## M L <br> D M <br> Chapter 9 <br> Support Vector Machines

## Learning Machines

- A machine to learn the mapping

$$
\mathbf{x}_{i} \mathbf{a} \quad y_{i}
$$

■ Defined as

$$
\mathbf{x} \text { a } \quad \begin{aligned}
& f(\mathbf{x}, \underbrace{\boldsymbol{\alpha})} \\
& \begin{array}{c}
\text { Learning by adjusting } \\
\text { this parameter? }
\end{array}
\end{aligned}
$$

## Generalization vs. Learning

- How a machine learns?
- Adjusting the parameters so as to partition the pattern (feature) space for classification.
- How to adjust?

Minimize the empirical risk (traditional approaches).

■ What the machine learned?

- Memorize the patterns it sees? or
- Memorize the rules it finds for different classes?
- What does the machine actually learn if it minimizes empirical risk only?


## Risks

Expected Risk (test error)

$$
R(\boldsymbol{\alpha})=\int \frac{1}{2}|y-f(\mathbf{x}, \boldsymbol{\alpha})| d P(\mathbf{x}, y)
$$

Empirical Risk (training error)

$$
\begin{gathered}
R_{e m p}(\boldsymbol{\alpha})=\frac{1}{2 l} \sum_{i=1}^{l}\left|y_{i}-f\left(\mathbf{x}_{i}, \boldsymbol{\alpha}\right)\right| \\
R(\boldsymbol{\alpha}) \approx R_{\text {emp }}(\boldsymbol{\alpha}) ?
\end{gathered}
$$

## More on Empirical Risk

■ How can make the empirical risk arbitrarily small?

- To let the machine have very large memorization capacity.

■ Does a machine with small empirical risk also get small expected risk?

- How to avoid the machine to strain to memorize training patterns, instead of doing generalization, only?
- How to deal with the straining-memorization capacity of a machine?
- What the new criterion should be?


## Structure Risk Minimization

## Goal: Learn both the right 'structure' and right `rules' for classification.

## Right Structure:

E.g., Right amount and right forms of components or parameters are to participate in a learning machine.

## Right Rules:

The empirical risk will also be reduced if right rules are learned.

## New Criterion

Risk due to the<br>Total Risk = Empirical Risk + structure of the learning machine

## The VC Dimension

- Consider a set of function $f(\mathbf{x}, \alpha) \in\{-1,1\}$.

■ A given set of $l$ points can be labeled in $2^{\prime}$ ways.

- If a member of the set $\{f(\alpha)\}$ can be found which correctly assigns the labels for all labeling, then the set of points is shattered by that set of functions.
- The VC dimension of $\{f(\alpha)\}$ is the maximum number of training points that can be shattered by $\{f(\alpha)\}$.

> VC: VapnikChervonenkis

## The VC Dimension for Oriented Lines in $\boldsymbol{R}^{2}$

- VC dimension $=3$

0





## More on VC Dimension

- In general, the VC dimension of a set of oriented hyperplanes in $R^{n}$ is $n+1$.

■ VC dimension is a measure of memorization capability.

- VC dimension is not directly related to number of parameters. Vapnik (1995) has an example with 1 parameter and infinite VC dimension.


## Bound on Expected Risk

Expected Risk $\quad R(\boldsymbol{\alpha})=\int \frac{1}{2}|y-f(\mathbf{x}, \boldsymbol{\alpha})| d P(\mathbf{x}, y)$
Empirical Risk $\quad R_{\text {emp }}(\boldsymbol{\alpha})=\frac{1}{2 l} \sum_{i=1}^{l}\left|y_{i}-f\left(\mathbf{x}_{i}, \boldsymbol{\alpha}\right)\right|$

$$
P(R(\alpha) \leq R_{\text {emp }}(\alpha)+\underbrace{\sqrt{\frac{h(\log (2 l / h)+1)-\log (\eta / 4)}{l}}}_{\text {VC Confidence }})=1-\eta
$$

$h$ is the VC dimension; $I$ is the number of samples

## Bound on Expected Risk

Consider small $\eta$ (e.g., $\eta \leq 0.05$ ).

$$
\begin{aligned}
& \longrightarrow R(\alpha) \leq R_{\text {emp }}(\alpha)+\sqrt{\frac{h(\log (2 l / h)+1)-\log (\eta / 4)}{l}} \\
& P(R(\alpha) \leq R_{\text {emp }}(\alpha)+\underbrace{\sqrt{\frac{h(\log (2 l / h)+1)-\log (\eta / 4)}{l}}}_{\text {VC Confidence }})=1-\eta
\end{aligned}
$$

## Bound on Expected Risk

Consider small $\eta$ (e.g., $\eta \leq 0.05$ ).
$\longrightarrow R(\alpha) \leq \underbrace{R_{\text {emp }}(\alpha)}+\sqrt{\frac{h(\log (2 l / h)+1)-\log (\eta / 4)}{l}}$
Traditional approaches minimize empirical risk only


Structure risk minimization want to minimize the bound

## VC Confidence

$$
R(\alpha) \leq R_{e m p}(\alpha)+\sqrt{\frac{h(\log (2 l / h)+1)-\log (\eta / 4)}{l}}
$$



## Structure Risk Minimization

$$
h_{1}<h_{2}<h_{3}<h_{4}
$$



Nested subset of functions with different VC dimensions.

## Structure Risk Minimization



## Linear SVM

- The linear separability


Linearly separable


Not linearly separable

## Linear SVM

- The linear separability


> How would you classify these points using a linear discriminant function in order to minimize the error rate?

Linearly separable

## Maximum Margin Classifier



Supporters

The linear discriminant
function (classifier) with the maximum margin is the best

Margin is defined as the width
that the boundary could be
increased by before hitting
a data point
$\square$ Why is it the best?

- Intuitively robust to outliners and thus strong generalization ability


## Relation Between VC Dimension and Margin ${ }_{\text {IMA }}$

- What is the relation btw. the margin width and VC dimension?
- Let $x$ belong to sphere of radius $R$. The set of margin separating hyperplanes has VC dimension h bounded by:

$$
\begin{aligned}
& \qquad \quad h \leq \min \left(\left(\frac{R}{\gamma}\right)^{2}, d\right)+1 \\
& \text { What doe dimession of } x
\end{aligned}
$$

## Linear SVM

- The linear separability



## Margin Width

$$
y_{i}\left(\mathbf{w} \mathbf{x}_{i}+b\right)-1 \geq 0 \quad \forall i
$$



$$
\begin{aligned}
d & =\frac{1-b}{\|\mathbf{w}\|}-\frac{-1-b}{\|\mathbf{w}\|} \\
& =\frac{2}{\|\mathbf{w}\|}
\end{aligned}
$$

How about maximize the margin?

