IIT KHARAGPUR

NPTEL ONLINE CERTIFICATION COURSES

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Data Mining

Week 5: Support Vector Machine

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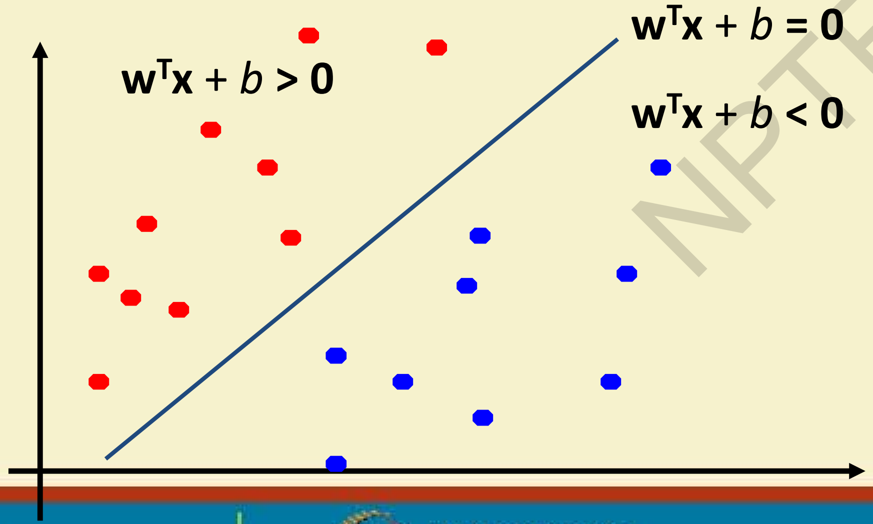
Support Vector Machines

Linear Separators

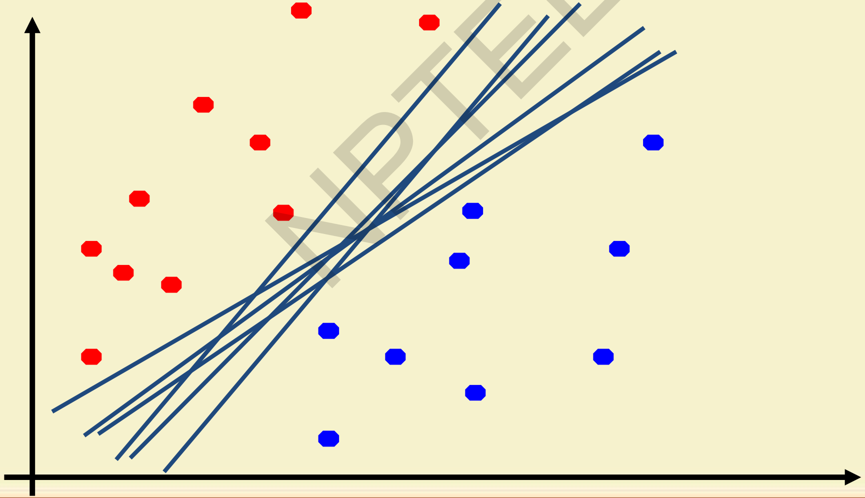
- Binary classification can be viewed as the task of separating classes in feature space:



$f(\mathbf{x}) = \text{sign}(\mathbf{w}^T\mathbf{x} + b)$

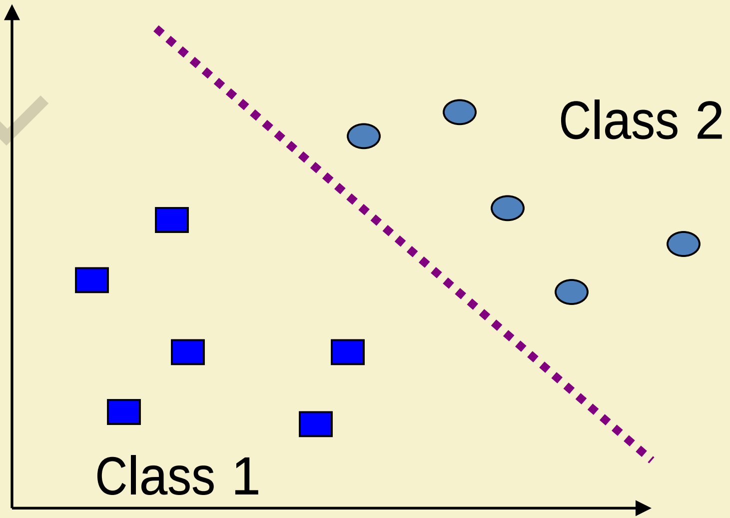
Linear Separators

- Which of the linear separators is optimal?

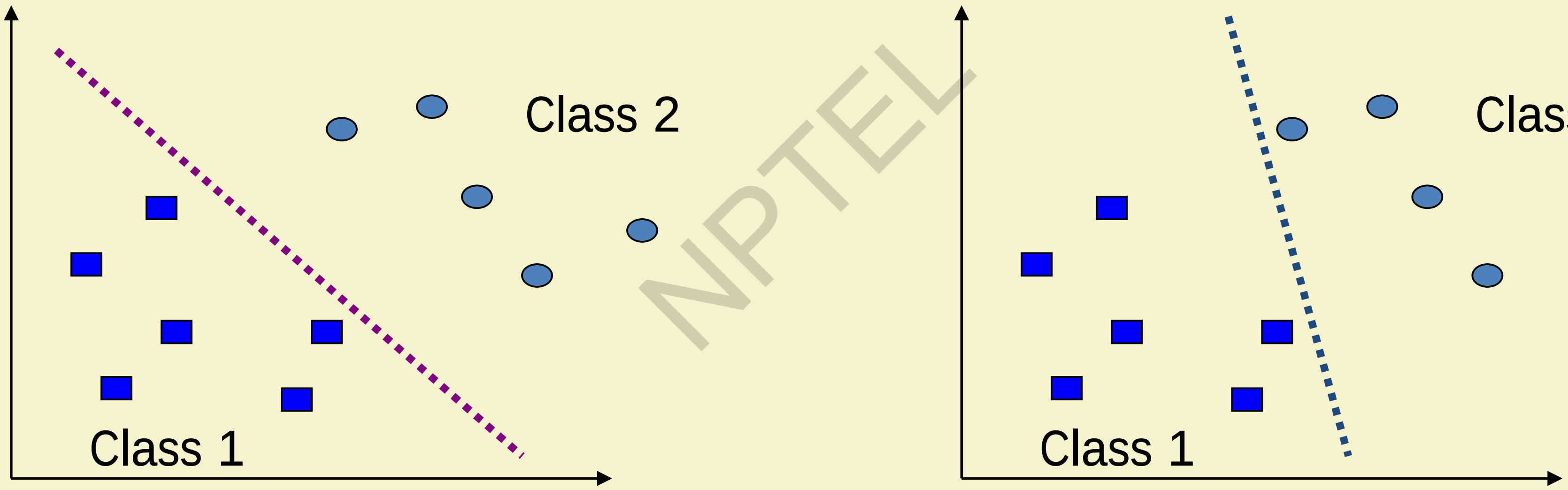


What is a good Decision Boundary?

