# Introduction to Machine Learning <br> Introduction to Support Vector Machines 

Andres Mendez-Vazquez

June 13, 2018

## Outline

(1) History

- The Beginning
(2) Separable Classes
- Separable Classes
- Hyperplanes
(3) Support Vectors
- Support Vectors
- Quadratic Optimization
- Rewriting The Optimization Problem
- Karush-Kuhn-Tucker Conditions
- Properties of the Dual

4 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?
(5) Soft Margins
- Introduction
- The Soft Margin Solution


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(1) History<br>- The Beginning

## 2 Separable Classes

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- She is currently the Head of Google Research, New York.
- Cortes is a recipient of the Paris Kanellakis Theory and Practice Award (ACM) for her work on theoretical foundations of support vector machines.


## In addition

## Alexey Yakovlevich Chervonenkis

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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## He died in September 22nd, 2014

At Losiny Ostrov National Park on 22 September 2014.

## Applications

## Partial List

(1) Predictive Control

- Control of chaotic systems.


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- AND counting....


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## Separable Classes

## Given

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\boldsymbol{x}_{i}, i=1, \cdots, N
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A set of samples belonging to two classes $\omega_{1}, \omega_{2}$.

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## Objective

We want to obtain a decision function as simple as

$$
g(\boldsymbol{x})=\boldsymbol{w}^{T} \boldsymbol{x}+w_{0}
$$

Such that we can do the following
A linear separation function $g(\boldsymbol{x})=\boldsymbol{w}^{t} \boldsymbol{x}+w_{0}$


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## In other words ...

## We have the following samples

- For $\boldsymbol{x}_{1}, \cdots, \boldsymbol{x}_{m} \in C_{1}$


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We want the following decision surfaces

- $\boldsymbol{w}^{T} \boldsymbol{x}_{i}+w_{0} \geq 0$ for $d_{i}=+1$ if $\boldsymbol{x}_{i} \in C_{1}$


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We want the following decision surfaces

- $\boldsymbol{w}^{T} \boldsymbol{x}_{i}+w_{0} \geq 0$ for $d_{i}=+1$ if $\boldsymbol{x}_{i} \in C_{1}$
- $\boldsymbol{w}^{T} \boldsymbol{x}_{j}+w_{0} \leq 0$ for $d_{j}=-1$ if $\boldsymbol{x}_{j} \in C_{2}$


## What do we want?

Our goal is to search for a direction $\boldsymbol{w}$ that gives the maximum possible margin


## Remember

We have the following


## A Little of Geometry

Thus


## A Little of Geometry

Thus


Then

$$
\begin{equation*}
d=\frac{\left|w_{0}\right|}{\sqrt{w_{1}^{2}+w_{2}^{2}}}, r=\frac{|g(\boldsymbol{x})|}{\sqrt{w_{1}^{2}+w_{2}^{2}}} \tag{1}
\end{equation*}
$$

First $d=\frac{\left|w_{0}\right|}{\sqrt{w_{1}^{2}+w_{2}^{2}}}$

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

$$
\begin{equation*}
\text { Area }=\frac{1}{2} C d \tag{2}
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In addition, the area can be calculated also as

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## Thus

$$
d=\frac{A B}{C}
$$

Remark: Can you get the rest of values?

What about $r=\frac{|g(x)|}{\sqrt{w_{1}^{2}+w_{2}^{2}}}$ ?
First, remember

$$
\begin{equation*}
g\left(\boldsymbol{x}_{p}\right)=0 \text { and } \boldsymbol{x}=\boldsymbol{x}_{p}+r \frac{\boldsymbol{w}}{\|\boldsymbol{w}\|} \tag{4}
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Thus, we have

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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

$$
r=\frac{g(\mathbf{x})}{\|\mathbf{w}\|}
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## This has the following interpretation

The distance from the projection


## Now

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

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\boldsymbol{w}^{T} x+w_{0}=0 \tag{5}
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## Clearly

This will be above or below the initial line $\boldsymbol{w}^{T} x+w_{0}=0$.