## Building SVM

# Minimize $\quad \frac{1}{2}\|\mathbf{w}\|^{2}$ <br> Subject to $\quad y_{i}\left(\mathbf{w}^{T} \mathbf{x}_{i}+b\right)-1 \geq 0 \quad \forall i$ 

This requires the knowledge about Lagrange Multiplier.

## The Method of Lagrange

Minimize $\quad \frac{1}{2}\|\mathbf{w}\|^{2}$
Subject to $\quad y_{i}\left(\mathbf{w}^{T} \mathbf{x}_{i}+b\right)-1 \geq 0 \quad \forall i$
The Lagrangian:

$$
L(\mathbf{w}, b ; \Lambda)=\frac{1}{2}\|\mathbf{w}\|^{2}-\sum_{i=1}^{l} \lambda_{i}\left[y_{i}\left(\mathbf{w}^{T} \mathbf{x}_{i}+b\right)-1\right] \quad \lambda_{i} \geq 0
$$

Minimize it w.r.t w \& b, while maximize it w.r.t. $\Lambda$.

## The Method of Lagrange

■ Why Lagrange?

- The constraints will be replaced by constraints on the Lagrange multipliers, which will be much easier to handle.
- In this reformulation of the problem, the training data will only appear in the form of dot products between vectors.


## The Method of Lagrange

How about if it is


Minimize it w.r.t w \& b, while maximize it w.r.t. $\Lambda$.

## The Method of Lagrange

$$
L(\mathbf{w}, b ; \Lambda)=\frac{1}{2}\|\mathbf{w}\|^{2}-\sum_{i=1}^{l} \lambda_{i} y_{i}\left(\mathbf{w}^{T} \mathbf{x}_{i}+b\right)+\sum_{i=1}^{l} \lambda_{i}
$$

Minimize $\quad \frac{1}{2}\|\mathbf{w}\|^{2}$
Subject to $\quad y_{i}\left(\mathbf{w}^{T} \mathbf{x}_{i}+b\right)-1 \geq 0 \quad \forall i$
The Lagrangian:

$$
\begin{aligned}
L(\mathbf{w}, b ; \Lambda) & =\frac{1}{2}\|\mathbf{w}\|^{2}-\sum_{i=1}^{l} \lambda_{i}\left[y_{i}\left(\mathbf{w}^{T} \mathbf{x}_{i}+b\right)-1\right] \quad \lambda_{i} \geq 0 \\
& =\frac{1}{2}\|\mathbf{w}\|^{2}-\sum_{i=1}^{l} \lambda_{i} y_{i}\left(\mathbf{w}^{T} \mathbf{x}_{i}+b\right)+\sum_{i=1}^{l} \lambda_{i}
\end{aligned}
$$

## Duality

$$
L(\mathbf{w}, b ; \Lambda)=\frac{1}{2}\|\mathbf{w}\|^{2}-\sum_{i=1}^{l} \lambda_{i} y_{i}\left(\mathbf{w}^{T} \mathbf{x}_{i}+b\right)+\sum_{i=1}^{l} \lambda_{i}
$$

Minimize $\quad \frac{1}{2}\|\mathbf{w}\|^{2}$
Subject to $\quad y_{i}\left(\mathbf{w}^{T} \mathbf{x}_{i}+b\right)-1 \geq 0 \quad \forall i$

Maximize $L\left(\mathbf{w}^{*}, b^{*} ; \Lambda\right)$
Subject to

$$
\begin{aligned}
& \nabla_{\mathbf{w}, b} L(\mathbf{w}, b ; \Lambda)=\mathbf{0} \\
& \lambda_{i} \geq 0, \quad i=1, \mathrm{~K}, l
\end{aligned}
$$

## Duality

$$
\begin{aligned}
& L(\mathbf{w}, b ; \Lambda)=\frac{1}{2}\|\mathbf{w}\|^{2}-\sum_{i=1}^{l} \lambda_{i} y_{i}\left(\mathbf{w}^{T} \mathbf{x}_{i}+b\right)+\sum_{i=1}^{l} \lambda_{i} \\
& \nabla_{\mathbf{w}} L(\mathbf{w}, b ; \Lambda)=\mathbf{w}-\sum_{i=1}^{l} \lambda_{i} y_{i} \mathbf{x}_{i}=\mathbf{0} \quad \square \quad \mathbf{w}^{*}=\sum_{i=1}^{l} \lambda_{i} y_{i} \mathbf{x}_{i} \\
& \nabla_{b} L(\mathbf{w}, b ; \Lambda)=\sum_{i=1}^{l} \lambda_{i} y_{i}=0 \quad \square \sum_{i=1}^{l} \lambda_{i} y_{i}=0
\end{aligned}
$$

Maximize $\quad L\left(\mathbf{w}^{*}, b^{*} ; \Lambda\right)$
Subject to

$$
\begin{aligned}
& \nabla_{\mathbf{w}, b} L(\mathbf{w}, b ; \Lambda)=\mathbf{0} \\
& \lambda_{i} \geq 0, \quad i=1, \mathrm{~K}, l
\end{aligned}
$$

## Duality

$$
\begin{gathered}
L(\mathbf{w}, b ; \Lambda)=\frac{1}{2}\|\mathbf{w}\|^{2}-\sum_{i=1}^{l} \lambda_{i} y_{i}\left(\mathbf{w}^{T} \mathbf{x}_{i}+b\right)+\sum_{i=1}^{l} \lambda_{i} \\
\nabla_{\mathbf{w}} L(\mathbf{w}, b ; \Lambda)=\mathbf{w}-\sum_{i=1}^{l} \lambda_{i} y_{i} \mathbf{x}_{i}=\mathbf{0} \quad \longrightarrow \mathbf{w}^{*}=\sum_{i=1}^{l} \lambda_{i} y_{i} \mathbf{x}_{i} \\
\nabla_{b} L(\mathbf{w}, b ; \Lambda)=\sum_{i=1}^{l} \lambda_{i} y_{i}=0 \\
\begin{array}{c}
L\left(\mathbf{w}^{*}, b^{*} ; \Lambda\right)= \\
=\frac{1}{2}\left(\sum_{i=1}^{l} \lambda_{i} y_{i} \mathbf{x}_{i}\right)^{T} \sum_{i=1}^{l} \lambda_{i} y_{i} \mathbf{x}_{i}-\left(\sum_{i=1}^{l} \lambda_{i} y_{i} \mathbf{x}_{i}\right)^{T} \sum_{i=1}^{l} \lambda_{i} y_{i} \mathbf{x}_{i}-b \sum_{i=1}^{l} \lambda_{i} y_{i}+\sum_{i=1}^{l} \lambda_{i} \\
=\sum_{i=1}^{l} \lambda_{i}-\frac{1}{2}\left(\sum_{i=1}^{l} \lambda_{i} y_{i} \mathbf{x}_{i}\right)^{T} \sum_{i=1}^{l} \lambda_{i} y_{i} \mathbf{x}_{i} \\
=\sum_{i=1}^{l} \lambda_{i}-\frac{1}{2} \sum_{i=1}^{l} \sum_{j=1}^{l} \lambda_{i} \lambda_{j} y_{i} y_{j}<\mathbf{x}_{i}, \mathbf{x}_{j}>
\end{array} \text { Maximize }
\end{gathered}
$$

