### Introduction to Machine Learning Introduction to Support Vector Machines

Andres Mendez-Vazquez

June 13, 2018

## Outline





#### Support Vectors

#### Support Vectors

- Quadratic Optimization
- Rewriting The Optimization Problem
- Karush-Kuhn-Tucker Conditions
- Properties of the Dual

#### Kernels

- Introduction Kernel Idea
- Higher Dimensional Space
- The Mercer Theorem for Kernels
  - Basic Idea
- From Inner products to Kernels
- Examples
- Now, How to select a Kernel?



Introduction

The Soft Margin Solution



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#### History • The Beginning



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He was a Soviet and Russian mathematician, and, with Vladimir Vapnik, was one of the main developers of the Vapnik–Chervonenkis theory, also known as the "**fundamental theory of learning**" an important part of computational learning theory.

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### Partial List

### Predictive Control

• Control of chaotic systems.

#### Inverse Geosounding Problem

▶ It is used to understand the internal structure of our planet.

#### Environmental Sciences

Spatio-temporal environmental data analysis and modeling.

#### Protein Fold and Remote Homology Detection

- In the recognition if two different species contain similar genes.
- Facial expression classification
- O Texture Classification
- E-Learning
- Handwritten Recognition
- AND counting....

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### Separable Classes

### Given

$$\boldsymbol{x}_i, \ i=1,\cdots,N$$

A set of samples belonging to two classes  $\omega_1$ ,  $\omega_2$ .



## Separable Classes

#### Given

$$\boldsymbol{x}_i, \ i=1,\cdots,N$$

A set of samples belonging to two classes  $\omega_1$ ,  $\omega_2$ .

#### Objective

We want to obtain a decision function as simple as

$$g\left(\boldsymbol{x}\right) = \boldsymbol{w}^T \boldsymbol{x} + w_0$$



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### Such that we can do the following



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### We have the following samples

- For  $oldsymbol{x}_1,\cdots,oldsymbol{x}_m\in C_1$
- For  $x_1, \cdots, x_n \in C_2$



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#### We want the following decision surfaces

### • $oldsymbol{w}^Toldsymbol{x}_i+w_0\geq 0$ for $d_i=+1$ if $oldsymbol{x}_i\in C_1$

•  $oldsymbol{w}^Toldsymbol{x}_j+w_0\leq 0$  for  $d_j=-1$  if  $oldsymbol{x}_j\in C_2$ 



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## What do we want?



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## Remember

#### We have the following



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# A Little of Geometry





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$$d = rac{|w_0|}{\sqrt{w_1^2 + w_2^2}}, \; r = rac{|g\left( x 
ight)|}{\sqrt{w_1^2 + w_2^2}}$$

## A Little of Geometry





### Then

$$d = \frac{|w_0|}{\sqrt{w_1^2 + w_2^2}}, \ r = \frac{|g(\boldsymbol{x})|}{\sqrt{w_1^2 + w_2^2}}$$
(1)

First 
$$d = \frac{|w_0|}{\sqrt{w_1^2 + w_2^2}}$$

### We can use the following rule in a triangle with a $90^o \ {\rm angle}$

$$Area = \frac{1}{2}Cd\tag{2}$$

#### In addition, the area can be calculated also as

$$Area = \frac{1}{2}AB$$

#### Thus

$$d = \frac{AB}{C}$$

Remark: Can you get the rest of values?

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# What about $\ r=rac{|g(m{x})|}{\sqrt{w_1^2+w_2^2}}$ ?

### First, remember

$$g(\boldsymbol{x}_p) = 0 \text{ and } \boldsymbol{x} = \boldsymbol{x}_p + r \frac{\boldsymbol{w}}{\|\boldsymbol{w}\|}$$
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$$g(\boldsymbol{x}) = \boldsymbol{w}^{T} \left[ \boldsymbol{x}_{p} + r \frac{\boldsymbol{w}}{\|\boldsymbol{w}\|} \right] + w_{0}$$

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### Then

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### Then

$$r = \frac{g(\mathbf{x})}{||\mathbf{w}||}$$

# This has the following interpretation





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### Now

### We know that the straight line that we are looking for looks like

$$\boldsymbol{w}^T \boldsymbol{x} + \boldsymbol{w}_0 = \boldsymbol{0}$$

#### What about something like this

$$\boldsymbol{w}^T \boldsymbol{x} + \boldsymbol{w}_0 = \boldsymbol{\delta}$$

#### Clearly

This will be above or below the initial line  $oldsymbol{w}^Tx+oldsymbol{w}_0=0$ 



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## Come back to the hyperplanes

We have then for each border support line an specific bias!!!