- Many decision boundaries!
  - The Perceptron algorithm can be used to find such a boundary
- Are all decision boundaries equally good?



Examples of Bad Decision Boundaries



Finding the Decision Boundary

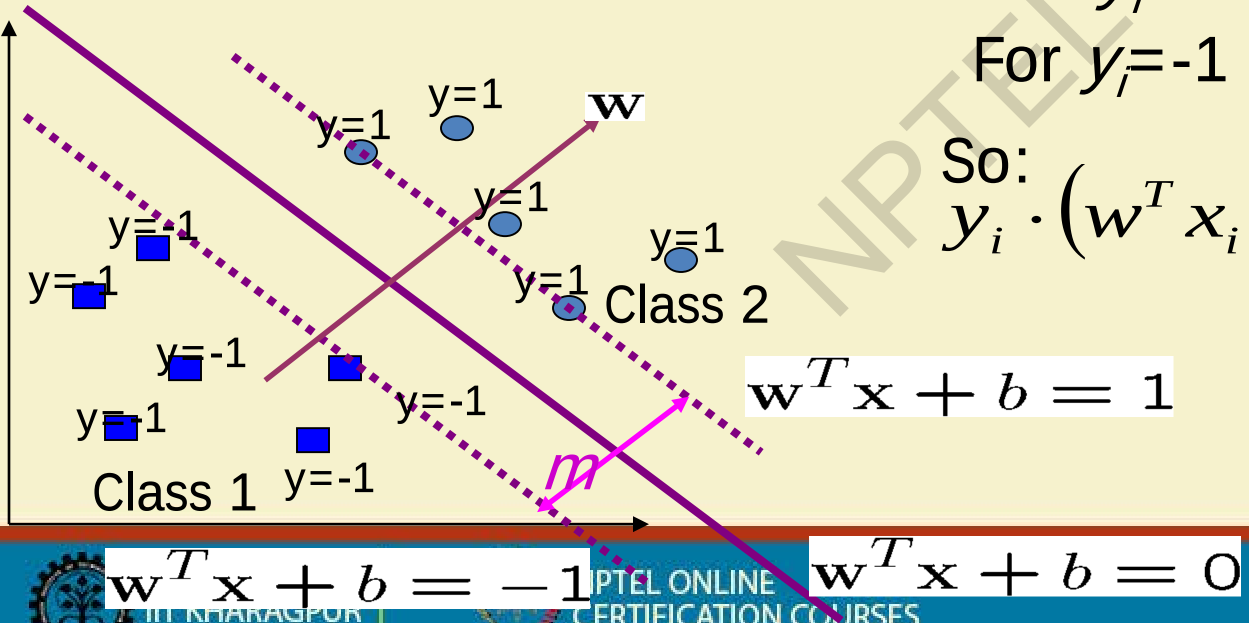
- Let $\{x_1, \ldots, x_n\}$ be our data set and let $y_i \in \{1,-1\}$ be the class label of x_i

For $y_i=1$ $\quad \mathbf{w}^T x_i + b \geq 1$

For $y_i=-1$ $\quad \mathbf{w}^T x_i + b \leq -1$

So:

$$y_i \cdot \left(\mathbf{w}^T x_i + b\right) \geq 1, \forall (x_i, y_i)$$



Large-margin Decision Boundary

- The decision boundary should be as far away from the data of both classes as possible
  - We should maximize the margin, *m*

$$m = \frac{2}{||\mathbf{w}||}$$

Finding the Decision Boundary

- The decision boundary should classify all points correctly $\Rightarrow$

$$y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1, \qquad \forall i$$

- The decision boundary can be found by solving the following constrained optimization problem

$$\text{Minimize } \frac{1}{2}||\mathbf{w}||^2$$

$$\text{subject to } y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1 \qquad \forall i$$

- This is a constrained optimization problem. Solving it requires to use Lagrange multipliers

Finding the Decision Boundary

$$\text{Minimize } \frac{1}{2}||\mathbf{w}||^2$$

$$\text{subject to } 1-y_i(\mathbf{w}^T\mathbf{x}_i+b) \leq 0 \qquad \text{for } i = 1, \ldots, n$$

- The Lagrangian is

$$\mathcal{L} = \frac{1}{2}\mathbf{w}^T\mathbf{w} + \sum_{i=1}^{n} \alpha_i \left(1 - y_i(\mathbf{w}^T\mathbf{x}_i + b)\right)$$

  - $\alpha_i \geq 0$
  - Note that $||\mathbf{w}||^2 = \mathbf{w}^T\mathbf{w}$

Gradient with respect to *w* and *b*

- Setting the gradient of w.r.t. **w** and b to zero, we have

$$L = \frac{1}{2}w^T w + \sum_{i=1}^{n} \alpha_i \left(1 - y_i \left(w^T x_i + b\right)\right) =$$

$$= \frac{1}{2}\sum_{k=1}^{m} w^k w^k + \sum_{i=1}^{n} \alpha_i \left(1 - y_i \left(\sum_{k=1}^{m} w^k x_i^{\,k} + b\right)\right)$$

n: no of examples, m: dimension of the space

$$\begin{cases} \dfrac{\partial L}{\partial w^k} = 0, \forall k \\ \dfrac{\partial L}{\partial b} = 0 \end{cases}$$

$$\mathbf{w} + \sum_{i=1}^{n} \alpha_i(-y_i)\mathbf{x}_i = \mathbf{0} \quad \Rightarrow \quad \mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i$$

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

The Dual Problem

- If we substitute $\mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i$, we have

$$
\begin{aligned}
\mathcal{L} &= \frac{1}{2} \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i^T \sum_{j=1}^{n} \alpha_j y_j \mathbf{x}_j + \sum_{i=1}^{n} \alpha_i \left(1 - y_i \Big(\sum_{j=1}^{n} \alpha_j y_j \mathbf{x}_j^T \mathbf{x}_i + b \Big) \right) \\
&= \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j + \sum_{i=1}^{n} \alpha_i - \sum_{i=1}^{n} \alpha_i y_i \sum_{j=1}^{n} \alpha_j y_j \mathbf{x}_j^T \mathbf{x}_i - b \sum_{i=1}^{n} \alpha_i y_i \\
&= -\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j + \sum_{i=1}^{n} \alpha_i
\end{aligned}
$$

