = +1 \\ \leq -1 & \text{if } y_i = -1 \end{array} \text{ for } i = 1 \ldots N$$

- Or equivalently

$$\min_{\mathbf{w}} ||\mathbf{w}||^2 \text{ subject to } y_i \left(\mathbf{w}^\top \mathbf{x}_i + b \right) \geq 1 \text{ for } i = 1 \ldots N$$

- This is a quadratic optimization problem subject to linear constraints and there is a unique minimum

Searching for MMH

- The above stated constrained optimization problem is popularly known as convex optimization problem, where objective function is quadratic and constraints are linear in the parameters W and b.
- The well known technique to solve a convex optimization problem is the standard Lagrange Multiplier method.
- First, we shall learn the Lagrange Multiplier method, then come back to the solving of our own SVM problem.

Lagrange Multiplier Method

- The Lagrange multiplier method follows two different steps depending on type of constraints.

  Equality constraint optimization problem: In this case, the problem is of the form:

  minimize f (x1, x2, …….. xd)

  subject to gi (x) = 0; i = 1, 2, …… p

  Inequality constraint optimization problem: In this case, the problem is of the form:

  minimize f (x1, x2, …….. xd)

  subject to hi (x) ≤ 0; i = 1, 2, …… p

Lagrange Multiplier Method

Equality constraint optimization problem solving

- The following steps are involved in this case:
  1. Define the Lagrangian as follows:

$$(X, \lambda) = f(X) + \sum_{i=1}^{p} \lambda_i . g_i(x) \tag{18}$$

where $\lambda_i' s$ are dummy variables called Lagrangian multipliers.

  2. Set the first order derivatives of the Lagrangian with respect to x and the Lagrangian multipliers $\lambda_i' s$ to zero's. That is

$$\frac{\delta L}{\delta x_i} = 0, i = 1, 2, ..., d$$
$$\frac{\delta L}{\delta \lambda_i} = 0, i = 1, 2, ..., p$$

  3. Solve the $(d + p)$ equations to find the optimal value of $X = [x_1, x_2....., x_d]$ and $\lambda_i' s$.

Lagrange Multiplier Method

Example: Equality constraint optimization problem

Suppose, minimize $f(x, y) = x + 2y$
subject to $x^2 + y^2 - 4 = 0$

1. Lagrangian $L(x, y, \lambda) = x + 2y + \lambda(x^2 + y^2 - 4)$
2. $\frac{\delta L}{\delta x} = 1 + 2\lambda x = 0$
   $\frac{\delta L}{\delta y} = 1 + 2\lambda y = 0$
   $\frac{\delta L}{\delta \lambda} = x^2 + y^2 - 4 = 0$
3. Solving the above three equations for x, y and λ, we get $x = \mp\frac{2}{\sqrt{5}}$, $y = \mp\frac{4}{\sqrt{5}}$ and $\lambda = \pm\frac{\sqrt{5}}{4}$

Lagrange Multiplier Method

Example : Equality constraint optimization problem

- When $\lambda = \frac{\sqrt{5}}{4}$,
  $x = -\frac{2}{\sqrt{5}}$,
  $y = -\frac{4}{\sqrt{5}}$,
  we get f$(x, y, \lambda) = -\frac{10}{\sqrt{5}}$
- Similarly, when $\lambda = -\frac{\sqrt{5}}{4}$,
  $x = \frac{2}{\sqrt{5}}$,
  $y = \frac{4}{\sqrt{5}}$,
  we get f$(x, y, \lambda) = \frac{10}{\sqrt{5}}$
- Thus, the function f(x, y) has its minimum value at
  $x = -\frac{2}{\sqrt{5}}, y = -\frac{4}{\sqrt{5}}$

Lagrange Multiplier Method

- **Inequality constraint optimization problem solving**

The method for solving this problem is quite similar to the Lagrange multiplier method described above.
It starts with the Lagrangian

$$L = f(x) + \sum_{i=1}^{p} \lambda_i . h_i(x) \qquad (19)$$

In addition to this, it introduces additional constraints, called **Karush-Kuhn-Tucker (KKT) constraints**,

Lagrange Multiplier Method

Inequality constraint optimization problem solving

$$\frac{\delta L}{\delta x_i} = 0, i = 1, 2, ..., d$$

$$\lambda_i \geq 0, i = 1, 2....., p$$

$$h_i(x) \leq 0, i = 1, 2....., p$$

$$\lambda_i . h_i(x) = 0, i = 1, 2....., p$$

Solving the above equations, we can find the optimal value of $f(x)$.

Lagrange Multiplier Method

Example: Inequality constraint optimization problem

Consider the following problem.

Minimize $f(x, y) = (x - 1)^2 + (y - 3)^2$
subject to $x + y \leq 2$,
$y \geq x$

- The Lagrangian for this problem is
  $L = (x - 1)^2 + (y - 3)^2 + \lambda_1(x + y - 2) + \lambda_2(x - y)$.

  subject to the KKT constraints, which are as follows:

Lagrange Multiplier Method

Example: Inequality constraint optimization problem

$$\frac{\delta L}{\delta x} = 2(x-1) + \lambda_1 + \lambda_2 = 0$$

$$\frac{\delta L}{\delta y} = 2(y-3) + \lambda_1 - \lambda_2 = 0$$

$$\lambda_1(x+y-2) = 0$$

$$\lambda_2(x-y) = 0$$

$$\lambda_1 \geq 0, \lambda_2 \geq 0$$

$$(x+y) \leq 2, y \geq x$$

Lagrange Multiplier Method

Example: Inequality constraint optimization problem

To solve KKT constraints, we have to check the following tests:

- Case 1: $\lambda_1 = 0, \lambda_2 = 0$

  $$2(x-1) = 0 \mid 2(y-3) = 0 \Rightarrow x = 1, y = 3$$

  since, $x + y = 4$, it violates $x + y \leq 2$; is not a feasible solution.

- Case 2: $\lambda_1 = 0, \lambda_2 \neq 0$ $2(x-y) = 0 \mid$
  $2(x-1) + \lambda_2 = 0 \mid$
  $2(y-3) - \lambda_2 = 0$
  $\Rightarrow x = 2, y = 2$ and $\lambda_2 = -2$
  since, $x + y \leq 4$, it violates $\lambda_2 \geq 0$; is not a feasible solution.

Lagrange Multiplier Method

Example: Inequality constraint optimization problem

- Case 3: $\lambda_1 \neq 0, \lambda_2 = 0$ $2(x+y) = 2$
  $2(x-1) + \lambda_1 = 0$
  $2(y-3) + \lambda_1 = 0$

  $\Rightarrow x = 0, y = 2$ and $\lambda_1 = 2$; this is a feasible solution.

- Case 4: $\lambda_1 \neq 0, \lambda_2 \neq 0$ $2(x+y) = 2$
  $2(x-y) = 0$
  $2(x-1) + \lambda_1 + \lambda_2 = 0$
  $2(y-3) + \lambda_1 - \lambda_2 = 0$

  $\Rightarrow x = 1, y = 1$ and $\lambda_1 = 2$ $\lambda_2 = -2$
  This is not a feasible solution.

LMM to Solve Linear SVM

- The optimization problem for the linear SVM is inequality constraint optimization problem.
- The Lagrangian multiplier for this optimization problem can be written as

$$L = \frac{||W||^2}{2} - \sum_{i=1}^{n} \lambda_i (y_i (W.x_i + b) - 1) \qquad (20)$$

where the parameters λ s are the Lagrangian multipliers, and
W = [w_1;w_2……w_m] and b are the model parameters.

LMM to Solve Linear SVM

- The KKT constraints are:

$$\frac{\delta L}{\delta w} = 0 \Rightarrow W = \sum_{i=1}^{n} \lambda_i . y_i . x_i$$

$$\frac{\delta L}{\delta b} = 0 \Rightarrow \sum_{i=1}^{n} \lambda_i . y_i = 0$$

$$\lambda \geq 0, i = 1, 2, ...n$$

$$\lambda_i [y_i (W.x_i + b) - 1] = 0, i = 1, 2, ...n$$

$$y_i (W.x_i + b) \geq 1, i = 1, 2, ...n$$

- Solving KKT constraints are computationally expensive and can be solved using a typical linear/ quadratic programming technique (or any other numerical technique).

LMM to Solve Linear SVM

- We first solve the above set of equations to find all the feasible solutions.
- Then, we can determine optimum value of μ(W, b).

Note:

1. Lagrangian multiplier λi must be zero unless the training instance xi satisfies the equation yi (W.xi + b) = 1. Thus, the training tuples with λi > 0 lie on the hyperplane margins and hence are support vectors.
2. The training instances that do not lie on the hyperplane margin have λi = 0.

Classifying a test sample using Linear SVM

- For a given training data, using SVM principle, we obtain MMH in the form of W, b and i ’s. This is the machine (i.e., the SVM).
- Now, let us see how this MMH can be used to classify a test tuple say X. This can be done as follows.

$$\delta(X) = W.X + b = \sum_{i=1}^{n} \lambda_i.y_i.x_i.X + b \qquad (21)$$

Note that

$$W = \sum_{i=1}^{n} \lambda_i.y_i.x_i$$

Classifying a test sample using Linear SVM

- This is famously called as “Representer Theorem” which states that the solution W always be represented as a linear combination of training data.

$$Thus, \delta(X) = W.X + b = \sum_{i=1}^{n} \lambda_i.y_i.x_i.X + b$$

Classifying a test sample using Linear SVM

- The above involves a dot product of xi :X, where xi is a support vector (this is so because (λi) = 0 for all training tuples except the support vectors), we can check the sign of (X).
- If it is positive, then X falls on or above the MMH and so the SVM predicts that X belongs to class label +. On the other hand, if the sign is negative, then X falls on or below MMH and the class prediction is -.
- **Note:**

1. Once the SVM is trained with training data, the complexity of the classifier is characterized by the number of support vectors.

   Dimensionality of data is not an issue in SVM unlike in other classifier.