### The new margin functions

• 
$$w'^T \mathbf{x} + w_{10} = 1$$

- $w'^T \mathbf{x} + w_{01} = -1$
- where  $w'=rac{w}{\delta}$ ,  $w_{10}=rac{w_0'}{\delta}$  , and  $w_{01}=rac{w_0'}{\delta}$



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### Now, we come back to the middle separator hyperplane, but with the normalized term

• 
$$oldsymbol{w}^T\mathbf{x}_i+w_0\geq oldsymbol{w}'^T\mathbf{x}+w_{10}$$
 for  $d_i=+1$ 

- ullet ullet  $oldsymbol{w}^T \mathbf{x}_i + w_0 \leq oldsymbol{w}^{\prime T} \mathbf{x} + w_{01}$  for  $d_i = -1$ 
  - · Where  $w_0$  is the bias of that central hyperplane!! And the  $m{w}$  is the normalized direction of  $m{w}'$



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,  $w_{10}=rac{w'_0}{\delta}$  , and  $w_{01}=rac{w''_0}{\delta}$ 

# Now, we come back to the middle separator hyperplane, but with the normalized term • $w^T \mathbf{x}_i + w_0 \ge w'^T \mathbf{x} + w_{10}$ for $d_i = +1$ • $w^T \mathbf{x}_i + w_0 \le w'^T \mathbf{x} + w_{01}$ for $d_i = -1$ • Where $w_0$ is the bias of that central hyperplanel! And the w is the normalized direction of w'



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► Where w<sub>0</sub> is the bias of that central hyperplane!! And the w is the normalized direction of w'

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# Come back to the hyperplanes

### The meaning of what I am saying!!!



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# A little about Support Vectors

### They are the vectors (Here, we assume that w)

 $oldsymbol{x}_i$  such that  $oldsymbol{w}^Toldsymbol{x}_i+w_0=1$  or  $oldsymbol{w}^Toldsymbol{x}_i+w_0=-1$ 



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### Properties

• The vectors nearest to the decision surface and the most difficult to classify.

Because of that, we have the name "Support Vector Machines".



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### Now, we can resume the decision rule for the hyperplane

#### For the support vectors

$$g\left(oldsymbol{x}_{i}
ight)=oldsymbol{w}^{T}oldsymbol{x}_{i}+w_{0}=-(+)1$$
 for  $d_{i}=-(+)1$ 

#### Implies

The distance to the support vectors is:

$$r = \frac{g(x_i)}{||w||} = \begin{cases} \frac{1}{||w||} & \text{if } d_i = +1 \\ -\frac{1}{||w||} & \text{if } d_i = -1 \end{cases}$$



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## Therefore ...

### We want the optimum value of the margin of separation as

$$\rho = \frac{1}{||\bm{w}||} + \frac{1}{||\bm{w}||} = \frac{2}{||\bm{w}||}$$

#### And the support vectors define the value of ,



(8)

## Therefore ...

We want the optimum value of the margin of separation as

$$\rho = \frac{1}{||\boldsymbol{w}||} + \frac{1}{||\boldsymbol{w}||} = \frac{2}{||\boldsymbol{w}||}$$
(8)

#### And the support vectors define the value of $\rho$



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## Thus

### If we want to maximize

$$\rho = \frac{2}{||\boldsymbol{w}||}$$

#### We instead to minimize

$$||\boldsymbol{w}|| = \sqrt{\boldsymbol{w}^T \boldsymbol{w}}$$

#### Or to minimize, after all we only need the direction of the vector $m{w}$

$$\frac{1}{2} \boldsymbol{w}^T \boldsymbol{w}$$



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### Under the restrictions

### Then, we have the samples with labels

 $T = \{(\boldsymbol{x}_i, d_i)\}_{i=1}^N$ 

Then we can put the decision rule as

 $d_i\left(\boldsymbol{w}^T\boldsymbol{x}_i + w_0\right) \ge 1 \ i = 1, \cdots, N$ 



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### Then, we have the optimization problem

### The optimization problem

$$min_{\boldsymbol{w}}\Phi\left(\boldsymbol{w}\right) = \frac{1}{2}\boldsymbol{w}^{T}\boldsymbol{w}$$

s.t. 
$$d_i(w^T x_i + w_0) \ge 1$$
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### Observations

• The cost functions  $\Phi(\boldsymbol{w})$  is convex.