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

Since

- This is a function of α_i only

The Dual Problem

- The new objective function is in terms of α_i only
- It is known as the dual problem: if we know **w**, we know all α_i; if we know all α_i, we know **w**
- The original problem is known as the primal problem
- The objective function of the dual problem needs to be maximized (comes out from the KKT theory)
- The dual problem is therefore:

$$\text{max. } W(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1,j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$

$$\text{subject to } \alpha_i \geq 0, \qquad \sum_{i=1}^{n} \alpha_i y_i = 0$$

The Dual Problem

$$\text{max.} \quad W(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1,j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$

$$\text{subject to } \alpha_i \geq 0, \sum_{i=1}^{n} \alpha_i y_i = 0$$

- This is a quadratic programming (QP) problem
  - A global maximum of α_i can always be found
- **w** can be recovered by

$$\mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i$$

Characteristics of the Solution

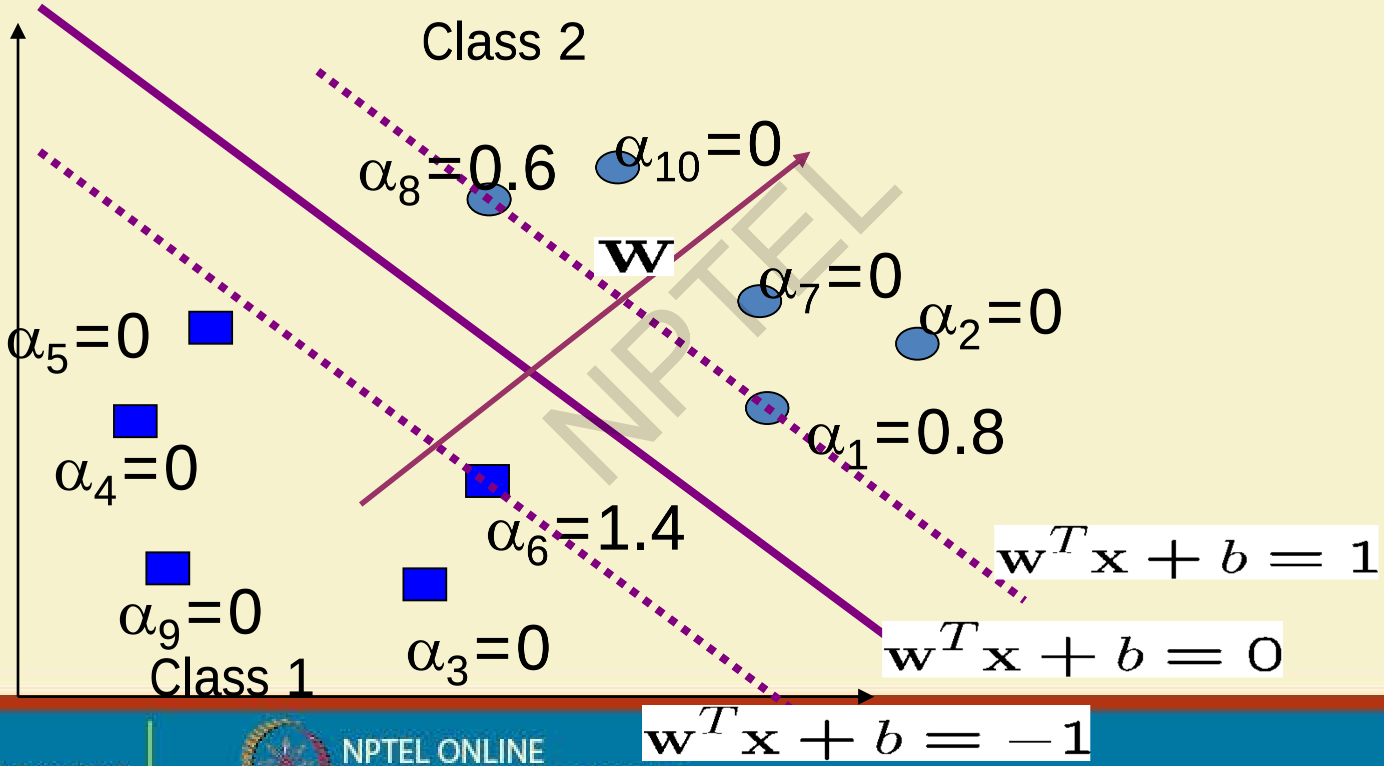
- Many of the α_i are zero
  - **w** is a linear combination of a small number of data points
  - This "sparse" representation can be viewed as data compression as in the construction of knn classifier

- $\mathbf{x}_i$ with non-zero α_i are called support vectors (SV)
  - The decision boundary is determined only by the SV
  - Let t_j (j=1, ..., s) be the indices of the s support vectors. We can write

$$\mathbf{w} = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} \mathbf{x}_{t_j}$$

  - Note: **w** need not be formed explicitly

A Geometrical Interpretation



Characteristics of the Solution

- For testing with a new data **z**
  - Compute $\mathbf{w}^T\mathbf{z} + b = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} (\mathbf{x}_{t_j}^T \mathbf{z}) + b$

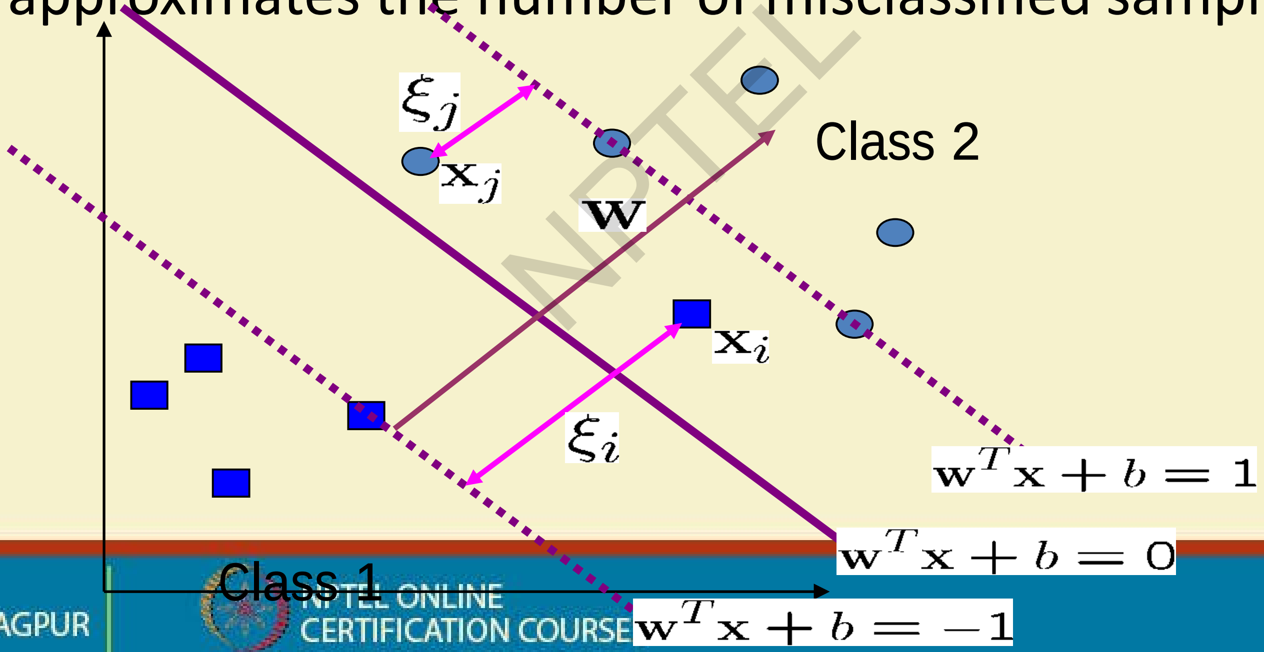
    and classify **z** as class 1 if the sum is positive, and class 2 otherwise
  - Note: **w** need not be formed explicitly