## Duality

$$
\begin{gathered}
L(\mathbf{w}, b ; \Lambda)=\frac{1}{2}\|\mathbf{w}\|^{2}-\sum_{i=1}^{l} \lambda_{i} y_{i}\left(\mathbf{w}^{T} \mathbf{x}_{i}+b\right)+\sum_{i=1}^{l} \lambda_{i} \\
\nabla_{\mathbf{w}} L(\mathbf{w}, b ; \Lambda)=\mathbf{w}-\sum_{i=1}^{l} \lambda_{i} y_{i} \mathbf{x}_{i}=\mathbf{0} \quad \square \mathbf{w}^{*}=\sum_{i=1}^{l} \lambda_{i} y_{i} \mathbf{x}_{i} \\
\nabla_{b} L(\mathbf{w}, b ; \Lambda)=\sum_{i=1}^{l} \lambda_{i} y_{i}=0 \\
L\left(\mathbf{w}^{*}, b^{*} ; \Lambda\right)=\frac{1}{2}\left(\sum_{i=1}^{l} \lambda_{i} y_{i} \mathbf{x}_{i}\right)^{T} \sum_{i=1}^{l} \lambda_{i} y_{i} \mathbf{x}_{i}-\left(\sum_{i=1}^{l} \lambda_{i} y_{i} \mathbf{x}_{i}\right)^{T} \sum_{i=1}^{l} \lambda_{i} y_{i} \mathbf{x}_{i}-b \sum_{i=1}^{l} \lambda_{i} y_{i}+\sum_{i=1}^{l} \lambda_{i} \\
=\sum_{i=1}^{l} \lambda_{i}-\frac{1}{2}\left(\sum_{i=1}^{l} \lambda_{i} y_{i} \mathbf{x}_{i}\right)^{T} \sum_{i=1}^{l} \lambda_{i} y_{i} \mathbf{x}_{i} \quad F(\Lambda)=\Lambda \cdot \mathbf{\Lambda}-\frac{1}{2} \Lambda^{T} D \Lambda=0 \\
\hline
\end{gathered}
$$

$$
=\sum_{i=1}^{l} \lambda_{i}-\frac{1}{2} \sum_{i=1}^{l} \sum_{j=1}^{l} \lambda_{i} \lambda_{j} y_{i} y_{j}\left\langle\mathbf{x}_{i}, \mathbf{x}_{j}\right\rangle \longleftrightarrow \text { Maximize }
$$

## Duality

Minimize $\quad \frac{1}{2}\|\mathbf{w}\|^{2}$
The Primal
Subject to $\quad y_{i}\left(\mathbf{w}^{T} \mathbf{x}_{i}+b\right)-1 \geq 0 \quad \forall i$

The Dual
Maximize $\quad F(\Lambda)=\Lambda \cdot \mathbf{1}-\frac{1}{2} \Lambda^{T} D \Lambda$
Subject to $\quad \Lambda^{T} \mathbf{y}=0$

$$
\Lambda \geq \mathbf{0}
$$

## The Solution

## Quadratic Programming

Find $\Lambda^{*}$ by $\ldots$
$\longmapsto \mathbf{w}^{*}=\sum_{i=1}^{l} \lambda_{i}^{*} y_{i} \mathbf{x}_{i} \quad b^{*}=?$
Maximize $\quad F(\Lambda)=\Lambda \cdot \mathbf{1}-\frac{1}{2} \Lambda^{T} D \Lambda$
Subject to

$$
\Lambda^{T} \mathbf{y}=0
$$

$$
\Lambda \geq \mathbf{0}
$$

## The Solution



$$
L(\mathbf{w}, b ; \Lambda)=\frac{1}{2}\|\mathbf{w}\|^{2}-\sum_{i=1}^{l} \lambda_{i}\left[y_{i}\left(\mathbf{w}^{T} \mathbf{x}_{i}+b\right)-1\right]
$$

## The Karush-Kuhn-Tucker Conditions

$$
\begin{gathered}
L(\mathbf{w}, b ; \Lambda)=\frac{1}{2}\|\mathbf{w}\|^{2}-\sum_{i=1}^{l} \lambda_{i}\left[y_{i}\left(\mathbf{w}^{T} \mathbf{x}_{i}+b\right)-1\right] \\
\nabla_{\mathbf{w}} L(\mathbf{w}, b ; \Lambda)=\mathbf{w}-\sum_{i=1}^{l} \lambda_{i} y_{i} \mathbf{x}_{i}=\mathbf{0} \\
\nabla_{b} L(\mathbf{w}, b ; \Lambda)=\sum_{i=1}^{l} \lambda_{i} y_{i}=0 \\
y_{i}\left(\mathbf{w}^{T} \mathbf{x}_{i}+b\right)-1 \geq 0, \quad i=1, \mathrm{~K}, l \\
\lambda_{i} \geq 0, \quad i=1, \mathrm{~K}, l \\
\lambda_{i}\left[y_{i}\left(\mathbf{w}^{T} \mathbf{x}_{i}+b\right)-1\right]=0, \quad i=1, \mathrm{~K}, l
\end{gathered}
$$

## Classification

$$
\begin{gathered}
\mathbf{w}^{*}=\sum_{i=1}^{l} \lambda_{i}^{*} y_{i} \mathbf{x}_{i} \\
f(\mathbf{x})=\operatorname{sgn}\left(\mathbf{w}^{* T} \mathbf{x}+b^{*}\right) \\
=\operatorname{sgn}\left(\sum_{i=1}^{l} \lambda_{i}^{*} y_{i}<\mathbf{x}_{i}, \mathbf{x}>+b^{*}\right) \\
=\operatorname{sgn}\left(\sum_{\lambda_{i}^{*} \neq 0} \lambda_{i}^{*} y_{i}<\mathbf{x}_{i}, \mathbf{x}>+b^{*}\right)
\end{gathered}
$$