The constrains are linear with respect to  $\boldsymbol{w}$ .



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# Then, Rewriting The Optimization Problem

### The optimization with equality constraints

$$min_{\boldsymbol{w}}\Phi\left(\boldsymbol{w}\right) = \frac{1}{2}\boldsymbol{w}^{T}\boldsymbol{w}$$

s.t. 
$$d_i(\boldsymbol{w}^T \boldsymbol{x}_i + w_0) \geq 1 \ i = 1, \cdots, N$$

### Using the Lagrange Multipliers (We will call them $\alpha_i$ )

We obtain the following cost function that we want to minimize

$$J(\boldsymbol{w}, w_0, \boldsymbol{\alpha}) = \frac{1}{2} \boldsymbol{w}^T \boldsymbol{w} - \sum_{i=1}^N \alpha_i [d_i(\boldsymbol{w}^T \mathbf{x}_i + w_0) - 1]$$



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### Observation

• Minimize with respect to  $\mathbf{w}$  and  $w_0$ .

• Maximize with respect to  $\alpha$  because it dominates

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$$-\sum_{i=1}^{N} \alpha_i [d_i (\boldsymbol{w}^T \boldsymbol{x}_i + w_0) - 1].$$
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### First An Inequality Constrained Problem P

$$\begin{array}{ll} \min & f\left(\boldsymbol{x}\right) \\ s.t & g_{1}\left(\boldsymbol{x}\right) &= 0 \\ & \vdots \\ & g_{N}\left(\boldsymbol{x}\right) &= 0 \end{array}$$

#### A really minimal version!!! Hey, it is a patch work!!!

A point  $\boldsymbol{x}$  is a local minimum of an equality constrained problem P only if a set of non-negative  $\alpha_i$ 's may be found such that:

$$abla L(\boldsymbol{x}, \boldsymbol{\alpha}) = 
abla f(\boldsymbol{x}) - \sum_{i=1}^{N} \alpha_i \nabla g_i(\boldsymbol{x}) = 0$$

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### Important

Think about this each constraint correspond to a sample in both classes, thus

• The corresponding  $\alpha_i$ 's are going to be zero after optimization, if a constraint is not active i.e.  $d_i \left( \boldsymbol{w}^T \boldsymbol{x}_i + w_0 \right) - 1 \neq 0$  (Remember Maximization).

#### Again the Support Vectors

This actually defines the idea of support vectors!!!

#### Thus

Only the  $lpha_i$ 's with active constraints (Support Vectors) will be different from zero when  $d_i\left(m{w}^Tm{x}_i+m{w}_0
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#### 

### The necessary conditions for optimality





### The necessary conditions for optimality

# Condition 1 $\frac{\partial J(\boldsymbol{w}, w_0, \boldsymbol{\alpha})}{\partial \boldsymbol{w}} = 0$ Condition 2 $\frac{\partial J(\boldsymbol{w}, w_0, \boldsymbol{\alpha})}{\partial w_0} = 0$

# Using the conditions







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# Using the conditions

### We have the first condition

$$\frac{\partial J(\boldsymbol{w}, w_0, \alpha)}{\partial \boldsymbol{w}} = \frac{\partial \frac{1}{2} \boldsymbol{w}^T \boldsymbol{w}}{\partial \boldsymbol{w}} - \frac{\partial \sum_{i=1}^N \alpha_i [d_i(\boldsymbol{w}^T \boldsymbol{x}_i + w_0) - 1]}{\partial \boldsymbol{w}} = 0$$
$$\frac{\partial J(\boldsymbol{w}, w_0, \alpha)}{\partial \boldsymbol{w}} = \frac{1}{2} (\boldsymbol{w} + \boldsymbol{w}) - \sum_{i=1}^N \alpha_i d_i \boldsymbol{x}_i$$

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Thus

### Using the conditions

### We have the first condition

$$\frac{\partial J(\boldsymbol{w}, w_0, \alpha)}{\partial \boldsymbol{w}} = \frac{\partial \frac{1}{2} \boldsymbol{w}^T \boldsymbol{w}}{\partial \boldsymbol{w}} - \frac{\partial \sum_{i=1}^N \alpha_i [d_i(\boldsymbol{w}^T \boldsymbol{x}_i + w_0) - 1]}{\partial \boldsymbol{w}} = 0$$
$$\frac{\partial J(\boldsymbol{w}, w_0, \alpha)}{\partial \boldsymbol{w}} = \frac{1}{2} (\boldsymbol{w} + \boldsymbol{w}) - \sum_{i=1}^N \alpha_i d_i \boldsymbol{x}_i$$

Thus

$$\boldsymbol{w} = \sum_{i=1}^{N} \alpha_i d_i \mathbf{x}_i \tag{10}$$

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# In a similar way ...