The Quadratic Programming Problem

- Many approaches have been proposed
  - Loqo, cplex, etc. (see http://www.numerical.rl.ac.uk/qp/qp.html)
- Most are “interior-point” methods
  - Start with an initial solution that can violate the constraints
  - Improve this solution by optimizing the objective function and/or reducing the amount of constraint violation
- For SVM, sequential minimal optimization (SMO) seems to be the most popular
  - A QP with two variables is trivial to solve
  - Each iteration of SMO picks a pair of (α_i,α_j) and solve the QP with these two variables; repeat until convergence
- In practice, we can just regard the QP solver as a “black-box” without bothering how it works

Non-linearly Separable Problems

- We allow "error" ξ_i in classification; it is based on the output of the discriminant function $\mathbf{w}^T\mathbf{x}+b$
- ξ_i approximates the number of misclassified samples



Soft Margin Hyperplane

- The new conditions become

$$\begin{cases} \mathbf{w}^T\mathbf{x}_i + b \geq 1 - \xi_i & y_i = 1 \\ \mathbf{w}^T\mathbf{x}_i + b \leq -1 + \xi_i & y_i = -1 \\ \xi_i \geq 0 & \forall i \end{cases}$$

  - ξ_i are "slack variables" in optimization
  - Note that ξ_i=0 if there is no error for $\mathbf{x}_i$
  - ξ_i is an upper bound of the number of errors
- We want to minimize

$$\frac{1}{2}\|w\|^2 + C\sum_{i=1}^{n}\xi_i$$

subject to $y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1 - \xi_i, \quad \xi_i \geq 0$

- C : tradeoff parameter between error and margin

The Optimization Problem

$$L = \frac{1}{2} w^T w + C \sum_{i=1}^{n} \xi_i + \sum_{i=1}^{n} \alpha_i \left(1 - \xi_i - y_i \left(w^T x_i + b\right)\right) - \sum_{i=1}^{n} \mu_i \xi_i$$

With α and μ Lagrange multipliers, POSITIVE

$$\frac{\partial L}{\partial w_j} = w_j - \sum_{i=1}^{n} \alpha_i y_i x_{ij} = 0$$

$$\vec{w} = \sum_{i=1}^{n} \alpha_i y_i \vec{x}_i = 0$$

$$\frac{\partial L}{\partial \xi_j} = C - \alpha_j - \mu_j = 0$$

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

The Dual Problem

$$L = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j y_i y_j \vec{x}_i^{\,T}\vec{x}_j + C\sum_{i=1}^{n}\xi_i +$$

$$+\sum_{i=1}^{n}\alpha_i\left(1-\xi_i - y_i\left(\sum_{j=1}^{n}\alpha_j y_j x_j^{\,T} x_i + b\right)\right) - \sum_{i=1}^{n}\mu_i\xi_i$$

With $\sum_{i=1}^{n} y_i\alpha_i = 0$ $\qquad C = \alpha_j + \mu_j$

$$L = -\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j y_i y_j \vec{x}_i^{\,T}\vec{x}_j + \sum_{i=1}^{n}\alpha_i$$

The Optimization Problem

- The dual of this new constrained optimization problem is

$$\text{max. } W(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1,j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$

$$\text{subject to } C \geq \alpha_i \geq 0, \sum_{i=1}^{n} \alpha_i y_i = 0$$

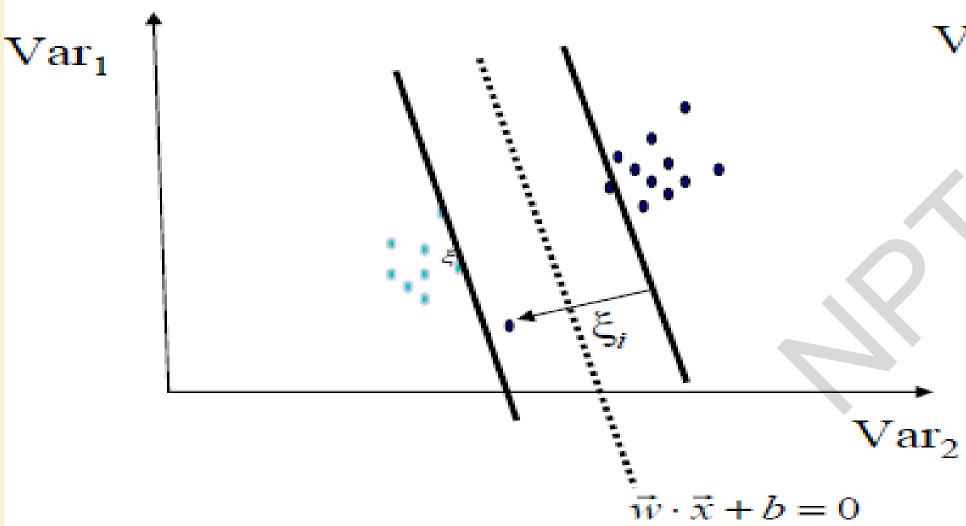
- New constrainsderive from $C = \alpha_j + \mu_j$ since μ and α are positive.
- **w** is recovered as $\mathbf{w} = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} \mathbf{x}_{t_j}$
- This is very similar to the optimization problem in the linear separable case, except that there is an upper bound *C* on α_i now
- Once again, a QP solver can be used to find α_i

$$\frac{1}{2}\|w\|^2 + C\sum_{i=1}^{n}\xi_i$$

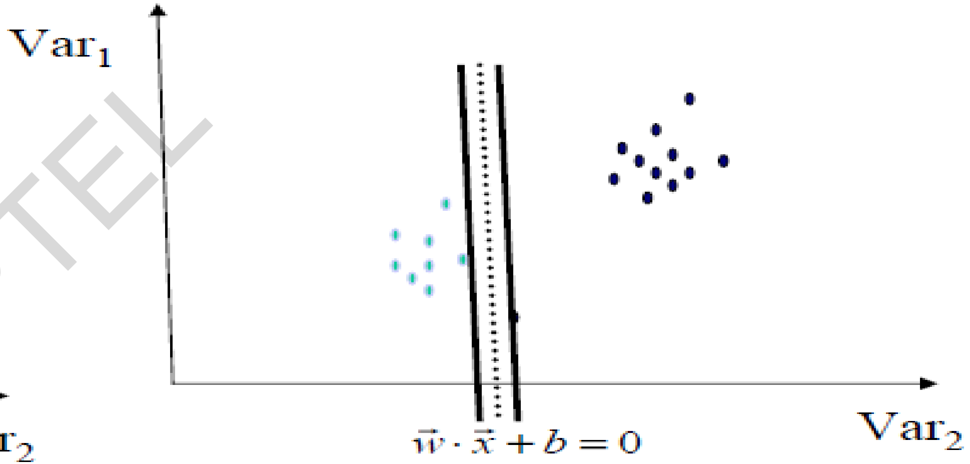
- The algorithm try to keep ξ null, maximising the margin
- The algorithm does not minimise the number of error. Instead, it minimises the sum of distances fron the hyperplane