- Consider the case of a binary classification starting with a training data of 8 tuples as shown in Table 1.
- Using quadratic programming, we can solve the KKT constraints to obtain the Lagrange multipliers λi for each training tuple, which is shown in Table 1.
- Note that only the first two tuples are support vectors in this case.
- Let W = (w1,w2) and b denote the parameter to be determined now. We can solve for w1 and w2 as follows:

$$w_1 = \sum_i \lambda_i . y_i . x_{i1} = 65.52 \times 1 \times 0.38 + 65.52 \times -1 \times 0.49 = -6.64 \quad (22)$$

$$w_2 = \sum_i \lambda_i . y_i . x_{i2} = 65.52 \times 1 \times 0.47 + 65.52 \times -1 \times 0.61 = -9.32 \quad (23)$$

Illustration : Linear SVM

Table 1: Training Data

A_1	A_2	y	λ_i
0.38	0.47	+	65.52
0.49	0.61	-	65.52
0.92	0.41	-	0
0.74	0.89	-	0
0.18	0.58	+	0
0.41	0.35	+	0
0.93	0.81	-	0
0.21	0.10	+	0

Illustration : Linear SVM

Figure 6: Linear SVM example.

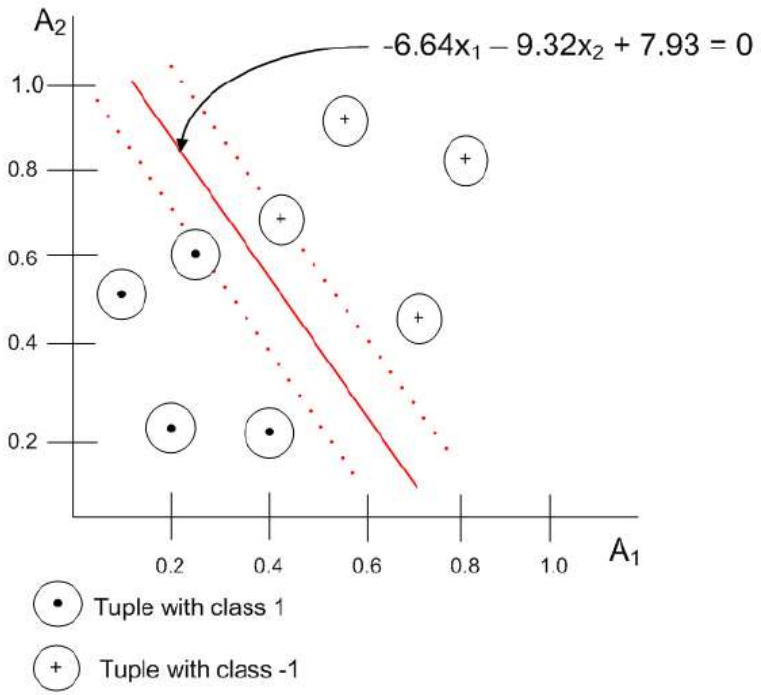


Illustration : Linear SVM

- The parameter b can be calculated for each support vector as follows
  $b_1 = 1 - W.x_1$ // for support vector x_1
  $= 1 - (-6.64) \times 0.38 - (-9.32) \times 0.47$ //using dot product
  $= 7.93$
  $b_2 = 1 - W.x_2$ // for support vector x_2
  $= 1 - (-6.64) \times 0.48 - (-9.32) \times 0.611$ //using dot product
  $= 7.93$

- Averaging these values of b_1 and b_2, we get $b = 7.93$.

Illustration : Linear SVM

- Thus, the MMH is $-6.64x_1 - 9.32x_2 + 7.93 = 0$ (also see Fig. 6).
- Suppose, test data is $X = (0.5, 0.5)$. Therefore,
  $\delta(X) = W.X + b$
  $= -6.64 \times 0.5 - 9.32 \times 0.5 + 7.93$
  $= -0.05$
  $= -ve$

- This implies that the test data falls on or below the MMH and SVM classifies that X belongs to class label -.

Classification of Multiple-class Data

- In the discussion of linear SVM, we have limited to binary classification (i.e., classification with two classes only).
- Note that the discussed linear SVM can handle any n-dimension, n 2. Now, we are to discuss a more generalized linear SVM to classify n-dimensional data belong to two or more classes.
- There are two possibilities: all classes are pairwise linearly separable, or classes are overlapping, that is, not linearly separable.
- If the classes are pair wise linearly separable, then we can extend the principle of linear SVM to each pair. There are two strategies:

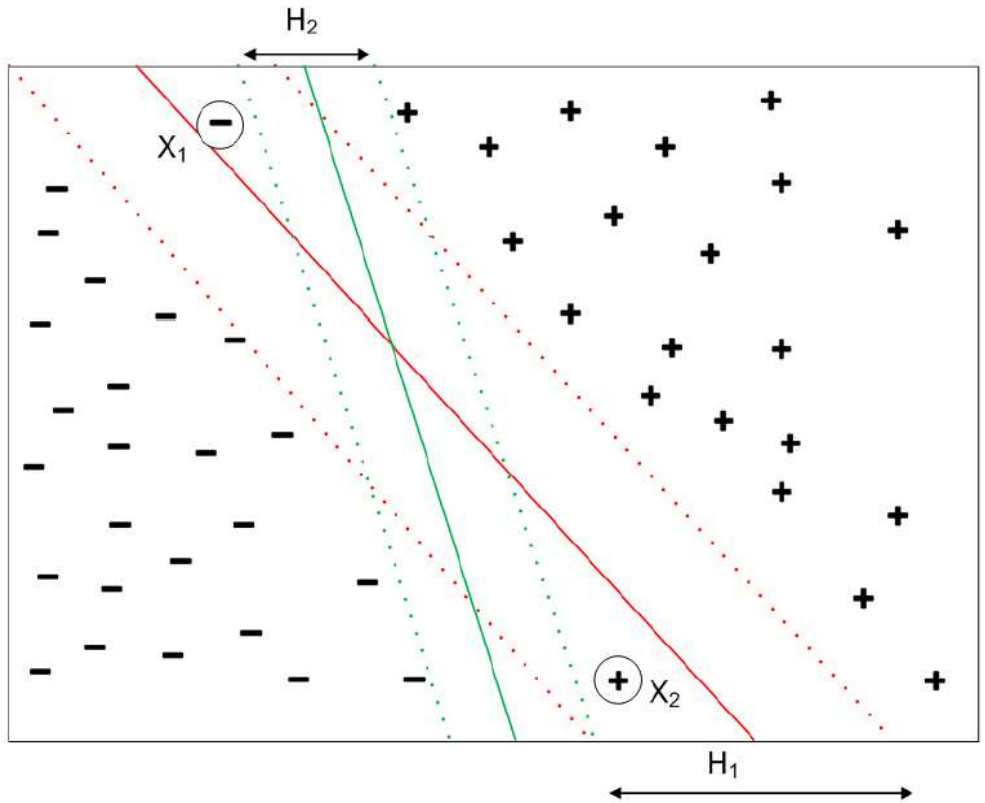
1. One versus one (OVO) strategy
2. One versus all (OVA) strategy

Multi-Class Classification: OVO Strategy

- In OVO strategy, we are to find MMHs for each pair of classes.
- Thus, if there are n classes, then nc2 pairs and hence so many classifiers possible (of course, some of which may be redundant).
- Also, see Fig. 7 for 3 classes (namely +, - and). Here, Hxy denotes MMH between class labels x and y.
- Similarly, you can think for 4 classes (namely +, -, *,÷) and more

- Note:
- The linear SVM that is used to classify multi-class data fails, if all classes are not linearly separable.
- If one class is linearly separable to remaining other classes and test data belongs to that particular class, then only it classifies accurately

Figure 10: Problem with linear SVM for linearly not separable data.



Linear SVM for Linearly Not Separable Data

- Suppose, X1 and X2 are two instances.
- We see that the hyperplane H1 classifies wrongly both X1 and X2.
- Also, we may note that with X1 and X2, we could draw another hyperplane namely H2, which could classify all training data correctly.
- However, H1 is more preferable than H2 as H1 has higher margin compared to H2 and thus H1 is less susceptible to over fitting.
- In other words, a linear SVM can be refitted to learn a hyperplane that is tolerable to a small number of non-separable training data.
- The approach of refitting is called soft margin approach (hence, the SVM is called Soft Margin SVM), where it introduces slack

  variables to the inseparable cases.
- More specifically, the soft margin SVM considers a linear SVM hyperplane (i.e., linear decision boundaries) even in situations

  where the classes are not linearly separable.
- The concept of Soft Margin SVM is presented in the following slides.

Soft Margin SVM

- Recall that for linear SVM, we are to determine a maximum margin hyperplane W.X + b = 0 with the following optimization:

$$minimize \frac{||W||^2}{2} \qquad (25)$$

$$subject\ to\ y_i.(W.x_i + b) \geq 1, i = 1, 2, ..., n$$

- In soft margin SVM, we consider the similar optimization technique except that a relaxation of inequalities, so that it also satisfies the case of linearly not separable data.

Soft Margin SVM

- To do this, soft margin SVM introduces slack variable (ξ), a positive-value into the constraint of optimization problem.
- Thus, for soft margin we rewrite the optimization problem as follows.

$$minimize \frac{||W||^2}{2}$$

$$subject\ to\ (W.x_i + b) \geq 1 - \xi_i, if\ y_i = +1$$

$$(W.x_i + b) \leq -1 + \xi_i,\ if\ y_i = -1 \qquad (26)$$

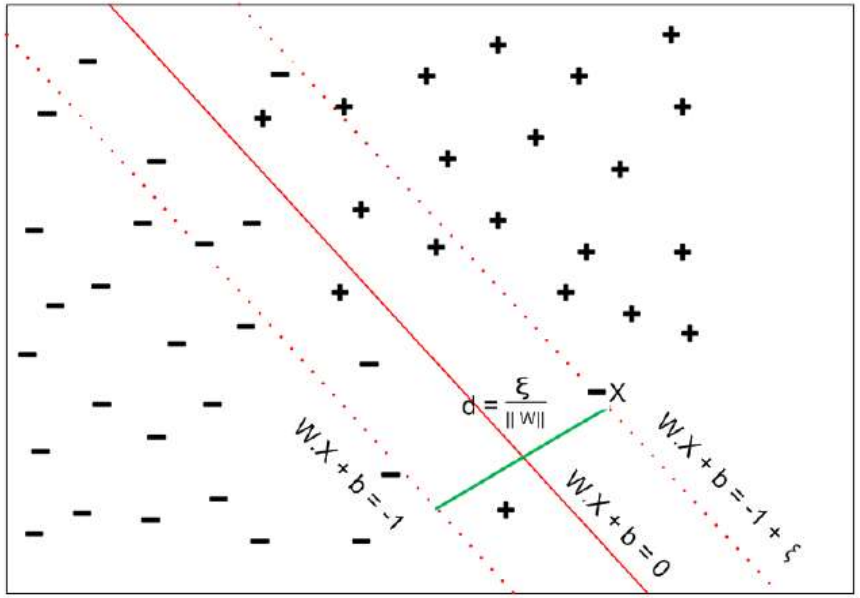
where $\forall_i, \xi_i \geq 0$.