## Classification Using Supporters



## Linear SVM

■ Then non-separable case


## Mathematic Formulation

For simplicity, we consider $k=1$.
Minimize $\quad \frac{1}{2}\|\mathbf{w}\|^{2}+C\left(\sum_{i} \xi_{i}\right)^{k}$
Subject to $\quad y_{i}\left(\mathbf{w}^{T} \mathbf{x}_{i}+b\right)-1+\xi_{i} \geq 0 \quad \forall i$

$$
\xi_{i} \geq 0 \quad \forall i
$$

## Mathematic Formulation

For simplicity, we consider $k=1$.
Minimize $\quad \frac{1}{2}\|\mathbf{w}\|^{2}+C\left(\sum_{i} \xi_{i}\right)^{k}$
Subject to $\quad y_{i}\left(\mathbf{w}^{T} \mathbf{x}_{i}+b\right)-1+\xi_{i} \geq 0 \quad \forall i$

$$
\xi_{i} \geq 0 \quad \forall i
$$

## The Lagrangian

Minimize $\quad \frac{1}{2}\|\mathbf{w}\|^{2}+C \sum_{i} \xi_{i}$

$$
\begin{array}{rlrl}
\text { Subject to } & y_{i}\left(\mathbf{w}^{T} \mathbf{x}_{i}+b\right)-1+\xi_{i} & \geq 0 & \forall i \\
\xi_{i} & \geq 0 & \forall i
\end{array}
$$

$$
\begin{aligned}
& L(\mathbf{w}, b, \Xi ; \Lambda, \mathrm{M}) \\
& \begin{aligned}
&=\frac{1}{2}\|\mathbf{w}\|^{2}+C \sum_{i} \xi_{i}-\sum_{i} \lambda_{i}\left[y_{i}\left(\mathbf{w}^{T} \mathbf{x}_{i}+b\right)-1+\xi_{i}\right]-\sum_{i} \mu_{i} \xi_{i} \\
& \quad \lambda_{i} \geq 0, \mu_{i} \geq 0
\end{aligned}
\end{aligned}
$$

## Duality

$$
L(\mathbf{w}, b, \Xi ; \Lambda, \mathrm{M})=\frac{1}{2}\|\mathbf{w}\|^{2}+C \sum_{i} \xi_{i}-\sum_{i} \lambda_{i}\left[y_{i}\left(\mathbf{w}^{T} \mathbf{x}_{i}+b\right)-1+\xi_{i}\right]-\sum_{i} \mu_{i} \xi_{i}
$$

Minimize $\quad \frac{1}{2}\|\mathbf{w}\|^{2}+C \sum_{i} \xi_{i} \quad \lambda_{i} \geq 0, \mu_{i} \geq 0$
Subject to $\quad y_{i}\left(\mathbf{w}^{T} \mathbf{x}_{i}+b\right)-1+\xi_{i} \geq 0 \quad \forall i$

$$
\xi_{i} \geq 0 \quad \forall i
$$

Maximize $\quad L\left(\mathbf{w}^{*}, b^{*}, \Xi^{*} ; \Lambda, M\right)$
Subject to $\quad \nabla_{\mathbf{w}, b, \Xi} L(\mathbf{w}, b, \Xi ; \Lambda, M)=0$

$$
\Lambda \geq \mathbf{0}, \mathrm{M} \geq \mathbf{0}
$$

## Duality

$$
\lambda_{i} \geq 0, \mu_{i} \geq 0
$$

$$
\begin{array}{cl}
\hline L(\mathbf{w}, b, \Xi ; \Lambda, \mathrm{M})=\frac{1}{2}\|\mathbf{w}\|^{2}+C \sum_{i} \xi_{i}-\sum_{i} \lambda_{i}\left[y_{i}\left(\mathbf{w}^{T} \mathbf{x}_{i}+b\right)-1+\xi_{i}\right]-\sum_{i} \mu_{i} \xi_{i} \\
\nabla_{\mathbf{w}} L(\mathbf{w}, b, \Xi ; \Lambda, \mathrm{M})=\mathbf{w}-\sum_{i} \lambda_{i} y_{i} \mathbf{x}_{i}=\mathbf{0} \square \mathbf{w}^{*}=\sum_{i} \lambda_{i} y_{i} \mathbf{x}_{i} \\
\nabla_{b} L(\mathbf{w}, b, \Xi ; \Lambda, \mathrm{M})=\sum_{i} \lambda_{i} y_{i}=0 \square \sum_{i} \lambda_{i} y_{i}=0 \\
\nabla_{\xi_{i}} L(\mathbf{w}, b, \Xi ; \Lambda, \mathrm{M})=C-\lambda_{i}-\mu_{i}=0 \square \mu_{i}=C-\lambda_{i} \\
& 0 \leq \lambda_{i} \leq C
\end{array}
$$

Maximize $\quad L\left(\mathbf{w}^{*}, b^{*}, \Xi^{*} ; \Lambda, \mathrm{M}\right)$
Subject to $\quad \nabla_{\mathbf{w}, b, \Xi} L(\mathbf{w}, b, \Xi ; \Lambda, \mathrm{M})=0$

$$
\Lambda \geq \mathbf{0}, \mathrm{M} \geq \mathbf{0}
$$

## Duality

$$
\lambda_{i} \geq 0, \mu_{i} \geq 0
$$

$$
L(\mathbf{w}, b, \Xi ; \Lambda, \mathbf{M})=\frac{1}{2}\|\mathbf{w}\|^{2}+C \sum_{i} \xi_{i}-\sum_{i} \lambda_{i}\left[y_{i}\left(\mathbf{w}^{T} \mathbf{x}_{i}+b\right)-1+\xi_{i}\right]-\sum_{i} \mu_{i} \xi_{i}
$$

$$
\nabla_{\mathbf{w}} L(\mathbf{w}, b, \Xi ; \Lambda, \mathbf{M})=\mathbf{w}-\sum_{i} \lambda_{i} y_{i} \mathbf{x}_{i}=\mathbf{0} \quad \mathbf{w}^{*}=\sum_{i} \lambda_{i} y_{i} \mathbf{x}_{i}
$$

$$
\nabla_{b} L(\mathbf{w}, b, \Xi ; \Lambda, \mathrm{M})=\sum_{i} \lambda_{i} y_{i}=0 \square \sum_{i} \lambda_{i} y_{i}=0
$$

$$
\nabla_{\xi_{i}} L(\mathbf{w}, b, \Xi ; \Lambda, \mathbf{M})=C-\lambda_{i}-\mu_{i}=0 \square \mu_{i}=C-\lambda_{i}
$$

$$
0 \leq \lambda_{i} \leq C
$$

$$
F(\Lambda, \mathrm{M})=L\left(\mathbf{w}^{*}, b^{*}, \Xi^{*} ; \Lambda, \mathrm{M}\right)=\sum_{i} \lambda_{i}-\frac{1}{2} \sum_{i} \sum_{j} \lambda_{i} \lambda_{j} y_{i} y_{j}<\mathbf{x}_{i}, \mathbf{x}_{j}>
$$