- When C increases the number of errors tend to lower. At the limit of C tending to infinite, the solution tend to that given by the hard margin formulation, with 0 errors

Soft margin is more robust



Soft Margin SVM



Hard Margin SVM

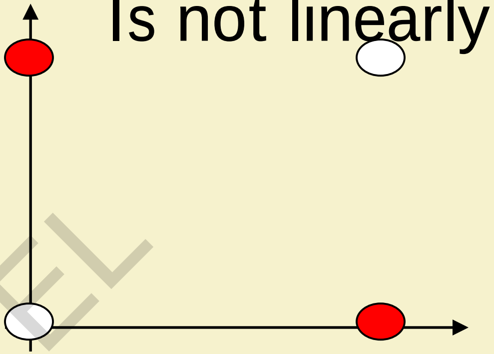
Extension to Non-linear Decision Boundary

- So far, we have only considered large-margin classifier with a linear decision boundary
- How to generalize it to become nonlinear?
- Key idea: transform $\mathbf{x}_i$ to a higher dimensional space to "make life easier"
  - Input space: the space the point $\mathbf{x}_i$ are located
  - Feature space: the space of $\phi(\mathbf{x}_i)$ after transformation
- Why transform?
  - Linear operation in the feature space is equivalent to non-linear operation in input space
  - Classification can become easier with a proper transformation. In the XOR problem, for example, adding a new feature of x_1x_2 make the problem linearly separable