- Thus, in soft margin SVM, we are to calculate W, b and ξ is as a solution to learn SVM.

Soft Margin SVM : Interpretation of ξ

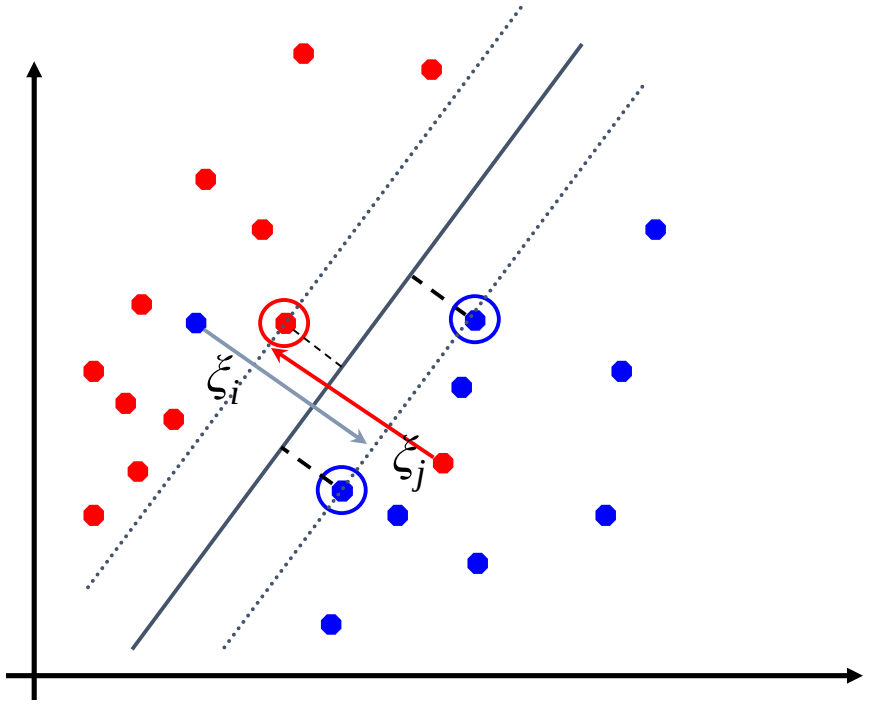
- Let us find an interpretation of , the slack variable in soft margin SVM. For this consider the data distribution shown in the Fig. 11.

Figure 11: Interpretation of slack variable ξ.



Soft Margin Classification

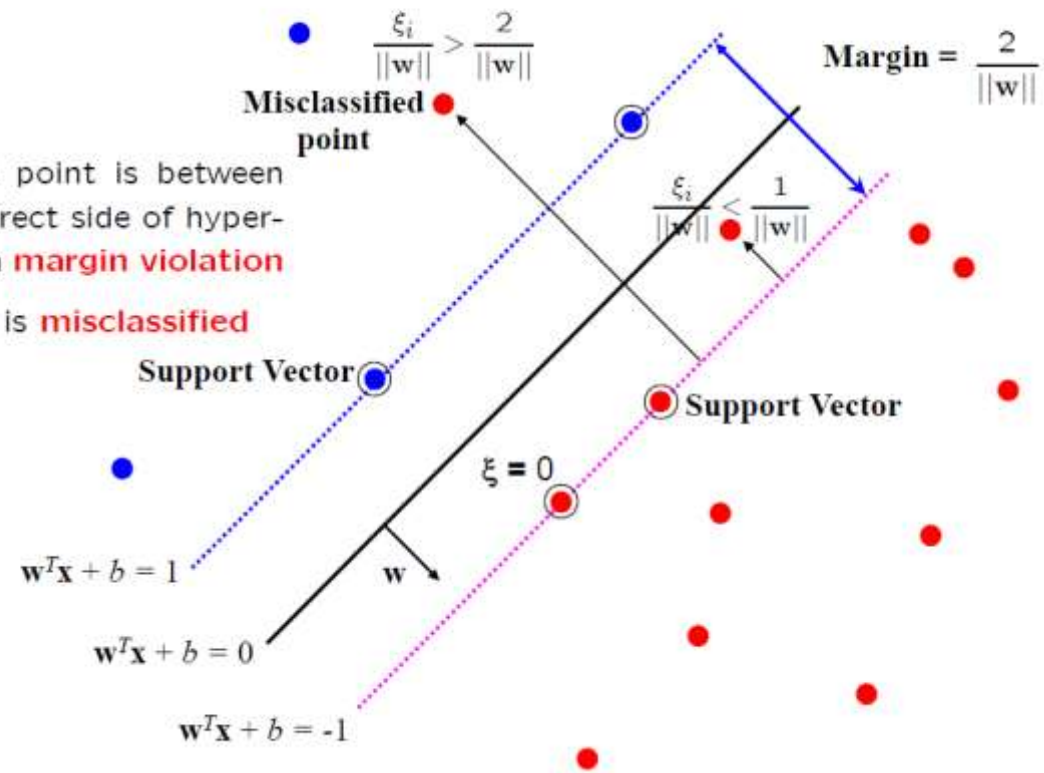
- If the training data is not linearly separable, *slack variables* ξ_i can be added to allow misclassification of difficult or noisy examples.
- Allow some errors
  - Let some points be moved to where they belong, at a cost
- Still, try to minimize training set errors, and to place hyperplane “far” from each class (large margin)



Introduce "slack" variables

$\xi_i \geq 0$

- for $0 < \xi \leq 1$ point is between margin and correct side of hyper-plane. This is a **margin violation**
- for $\xi > 1$ point is **misclassified**



Soft Margin SVM : Interpretation of ξ

- The data X is one of the instances that violates the constraints to be satisfied for linear SVM.
- Thus, W.X + b = -1+ξ represents a hyperplane that is parallel to the decision boundaries for class - and passes through X.
- It can be shown that the distance between the hyperplanes is

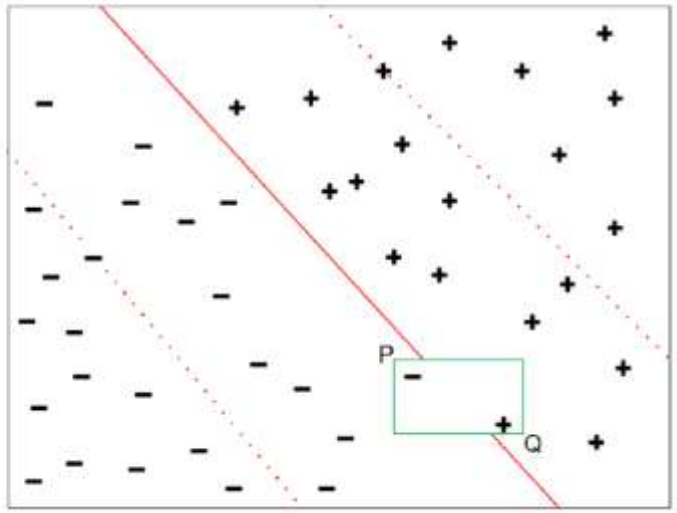
$$d = \frac{\xi}{||w||}.$$

- In other words, provides an estimate of the error of decision boundary on the training example X.

Soft Margin SVM : Interpretation of ξ

- In principle, Eqn. 25 and 26 can be chosen as the optimization problem to train a soft margin SVM.
- However, the soft margin SVM should impose a constraint on the number of such non linearly separable data it takes into account.
- This is so because a SVM may be trained with decision boundaries with very high margin thus, chances of misclassifying many of the training data.
- This is explained in Fig. 12. Here, if we increase margin further, then P and Q will be misclassified.
- Thus, there is a trade-off between the length of margin and training error.

Figure 12: MMH with wide margin and large training error.



Soft Margin SVM : Interpretation of ξ

- To avoid this problem, it is therefore necessary to modify the objective function, so that penalizing for margins with a large gap, that is, large values of slack variables.
- The modified objective function can be written as

  - The modified objective function can be written as

$$f(W) = \frac{||W||^2}{2} + c.\sum_{i=1}^{n}(\xi_i)^{\phi} \tag{27}$$

    where c and ϕ are user specified parameters representing the penalty of misclassifying the training data.

  - Usually, $\phi = 1$. The larger value of c implies more penalty.