## Maximize this

## Duality

$$
\lambda_{i} \geq 0, \mu_{i} \geq 0
$$

$$
L(\mathbf{w}, b, \Xi ; \Lambda, \mathbf{M})=\frac{1}{2}\|\mathbf{w}\|^{2}+C \sum_{i} \xi_{i}-\sum_{i} \lambda_{i}\left[y_{i}\left(\mathbf{w}^{T} \mathbf{x}_{i}+b\right)-1+\xi_{i}\right]-\sum_{i} \mu_{i} \xi_{i}
$$

$$
\nabla_{\mathbf{w}} L(\mathbf{w}, b, \Xi ; \Lambda, \mathbf{M})=\mathbf{w}-\sum_{i} \lambda_{i} y_{i} \mathbf{x}_{i}=\mathbf{0} \square \mathbf{w}^{*}=\sum_{i} \lambda_{i} y_{i} \mathbf{x}_{i}
$$

$$
\nabla_{b} L(\mathbf{w}, b, \Xi ; \Lambda, \mathbf{M})=\sum_{i} \lambda_{i} y_{i}=0 \square \sum_{i} \lambda_{i} y_{i}=0
$$

$$
\Lambda^{T} \mathbf{y}=0
$$

$$
\nabla_{\xi_{i}} L(\mathbf{w}, b, \Xi ; \Lambda, \mathbf{M})=C-\lambda_{i}-\mu_{i}=0 \square \mu_{i}=C-\lambda_{i}
$$

$$
0 \leq \Lambda \leq C \quad 0 \leq \lambda_{i} \leq C
$$

$$
F(\Lambda, \mathrm{M})=L\left(\mathbf{w}^{*}, b^{*}, \Xi^{*} ; \Lambda, \mathrm{M}\right)=\sum_{i} \lambda_{i}-\frac{1}{2} \sum_{i} \sum_{j} \lambda_{i} \lambda_{j} y_{i} y_{j}<\mathbf{x}_{i}, \mathbf{x}_{j}>
$$

$$
F(\Lambda)=\Lambda \cdot \mathbf{1}-\frac{1}{2} \Lambda^{T} D \Lambda
$$

## Duality

The Primal
Subject to $\quad y_{i}\left(\mathbf{w}^{T} \mathbf{x}_{i}+b\right)-1+\xi_{i} \geq 0 \quad \forall i$

$$
\xi_{i} \geq 0 \quad \forall i
$$

Maximize $\quad F(\Lambda)=\Lambda \cdot \mathbf{1}-\frac{1}{2} \Lambda^{T} D \Lambda$
Subject to

$$
\Lambda^{T} \mathbf{y}=0
$$

$$
\mathbf{0} \leq \Lambda \leq C \mathbf{1}
$$

## The Karush-Kuhn-Tucker Conditions

$$
\begin{aligned}
& L(\mathbf{w}, b, \Xi ; \Lambda, \mathrm{M})=\frac{1}{2}\|\mathbf{w}\|^{2}+C \sum_{i} \xi_{i}-\sum_{i} \lambda_{i}\left[y_{i}\left(\mathbf{w}^{T} \mathbf{x}_{i}+b\right)-1+\xi_{i}\right]-\sum_{i} \mu_{i} \xi_{i} \\
& \nabla_{\mathbf{w}} L(\mathbf{w}, b, \Xi ; \Lambda, \mathrm{M})=\mathbf{w}-\sum_{i} \lambda_{i} y_{i} \mathbf{x}_{i}=\mathbf{0} \\
& \nabla_{b} L(\mathbf{w}, b, \Xi ; \Lambda, \mathrm{M})=\sum_{i} \lambda_{i} y_{i}=0 \\
& \nabla_{\xi_{i}} L(\mathbf{w}, b, \Xi ; \Lambda, \mathrm{M})=C-\lambda_{i}-\mu_{i}=0 \\
& y_{i}\left(\mathbf{w}^{T} \mathbf{x}_{i}+b\right)-1+\xi_{i} \geq 0 \\
& \xi_{i} \geq 0 \\
& \mu_{i} \geq 0 \\
& \lambda_{i} \geq 0 \\
& \lambda_{i}\left[y_{i}\left(\mathbf{w}^{T} \mathbf{x}_{i}+b\right)-1+\xi_{i}\right]=0 \\
& \mu_{i} \xi_{i}=0
\end{aligned}
$$

## The Solution

## Quadratic Programming

Find $\Lambda^{*}$ by $\ldots$
$\longrightarrow \mathbf{w}^{*}=\sum_{i=1}^{l} \lambda_{i}^{*} y_{i} \mathbf{x}_{i}$

$$
\begin{aligned}
b^{*} & =? \\
\Xi & =?
\end{aligned}
$$

The Dual
Maximize $\quad F(\Lambda)=\Lambda \cdot \mathbf{1}-\frac{1}{2} \Lambda^{T} D \Lambda$
Subject to $\quad \Lambda^{T} \mathbf{y}=0$

$$
\mathbf{0} \leq \Lambda \leq C \mathbf{1}
$$

## The Solution

Find $\Lambda^{*}$ by $\ldots$

## Call it a support

$$
\mathbf{w}^{*}=\sum_{i=1}^{l} \lambda_{i}^{*} y_{i} \mathbf{x}_{i}
$$

$$
\Longrightarrow b^{*}=y_{i}-\mathbf{w}^{*^{T}} \mathbf{x}_{i}^{\circ}, \quad 0<\lambda_{i}<C
$$

The Lagrangian:

$$
\begin{aligned}
& L(\mathbf{w}, b, \Xi ; \Lambda, \mathrm{M}) \\
& =\frac{1}{2}\|\mathbf{w}\|^{2}+C \sum_{i} \xi_{i}-\sum_{i} \lambda_{i}\left[y_{i}\left(\mathbf{w}^{T} \mathbf{x}_{i}+b\right)-1+\xi_{i}\right]-\sum_{i} \mu_{i} \xi_{i}
\end{aligned}
$$

## The Solution

Find $\Lambda^{*}$ by $\ldots$

$$
\mathbf{w}^{*}=\sum_{i=1}^{l} \lambda_{i}^{*} y_{i} \mathbf{x}_{i}
$$

$$
b^{*}=y_{i}-\mathbf{w}^{*^{T}} \mathbf{x}_{i}, \quad 0<\lambda_{i}<C
$$

$$
\xi_{i}=\max \left[0,1-y_{i}\left(\mathbf{w}^{*} \mathbf{x}_{i}+b^{*}\right)\right]
$$

A false classification pattern if $\xi_{i}>1$.

## Classification

$$
\mathbf{w}^{*}=\sum_{i=1}^{l} \lambda_{i}^{*} y_{i} \mathbf{x}_{i}
$$

$$
\begin{aligned}
f(\mathbf{x}) & =\operatorname{sgn}\left(\mathbf{w}^{* T} \mathbf{x}+b^{*}\right) \\
& =\operatorname{sgn}\left(\sum_{i=1}^{l} \lambda_{i}^{*} y_{i}<\mathbf{x}_{i}, \mathbf{x}>+b^{*}\right) \\
& =\operatorname{sgn}\left(\sum_{\lambda_{i}^{*} \neq 0} \lambda_{i}^{*} y_{i}<\mathbf{x}_{i}, \mathbf{x}>+b^{*}\right)
\end{aligned}
$$

## Classification Using Supporters



## Lagrange Multiplier

■ "Lagrange Multiplier Method" is a powerful tool for constraint optimization.