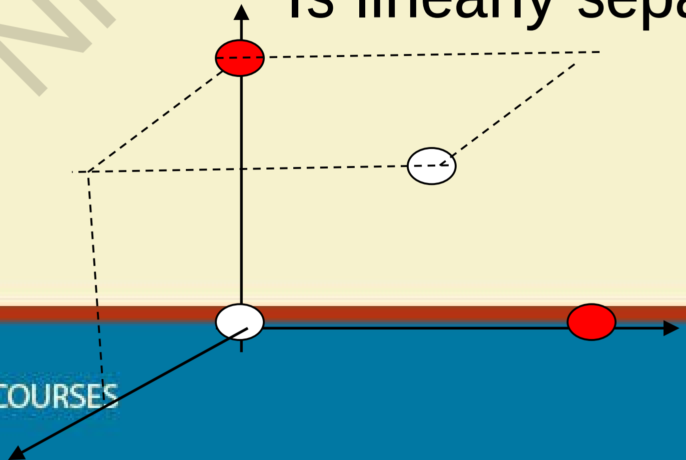
XOR

X	Y	
0	0	0
0	1	1
1	0	1
1	1	0

Is not linearly separable

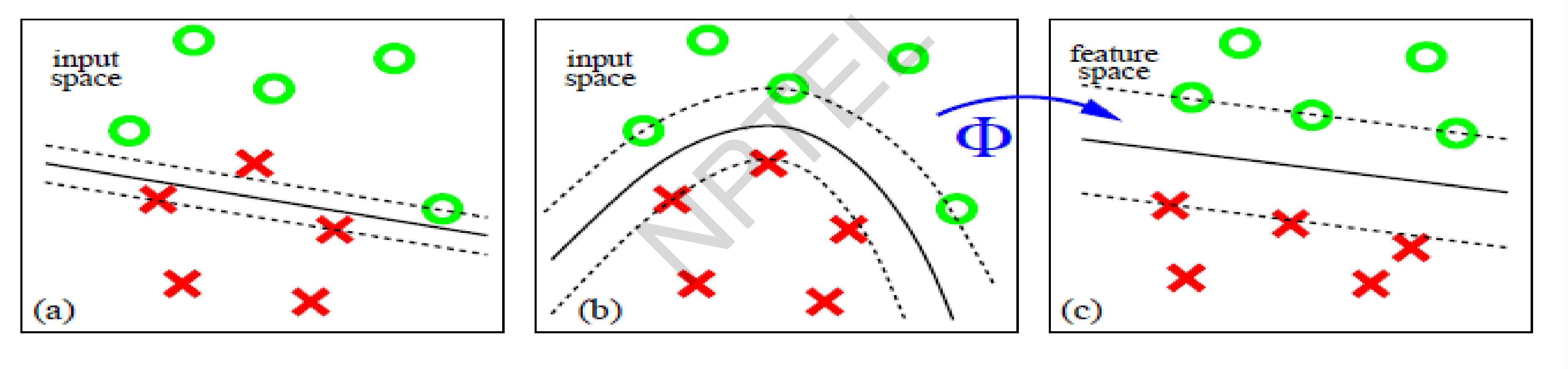


Is linearly separable

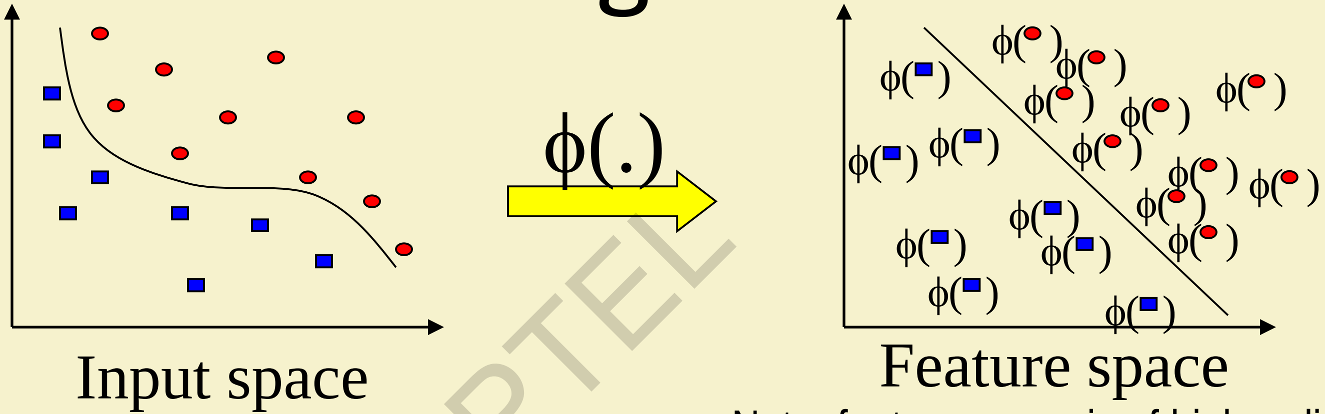


X	Y	XY	
0	0	0	0
0	1	0	1
1	0	0	1
1	1	1	0

Find a feature space



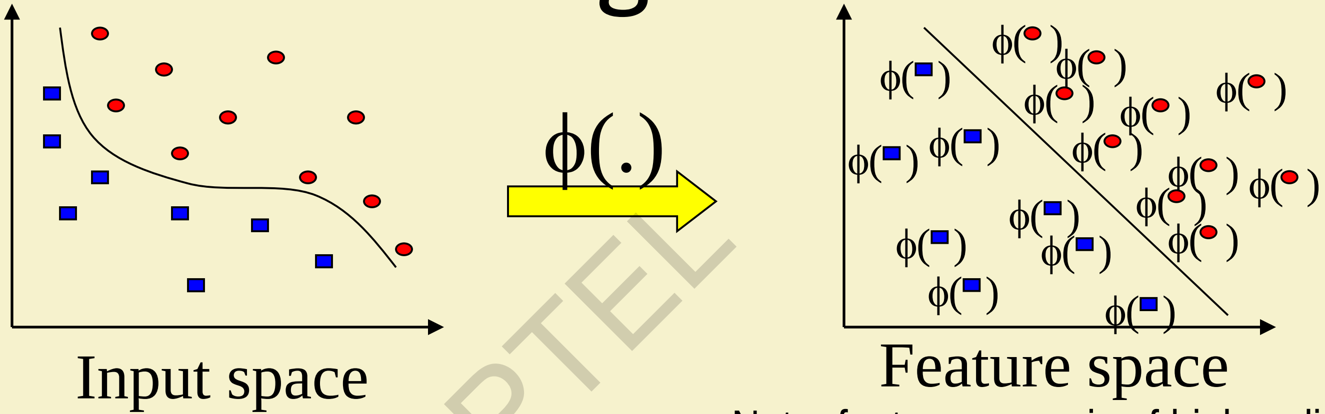
Transforming the Data



Note: feature space is of higher dimension than the input space in practice

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

Transforming the Data



Note: feature space is of higher dimension than the input space in practice

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

The Kernel Trick

- Recall the SVM optimization problem

$$\max.\ W(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1,j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$

$$\text{subject to } C \geq \alpha_i \geq 0,\ \sum_{i=1}^{n} \alpha_i y_i = 0$$

- The data points only appear as inner product
- As long as we can calculate the inner product in the feature space, we do not need the mapping explicitly
- Many common geometric operations (angles, distances) can be expressed by inner products
- Define the kernel function *K* by $K(\mathbf{x}_i, \mathbf{x}_j) = \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$

An Example for ϕ(.) and K(.,.)

- Suppose ϕ(.) is given as follows

$$\phi(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}) = (1, \sqrt{2}x_1, \sqrt{2}x_2, x_1^2, x_2^2, \sqrt{2}x_1x_2)$$

- An inner product in the feature space is

$$\langle \phi(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}), \phi(\begin{bmatrix} y_1 \\ y_2 \end{bmatrix}) \rangle = (1 + x_1y_1 + x_2y_2)^2$$

- So, if we define the kernel function as follows, there is no need to carry out ϕ(.) explicitly

$$K(\mathbf{x}, \mathbf{y}) = (1 + x_1y_1 + x_2y_2)^2$$

- This use of kernel function to avoid carrying out ϕ(.) explicitly is known as the kernel trick

Kernels

- Given a mapping: $\mathbf{x} \rightarrow \boldsymbol{\varphi}(\mathbf{x})$

a kernel is represented as the inner product

$$K(\mathbf{x},\mathbf{y}) \rightarrow \sum_i \varphi_i(\mathbf{x})\varphi_i(\mathbf{y})$$

A kernel must satisfy the Mercer's condition:

$$\forall g(\mathbf{x}) \text{ such that } \int g^2(\mathbf{x})d\mathbf{x} \geq 0 \Rightarrow \int K(\mathbf{x},\mathbf{y})g(\mathbf{x})g(\mathbf{y})d\mathbf{x}d\mathbf{y} \geq 0$$

Modification Due to Kernel Function

- Change all inner products to kernel functions
- For training,

Original

$$\text{max. } W(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1,j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$

$$\text{subject to } C \geq \alpha_i \geq 0, \sum_{i=1}^{n} \alpha_i y_i = 0$$

With kernel function

$$\text{max. } W(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1,j=1}^{n} \alpha_i \alpha_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j)$$

$$\text{subject to } C \geq \alpha_i \geq 0, \sum_{i=1}^{n} \alpha_i y_i = 0$$

Modification Due to Kernel Function

- For testing, new data **z** is classified as class 1 if *f* ≥0, and as class 2 if *f* <0

Original

$$\mathbf{w} = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} \mathbf{x}_{t_j}$$

$$f = \mathbf{w}^T \mathbf{z} + b = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} \mathbf{x}_{t_j}^T \mathbf{z} + b$$

With kernel function

$$\mathbf{w} = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} \phi(\mathbf{x}_{t_j})$$

$$f = \langle \mathbf{w}, \phi(\mathbf{z}) \rangle + b = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} K(\mathbf{x}_{t_j}, \mathbf{z}) + b$$

More on Kernel Functions

- Since the training of SVM only requires the value of $K(\mathbf{x}_i, \mathbf{x}_j)$, there is no restriction of the form of $\mathbf{x}_i$ and $\mathbf{x}_j$
  - $\mathbf{x}_i$ can be a sequence or a tree, instead of a feature vector
- $K(\mathbf{x}_i, \mathbf{x}_j)$ is just a similarity measure comparing $\mathbf{x}_i$ and $\mathbf{x}_j$

$$f(\mathbf{z}) = \sum_{\mathbf{x}_i \in \mathcal{S}} \alpha_i y_i K(\mathbf{z}, \mathbf{x}_i) + b$$

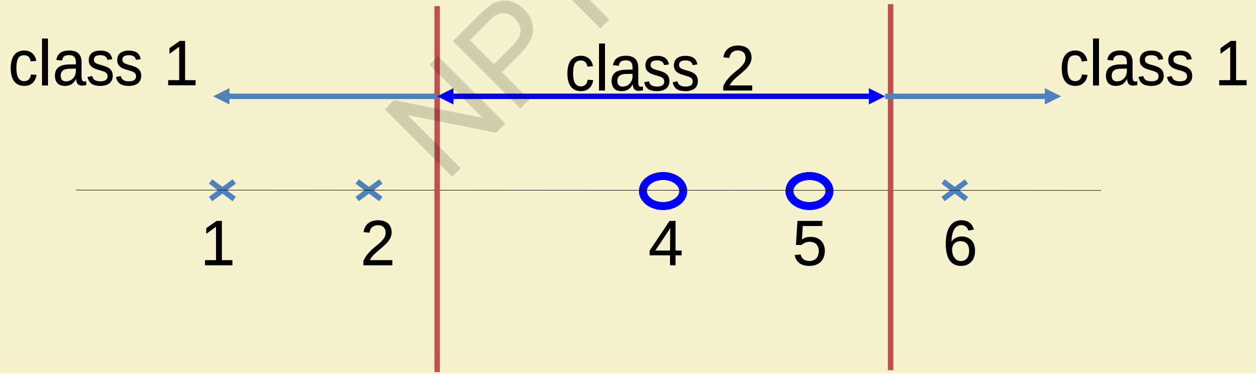
$\mathcal{S}$: the set of support vectors