Solving for Soft Margin SVM

- We can follow the Lagrange multiplier method to solve the inequality constraint optimization problem, which can be reworked as follows:

$$L = \frac{||W||^2}{2} + c.\sum_{i=1}^{n} \xi_i - \sum_{i=1}^{n} \lambda_i (y_i(W.x_i + b) - 1 + \xi_i) - \sum_{i=1}^{n} \mu_i.\xi_i \quad (28)$$

- Here, λ_i's and μ_i's are Lagrange multipliers.
- The inequality constraints are:

$$\xi_i \geq 0, \lambda_i \geq 0, \mu_i \geq 0.$$

$$\lambda_i\{y_i(W.x_i + b) - 1 + \xi_i\} = 0$$

$$\mu_i.\xi_i = 0$$

"Soft" margin solution

The optimization problem becomes

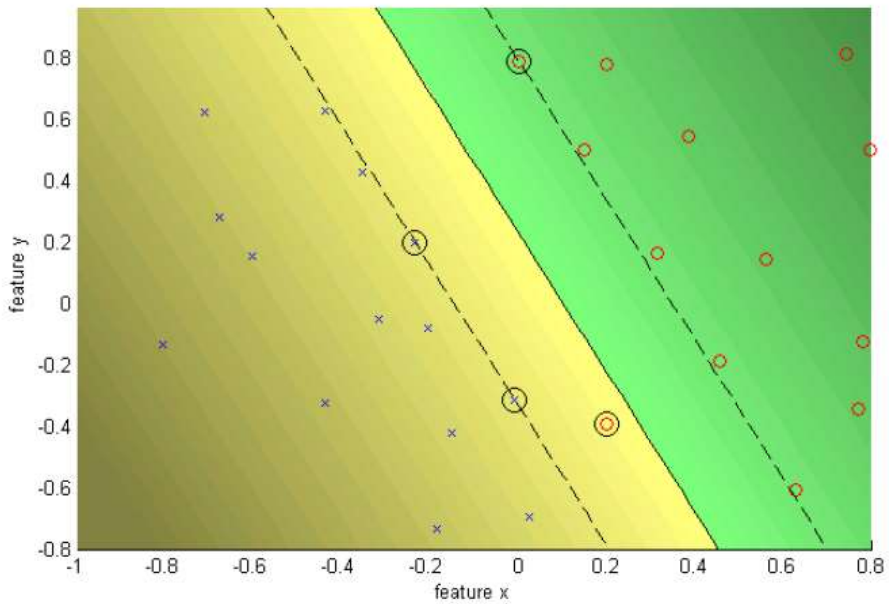
$$\min_{\mathbf{w}\in\mathbb{R}^d,\xi_i\in\mathbb{R}+} ||\mathbf{w}||^2+C\sum_i^N \xi_i$$

subject to

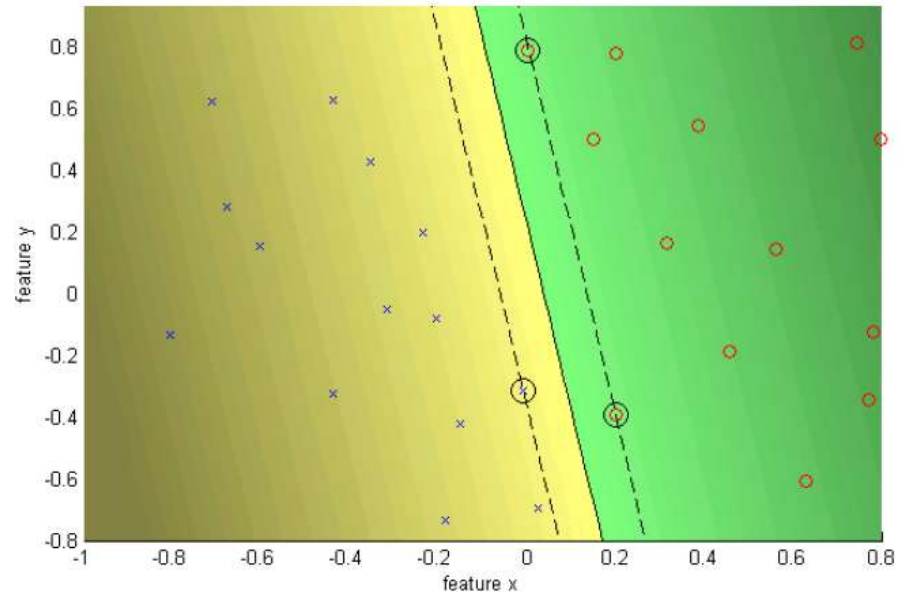
$$y_i\left(\mathbf{w}^\top\mathbf{x}_i+b\right)\geq 1-\xi_i \text{ for } i=1\ldots N$$

- Every constraint can be satisfied if ξ_i is sufficiently large
- C is a regularization parameter:
  - small C allows constraints to be easily ignored $\rightarrow$ large margin
  - large C makes constraints hard to ignore $\rightarrow$ narrow margin
  - $C=\infty$ enforces all constraints: hard margin
- This is still a quadratic optimization problem and there is a unique minimum. Note, there is only one parameter, C.

C = 10 soft margin



C = Infinity hard margin



Solving for Soft Margin SVM

- The KKT constraints (in terms of first order derivative of L with respect to different parameters) are:

$$\frac{\delta L}{\delta w_j} = w_j - \sum_{i=1}^{n} \lambda_i . y_i . x_{ij} = 0$$

$$w_j = \sum_{i=1}^{n} \lambda_i . y_i . x_{ij} = 0 \, \forall_i = 1, 2 .... n$$

$$\frac{\delta L}{\delta b} = -\sum_{i=1}^{n} \lambda_i . y_i = 0$$

$$\sum_{i=1}^{n} \lambda_i . y_i = 0$$

Solving for Soft Margin SVM

$$\frac{\delta L}{\delta \xi_i} = c - \lambda_i - \mu_i = 0$$

$$\lambda_i + \mu_i = c \text{ and } \mu_i.\xi_i = 0 \forall_i = 1, 2, ...n. \tag{29}$$

- The above set of equations can be solved for values of $W = [w_1, w_2.....w_m], b, \lambda_i's, \ \mu_i's$ and $\xi_i's$.
- **Note:**
  1. $\lambda_i \neq 0$ for support vectors or has $\xi_i > 0$ and
  2. $\mu_i = 0$ for those training data which are misclassified, that is, $\xi_i > 0$.

Optimization

Learning an SVM has been formulated as a constrained optimization problem over $\mathbf{w}$ and ξ

$$\min_{\mathbf{w}\in\mathbb{R}^d,\xi_i\in\mathbb{R}^+} ||\mathbf{w}||^2 + C\sum_i^N \xi_i \text{ subject to } y_i\left(\mathbf{w}^\top\mathbf{x}_i + b\right) \geq 1 - \xi_i \text{ for } i = 1\ldots N$$

The constraint $y_i\left(\mathbf{w}^\top\mathbf{x}_i + b\right) \geq 1 - \xi_i$, can be written more concisely as

$$y_i f(\mathbf{x}_i) \geq 1 - \xi_i$$

which, together with $\xi_i \geq 0$, is equivalent to

$$\xi_i = \max(0, 1 - y_i f(\mathbf{x}_i))$$

Hence the learning problem is equivalent to the unconstrained optimization problem over $\mathbf{w}$

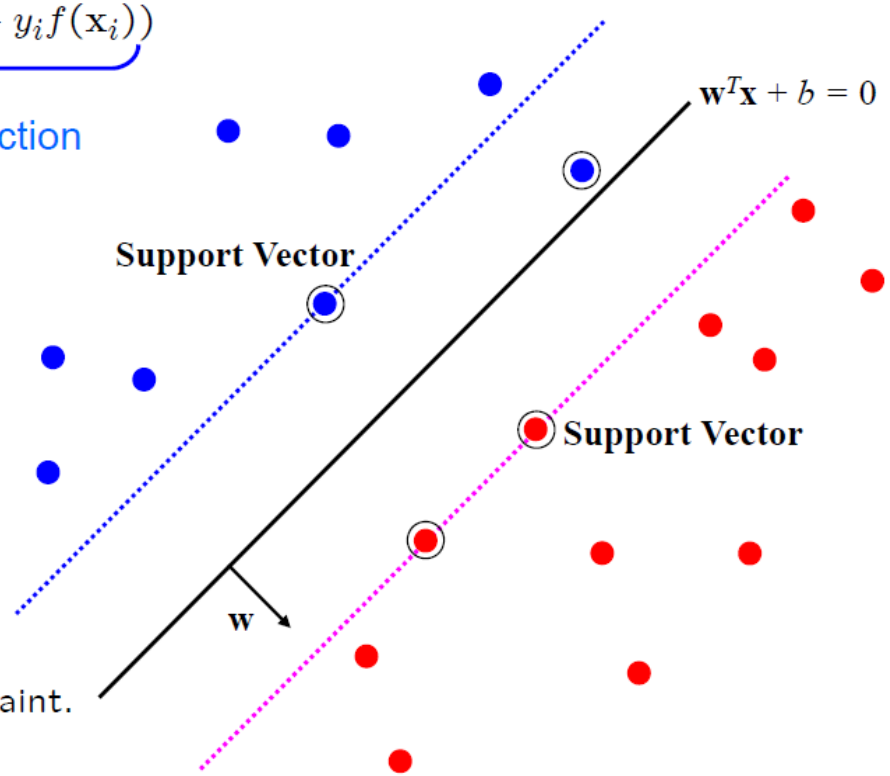
$$\min_{\mathbf{w}\in\mathbb{R}^d} \underbrace{||\mathbf{w}||^2}_{\text{regularization}} + C\sum_i^N \underbrace{\max(0, 1 - y_i f(\mathbf{x}_i))}_{\text{loss function}}$$

Loss function

$$\min_{\mathbf{w}\in\mathbb{R}^d} ||\mathbf{w}||^2 + C\sum_i^N \underbrace{\max(0, 1 - y_i f(\mathbf{x}_i))}_{\text{loss function}}$$

Points are in three categories:

1. $y_i f(x_i) > 1$
   Point is outside margin.
   No contribution to loss
2. $y_i f(x_i) = 1$
   Point is on margin.
   No contribution to loss.
   As in hard margin case.
3. $y_i f(x_i) < 1$
   Point violates margin constraint.
   Contributes to loss



SVM Testing

$$f(x) = \sum_i \alpha_i y_i (\mathbf{x}_i{}^\top \mathbf{x}) + b$$

support vectors

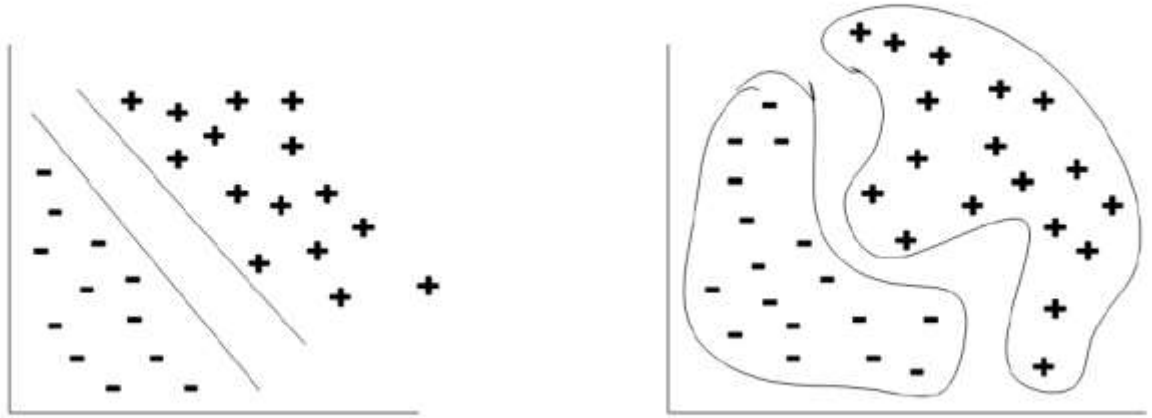
SVM classification for non separable data

- Such a linearly not separable data can be classified using two approaches.
  1 Linear SVM with soft margin
  2 Non-linear SVM
- In the following, we discuss the extension of linear SVM to classify linearly not separable data.
- We discuss non-linear SVM in detail later.
- If the number of training data instances violating linear separability is less, then we can use linear SVM classifier to classify them.
- The rational behind this approach can be better understood from Fig. 10.