### We have by the second optimality condition

$$\sum_{i=1}^{N} \alpha_i d_i = 0$$

#### Note

$$\alpha_i \left[ d_i \left( \boldsymbol{w}^T \boldsymbol{x}_i + \boldsymbol{w}_0 \right) - 1 \right] = 0$$

Because the constraint vanishes in the optimal solution i.e.  $\alpha_i = 0$  or  $d_i \left( \boldsymbol{w}^T \boldsymbol{x}_i + \boldsymbol{w}_0 \right) - 1 = 0.$ 



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### We need something extra

Our classic trick of transforming a problem into another problem

#### In this case

We use the Primal-Dual Problem for Lagrangian

#### Where

We move from a minimization to a maximization!!!





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Our classic trick of transforming a problem into another problem

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# **Duality Theorem**

### First Property

If the Primal has an optimal solution (w\* and  $\alpha*$ ), the dual too.

In order to *w* \* and *α*\* to be optimal solutions for the primal and dual problem respectively, It is necessary and sufficient that *w*\*:

 $\begin{aligned} \Phi(\boldsymbol{w}*) &= J\left(\boldsymbol{w}*, w_0*, \boldsymbol{\alpha}*\right) \\ &= \min_{\boldsymbol{w}} J\left(\boldsymbol{w}*, w_0*, \boldsymbol{\alpha}*\right) \end{aligned}$ 



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# **Duality Theorem**

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If the Primal has an optimal solution (w\* and  $\alpha*)$ , the dual too.

### Thus

In order to w\* and  $\alpha*$  to be optimal solutions for the primal and dual problem respectively, It is necessary and sufficient that w\*:

• It is a feasible solution for the primal problem and

$$\Phi(\boldsymbol{w}*) = J(\boldsymbol{w}*, w_0*, \boldsymbol{\alpha}*)$$
$$= \min_{\boldsymbol{w}} J(\boldsymbol{w}*, w_0*, \boldsymbol{\alpha}*)$$



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# Reformulate our Equations

### We have then

$$J(\boldsymbol{w}, w_0, \boldsymbol{\alpha}) = \frac{1}{2} \boldsymbol{w}^T \boldsymbol{w} - \sum_{i=1}^N \alpha_i d_i \boldsymbol{w}^T \mathbf{x}_i - w_0 \sum_{i=1}^N \alpha_i d_i + \sum_{i=1}^N \alpha_i$$

Now for our 2nd optimality condition





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# Reformulate our Equations

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We have finally for the 1st Optimality Condition:



Second, setting  $J(\boldsymbol{w}, w_0, \boldsymbol{\alpha}) = Q(\boldsymbol{\alpha})$ 

 $Q\left(\boldsymbol{\alpha}\right) = \sum_{i=1}^{N} \alpha_{i} - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_{i} \alpha_{j} d_{i} d_{j} \boldsymbol{x}_{j}^{T} \boldsymbol{x}_{i}$ 



We have finally for the 1st Optimality Condition:

First  

$$\boldsymbol{w}^T \boldsymbol{w} = \sum_{i=1}^N \alpha_i d_i \boldsymbol{w}^T \boldsymbol{x}_i = \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j d_i d_j \boldsymbol{x}_j^T \boldsymbol{x}_i$$

Second, setting  $J(\boldsymbol{w}, w_0, \boldsymbol{\alpha}) = Q(\boldsymbol{\alpha})$ 

$$Q(\boldsymbol{\alpha}) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j d_i d_j \boldsymbol{x}_j^T \boldsymbol{x}_i$$



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### From here, we have the problem

### This is the problem that we really solve

Given the training sample  $\{(\mathbf{x}_i, d_i)\}_{i=1}^N$ , find the Lagrange multipliers  $\{\alpha_i\}_{i=1}^N$  that maximize the objective function

$$Q(\alpha) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j d_i d_j \boldsymbol{x}_j^T \boldsymbol{x}_i$$

subject to the constraints

$$\sum_{i=1}^{N} \alpha_i d_i = 0 \tag{11}$$

$$\alpha_i \ge 0 \text{ for } i = 1, \cdots, N \tag{12}$$

#### Note

In the Primal, we were trying to minimize the cost function, for this it is necessary to maximize  $\alpha$ . That is the reason why we are maximizing  $Q(\alpha)$ .