- Contributed by Riemann.


## Milkmaid Problem



## Milkmaid Problem

## Milkmaid Problem

Goal:
Minimize

$$
f(x, y)
$$

Subject to

$$
g(x, y)=0
$$

$$
f(x, y)=\sum_{i=1}^{2} \sqrt{\left(x-x_{i}\right)^{2}+\left(y-y_{i}\right)^{2}}
$$

## Observation

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Goal:
Minimize

$$
f(x, y)
$$

Subject to

$$
f(x, y)=\sum_{i=1}^{2} \sqrt{\left(x-x_{i}\right)^{2}+\left(y-y_{i}\right)^{2}}
$$

At the extreme point, say, $\left(x^{*}, y^{*}\right)$

$$
g(x, y)=0
$$

## Optimization with Equality Constraints

Goal: Min/Max $\quad f(\mathbf{x})$
Subject to $\quad g(\mathbf{x})=0$
Lemma:
At an extreme point, say, $\mathrm{x}^{*}$, we have

$$
\nabla f\left(\mathbf{x}^{*}\right)=\lambda \nabla g\left(\mathbf{x}^{*}\right) \text { if } \nabla g\left(\mathbf{x}^{*}\right) \neq 0
$$

## Proof

$$
\nabla f\left(\mathbf{x}^{*}\right)=\lambda \nabla g\left(\mathbf{x}^{*}\right) \text { if } \nabla g\left(\mathbf{x}^{*}\right) \neq 0
$$

x* be an extreme point.
Let $\quad \mathbf{r}(t)$ be any differentiable path on surface $g(x)=0$ such that $\mathbf{r}\left(t_{0}\right)=x^{*}$.
$\square \mathbf{r}^{\prime}\left(t_{0}\right) \begin{aligned} & \text { is a vector tangent to the } \\ & \text { surface } g(\mathbf{x})=0 \text { at } \mathbf{x}^{*}\end{aligned}$
$\longrightarrow f\left(\mathbf{x}^{*}\right)=\left.f(\mathbf{r}(t))\right|_{t=t_{0}}$

$$
\frac{d}{d t} f(\mathbf{r}(t))=\nabla f(\mathbf{r}(t)) \cdot \mathbf{r}^{\prime}(t)
$$

Since $\mathbf{x}^{*}$ be an extreme point,

$$
0=\nabla f\left(\mathbf{r}\left(t_{0}\right)\right) \cdot \mathbf{r}^{\prime}\left(t_{0}\right)=\nabla f\left(\mathbf{x}^{*}\right) \cdot \mathbf{r}^{\prime}\left(t_{0}\right)
$$

## Proof

$$
\nabla f\left(\mathbf{x}^{*}\right)=\lambda \nabla g\left(\mathbf{x}^{*}\right) \text { if } \nabla g\left(\mathbf{x}^{*}\right) \neq 0
$$

$$
\nabla f\left(\mathbf{x}^{*}\right) \perp \mathbf{r}^{\prime}\left(t_{0}\right)
$$

This is true for any $r$ pass through $x^{*}$ on surface $g(\mathbf{x})=0$.

It implies that

$$
\nabla f\left(\mathbf{x}^{*}\right) \perp \Gamma,
$$


where $\Gamma$ is the tangential plane of surface $g(\mathbf{x})=0$ at $\mathbf{x}^{*}$.

$$
0=\nabla f\left(\mathbf{r}\left(t_{0}\right)\right) \cdot \mathbf{r}^{\prime}\left(t_{0}\right)=\nabla f\left(\mathbf{x}^{*}\right) \cdot \mathbf{r}^{\prime}\left(t_{0}\right)
$$

$$
g(\mathbf{x})=0
$$

## Optimization with Equality Constraints

Goal: Min/Max $\quad f(\mathbf{x})$
Subject to $\quad g(\mathbf{x})=0$
Lemma:
At an extreme point, say, $x^{*}$, we have

$$
\nabla f\left(\mathbf{x}^{*}\right)=\lambda \nabla g\left(\mathbf{x}^{*}\right) \text { if } \nabla g\left(\mathbf{x}^{*}\right) \neq 0
$$

## The Method of Lagrange

## x: dimension $n$.

## Goal: Min/Max <br> $f(\mathbf{x})$ <br> 

Find the extreme points by solving the following equations.

$$
\left.\begin{array}{rl}
\nabla f(\mathbf{x}) & =\lambda \nabla g(\mathbf{x}) \\
g(\mathbf{x}) & =0
\end{array}\right\} \begin{aligned}
& n+1 \text { equations } \\
& \text { with } n+1 \text { variables }
\end{aligned}
$$

## Lagrangian

## Goal: Min/Max <br> Subject to $f(\mathbf{x})$ $g(\mathbf{x})=0)^{\text {constrant }}$ Opimization

Define $L(\mathbf{x} ; \lambda)=f(\mathbf{x})+\lambda g(\mathbf{x})$ - Lagrangian

Solve

$$
\left.\begin{array}{l}
\nabla_{\mathbf{x}} L(\mathbf{x} ; \lambda)=\mathbf{0} \\
\nabla_{\lambda} L(\mathbf{x} ; \lambda)=\mathbf{0}
\end{array}\right\} \begin{gathered}
\text { Unconstraint } \\
\text { Optimization }
\end{gathered}
$$

## Optimization with <br> Multiple Equality Constraints

$$
\Lambda=\left(\lambda_{1}, \mathrm{~K}, \lambda_{m}\right)^{T}
$$

Min/Max $\quad f(\mathbf{x})$
Subject to $\quad g_{i}(\mathbf{x})=0, \quad i=1, \mathrm{~K}, m$
Define $L(\mathbf{x} ; \Lambda)=f(\mathbf{x})+\sum_{i=1}^{m} \lambda_{i} g_{i}(\mathbf{x})$ - Lagrangian
Solve $\nabla_{\mathbf{x}, \Lambda} L(\mathbf{x} ; \Lambda)=\mathbf{0}$

## Optimization with Inequality Constraints

## Minimize $\quad f(\mathbf{x})$

Subject to

$$
\begin{array}{ll}
g_{i}(\mathbf{x})=0, & i=1, \mathrm{~K}, m \\
h_{j}(\mathbf{x}) \leq 0, & j=1, \mathrm{~K}, n
\end{array}
$$

You can always reformulate your problems into the about form.