## Come back to the hyperplanes

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


## Then, normalize by $\delta$

The new margin functions

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

- $\boldsymbol{w}^{T} \mathbf{x}_{i}+w_{0} \geq \boldsymbol{w}^{T} \mathbf{x}+w_{10}$ for $d_{i}=+1$

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- Where $w_{0}$ is the bias of that central hyperplane!! And the $\boldsymbol{w}$ is the normalized direction of $\boldsymbol{w}^{\prime}$


## 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 $w$ )
$\boldsymbol{x}_{i}$ such that $\boldsymbol{w}^{T} \boldsymbol{x}_{i}+w_{0}=1$ or $\boldsymbol{w}^{T} \boldsymbol{x}_{i}+w_{0}=-1$

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## Properties

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


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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".

Now, we can resume the decision rule for the hyperplane

For the support vectors

$$
\begin{equation*}
g\left(\boldsymbol{x}_{i}\right)=\boldsymbol{w}^{T} \boldsymbol{x}_{i}+w_{0}=-(+) 1 \text { for } d_{i}=-(+) 1 \tag{7}
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\end{equation*}
$$

## Implies

The distance to the support vectors is:

$$
r=\frac{g\left(\boldsymbol{x}_{i}\right)}{\|\boldsymbol{w}\|}= \begin{cases}\frac{1}{\|\boldsymbol{w}\|} & \text { if } d_{i}=+1 \\ -\frac{1}{\|\boldsymbol{w}\|} & \text { if } d_{i}=-1\end{cases}
$$

## Therefore ...

We want the optimum value of the margin of separation as

$$
\begin{equation*}
\rho=\frac{1}{\|\boldsymbol{w}\|}+\frac{1}{\|\boldsymbol{w}\|}=\frac{2}{\|\boldsymbol{w}\|} \tag{8}
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And the support vectors define the value of $\rho$


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

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

## Under the restrictions

Then, we have the samples with labels

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T=\left\{\left(\boldsymbol{x}_{i}, d_{i}\right)\right\}_{i=1}^{N}
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Then we can put the decision rule as

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d_{i}\left(\boldsymbol{w}^{T} \boldsymbol{x}_{i}+w_{0}\right) \geq 1 i=1, \cdots, N
$$

Then, we have the optimization problem

The optimization problem

$$
\begin{gathered}
\min _{\boldsymbol{w}} \Phi(\boldsymbol{w})=\frac{1}{2} \boldsymbol{w}^{T} \boldsymbol{w} \\
\text { s.t. } d_{i}\left(\boldsymbol{w}^{T} \boldsymbol{x}_{i}+w_{0}\right) \geq 1 i=1, \cdots, N
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## Observations

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

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## Observations

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


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Hyperplanes

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## Then, Rewriting The Optimization Problem

The optimization with equality constraints

$$
\begin{aligned}
\min _{\boldsymbol{w}} \Phi(\boldsymbol{w}) & =\frac{1}{2} \boldsymbol{w}^{T} \boldsymbol{w} \\
\text { s.t. } d_{i}\left(\boldsymbol{w}^{T} \boldsymbol{x}_{i}+w_{0}\right) & \geq 1 i=1, \cdots, N
\end{aligned}
$$

## Then, for our problem

## Using the Lagrange Multipliers (We will call them $\alpha_{i}$ )

We obtain the following cost function that we want to minimize

$$
J\left(\boldsymbol{w}, w_{0}, \boldsymbol{\alpha}\right)=\frac{1}{2} \boldsymbol{w}^{T} \boldsymbol{w}-\sum_{i=1}^{N} \alpha_{i}\left[d_{i}\left(\boldsymbol{w}^{T} \mathbf{x}_{i}+w_{0}\right)-1\right]
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## Observation

- Minimize with respect to $\mathbf{w}$ and $w_{0}$.


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$$

## Observation

- Minimize with respect to $\mathbf{w}$ and $w_{0}$.
- Maximize with respect to $\alpha$ because it dominates

$$
\begin{equation*}
-\sum_{i=1}^{N} \alpha_{i}\left[d_{i}\left(\boldsymbol{w}^{T} \boldsymbol{x}_{i}+w_{0}\right)-1\right] \tag{9}
\end{equation*}
$$

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## Karush-Kuhn-Tucker Conditions

First An Inequality Constrained Problem $P$

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

## 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 $\alpha_{j}$ 's may be found such that:

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

## Karush-Kuhn-Tucker Conditions

## 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).


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This actually defines the idea of support vectors!!!

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## Again the Support Vectors

This actually defines the idea of support vectors!!!