Non-Linear SVM

- **SVM classification for non separable data**
- Figure 9 shows a 2-D views of data when they are linearly separable and not separable.
- In general, if data are linearly separable, then there is a hyperplane otherwise no hyperplane.

Figure 9: Two types of training data.



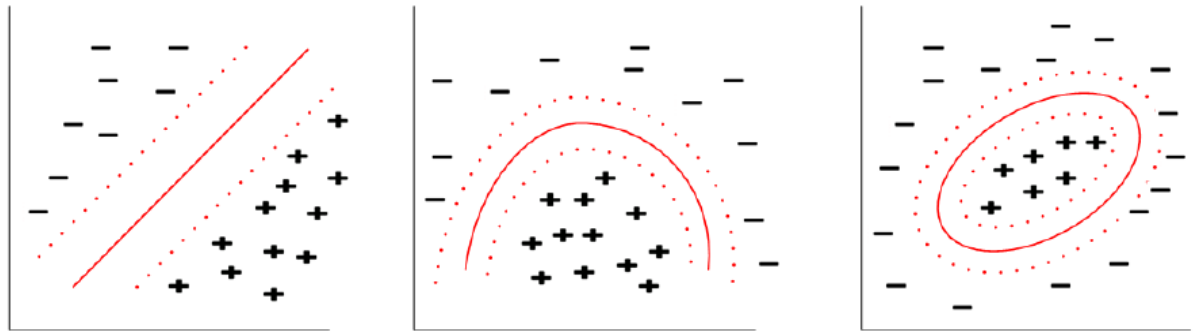
(a) Linearly separable

(b) Linearly non-separable

Non-Linear SVM

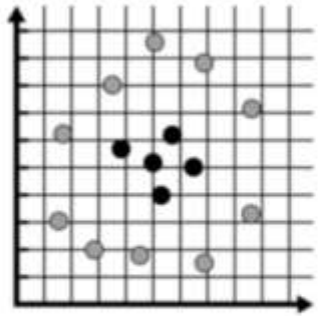
- Linear SVM undoubtedly better to classify data if it is trained by linearly separable data.
- Linear SVM also can be used for non-linearly separable data, provided that number of such instances is less.
- However, in real life applications, number of data overlapping is so high that soft margin SVM cannot cope to yield accurate classifier.
- As an alternative to this there is a need to compute a decision boundary, which is not linear (i.e., not a hyperplane rather hypersurface).
- Note that a linear hyperplane is expressed as a linear equation in terms of n-dimensional component, whe

Figure 13: 2D view of few class separabilities.



(a) Linear hyperplane (b) Nonlinear hyperplane (c) Nonlinear hypersurface

Non-Linear Support Vector Machines

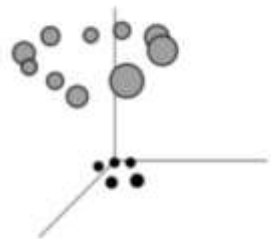


Our original data not linearly separable.

Using a plain SVM here would give us a predictor with terrible performance.

Non-Linear Support Vector Machines

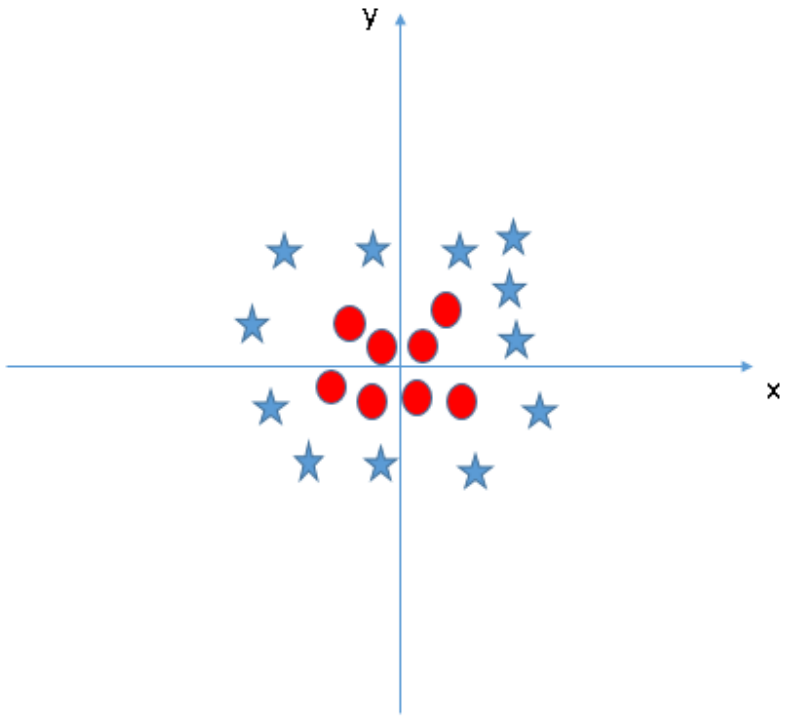
Transform the given data using a **kernel function**.



We **hope** that after applying a non-linear kernel to the data, we can apply a regular SVM and get good accuracy

Find the hyperplane to segregate to classes (Scenario-5)

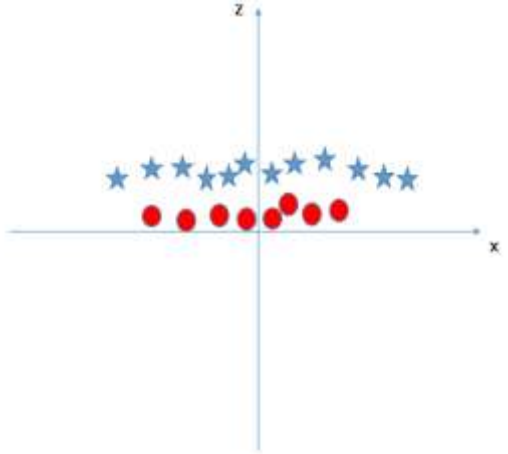
- In the scenario below, we can't have linear hyperplane between the two classes, so how does SVM classify these two classes? Till now, we have only looked at the linear hyperplane.



SVM can solve this problem. It solves this problem by introducing additional feature. Here, we will add a new feature $z=x^2+y^2$.

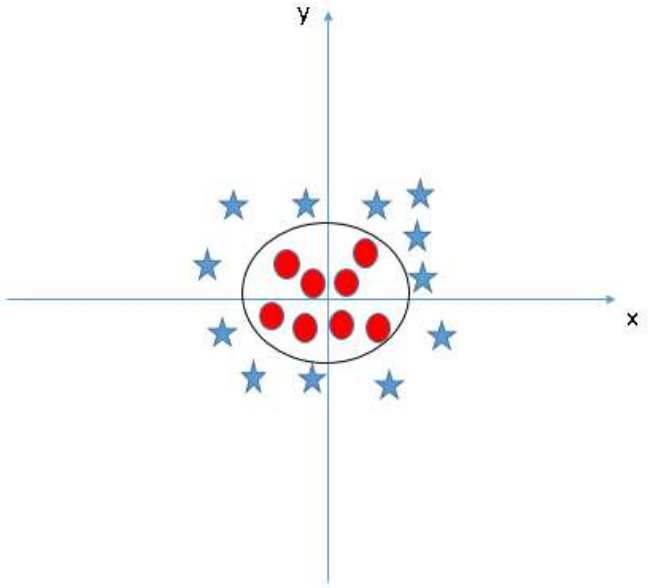
Scenario-5

- Now, let’s plot the data points on axis x and z:



- In above plot, points to consider are:
  - All values for z would be positive always because z is the squared sum of both x and y
  - In the original plot, red circles appear close to the origin of x and y axes, leading to lower value of z and star relatively away from the origin result to higher value of z.

- In SVM, it is easy to have a linear hyperplane between these two classes. But, another burning question which arises is, should we need to add this feature manually to have a hyperplane. No, SVM has a technique called the **kernel trick**. These are functions which takes low dimensional input space and transform it to a higher dimensional space i.e. it converts not separable problem to separable problem, these functions are called **kernels**. It is mostly useful in non-linear separation problem. Simply put, it does some extremely complex data transformations, then find out the process to separate the data based on the labels or outputs you've defined.
- When we look at the hyperplane in original input space it looks like a circle:



Non-Linear SVM

- A hyperplane is expressed as linear : w1x1 + w2x2 + w3x3 + c = 0 ----------(30)
- Whereas a non-linear hypersurface is expressed as.

$$Nonlinear: \; w_1 x_1^2 + w_2 x_2^2 + w_3 x_1 x_2 + w_4 x_3^2 + w_5 x_1 x_3 + c = 0 \qquad (31)$$

- The task therefore takes a turn to find a nonlinear decision boundaries, that is, nonlinear hypersurface in input space comprising with linearly not separable data.
- This task indeed neither hard nor so complex, and fortunately can be accomplished extending the formulation of linear SVM, we have already learned.