## Lagrange Multipliers

$$
\begin{aligned}
\Lambda & =\left(\lambda_{1}, \mathrm{~K}, \lambda_{m}\right)^{T} \\
\mathrm{M} & =\left(\mu_{1}, \mathrm{~K}, \mu_{n}\right)^{T} \quad \mu_{i} \geq 0
\end{aligned}
$$

Minimize $\quad f(\mathbf{x})$
Subject to

$$
\begin{array}{ll}
g_{i}(\mathbf{x})=0, & i=1, \mathrm{~K}, m \\
h_{j}(\mathbf{x}) \leq 0, & j=1, \mathrm{~K}, n
\end{array}
$$

Lagrangian:

$$
L(\mathbf{x} ; \Lambda, \mathrm{M})=f(\mathbf{x})+\sum_{i=1}^{m} \lambda_{i} g_{i}(\mathbf{x})+\sum_{j=1}^{n} \mu_{j} h_{j}(\mathbf{x})
$$

## Lagrange Multipliers

$$
\begin{aligned}
\Lambda & =\left(\lambda_{1}, \mathrm{~K}, \lambda_{m}\right)^{T} \\
\mathrm{M} & =\left(\mu_{1}, \mathrm{~K}, \mu_{n}\right)^{T} \quad \mu_{i} \geq 0
\end{aligned}
$$

Minimize $\quad f(\mathbf{x})$
Subject to
$g_{i}(\mathbf{x})=0, \underbrace{\text { feasible solutions }}_{l \rightarrow 1, \mathbb{R}_{l}, m}$

0 for feasible solutions

Lagrangian:

$$
L(\mathbf{x} ; \Lambda, \mathrm{M})=f(\mathbf{x})+\sum_{i=1}^{\circ} \lambda_{i} g_{i}(\mathbf{x})+\sum_{j=1}^{n} \mu_{j} h_{j}(\mathbf{x})
$$

## Duality

$$
L(\mathbf{x} ; \Lambda, \mathrm{M})=f(\mathbf{x})+\sum_{i=1}^{m} \lambda_{i} g_{i}(\mathbf{x})+\sum_{j=1}^{n} \mu_{j} h_{j}(\mathbf{x})
$$

Let $x^{*}$ be a local extreme.

$$
\Longrightarrow \mathbf{0}=\left.\nabla_{\mathbf{x}} L(\mathbf{x} ; \Lambda, \mathrm{M})\right|_{\mathbf{x}=\mathbf{x}^{*}}
$$

Define $\quad D(\Lambda, \mathrm{M})=L\left(\mathbf{x}^{*} ; \Lambda, \mathrm{M}\right)$

$$
D(\Lambda, \mathrm{M})=f\left(\mathbf{x}^{*}\right)+\sum_{i=1}^{m} \lambda_{i} g_{i}\left(\mathbf{x}^{*}\right)+\sum_{j=1}^{n} \mu_{j} h_{j}\left(\mathbf{x}^{*}\right) \leq f\left(\mathbf{x}^{*}\right)
$$

Maximize it w.r.t. $\Lambda, M$

## Duality

$$
L(\mathbf{x} ; \Lambda, \mathrm{M})=\sqrt{\text { To minimize the Lagrangian w.r.t } \mathbf{x},} \begin{aligned}
& \text { while to maximize it w.r.t. } \Lambda \text { and } \mathrm{M} .
\end{aligned}
$$

Let $x^{*}$ be a local extreme.
$\Longrightarrow \mathbf{0}=\left.\nabla_{\mathbf{x}} L(\mathbf{x} ; \Lambda, \mathrm{M})\right|_{\mathbf{x}=\mathbf{x}^{*}}$ What are we doing?
Define $D(\Lambda, \mathrm{M})=L\left(\mathbf{x}^{*} ; \Lambda, \mathrm{M}\right)$

$$
D(\Lambda, \mathrm{M})=f\left(\mathbf{x}^{*}\right)+\sum_{i=1}^{m} \lambda_{i} g_{i}\left(\mathbf{x}^{*}\right)+\sum_{j=1}^{n} \mu_{j} h_{j}\left(\mathbf{x}^{*}\right) \leq f\left(\mathbf{x}^{*}\right)
$$

Maximize it w.r.t. $\Lambda, \mathrm{M}$

## Saddle Point Determination

$$
L(\mathbf{x} ; \Lambda, \mathrm{M})=f(\mathbf{x})+\sum_{i=1}^{m} \lambda_{i} g_{i}(\mathbf{x})+\sum_{j=1}^{n} \mu_{j} h_{j}(\mathbf{x})
$$



## Saddle Point Determination

$$
L(\mathbf{x} ; \Lambda, \mathrm{M})=f(\mathbf{x})+\sum_{i=1}^{m} \lambda_{i} g_{i}(\mathbf{x})+\sum_{j=1}^{n} \mu_{j} h_{j}(\mathbf{x})
$$

Minimize $\quad f(\mathbf{x})$
The primal
Subject to $\quad g_{i}(\mathbf{x})=0, \quad i=1, K, m$

$$
h_{j}(\mathbf{x}) \leq 0, \quad j=1, \mathrm{~K}, n
$$

Maximize $L\left(\mathbf{x}^{*} ; \Lambda, \mathrm{M}\right)$
The dual
Subject to $\quad \nabla_{\mathbf{x}, \Lambda} L(\mathbf{x} ; \Lambda, M)=\mathbf{0}$

$$
\mathrm{M} \geq \mathbf{0}
$$

## The Karush-Kuhn-Tucker Conditions

$$
\begin{gathered}
L(\mathbf{x} ; \Lambda, \mathrm{M})=f(\mathbf{x})+\sum_{i=1}^{m} \lambda_{i} g_{i}(\mathbf{x})+\sum_{j=1}^{n} \mu_{j} h_{j}(\mathbf{x}) \\
\nabla_{\mathbf{x}} L(\mathbf{x} ; \Lambda, \mathrm{M})=\nabla_{\mathbf{x}} f(\mathbf{x})+\sum_{i=1}^{m} \lambda_{i} \nabla_{\mathbf{x}} g_{i}(\mathbf{x})+\sum_{j=1}^{n} \mu_{j} \nabla_{\mathbf{x}} h_{j}(\mathbf{x})=\mathbf{0} \\
g_{i}(\mathbf{x})=0, \quad i=1, \mathrm{~K}, m \\
\mu_{j} \geq 0, \quad j=1, \mathrm{~K}, n \\
h_{j}(\mathbf{x}) \leq 0, \quad j=1, \mathrm{~K}, n \\
\mu_{j} h_{j}(\mathbf{x})=0, \quad j=1, \mathrm{~K}, n
\end{gathered}
$$

## Non-linear SVMs

$\square$ Datasets that are linearly separable with noise work out great:

$\square$ But what are we going to do if the dataset is just too hard?