## Thus

Only the $\alpha_{i}$ 's with active constraints (Support Vectors) will be different from zero when $d_{i}\left(\boldsymbol{w}^{T} \boldsymbol{x}_{i}+w_{0}\right)-1=0$.

## The necessary conditions for optimality

## Condition 1

$$
\frac{\partial J\left(\boldsymbol{w}, w_{0}, \boldsymbol{\alpha}\right)}{\partial \boldsymbol{w}}=0
$$

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Condition 2

$$
\frac{\partial J\left(\boldsymbol{w}, w_{0}, \boldsymbol{\alpha}\right)}{\partial w_{0}}=0
$$

## Using the conditions

## We have the first condition

$$
\frac{\partial J\left(\boldsymbol{w}, w_{0}, \alpha\right)}{\partial \boldsymbol{w}}=\frac{\partial \frac{1}{2} \boldsymbol{w}^{T} \boldsymbol{w}}{\partial \boldsymbol{w}}-\frac{\partial \sum_{i=1}^{N} \alpha_{i}\left[d_{i}\left(\boldsymbol{w}^{T} \boldsymbol{x}_{i}+w_{0}\right)-1\right]}{\partial \boldsymbol{w}}=0
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\frac{\partial J\left(\boldsymbol{w}, w_{0}, \alpha\right)}{\partial \boldsymbol{w}}=\frac{1}{2}(\boldsymbol{w}+\boldsymbol{w})-\sum_{i=1}^{N} \alpha_{i} d_{i} \boldsymbol{x}_{i}
\end{gathered}
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## Thus

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## We have the first condition

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\end{gathered}
$$

## Thus

$$
\begin{equation*}
\boldsymbol{w}=\sum_{i=1}^{N} \alpha_{i} d_{i} \mathbf{x}_{i} \tag{10}
\end{equation*}
$$

## In a similar way ...

## We have by the second optimality condition

$$
\sum_{i=1}^{N} \alpha_{i} d_{i}=0
$$

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$$

## Note

$$
\alpha_{i}\left[d_{i}\left(\boldsymbol{w}^{T} \boldsymbol{x}_{i}+w_{0}\right)-1\right]=0
$$

Because the constraint vanishes in the optimal solution i.e. $\alpha_{i}=0$ or $d_{i}\left(\boldsymbol{w}^{T} \boldsymbol{x}_{i}+w_{0}\right)-1=0$.

## Thus

## We need something extra

Our classic trick of transforming a problem into another problem

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In this case<br>We use the Primal-Dual Problem for Lagrangian

## Thus

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## Where

We move from a minimization to a maximization!!!

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## Duality Theorem

## First Property

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

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

## Thus

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

- It is a feasible solution for the primal problem and

$$
\begin{aligned}
\Phi(\boldsymbol{w} *) & =J\left(\boldsymbol{w} *, w_{0} *, \boldsymbol{\alpha} *\right) \\
& =\min _{\boldsymbol{w}} J\left(\boldsymbol{w} *, w_{0} *, \boldsymbol{\alpha} *\right)
\end{aligned}
$$

## Reformulate our Equations

## We have then

$$
J\left(\boldsymbol{w}, w_{0}, \boldsymbol{\alpha}\right)=\frac{1}{2} \boldsymbol{w}^{T} \boldsymbol{w}-\sum_{i=1}^{N} \alpha_{i} d_{i} \boldsymbol{w}^{T} \mathbf{x}_{i}-w_{0} \sum_{i=1}^{N} \alpha_{i} d_{i}+\sum_{i=1}^{N} \alpha_{i}
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$$

Now for our 2nd optimality condition

$$
J\left(\boldsymbol{w}, w_{0}, \boldsymbol{\alpha}\right)=\frac{1}{2} \boldsymbol{w}^{T} \boldsymbol{w}-\sum_{i=1}^{N} \alpha_{i} d_{i} \boldsymbol{w}^{T} \boldsymbol{x}_{i}+\sum_{i=1}^{N} \alpha_{i}
$$

We have finally for the 1st Optimality Condition:

## First

$$
\boldsymbol{w}^{T} \boldsymbol{w}=\sum_{i=1}^{N} \alpha_{i} d_{i} \boldsymbol{w}^{T} \boldsymbol{x}_{i}=\sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_{i} \alpha_{j} d_{i} d_{j} \boldsymbol{x}_{j}^{T} \boldsymbol{x}_{i}
$$