Non-Linear SVM

- This can be achieved in two major steps.

  1 Transform the original (non-linear) input data into a higher dimensional space (as a linear representation of data). Note that this is feasible because SVM's performance is decided by number of support vectors (i.e., training data) not by the dimension of data.

  2 Search for the linear decision boundaries to separate the transformed higher dimensional data.

The above can be done in the same line as we have done for linear SVM.

- In nutshell, to have a nonlinear SVM, the trick is to transform non-linear data into higher dimensional linear data.
- This transformation is popularly called non linear mapping or attribute transformation. The rest is same as the linear SVM.

Concept of Non-Linear Mapping

- In order to understand the concept of non-linear transformation of original input data into a higher dimensional space, let us consider a non-linear second order polynomial in a 3-D input space.

$$X(x_1, x_2, x_3) = w_1 x_1 + w_2 x_2 + w_3 x_3 + w_4 x_1^2 + w_5 x_1 x_2 + w_6 x_1 x_3 + c$$

The 3-D input vector $X(x_1, x_2, x_3)$ can be mapped into a 6-D space $Z(z_1, z_2, z_3, z_4, z_5, z_6)$ using the following mappings:

$$z_1 = \phi_1(x) = x_1$$

$$z_2 = \phi_2(x) = x_2$$

$$z_3 = \phi_3(x) = x_3$$

$$z_4 = \phi_4(x) = x_1^2$$

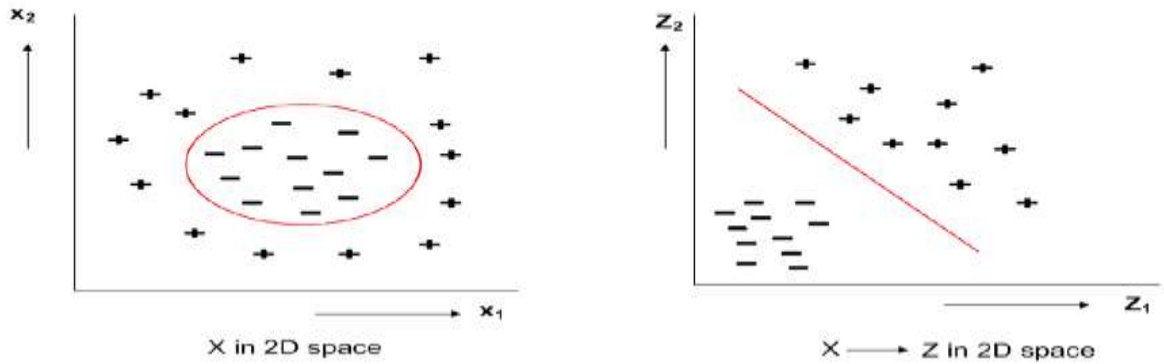
$$z_5 = \phi_5(x) = x_1.x_2$$

$$z_6 = \phi_6(x) = x_1.x_3$$

Concept of Non-Linear Mapping

- The transformed form of linear data in 6-D space will look like.
- Z : w1z1 + w2z2 + w3z3 + w4z4 + w5z5 + w6x1z6 + c
- Thus, if Z space has input data for its attributes x1; x2; x3 (and hence Z's values), then we can classify them using linear decision boundaries.
- **Example: Non-linear mapping to linear SVM**
- The below figure shows an example of 2-D data set consisting of class label +1 (as +) and class label -1 (as -).

Figure 14: Non-linear mapping to Linear SVM.



Concept of Non-Linear Mapping

All instances of class -1 can be separated from instances of class +1 by a circle, The following equation of the decision boundary can be thought of:

Example: Non-linear mapping to linear SVM

We see that

$$X(x_1, x_2) = +1 \text{ if } \sqrt{(x_1 - 0.5)^2 + (x_2 - 0.5)^2} > 2$$

$$X(x_1, x_2) = -1 \text{ otherwise} \tag{32}$$

Concept of Non-Linear Mapping

Example: Non-linear mapping to linear SVM

- The decision boundary can be written as:

$$X = \sqrt{(x_1 - 0.5)^2 + (x_2 - 0.5)^2} = 0.2$$

$$or\ x_1^2 - x_1 + x_2^2 - x_2 = 0.46$$

- A non-linear transformation in 2-D space is proposed as follows:

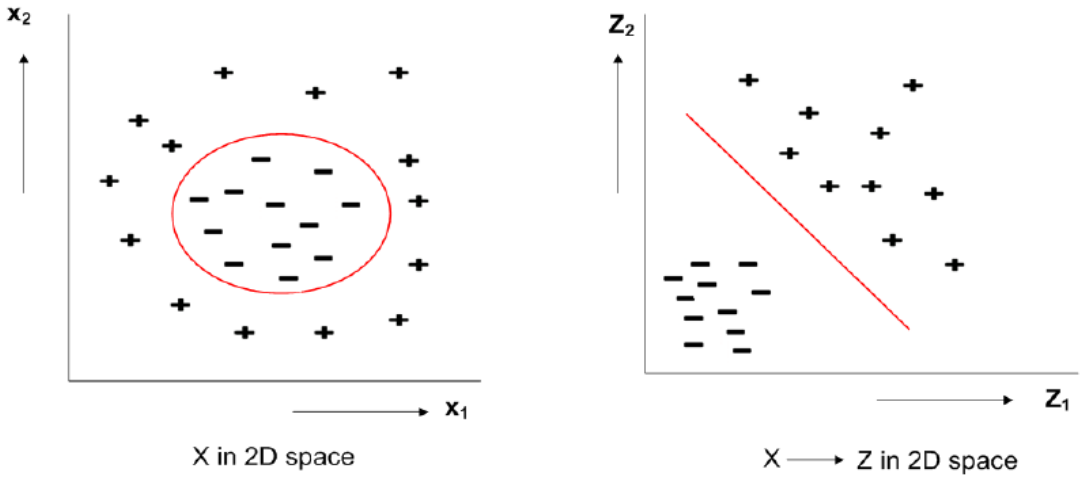
$$Z(z_1, z_2) : \phi_1(x) = x_1^2 - x_1, \phi_2(x) = x_2^2 - x_2 \qquad (33)$$

Concept of Non-Linear Mapping

Example: Non-linear mapping to linear SVM

- The Z space when plotted will take view as shown in Fig. 15, where data are separable with linear boundary, namely $Z : z_1 + z_2 = -0.46$

Figure 15: Non-linear mapping to Linear SVM.



Non-Linear to Linear Transformation: Issues

The non linear mapping and hence a linear decision boundary
concept looks pretty simple. But there are many potential problems to do so.

Mapping: How to choose the non linear mapping to a higher dimensional space?

In fact, the – Ø transformation works fine for small example.

But, it fails for realistically sized problems.

Cost of mapping: For n-dimensional input instances there exist

$$N_H = \frac{(N+d-1)!}{d!(N-1)!}$$

different monomials comprising a feature space dimensionality N_H. Here, d is the maximum degree of monomial

Non-Linear to Linear Transformation: Issues

- Dimensionality problem: It may suffer from the curse of dimensionality problem often associated with a high dimensional data.
- More specifically, in the calculation of W.X or Xi :X (in (X) see Eqn. 18), we need n multiplications and n additions (in their dot products) for each of the n-dimensional input instances and support vectors, respectively.
- As the number of input instances as well as support vectors are enormously large, it is therefore, computationally expensive.
- Computational cost: Solving the quadratic constrained optimization problem in the high dimensional feature space is too a computationally expensive task.

Non-Linear to Linear Transformation: Issues

- Fortunately, mathematicians have cleverly proposes an elegant solution to the above problems.
- Their solution consist of the following:

  Dual formulation of optimization problem

  Kernel trick
- In the next few slides, we shall learn about the above-mentioned two topics.

Dual Formulation of Optimization Problem

- We have already learned the Lagrangian formulation to find the maximum margin hyperplane as a linear SVM classifier.
- Such a formulation is called primal form of the constraint optimization problem.
- Primal form of Lagrangian optimization problem is reproduced further

$$Minimize \frac{||W||^2}{2}$$

$$Subject\ to\ y_i(W.x_i + b) \geq 1,\ i = 1, 2, 3.....n. \qquad (34)$$

Dual Formulation of Optimization Problem

The primal form of the above mentioned inequality constraint optimization problem(according to Lagrange multiplier method) is given by

$$L_p = \frac{||W||^2}{2} - \sum_{i=1}^{n} \lambda_i (y_i (W.x_i + b) - 1) \qquad (35)$$

This Lp is called the primal form of the Lagrangian optimization problem.

Dual Formulation of Optimization Problem

- The dual form of the same problem can be derived as follows.
- To minimize the Lagrangian, we must take the derivative of L_p with respect to W, b and set them to zero.

$$\frac{\delta L_p}{\delta W} = 0 \Rightarrow W = \sum_{i=1}^{n} \lambda_i . y_i . x_i \qquad (36)$$

$$\frac{\delta L_p}{\delta b} = 0 \Rightarrow \sum_{i=1}^{n} \lambda_i . y_i = 0 \qquad (37)$$

Dual Formulation of Optimization Problem

- From above two equation we get Lagrangian L as

$$L = \sum_{i=1}^{n} \lambda_i + \frac{1}{2} \sum_{i,j} \lambda_i . y_i . \lambda_j . y_j . x_i . x_j - \sum_{i=1}^{n} \lambda_i . y_i \sum_{j=1}^{n} (\lambda_j . y_j . x_j) x_i$$

$$= \sum_{i=1}^{n} \lambda_i - \frac{1}{2} \sum_{i,j} \lambda_i . \lambda_j . y_i . y_j . x_i . x_j$$

- This form is called the dual form of Lagrangian and distinguishably written as:

$$L_D = \sum_{i=1}^{n} \lambda_i - \frac{1}{2} \sum_{i,j} \lambda_i . \lambda_j . y_i . y_j . x_i . x_j \tag{38}$$

  - This form is called the dual form of Lagrangian and distinguishably written as:

$$L_D = \sum_{i=1}^{n} \lambda_i - \frac{1}{2} \sum_{i,j} \lambda_i . \lambda_j . y_i . y_j . x_i . x_j \tag{39}$$

Dual Formulation of Optimization Problem

- There are key differences between primal (Lp) and dual (LD) forms of Lagrangian optimization problem as follows.