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# Solving for lpha

We can compute  $w^*$  once we get the optimal  $\alpha_i^*$  by using (Eq. 10)

$$\boldsymbol{w}^* = \sum_{i=1}^N \alpha_i^* d_i \boldsymbol{x}_i$$

In addition, we can compute the optimal bias  $w^*_0$  using the optimal weight,  $oldsymbol{w}^*$ 

For this, we use the positive margin equation:

$$g\left(oldsymbol{x}^{(s)}
ight) = oldsymbol{w}^Toldsymbol{x}^{(s)} + w_0 = 1$$

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corresponding to a positive support vector.

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### Then

$$w_0 = 1 - (\boldsymbol{w}^*)^T \, \boldsymbol{x}^{(s)}$$
 for  $d^{(s)} = 1$  (13)

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### What do we need?

### Until now, we have only a maximal margin algorithm

### • All this work fine when the classes are separable

- Problem, What when they are not separable?
- What we can do?


### Until now, we have only a maximal margin algorithm

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# Map to a higher Dimensional Space

### Assume that exist a mapping

$$oldsymbol{x} \in \mathbb{R}^l o oldsymbol{y} \in \mathbb{R}^k$$

#### Then, it is possible to define the following mapping



# Map to a higher Dimensional Space

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# Define a map to a higher Dimension

### Nonlinear transformations

Given a series of nonlinear transformations

 $\{\phi_i\left(\boldsymbol{x}\right)\}_{i=1}^m$ 

from input space to the feature space.

#### We can define the decision surface as

 $\sum_{i=1}^{m} w_i \phi_i\left(x\right) + w_0 = 0$ 



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# Define a map to a higher Dimension

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# This allows us to define

### The following vector

$$\phi\left(\boldsymbol{x}\right) = \left(\phi_{0}\left(\boldsymbol{x}\right), \phi_{1}\left(\boldsymbol{x}\right), \cdots, \phi_{m}\left(\boldsymbol{x}\right)\right)^{T}$$

that represents the mapping.

#### From this mapping

We can define the following kernel function

 $K:\mathbf{X}\times\mathbf{X}\to\mathbb{R}$ 

$$K\left(\boldsymbol{x}_{i}, \boldsymbol{x}_{j}\right) = \phi\left(\boldsymbol{x}_{i}\right)^{T} \phi\left(\boldsymbol{x}_{j}\right)$$



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- Introduction Kernel Idea
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- The Mercer Theorem for Kernels
   Basic Idea
  - From Inner products to Kernels
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- Now, How to select a Kernel?

#### Soft Margin

Introduction

The Soft Margin Solution



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# Basic Idea

### Something Notable

• The SVM uses the scalar product  $\langle x_i, x_j \rangle$  as a measure of similarity between  $x_i$  and  $x_j$ , and of distance to the hyperplane.



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- Since the scalar product is linear, the SVM is a linear method.

Using a nonlinear function instead, we can make the classifier nonlinear.



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Using a nonlinear function instead, we can make the classifier nonlinear.



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# We do this by defining the following map

#### Nonlinear transformations

Given a series of nonlinear transformations

 $\left\{\phi_{i}\left(\boldsymbol{x}\right)\right\}_{i=1}^{m}$ 

from input space to the feature space.

#### We can define the decision surface as

 $\sum_{i=1}^{m}w_{i}\phi_{i}\left(oldsymbol{x}
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## This allows us to define

### The following vector

$$\phi(\boldsymbol{x}) = (\phi_0(\boldsymbol{x}), \phi_1(\boldsymbol{x}), \cdots, \phi_m(\boldsymbol{x}))^T$$

That represents the mapping.



# Outline

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# Finally

### We define the decision surface as

$$\boldsymbol{w}^{T}\boldsymbol{\phi}\left(\boldsymbol{x}\right)=0\tag{14}$$

#### We now seek "linear" separability of features, we may write

$$\boldsymbol{w} = \sum_{i=1}^{N} \alpha_i d_i \phi\left(\boldsymbol{x}_i\right) \tag{15}$$

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#### Thus, we finish with the following decision surface

$$\sum_{i=1}^{N} \alpha_{i} d_{i} \phi^{T}\left(\boldsymbol{x}_{i}\right) \phi\left(\boldsymbol{x}\right) = 0$$



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$$\sum_{i=1}^{N} \alpha_{i} d_{i} \phi^{T} \left( \boldsymbol{x}_{i} \right) \phi \left( \boldsymbol{x} \right) = 0$$
(16)

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# Thus

## The term $\phi^{T}\left(oldsymbol{x}_{i} ight)\overline{\phi\left(oldsymbol{x} ight)}$

It represents the inner product of two vectors induced in the feature space induced by the input patterns.