We have finally for the 1st Optimality Condition:

## First

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\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 $J\left(\boldsymbol{w}, w_{0}, \boldsymbol{\alpha}\right)=Q(\boldsymbol{\alpha})$

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

## From here, we have the problem

## This is the problem that we really solve

Given the training sample $\left\{\left(\mathbf{x}_{i}, d_{i}\right)\right\}_{i=1}^{N}$, find the Lagrange multipliers $\left\{\alpha_{i}\right\}_{i=1}^{N}$ 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

$$
\begin{gather*}
\sum_{i=1}^{N} \alpha_{i} d_{i}=0  \tag{11}\\
\alpha_{i} \geq 0 \text { for } i=1, \cdots, N \tag{12}
\end{gather*}
$$

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\end{gather*}
$$

## Note

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

## Solving for $\boldsymbol{\alpha}$

We can compute $\boldsymbol{w}^{*}$ once we get the optimal $\alpha_{i}^{*}$ by using (Eq. 10)

$$
\boldsymbol{w}^{*}=\sum_{i=1}^{N} \alpha_{i}^{*} d_{i} \boldsymbol{x}_{i}
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In addition, we can compute the optimal bias $w_{0}^{*}$ using the optimal weight, $w^{*}$
For this, we use the positive margin equation:

$$
g\left(\boldsymbol{x}^{(s)}\right)=\boldsymbol{w}^{T} \boldsymbol{x}^{(s)}+w_{0}=1
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corresponding to a positive support vector.

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## Then

$$
\begin{equation*}
w_{0}=1-\left(\boldsymbol{w}^{*}\right)^{T} \boldsymbol{x}^{(s)} \text { for } d^{(s)}=1 \tag{13}
\end{equation*}
$$

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## What do we need?

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

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- All this work fine when the classes are separable
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## Map to a higher Dimensional Space

Assume that exist a mapping

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Then, it is possible to define the following mapping


## Define a map to a higher Dimension

Nonlinear transformations
Given a series of nonlinear transformations

$$
\left\{\phi_{i}(\boldsymbol{x})\right\}_{i=1}^{m}
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from input space to the feature space.

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## We can define the decision surface as

$$
\sum_{i=1}^{m} w_{i} \phi_{i}(\boldsymbol{x})+w_{0}=0
$$

## This allows us to define

## The following vector

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

that represents the mapping.

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## From this mapping

We can define the following kernel function

$$
\begin{gathered}
K: \mathbf{X} \times \mathbf{X} \rightarrow \mathbb{R} \\
K\left(\boldsymbol{x}_{i}, \boldsymbol{x}_{j}\right)=\phi\left(\boldsymbol{x}_{i}\right)^{T} \phi\left(\boldsymbol{x}_{j}\right)
\end{gathered}
$$

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## - Basic Idea

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## Basic Idea

## Something Notable

- The SVM uses the scalar product $\left\langle\boldsymbol{x}_{i}, \boldsymbol{x}_{j}\right\rangle$ as a measure of similarity between $\boldsymbol{x}_{i}$ and $\boldsymbol{x}_{j}$, and of distance to the hyperplane.


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


## But

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

We do this by defining the following map

Nonlinear transformations
Given a series of nonlinear transformations

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That represents the mapping.

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## Finally

## We define the decision surface as

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

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\begin{equation*}
\boldsymbol{w}=\sum_{i=1}^{N} \alpha_{i} d_{i} \phi\left(\boldsymbol{x}_{i}\right) \tag{15}
\end{equation*}
$$

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## We define the decision surface as

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\boldsymbol{w}=\sum_{i=1}^{N} \alpha_{i} d_{i} \phi\left(\boldsymbol{x}_{i}\right) \tag{15}
\end{equation*}
$$

Thus, we finish with the following decision surface

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

## Thus

The term $\phi^{T}\left(\boldsymbol{x}_{i}\right) \phi(\boldsymbol{x})$
It represents the inner product of two vectors induced in the feature space induced by the input patterns.