- For a test object **z**, the discriminant function essentially is a weighted sum of the similarity between z and a pre-selected set of objects (the support vectors)

Example

- Suppose we have 5 1D data points
  - $x_1=1$, $x_2=2$, $x_3=4$, $x_4=5$, $x_5=6$, with 1, 2, 6 as class 1 and 4, 5 as class 2 $\Rightarrow$ $y_1=1$, $y_2=1$, $y_3=-1$, $y_4=-1$, $y_5=1$

Example



Example

- We use the polynomial kernel of degree 2
  - $K(x,y) = (xy+1)^2$
  - C is set to 100

$$\max. \sum_{i=1}^{5} \alpha_i - \frac{1}{2} \sum_{i=1}^{5} \sum_{j=1}^{5} \alpha_i \alpha_j y_i y_j (x_i x_j + 1)^2$$

$$\text{subject to } 100 \geq \alpha_i \geq 0, \sum_{i=1}^{5} \alpha_i y_i = 0$$

- We first find α_i (i=1, …, 5) by

Example

- By using a QP solver, we get
  - α_1=0, α_2=2.5, α_3=0, α_4=7.333, α_5=4.833
  - Note that the constraints are indeed satisfied
  - The support vectors are {x_2=2, x_4=5, x_5=6}
- The discriminant function is

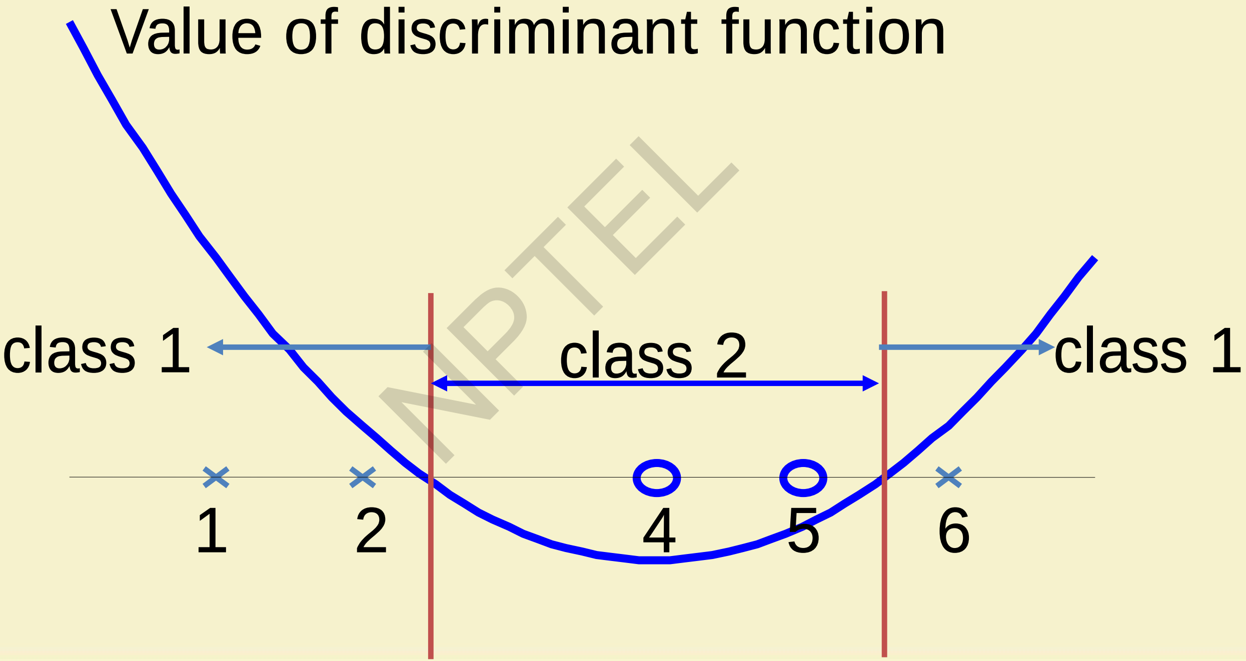
$$\begin{aligned} f(z) &= 2.5(1)(2z+1)^2 + 7.333(-1)(5z+1)^2 + \overbrace{4.833}^{\alpha_5}\overbrace{(1)}^{y_5}\overbrace{(6z+1)^2}^{K(z,x_5)} + b \\ &= 0.6667z^2 - 5.333z + b \end{aligned}$$

- *b* i

- All three give b=9

$$\Rightarrow \quad f(z) = 0.6667z^2 - 5.333z + 9$$

Example


Value of discriminant function
class 1
class 2
class 1
1
2
4
5
6

Kernel Functions

- In practical use of SVM, the user specifies the kernel function; the transformation $\phi(.)$ is not explicitly stated
- Given a kernel function $K(\mathbf{x}_i, \mathbf{x}_j)$, the transformation $\phi(.)$ is given by its eigenfunctions (a concept in functional analysis)
  - Eigenfunctions can be difficult to construct explicitly
  - This is why people only specify the kernel function without worrying about the exact transformation
- Another view: kernel function, being an inner product, is really a similarity measure between the objects

A kernel is associated to a transformation

- Given a kernel, in principle it should be recovered the transformation in the feature space that originates it.