#### We can introduce the inner-product kernel

$$K\left(\boldsymbol{x_{i}}, \boldsymbol{x}\right) = \phi^{T}\left(\boldsymbol{x_{i}}\right)\phi\left(\boldsymbol{x}\right) = \sum_{j=0}^{m} \phi_{j}\left(\boldsymbol{x_{i}}\right)\phi_{j}\left(\boldsymbol{x}\right)$$

Property: Symmetry

$$K(\boldsymbol{x}_i, \boldsymbol{x}) = K(\boldsymbol{x}, \boldsymbol{x}_i)$$



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# This allows to redefine the optimal hyperplane

# We get N $\sum \alpha_i d_i K\left(\boldsymbol{x}_i, \boldsymbol{x}\right) = 0$ (19)i=1

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Using kernels, we can avoid to go from:

$$\mathsf{Input Space} \Longrightarrow \mathsf{Mapping Space} \Longrightarrow \mathsf{Inner Product} \tag{20}$$

#### By directly going from

#### nput Space $\implies$ Inner Product



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#### Input Space $\implies$ Inner Product

(21)

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### Important

### Something Notable

The expansion of (Eq. 17) for the inner-product kernel  $K(x_i, x)$  is an important special case of that arises in functional analysis.



# Mercer's Theorem

#### Mercer's Theorem

Let K(x, x') be a continuous symmetric kernel that is defined in the closed interval  $a \le x \le b$  and likewise for x'. The kernel K(x, x') can be expanded in the series

$$K(\boldsymbol{x}, \boldsymbol{x'}) = \sum_{i=1}^{\infty} \lambda_i \phi_i(\boldsymbol{x}) \phi_i(\mathbf{x'})$$
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Positive coefficients,  $\lambda_i > 0$  for all i.



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#### With

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# Mercer's Theorem

# For this expression to be valid and or it to converge absolutely and uniformly

It is necessary and sufficient that the condition

$$\int_{a}^{b} \int_{a}^{b} K(\boldsymbol{x}, \boldsymbol{x'}) \psi(\boldsymbol{x}) \psi(\boldsymbol{x'}) d\boldsymbol{x} d\boldsymbol{x'} \ge 0$$
(23)

holds for all  $\psi$  such that  $\int_{a}^{b} \psi^{2}(x) dx < \infty$  (Example of a quadratic norm for functions).



# Remarks

### First

The functions  $\phi_i(x)$  are called eigenfunctions of the expansion and the numbers  $\lambda_i$  are called eigenvalues.

#### Second

The fact that all of the eigenvalues are positive means that the kernel  $K\left(m{x},m{x}'
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# Not only that

#### We have that

For  $\lambda_i \neq 1$ , the *i*th image of  $\sqrt{\lambda_i}\phi_i(x)$  induced in the feature space by the input vector x is an eigenfunction of the expansion.

#### In theory

The dimensionality of the feature space (i.e., the number of eigenvalues/ eigenfunctions) can be infinitely large.



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## Example

## Assume

$$oldsymbol{x} \in \mathbb{R} o oldsymbol{y} = \left[ egin{array}{c} x_1^2 \ \sqrt{2} x_1 x_2 \ x_2^2 \end{array} 
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#### We can show that

 $oldsymbol{y}_i^Toldsymbol{y}_j = ig(oldsymbol{x}_i^Toldsymbol{x}_jig)^{ au}$ 



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## Example of Kernels

## Polynomials

$$k\left(\boldsymbol{x},\boldsymbol{z}\right) = (\boldsymbol{x}^T\boldsymbol{z}+1)^q \ q > 0$$

#### Radial Basis Functions

$$k\left(\boldsymbol{x}, \boldsymbol{z}\right) = \exp\left(-\frac{||\boldsymbol{x} - \boldsymbol{z}||^2}{\sigma^2}\right)$$

#### Hyperbolic Tangents

$$k\left(oldsymbol{x},oldsymbol{z}
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Now, How to select a Kernel?

### We have a problem

Selecting a specific kernel and parameters is usually done in a try-and-see manner.

#### Thus

In general, the Radial Basis Functions kernel is a reasonable first choice.

#### Then

if this fails, we can try the other possible kernels.