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We can introduce the inner-product kernel

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K\left(\boldsymbol{x}_{i}, \boldsymbol{x}\right)=\phi^{T}\left(\boldsymbol{x}_{i}\right) \phi(\boldsymbol{x})=\sum_{j=0}^{m} \phi_{j}\left(\boldsymbol{x}_{i}\right) \phi_{j}(\boldsymbol{x}) \tag{17}
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\end{equation*}
$$

## Property: Symmetry

$$
\begin{equation*}
K\left(\boldsymbol{x}_{i}, \boldsymbol{x}\right)=K\left(\boldsymbol{x}, \boldsymbol{x}_{i}\right) \tag{18}
\end{equation*}
$$

This allows to redefine the optimal hyperplane

We get

$$
\begin{equation*}
\sum_{i=1}^{N} \alpha_{i} d_{i} K\left(\boldsymbol{x}_{i}, \boldsymbol{x}\right)=0 \tag{19}
\end{equation*}
$$

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## Something Notable

Using kernels, we can avoid to go from:

$$
\text { Input Space } \Longrightarrow \text { Mapping Space } \Longrightarrow \text { Inner Product }
$$

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## Something Notable

Using kernels, we can avoid to go from:

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## By directly going from

$$
\text { Input Space } \Longrightarrow \text { Inner Product }
$$

## Important

## Something Notable

The expansion of (Eq. 17) for the inner-product kernel $K\left(\boldsymbol{x}_{i}, \boldsymbol{x}\right)$ is an important special case of that arises in functional analysis.

## Mercer's Theorem

## Mercer's Theorem

Let $K\left(\boldsymbol{x}, \boldsymbol{x}^{\prime}\right)$ be a continuous symmetric kernel that is defined in the closed interval $\boldsymbol{a} \leq \boldsymbol{x} \leq \boldsymbol{b}$ and likewise for $\boldsymbol{x}^{\prime}$. The kernel $K\left(\boldsymbol{x}, \boldsymbol{x}^{\prime}\right)$ can be expanded in the series

$$
\begin{equation*}
K\left(\boldsymbol{x}, \boldsymbol{x}^{\prime}\right)=\sum_{i=1}^{\infty} \lambda_{i} \phi_{i}(\boldsymbol{x}) \phi_{i}\left(\mathbf{x}^{\prime}\right) \tag{22}
\end{equation*}
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\end{equation*}
$$

## With

Positive coefficients, $\lambda_{i}>0$ for all $i$.

## 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

$$
\begin{equation*}
\int_{a}^{b} \int_{a}^{b} K\left(\boldsymbol{x}, \boldsymbol{x}^{\prime}\right) \psi(\boldsymbol{x}) \psi\left(\boldsymbol{x}^{\prime}\right) d \boldsymbol{x} d \boldsymbol{x}^{\prime} \geq 0 \tag{23}
\end{equation*}
$$

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

## Remarks

## First

The functions $\phi_{i}(\boldsymbol{x})$ are called eigenfunctions of the expansion and the numbers $\lambda_{i}$ are called eigenvalues.

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The functions $\phi_{i}(\boldsymbol{x})$ 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 $K\left(\boldsymbol{x}, \boldsymbol{x}^{\prime}\right)$ is positive definite.

## Not only that

## We have that

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

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## In theory

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

## Outline

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## - Examples

O Now, How to select a Kernel?
(5) Soft Margins

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## Example

## Assume

$$
\boldsymbol{x} \in \mathbb{R} \rightarrow \boldsymbol{y}=\left[\begin{array}{c}
x_{1}^{2} \\
\sqrt{2} x_{1} x_{2} \\
x_{2}^{2}
\end{array}\right]
$$

## Example

## Assume

$$
\boldsymbol{x} \in \mathbb{R} \rightarrow \boldsymbol{y}=\left[\begin{array}{c}
x_{1}^{2} \\
\sqrt{2} x_{1} x_{2} \\
x_{2}^{2}
\end{array}\right]
$$

## We can show that

$$
\boldsymbol{y}_{i}^{T} \boldsymbol{y}_{j}=\left(\boldsymbol{x}_{i}^{T} \boldsymbol{x}_{j}\right)^{2}
$$

## Example of Kernels

## Polynomials

$$
k(\boldsymbol{x}, \boldsymbol{z})=\left(\boldsymbol{x}^{T} \boldsymbol{z}+1\right)^{q} q>0
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k(\boldsymbol{x}, \boldsymbol{z})=\exp \left(-\frac{\|\boldsymbol{x}-\boldsymbol{z}\|^{2}}{\sigma^{2}}\right)
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## Radial Basis Functions

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

Hyperbolic Tangents

$$
k(\boldsymbol{x}, \boldsymbol{z})=\tanh \left(\beta \boldsymbol{x}^{T} \boldsymbol{z}+\gamma\right)
$$

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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.