$\square$ How about... mapping data to a higher-dimensional space:


## Non-linear SVMs: Feature Space

$\square$ General idea: the original input space can be mapped to some higher-dimensional feature space where the training set is separable:


## Nonlinear SVMs: The Kernel Trick

$\square$ With this mapping, our discriminant function is now:

$$
g(x)=w^{T} \phi(x)+b=\sum_{x_{i} \in S V} \lambda_{i} y_{i} \phi\left(x_{i}\right) \phi(x)+b
$$

$\square$ No need to know this mapping explicitly, because we only use the dot product of feature vectors in both the training and test.
$\square$ A kernel function is defined as a function that corresponds to a dot product of two feature vectors in some expanded feature space:

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

## Nonlinear SVMs: The Kernel Trick

## $\square$ An example:

2-dimensional vectors $\mathrm{x}=\left[\begin{array}{ll}x_{1} & x_{2}\end{array}\right]$;
let $K\left(\mathrm{x}_{\mathrm{i}}, \mathrm{x}_{\mathrm{j}}\right)=\left(1+\mathrm{x}_{\mathrm{i}}{ }^{\mathrm{T}} \mathrm{x}_{\mathrm{j}}\right)^{2}$,
Need to show that $K\left(\mathrm{x}_{\mathrm{i}}, \mathrm{x}_{\mathrm{j}}\right)=\varphi\left(\mathrm{x}_{\mathrm{i}}\right)^{\mathrm{T}} \varphi\left(\mathrm{x}_{\mathrm{j}}\right)$ :

$$
\begin{aligned}
& K\left(\mathrm{x}_{\mathrm{i}} \mathrm{x} \mathrm{x}_{\mathrm{j}}\right)=\left(1+\mathrm{x}_{\mathrm{i}} \mathrm{~T}_{\mathrm{i}}\right)^{2}, \\
& =1+x_{i 1}{ }^{2} x_{j 1}{ }^{2}+2 x_{i 1} x_{j 1} x_{i 2} x_{j 2}+x_{i 2}{ }^{2} x_{j 2}{ }^{2}+2 x_{i 1} x_{j 1}+2 x_{i 2} x_{j 2} \\
& =\left[\begin{array}{lllll}
1 & x_{i 1}{ }^{2} & \sqrt{ } 2 x_{i 1} x_{i 2} & x_{i 2}{ }^{2} & \sqrt{ } 2 x_{i 1} \\
\sqrt{ } 2 x_{i 2}
\end{array}\right]\left[\begin{array}{llll}
1 & x_{j 1}{ }^{2} \sqrt{ } 2 x_{j 1} x_{j 2} & x_{j 2}{ }^{2} \sqrt{ } 2 x_{j 1} & \sqrt{ } 2 x_{j 2}
\end{array}\right]^{\mathrm{T}} \\
& =\varphi\left(\mathrm{x}_{\mathrm{i}}\right)^{\mathrm{T}} \varphi\left(\mathrm{x}_{\mathrm{j}}\right), \quad \text { where } \varphi(\mathrm{x})=\left[\begin{array}{lllll}
1 & x_{1}{ }^{2} & \sqrt{ } 2 x_{1} x_{2} & x_{2}^{2} & \sqrt{ } 2 x_{1} \\
\sqrt{ } 2 x_{2}
\end{array}\right]^{\mathrm{T}}
\end{aligned}
$$

## Nonlinear SVMs: The Kernel Trick мпма

$\square$ Examples of commonly-used kernel functions:

- Linear kernel: $K\left(\mathbf{x}_{i}, \mathbf{x}_{j}\right)=\mathbf{x}_{i}^{T} \mathbf{x}_{j}$
- Polynomial kernel: $K\left(\mathbf{x}_{i}, \mathbf{x}_{j}\right)=\left(1+\mathbf{x}_{i}^{T} \mathbf{x}_{j}\right)^{p}$
- Gaussian (Radial-Basis Function (RBF) ) kernel:

$$
K\left(\mathbf{x}_{i}, \mathbf{x}_{j}\right)=\exp \left(-\frac{\left\|\mathbf{x}_{i}-\mathbf{x}_{j}\right\|^{2}}{2 \sigma^{2}}\right)
$$

- Sigmoid:

$$
K\left(\mathbf{x}_{i}, \mathbf{x}_{j}\right)=\tanh \left(\beta_{0} \mathbf{x}_{i}^{T} \mathbf{x}_{j}+\beta_{1}\right)
$$

$\square$ In general, functions that satisfy Mercer's condition can be kernel functions.

## Nonlinear SVM: Optimization

$\square$ Formulation: (Lagrangian Dual Problem)

$$
\begin{aligned}
& \max \sum_{i} \lambda_{i}-\frac{1}{2} \sum_{i} \sum_{j} \lambda_{i} \lambda_{j} y_{i} y_{j} K\left(x_{i}, x_{j}\right) \\
& \text { such that } \\
& 0 \leq \lambda_{i} \leq C \\
& \sum_{i} \lambda_{i} y_{i}=0
\end{aligned}
$$

$\square$ The solution of the discriminant function is

$$
g(x)=w^{T} \phi(x)+b=\sum_{x_{i} \in S V} \lambda_{i} y_{i} K\left(x, x_{i}\right)+b
$$

$\square \quad$ The optimization technique is the same.

## Support Vector Machine: Algorithm $M_{V A}$

- 1. Choose a kernel function
- 2. Choose a value for $C$
$\square$ 3. Solve the quadratic programming problem (many software packages available)
- 4. Construct the discriminant function from the support vectors


## Other issues

- Choice of kernel
- Gaussian or polynomial kernel is default
- if ineffective, more elaborate kernels are needed
- domain experts can give assistance in formulating appropriate similarity measures
- Choice of kernel parameters
- e.g. $\sigma$ in Gaussian kernel
- $\sigma$ is the distance between closest points with different classifications
- In the absence of reliable criteria, applications rely on the use of a validation set or cross-validation to set such parameters.
- Optimization criterion - Hard margin v.s. Soft margin
- a lengthy series of experiments in which various parameters are tested


## Comparison with Neural Networks

- Neural Networks
- Hidden Layers map to lower dimensional spaces
- Search space has multiple local minima
- Training is expensive
- Classification extremely efficient
- Requires number of hidden units and layers
- Very good accuracy in typical domains
$\square$ SVMs
- Kernel maps to a veryhigh dimensional space
- Search space has a unique minimum
- Training is extremely efficient
- Classification extremely efficient
- Kernel and cost the two parameters to select
- Very good accuracy in typical domains
- Extremely robust

■ UCI datasets: http://archive.ics.uci.edu/ml/datasets.html

- Reuters-21578 Text Categorization Collection
- Wine
- Credit Approval
- Requirements
- Use different kernels(>=3)
- Choose best values for parameters
- You can also use dimension reduction method, e.g., PCA

■ 针对UCI数据集（
http：／／archive．ics．uci．edu／ml／datasets．html）中的 Musk（version2），Wine，采用三种SVM来对其进行分类，计算准确率。其中每种SVM要求用不同的核函数。另外，采用一种集成学习方法，将不同模型集成，集成的模型可以是不同核函数的 SVM，也可以加上神经网络，KNN，线性模型，多项式模型等。比较集成模型与SVM模型及其他模型的结果。
－要求：6月17日 24 时之前提交代码和报告。

## MIMA Groun

## [ Thank You! ]

Any Question?