- $K(x,y) = (xy+1)^2 = x^2y^2+2xy+1$

It corresponds the transformation $x \rightarrow \begin{pmatrix} x^2 \\ \sqrt{2}x \\ 1 \end{pmatrix}$

Examples of Kernel Functions

- Polynomial kernel up to degree *d*

$$K(\mathbf{u}, \mathbf{v}) = (\mathbf{u} \cdot \mathbf{v})^d$$

- Polynomial kernel up to degree *d*

$$K(\mathbf{x}, \mathbf{y}) = (\mathbf{x}^T\mathbf{y} + 1)^d$$

- Radial basis function kernel with width σ

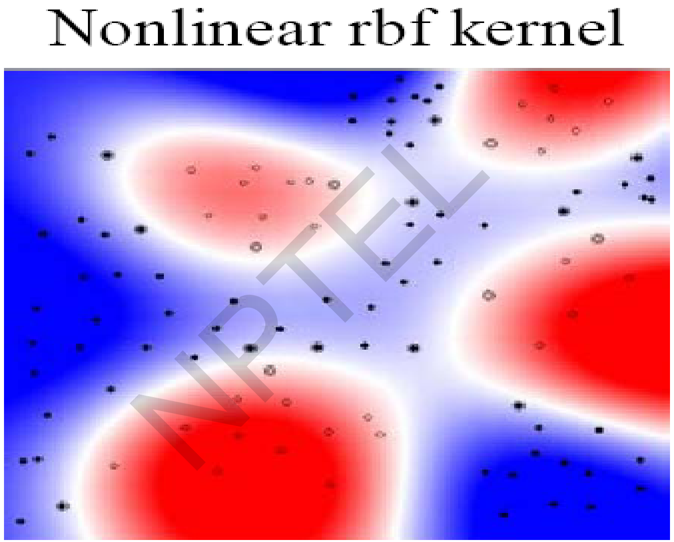
$$K(\mathbf{x}, \mathbf{y}) = \exp(-||\mathbf{x} - \mathbf{y}||^2/(2\sigma^2))$$

  - The feature space is infinite-dimensional
- Sigmoid with parameter κ and θ

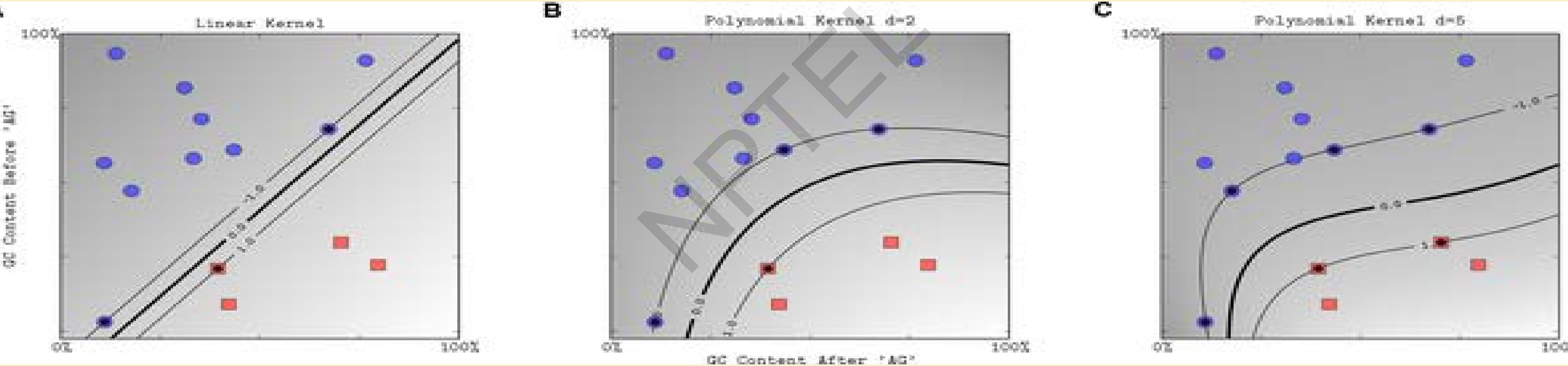
$$K(\mathbf{x}, \mathbf{y}) = \tanh(\kappa\mathbf{x}^T\mathbf{y} + \theta)$$

  - It does not satisfy the Mercer condition on all κ and θ

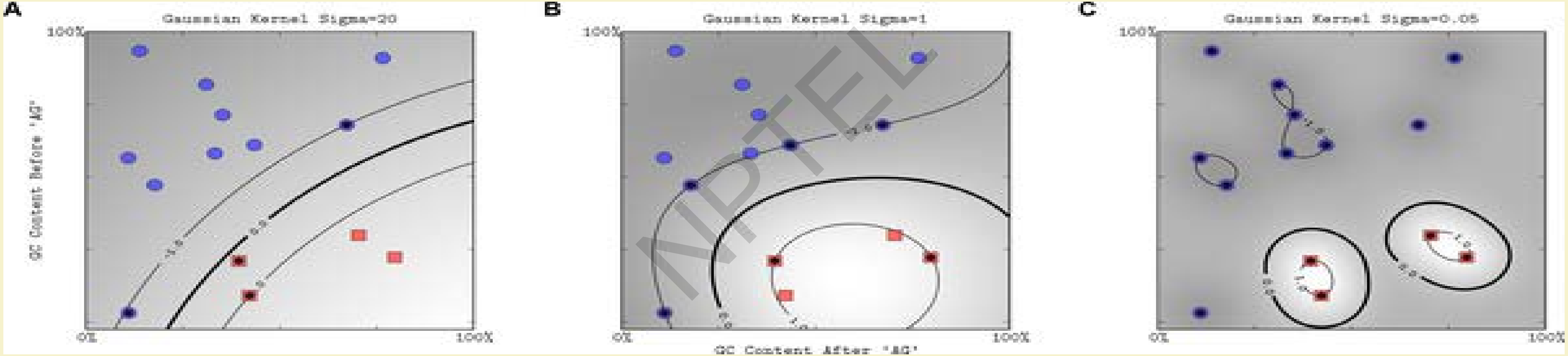
Example



Ploynomial kernel



Gaussian RBF kernel



Choosing the Kernel Function

- Probably the most tricky part of using SVM.
- The kernel function is important because it creates the kernel matrix, which summarizes all the data
- Many principles have been proposed (diffusion kernel, Fisher kernel, string kernel, …)
- There is even research to estimate the kernel matrix from available information

- In practice, a low degree polynomial kernel or RBF kernel with a reasonable width is a good initial try
- Note that SVM with RBF kernel is closely related to RBF neural networks, with the centers of the radial basis functions automatically chosen for SVM

Software

- A list of SVM implementation can be found at http://www.kernel-machines.org/software.html
- Some implementation (such as LIBSVM) can handle multi-class classification
- SVMLight is among one of the earliest implementation of SVM
- Several Matlab toolboxes for SVM are also available

Summary: Steps for Classification

- Prepare the pattern matrix
- Select the kernel function to use
- Select the parameter of the kernel function and the value of *C*
  - You can use the values suggested by the SVM software, or you can set apart a validation set to determine the values of the parameter
- Execute the training algorithm and obtain the α_i
- Unseen data can be classified using the α_i and the support vectors

Strengths and Weaknesses of SVM

- Strengths
  - Training is relatively easy
    - No local optimal, unlike in neural networks
  - It scales relatively well to high dimensional data
  - Tradeoff between classifier complexity and error can be controlled explicitly
  - Non-traditional data like strings and trees can be used as input to SVM, instead of feature vectors
- Weaknesses
  - Need to choose a “good” kernel function.

Conclusion

- SVM is a useful alternative to neural networks
- Two key concepts of SVM: maximize the margin and the kernel trick
- Many SVM implementations like libSVM are available on the web for you to try on your data set!

End of Support Vector Machine