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if this fails, we can try the other possible kernels.



# Thus, we have something like this

## Step 1

Normalize the data.

#### Step 2

Use cross-validation to adjust the parameters of the selected kernel.

### Step 3

Train against the entire dataset.



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Optimal Hyperplane for non-separable patterns

### Important

We have been considering only problems where the classes are linearly separable.

#### Now

What happen when the patterns are not separable?

#### Thus, we can still build a separating hyperplane

But errors will happen in the classification... We need to minimize them..



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What happen when the patterns are not separable?

## Thus, we can still build a separating hyperplane

But errors will happen in the classification... We need to minimize them...



# What if the following happens

## Some data points invade the "margin" space



# Fixing the Problem - Corinna's Style

The margin of separation between classes is said to be soft if a data point  $(x_i, d_i)$  violates the following condition

$$d_i\left(\boldsymbol{w}^T\boldsymbol{x}_i+b\right) \ge +1 \ i=1,2,...,N$$
(24)

#### I his violation can arise in one of two ways

The data point  $(x_i, d_i)$  falls inside the region of separation but on the right side of the decision surface - still correct classification.



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## Example



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Example



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# Solving the problem

#### What to do?

We introduce a set of nonnegative scalar values {ξ<sub>i</sub>}<sup>N</sup><sub>i=1</sub>.

#### Introduce this into the decision rule

 $d_i \left( \boldsymbol{w}^T \boldsymbol{x}_i + b \right) \ge 1 - \xi_i \ i = 1, 2, ..., N$ 



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# The $\xi_i$ are called slack variables

### What?

In 1995, Corinna Cortes and Vladimir N. Vapnik suggested a modified maximum margin idea that allows for mislabeled examples.

#### Ok!!!

Instead of expecting to have constant margin for all the samples, the margin can change depending of the sample.

#### What do we have?

 $\xi_i$  measures the deviation of a data point from the ideal condition of pattern separability.



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## What if?

## • You have $0 \le \xi_i \le 1$



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## Support Vectors

#### We want

• Support vectors that satisfy equation (Eq. 25) even when  $\xi_i > 0$ 

$$d_i \left( \boldsymbol{w}^T \boldsymbol{x}_i + b \right) \ge 1 - \xi_i \ i = 1, 2, ..., N$$

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# We want the following

## We want to find an hyperplane

### Such that average error is misclassified over all the samples

$$\frac{1}{N}\sum_{i=1}^{N}\mathsf{e}^2$$

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(26)

# First Attempt Into Minimization

## We can try the following

Given

$$I\left(x\right) = \begin{cases} 0 & \text{ if } x \leq 0\\ 1 & \text{ if } x > 0 \end{cases}$$

### Minimize the following

$$\Phi\left(\boldsymbol{\xi}\right) = \sum_{i=1}^{N} I\left(\xi_{i} - 1\right)$$

with respect to the weight vector w subject to •  $d_i \left( w^T x_i + b \right) \ge 1 - \xi_i \ i = 1, 2, ..., N$ •  $\|w\|^2 \le C$  for a given C.

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(27)

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**9** 
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 $\| \boldsymbol{w} \|^{2} \leq C \text{ for a given } C.$
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### Using this first attempt

Minimization of  $\Phi\left(\boldsymbol{\xi}\right)$  with respect to  $\mathbf{w}$  is a non-convex optimization problem that is NP-complete.



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Minimization of  $\Phi\left(\boldsymbol{\xi}\right)$  with respect to  $\mathbf{w}$  is a non-convex optimization problem that is NP-complete.

### Thus, we need to use an approximation, maybe

$$\Phi\left(\boldsymbol{\xi}\right) = \sum_{i=1}^{N} \xi_i$$

Now, we simplify the computations by integrating the vector  $m{w}$ 

$$\Phi(\boldsymbol{w}, \boldsymbol{\xi}) = rac{1}{2} \boldsymbol{w}^T \boldsymbol{w} + C \sum_{i=1}^N \xi_i$$



(29)

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(30)

(29)

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### Important

#### First

Minimizing the first term in (Eq. 30) is related to minimize the Vapnik–Chervonenkis dimension.

 Which is a measure of the capacity (complexity, expressive power, richness, or flexibility) of a statistical classification algorithm.



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The second term  $\sum_{i=1}^N \xi_i$  is an upper bound on the number of test errors.



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The second term  $\sum_{i=1}^{N} \xi_i$  is an upper bound on the number of test errors.