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## Thus

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

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## We have a problem

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

## Thus <br> In general, the Radial Basis Functions kernel is a reasonable first choice.

## Then

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

## Thus, we have something like this

Step 1
Normalize the data.

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## Step 2

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

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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.

## Outline

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## Optimal Hyperplane for non-separable patterns

## Important

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

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## Now

What happen when the patterns are not separable?

## Optimal Hyperplane for non-separable patterns

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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...

## 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 $\left(x_{i}, d_{i}\right)$ violates the following condition

$$
\begin{equation*}
d_{i}\left(\boldsymbol{w}^{T} \boldsymbol{x}_{i}+b\right) \geq+1 i=1,2, \ldots, N \tag{24}
\end{equation*}
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$$

## This violation can arise in one of two ways

The data point $\left(\boldsymbol{x}_{i}, d_{i}\right)$ falls inside the region of separation but on the right side of the decision surface - still correct classification.

## We have then

## Example



## Or...

This violation can arise in one of two ways
The data point $\left(\boldsymbol{x}_{i}, d_{i}\right)$ falls on the wrong side of the decision surface incorrect classification.

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## Example



## Solving the problem

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## What to do?

- We introduce a set of nonnegative scalar values $\left\{\xi_{i}\right\}_{i=1}^{N}$.


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- We introduce a set of nonnegative scalar values $\left\{\xi_{i}\right\}_{i=1}^{N}$.

Introduce this into the decision rule

$$
\begin{equation*}
d_{i}\left(\boldsymbol{w}^{T} \boldsymbol{x}_{i}+b\right) \geq 1-\xi_{i} i=1,2, \ldots, N \tag{25}
\end{equation*}
$$

## 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.

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## Ok!!!

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

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## 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．

## Properties of $\xi_{i}$

## What if?

- You have $0 \leq \xi_{i} \leq 1$


## Properties of $\xi_{i}$

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## Properties of $\xi_{i}$

## What if?

- You have $\xi_{i}>1$


## We have



## Support Vectors

## We want

- Support vectors that satisfy equation (Eq. 25) even when $\xi_{i}>0$

$$
d_{i}\left(\boldsymbol{w}^{T} \boldsymbol{x}_{i}+b\right) \geq 1-\xi_{i} i=1,2, \ldots, N
$$

## We want the following

## We want to find an hyperplane

Such that average error is misclassified over all the samples

$$
\begin{equation*}
\frac{1}{N} \sum_{i=1}^{N} \mathrm{e}^{2} \tag{26}
\end{equation*}
$$

## First Attempt Into Minimization

We can try the following
Given

$$
I(x)= \begin{cases}0 & \text { if } x \leq 0  \tag{27}\\ 1 & \text { if } x>0\end{cases}
$$

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## We can try the following

## Given

$$
I(x)= \begin{cases}0 & \text { if } x \leq 0  \tag{27}\\ 1 & \text { if } x>0\end{cases}
$$

## Minimize the following

$$
\begin{equation*}
\Phi(\boldsymbol{\xi})=\sum_{i=1}^{N} I\left(\xi_{i}-1\right) \tag{28}
\end{equation*}
$$

with respect to the weight vector $\boldsymbol{w}$ subject to
(1) $d_{i}\left(\boldsymbol{w}^{T} \boldsymbol{x}_{i}+b\right) \geq 1-\xi_{i} i=1,2, \ldots, N$
(2) $\|\boldsymbol{w}\|^{2} \leq C$ for a given $C$.

## Problem

## Using this first attempt

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

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Thus, we need to use an approximation, maybe

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\Phi(\boldsymbol{\xi})=\sum_{i=1}^{N} \xi_{i} \tag{29}
\end{equation*}
$$

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

$$
\begin{equation*}
\Phi(\boldsymbol{w}, \boldsymbol{\xi})=\frac{1}{2} \boldsymbol{w}^{T} \boldsymbol{w}+C \sum_{i=1}^{N} \xi_{i} \tag{30}
\end{equation*}
$$

## Important

## First

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

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## 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.