1 Lp involves a large number of parameters namely W, b and i ’s. On the other hand, LD involves only i ’s, that is, Lagrange multipliers.

2 Lp is the minimization problem as the quadratic term is positive. However, the quadratic term in LD is negative sign, Hence it is turned out to be a maximization problem.

3 Lp involves the calculation of W:x, whereas LD involves the calculation of xi :xj . This, in fact, advantageous, and we will realize it when we learn Kernel-based calculation.

Dual Formulation of Optimization Problem

4. The SVM classifier with primal form is $\delta_p(x) = W.x + b$ with $W = \sum_{i=1}^{n} \lambda_i.y_i.x_i$ whereas the dual version of the classifier is

$$\delta_D(X) = \sum_{i=1}^{m} \lambda_i.y_i.(x_i.x) + b$$

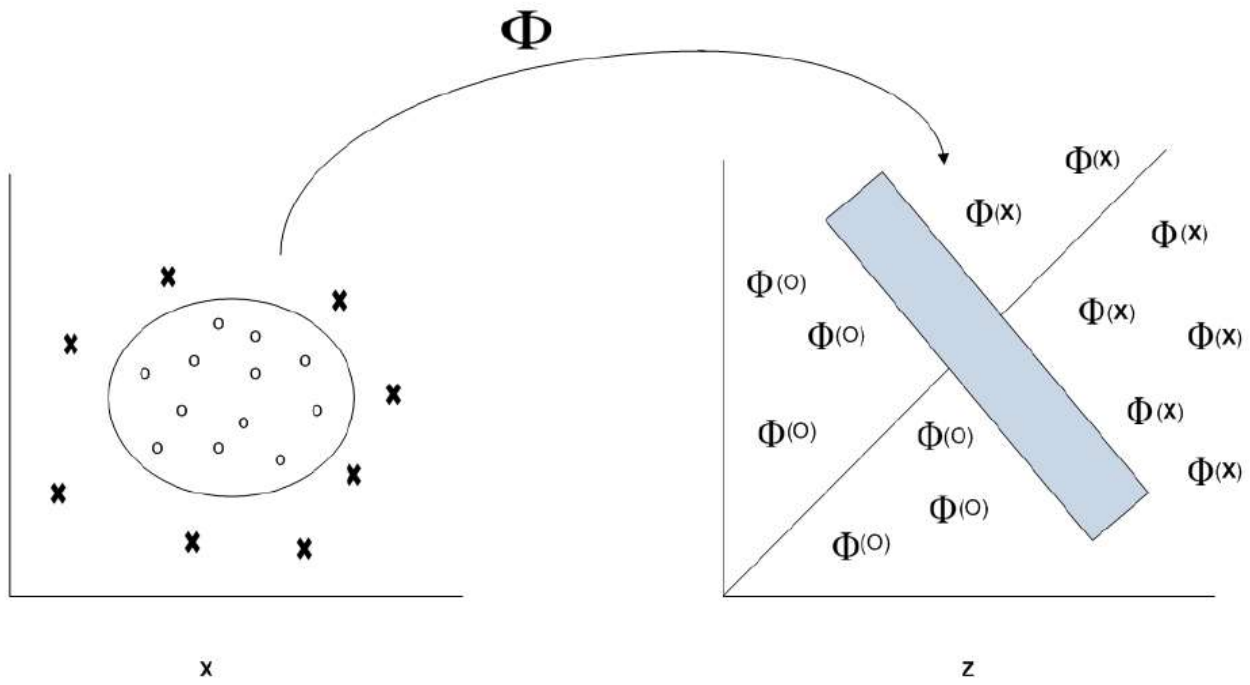
where x_i being the i^{th} support vector, and there are m support vectors. Thus, both L_p and L_D are equivalent.

Kernel Trick

- We have already covered an idea that training data which are not linearly separable, can be transformed into a higher dimensional feature space such that in higher dimensional transformed space a hyperplane can be decided to separate the transformed data and hence original data(also see Fig.16).
- Clearly the data on the left in the figure is not linearly separable.
- Yet if we map it to a 3D space using and the mapped data, then it is possible to have a decision boundaries and hence hyperplane in 3D space.

Kernel Trick

Figure 16: SVM classifier in transformed feature space



Kernel Trick

Example: SVM classifier for non-linear data

- Suppose, there are a set of data in R^2(i.e., in 2-D space), ϕ is the mapping for $X \epsilon R^2$ to $Z(z_1, z_2, z_3) \epsilon R^3$, in the 3-D space.

$$R^2 \Rightarrow X(x_1, x_2)$$

$$R^3 \Rightarrow Z(z_1, z_2, z_3)$$

Kernel Trick

Example: SVM classifier for non-linear data

- $$\phi(X) \Rightarrow Z$$

$$z_1 = x_1^2, z_2 = \sqrt{2}x_1x_2, z_3 = x_2^2$$

- The hyperplane in R^2 is of the form

$$w_1x_1^2 + w_2\sqrt{2}x_1x_2 + w_3x_2^2 = 0$$

- Which is the equation of an ellipse in 2D.

Kernel Trick

Example: SVM classifier for non-linear data

- After the transformation, ϕ as mentioned above, we have the decision boundary of the form

$$w_1 z_1 + w_2 z_2 + w_3 z_2 = 0$$

- This is clearly a linear form in 3-D space. In other words, $W.x + b = 0$ in R^2 has a mapped equivalent $W.z + b' = 0$ in R^3

- This means that data which are not linearly separable in 2-D are separable in 3-D, that is, non linear data can be classified by a linear SVM classifier.

Kernel Trick

- The above can be generalized in the following.
  - **Classifier:**

$$\delta(x) = \sum_{i=1}^{n} \lambda_i y_i y_i . x + b$$

$$\delta(z) = \sum_{i=1}^{n} \lambda_i y_i \phi(x_i).\phi(x) + b$$

  - **Learning:**

$$\textit{Maximize} \sum_{i=1}^{n} \lambda_i - \frac{1}{2} \sum_{i,j} \lambda_i \lambda_j . y_i . y_j . x_i . x_j$$

$$\textit{Maximize} \sum_{i=1}^{n} \lambda_i - \frac{1}{2} \sum_{i,j} \lambda_i \lambda_j . y_i . y_j \phi(x_i).\phi(x_j)$$

Subject to: $\lambda_i \geq 0$, $\sum_i \lambda_i . y_i = 0$

Kernel Trick

- Now, question here is how to choose , the mapping function X) Z, so that linear SVM can be directly applied to.
- A breakthrough solution to this problem comes in the form of a method as the kernel trick.
- We discuss the kernel trick in the following.
- We know that (.) dot product is often regarded as a measure of
- similarity between two input vectors.

  - For example, if X and Y are two vectors, then

$$X.Y = |X||Y|cos\theta$$

  - Here, similarity between X and Y is measured as cosine similarity.
  - If θ=0 (i.e., cosθ=1), then they are most similar, otherwise orthogonal means dissimilar.

Kernel Trick

- Analogously, if X_i and X_j are two tuples, then $X_i.X_j$ is regarded as a measure of similarity between X_i and X_j.
- Again, $\phi(X_i)$ and $\phi(X_j)$ are the transformed features of X_i and X_j, respectively in the transformed space; thus, $\phi(X_i).\phi(X_j)$ is also should be regarded as the similarity measure between $\phi(X_i)$ and $\phi(X_j)$ in the transformed space.
- This is indeed an important revelation and is the basic idea behind the kernel trick.
- Now, naturally question arises, if both measures the similarity, then what is the correlation between them (i.e., $X_i.X_j$ and $\phi(X_i).\phi(X_j)$).
- Let us try to find the answer to this question through an example.

Kernel Trick

Example: Correlation between $X_i.X_j$ and $\phi(X_i).\phi(X_j)$

- Without any loss of generality, let us consider a situation stated below.

$$\phi : R^2 \Rightarrow R^3 = x_1^2 \Rightarrow z, x_2^2 \Rightarrow z_2, \sqrt{2}x_1x_2 \Rightarrow z_3 \qquad (40)$$

- Suppose, $X_i = [x_{i1}, x_{i2}]$ and $X_j = [x_{j1}, x_{j2}]$ are any two vectors in R^2.

- Similarly, $\phi(X_i) = [x_{i1}^2, \sqrt{2}.x_{i1}.x_{i2}, x_{i2}^2]$ and $\phi(X_j) = [x_{j1}^2, \sqrt{2}.x_{j1}.x_{j2}, x_{j2}^2]$ are two transformed version of X_i and X_j but in R^3.

Kernel Trick

Example: Correlation between $X_i.X_j$ and $\phi(X_i).\phi(X_j)$

- Now,

$$\phi(X_i).\phi(X_j) = [x_{i1}^2, \sqrt{2}.x_{i1}.x_{i2}, x_{i2}^2] \begin{bmatrix} x_{j1}^2 \\ \sqrt{2}x_{j1}x_{j2} \\ x_{j2}^2 \end{bmatrix}$$

$$= x_{i1}^2.x_{j1}^2 + 2x_{i1}x_{i2}x_{j1}x_{j2} + x_{i2}^2.x_{j2}^2$$

$$= (x_{i1}.x_{j1} + x_{i2}.x_{j2})^2$$

$$= \{[x_{i1}, x_{i2}] \begin{bmatrix} x_{j1} \\ x_{j2} \end{bmatrix}\}^2$$

$$= (X_i.X_j)^2$$

Kernel Trick

- With reference to the above example, we can conclude that $\phi(X_i).\phi(X_j)$ are correlated to $X_i.X_j$.
- In fact, the same can be proved in general, for any feature vectors and their transformed feature vectors.
- A formal proof of this is beyond the scope of this course.
- More specifically, there is a correlation between dot products of original data and transformed data.
- Based on the above discussion, we can write the following implications.

$$X_i.X_j \Rightarrow \phi(X_i).\phi(X_j) \Rightarrow K(X_i, X_j) \tag{41}$$

- Here, $K(X_i, X_j$ denotes a function more popularly called as kernel function

Kernel Trick : Significance

- This kernel function $K(X_i, X_j)$ physically implies the similarity in the transformed space (i.e., nonlinear similarity measure) using the original attribute X_i, X_j. In other words, K, the similarity function compute a similarity of both whether data in original attribute space or transformed attribute space.
- **Implicit transformation**
  - The first and foremost significance is that we do not require any ϕ transformation to the original input data at all. This is evident from the following re-writing of our SVM classification problem.

$$\textit{Classifier}: \ \delta(X) = \sum_{i=1}^{n} \lambda_i . Y_i . K(X_i, X) + b \tag{42}$$

$$\textit{Learning}: \ \textit{maximize} \sum_{i=1} \lambda_i - \frac{1}{2} \sum_{i,j} \lambda_i . \lambda_j Y_i Y_j . K(X_i . X_j) \tag{43}$$

$$\textit{Subject to } \lambda_i \geq 0 \textit{ and } \sum_{i}^{n} \lambda_i . Y_i = 0 \tag{44}$$

Kernel Trick : Significance

- **Computational efficiency:**
- Another important significance is easy and efficient computability.
- We know that in the discussed SVM classifier, we need several and repeated round of computation of dot products both in learning phase as well as in classification phase.
- On other hand, using kernel trick, we can do it once and with fewer dot products.
- This is explained in the following.