Some problems for the Parameter C

#### Little Problem

The parameter C has to be selected by the user.



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Some problems for the Parameter C

### Little Problem

The parameter C has to be selected by the user.

#### This can be done in two ways

- The parameter C is determined experimentally via the standard use of a training! (validation) test set.
- It is determined analytically by estimating the Vapnik–Chervonenkis dimension.



### Primal Problem

# Problem, given samples $\{(\boldsymbol{x}_i, d_i)\}_{i=1}^N$

$$\begin{split} \min_{\boldsymbol{w},\boldsymbol{\xi}} \Phi\left(\boldsymbol{w},\boldsymbol{\xi}\right) &= \min_{\boldsymbol{w},\boldsymbol{\xi}} \left\{ \frac{1}{2} \boldsymbol{w}^T \boldsymbol{w} + C \sum_{i=1}^N \xi_i \right\} \\ \text{s.t. } d_i(\boldsymbol{w}^T \boldsymbol{x}_i + w_0) \geq 1 - \xi_i \text{ for } i = 1, \cdots, N \\ \xi_i \geq 0 \text{ for all } i \end{split}$$

With C a user-specified positive parameter.



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#### Support Vectors

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- Rewriting The Optimization Problem
- Karush-Kuhn-Tucker Conditions
- Properties of the Dual

#### Kernels

- Introduction Kernel Idea
- Higher Dimensional Space
- The Mercer Theorem for Kernels
  - Basic Idea
- From Inner products to Kernels
- Examples
- Now, How to select a Kernel?





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# Final Setup

Using Lagrange Multipliers and dual-primal method is possible to obtain the following setup

Given the training sample  $\{(\mathbf{x}_i, d_i)\}_{i=1}^N$ , find the Lagrange multipliers  $\{\alpha_i\}_{i=1}^N$  that maximize the objective function

$$\min_{\alpha} Q(\alpha) = \min_{\alpha} \left\{ \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j d_i d_j \boldsymbol{x}_j^T \boldsymbol{x}_i \right\}$$

subject to the constraints

$$\sum_{i=1}^{N} \alpha_i d_i = 0 \tag{31}$$

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$$0 \le \alpha_i \le C \text{ for } i = 1, \cdots, N \tag{32}$$

where C is a user-specified positive parameter.

### Something Notable

- Note that neither the slack variables nor their Lagrange multipliers appear in the dual problem.
- The dual problem for the case of non-separable patterns is thus similar to that for the simple case of linearly separable patterns



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### Note the following

$$\xi_i = 0$$
 if  $\alpha_i < C$ 

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### The optimal solution for the weight vector $oldsymbol{w}^*$

$$oldsymbol{w}^* = \sum_{i=1}^{N_s} lpha_i^* d_i oldsymbol{x}_i$$

Where  $N_s$  is the number of support vectors.



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### The KKT conditions are as follow

• 
$$\alpha_i \left[ d_i \left( \boldsymbol{w}^T \boldsymbol{x}_i + w_o \right) - 1 + \xi_i \right] = 0$$
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•  $\mu_i \xi_i = 0$  for  $i = 1, 2, ..., N$ .

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### The $\mu_i$ are Lagrange multipliers

They are used to enforce the non-negativity of the slack variables  $\xi_i$  for all i.

#### Something Notable

At saddle point, the derivative of the Lagrangian function for the primal problem:

$$\frac{1}{2}\boldsymbol{w}^{T}\boldsymbol{w} + C\sum_{i=1}^{N}\xi_{i} - \sum_{i=1}^{N}\alpha_{i}\left[d_{i}\left(\boldsymbol{w}^{T}\boldsymbol{x}_{i} + w_{o}\right) - 1 + \xi_{i}\right] - \sum_{i=1}^{N}\mu_{i}\xi_{i} \quad (34)$$



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# Thus

### We get

$$\alpha_i + \mu_i = C \tag{35}$$

#### Thus, we get if

Then  $\mu_i > 0 \Rightarrow \xi_i = 0$ 

#### We may determine $w_0$

Using any data point  $(x_i, d_i)$  in the training set such that  $0 \le \alpha_i^* \le C$ . Then, given  $\xi_i = 0$ ,

$$w_0^* = rac{1}{d_i} - \left( oldsymbol{w}^* 
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### Nevertheless

#### It is better

To take the mean value of  $w_0^*$  from all such data points in the training sample (Burges, 1998).

• BTW He has a great book in SVM's "An Introduction to Support Vector Machines and Other Kernel-based Learning Methods"



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