## Second

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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This can be done in two ways
(1) The parameter $C$ is determined experimentally via the standard use of a training! (validation) test set.

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

## Primal Problem

Problem, given samples $\left\{\left(\boldsymbol{x}_{i}, d_{i}\right)\right\}_{i=1}^{N}$

$$
\begin{aligned}
& \min _{\boldsymbol{w}, \boldsymbol{\xi}} \Phi(\boldsymbol{w}, \boldsymbol{\xi})=\min _{\mathbf{w}, \boldsymbol{\xi}}\left\{\frac{1}{2} \boldsymbol{w}^{T} \boldsymbol{w}+C \sum_{i=1}^{N} \xi_{i}\right\} \\
& \text { s.t. } d_{i}\left(\boldsymbol{w}^{T} \boldsymbol{x}_{i}+w_{0}\right) \geq 1-\xi_{i} \text { for } i=1, \cdots, N \\
& \xi_{i} \geq 0 \text { for all } i
\end{aligned}
$$

With $C$ a user-specified positive parameter.

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## Final Setup

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

Given the training sample $\left\{\left(\mathbf{x}_{i}, d_{i}\right)\right\}_{i=1}^{N}$, find the Lagrange multipliers $\left\{\alpha_{i}\right\}_{i=1}^{N}$ 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

$$
\begin{gather*}
\sum_{i=1}^{N} \alpha_{i} d_{i}=0  \tag{31}\\
0 \leq \alpha_{i} \leq C \text { for } i=1, \cdots, N \tag{32}
\end{gather*}
$$

where $C$ is a user-specified positive parameter.

## Remarks

## Something Notable

- Note that neither the slack variables nor their Lagrange multipliers appear in the dual problem.


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## The only big difference

Instead of using the constraint $\alpha_{i} \geq 0$, the new problem use the more stringent constraint $0 \leq \alpha_{i} \leq C$.

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## The only big difference

Instead of using the constraint $\alpha_{i} \geq 0$, the new problem use the more stringent constraint $0 \leq \alpha_{i} \leq C$.

## Note the following

$$
\begin{equation*}
\xi_{i}=0 \text { if } \alpha_{i}<C \tag{33}
\end{equation*}
$$

## Finally

The optimal solution for the weight vector $\boldsymbol{w}^{*}$

$$
\boldsymbol{w}^{*}=\sum_{i=1}^{N_{s}} \alpha_{i}^{*} d_{i} \boldsymbol{x}_{i}
$$

Where $N_{s}$ is the number of support vectors.

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## In addition

The determination of the optimum values to that described before.

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The determination of the optimum values to that described before.
The KKT conditions are as follow

- $\alpha_{i}\left[d_{i}\left(\boldsymbol{w}^{T} \boldsymbol{x}_{i}+w_{o}\right)-1+\xi_{i}\right]=0$ for $i=1,2, \ldots, N$.


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- $\alpha_{i}\left[d_{i}\left(\boldsymbol{w}^{T} \boldsymbol{x}_{i}+w_{o}\right)-1+\xi_{i}\right]=0$ for $i=1,2, \ldots, N$.
- $\mu_{i} \xi_{i}=0$ for $i=1,2, \ldots, N$.


## Where...

The $\mu_{i}$ are Lagrange multipliers
They are used to enforce the non-negativity of the slack variables $\xi_{i}$ for all $i$.

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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:

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

## Thus

We get

$$
\alpha_{i}+\mu_{i}=C
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\alpha_{i}+\mu_{i}=C \tag{35}
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Thus, we get if $\alpha_{i}<C$
Then $\mu_{i}>0 \Rightarrow \xi_{i}=0$

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We get

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\begin{equation*}
\alpha_{i}+\mu_{i}=C \tag{35}
\end{equation*}
$$

Thus, we get if $\alpha_{i}<C$
Then $\mu_{i}>0 \Rightarrow \xi_{i}=0$

## We may determine $w_{0}$

Using any data point $\left(\boldsymbol{x}_{i}, d_{i}\right)$ in the training set such that $0 \leq \alpha_{i}^{*} \leq C$. Then, given $\xi_{i}=0$,

$$
\begin{equation*}
w_{0}^{*}=\frac{1}{d_{i}}-\left(\boldsymbol{w}^{*}\right)^{T} \boldsymbol{x}_{i} \tag{36}
\end{equation*}
$$

## 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"