- We define a matrix called design matrix(X), which contains all data and gram matrix (K), which contains all dot products are as follows:

$$\textit{Design matrix}: \; X = \begin{bmatrix} X_1 \\ X_2 \\ . \\ . \\ . \\ X_n \end{bmatrix}_{n \times N} \tag{45}$$

  where n denotes the number of training data in N-dimensional data space.
- Note that X contains all input data in the original attribute space.

Kernel Trick : Significance

In nutshell, we have the following.

- Instead of mapping our data via ϕ and computing the dot products, we can accomplish everything in one operation.
- Classifier can be learnt and applied without explicitly computing $\phi(X)$.
- Complexity of learning depends on n (typically it is $O(n^3)$), not on N, the dimensionality of data space.
- All that is required is the kernel $K(X_i, X_j)$
- Next, we discuss the aspect of deciding kernel functions.

Kernel Functions

Before going to learn the popular kernel functions adopted in SVM classification, we give a precise and formal definition of kernel $k(X_i, X_j)$.

Definition 10.1:

A kernel function $K(X_i, X_j)$ is a real valued function defined on R such that there is another function $\phi : X \to Z$ such that $K(X_i, X_j) = \phi(X_i).\phi(X_j)$. Symbolically we write $\phi : R^m \to R^n : K(X_i, X_j) = \phi(X_i).\phi(X_j)$ where $n > m$.

Kernel Functions : Example

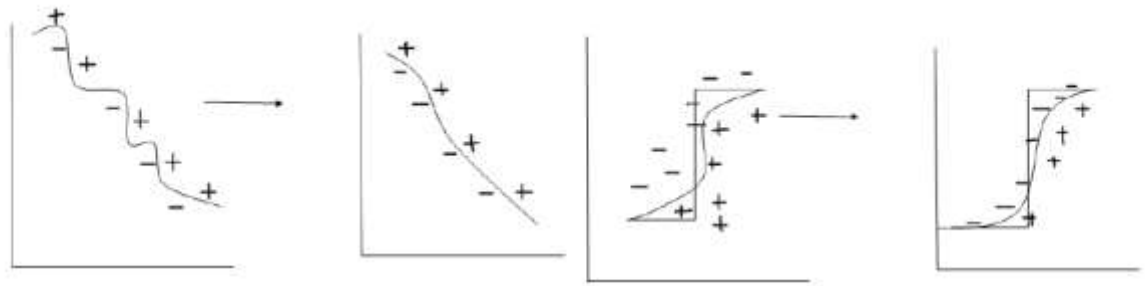
Table 2: Some standard kernel functions

Kernel name	Functional form	Remark
Linear kernel	$K(X, Y) = X^T Y$	The simplest kernel used in linear SVM
Polynomial kernel of degree p	$K(X, Y) = (X^T Y + 1)^\rho, \rho > 0$	It produces a large dot products. Power ρ is specified apriori by the user.
Gaussian (RBF) kernel	$K(X, Y) = e^{\frac{c\|\|x-y\|\|^2}{2\sigma^2}}$	It is a nonlinear kernel called Gaussian Radia Bias function kernel
Laplacian kernel	$K(X, Y) = e^{-\lambda\|\|x-y\|\|}$	Follows laplacian mapping
Sigmoid kernel	$K(X, Y) = tanh(\beta_0 X^T y + \beta_1)$	Followed when statistical test data is known
Mahalanobis kernel	$K(X, Y) = e^{-(X-y)^T A(x-y)}$	Followed when statistical test data is known

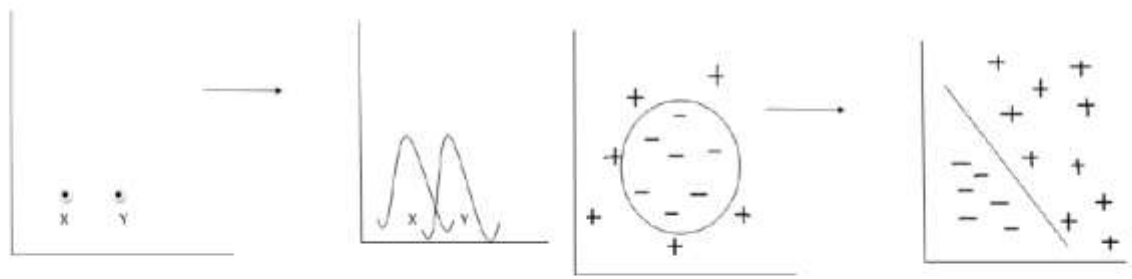
Kernel Functions : Example

- Different kernel functions follow different parameters. Those parameters are called magic parameters and to be decided a priori.
- Further, which kernels to be followed also depends on the pattern of data as well as prudent of user.
- In general, polynomial kernels result in a large dot products, Gaussian RBF produces more support vectors than other kernels.
- To have an intuitive idea of kernels to be used in non-linear data handling is shown in Fig. 17.

Kernel Functions : Example



(a) Polynomial kernel (b) Sigmoid kernel



(c) Laplacian kernel (d) Gaussian RBF kernel

Figure 17: Visual interpretation of few kernel functions.

Why are SVMs fast?

1.Quadratic optimization (convex!)

2. They work in the dual, with relatively few points

3. The kernel trick

Why are SVMs often more accurate than logistic regression?

1. SVMs use kernels –but regression can, too

2.SVMs assume less about the model form

3. Logistic regression uses all the data points, assuming a probabilistic model, while SVMs ignore the points that are clearly correct, and give less weight to ones that are wrong

Characteristics of SVM

- The SVM learning problem can be formulated as a convex
- optimization problem, in which efficient algorithms are available to
- find the global minimum of the objective function. Other methods
- namely rule based classifier, ANN classifier etc. find only local
- optimum solutions.
- 2 SVM is the best suitable to classify both linear as well as
- non-linear training data efficiently.
- 3 SVM can be applied to categorical data by introducing a suitable
- similarity measures.
- 4 Computational complexity is influenced by number of training data
- not the dimension of data. In fact, learning is a bit computationally
- heavy and hence slow, but classification of test is extremely fast
- and accurate.

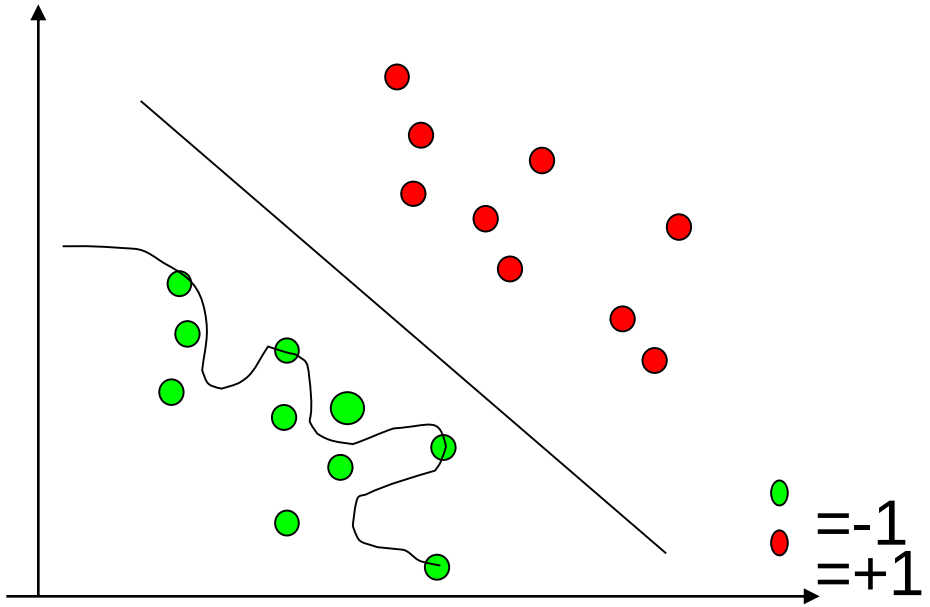
Main Ideas

- Formalize notion of the best linear separator
- Way to convert a constrained optimization problem to one that is easier to solve
- Projecting data into higher-dimensional space makes it linearly separable
- Depends only on the number of training examples, not on dimensionality of the kernel space!

Overtraining/overfitting

A well known problem with machine learning methods is overtraining. This means that we have learned the training data very well, but we can not classify unseen examples correctly.

An example: A botanist really knowing trees.Everytime he sees a new tree, he claims it is not a tree.



Overtraining/overfitting 2

A measure of the risk of overtraining with SVM (there are also other measures).

It can be shown that: The portion, n, of unseen data that will be missclassified is bounded by:

$n \leq$ Number of support vectors / number of training examples

Ockham´s razor principle: Simpler system are better than more complex ones. In SVM case: fewer support vectors mean a simpler representation of the hyperplane.

Example: Understanding a certain cancer if it can be described by one gene is easier than if we have to describe it with 5000.