## MIMA Group

#### M L D M Chapter 9 Support Vector Machines

## **Learning Machines**

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• A machine to learn the mapping

$$\mathbf{x}_i \mathbf{a} \quad y_i$$

Defined as

**X** a 
$$f(\mathbf{X}, \mathbf{0})$$
  
Learning by adjusting  
this parameter?

## **Generalization vs. Learning**

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- 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**

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Expected Risk (test error)

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

Empirical Risk (training error)

$$R_{emp}(\boldsymbol{\alpha}) = \frac{1}{2l} \sum_{i=1}^{l} |y_i - f(\mathbf{x}_i, \boldsymbol{\alpha})|$$
$$R(\boldsymbol{\alpha}) \approx R_{emp}(\boldsymbol{\alpha})?$$

## **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.



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# Total Risk=Empirical Risk+Risk due to theTotal Risk=Empirical Risk+structure ofthe learning machine

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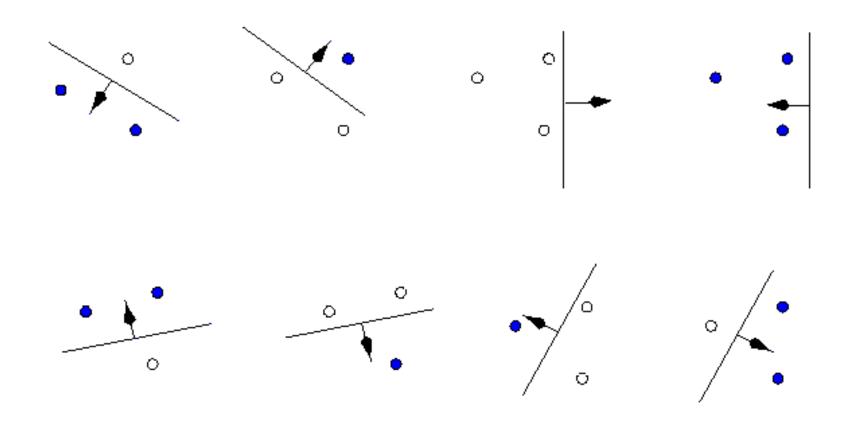
## **The VC Dimension**

- Consider a set of function  $f(\mathbf{x}, \alpha) \in \{-1, 1\}$ .
- A given set of *l* points can be labeled in 2<sup>l</sup> ways.
- If a member of the set {f (α)} 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 (α)} is the maximum number of training points that can be shattered by {f (α)}.

VC: Vapnik Chervonenkis

#### The VC Dimension for Oriented Lines in R<sup>2</sup>

VC dimension = 3



## More on VC Dimension

- In general, the VC dimension of a set of oriented hyperplanes in R<sup>n</sup> 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 
$$R(\boldsymbol{\alpha}) = \int \frac{1}{2} |y - f(\mathbf{x}, \boldsymbol{\alpha})| dP(\mathbf{x}, y)$$
  
Empirical Risk  $R_{emp}(\boldsymbol{\alpha}) = \frac{1}{2l} \sum_{i=1}^{l} |y_i - f(\mathbf{x}_i, \boldsymbol{\alpha})|$ 

$$P\left(R(\alpha) \leq R_{emp}(\alpha) + \sqrt{\frac{h(\log(2l/h) + 1) - \log(\eta/4)}{l}}\right) = 1 - \eta$$
  
VC Confidence  
h is the VC dimension; I is the number of samples

Xin-Shun Xu @ SDU

## **Bound on Expected Risk**

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

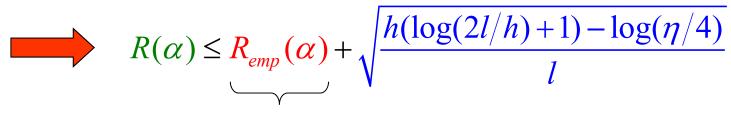
$$R(\alpha) \le R_{emp}(\alpha) + \sqrt{\frac{h(\log(2l/h) + 1) - \log(\eta/4)}{l}}$$

$$P\left(R(\alpha) \le R_{emp}(\alpha) + \sqrt{\frac{h(\log(2l/h) + 1) - \log(\eta/4)}{l}}\right) = 1 - \eta$$
  
VC Confidence

## **Bound on Expected Risk**

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



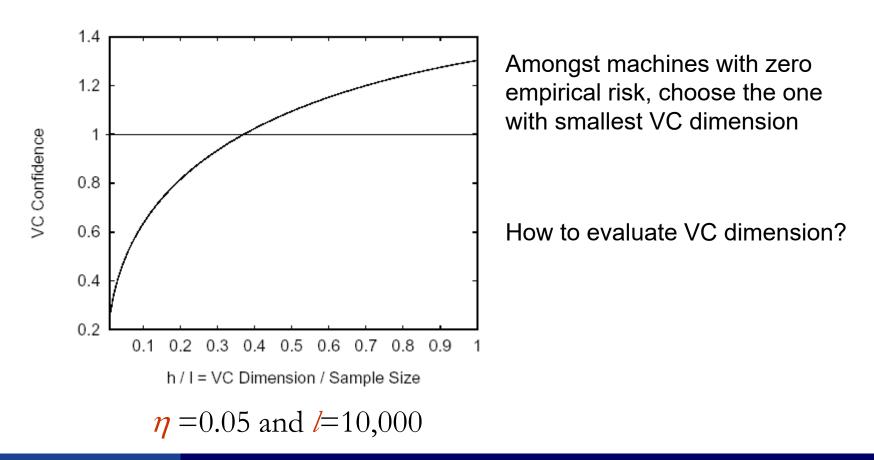
Traditional approaches minimize empirical risk only



## **VC Confidence**

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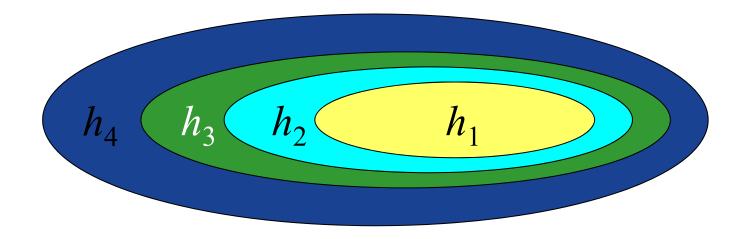
$$R(\alpha) \le R_{emp}(\alpha) + \sqrt{\frac{h(\log(2l/h) + 1) - \log(\eta/4)}{l}}$$



## **Structure Risk Minimization**

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#### $h_1 < h_2 < h_3 < h_4$



Nested subset of functions with different VC dimensions.

## **Structure Risk Minimization**

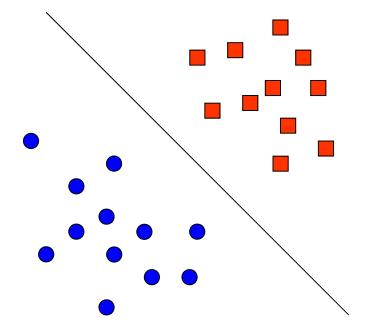
underfitting bestmodel overfitting error bound on test error \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* capacity term training error h structure H2 H3 H.

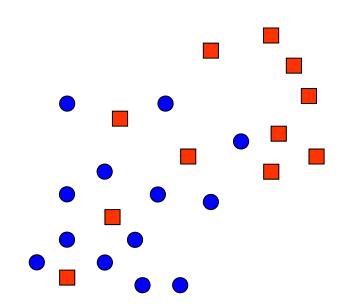
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## Linear SVM

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#### The linear separability





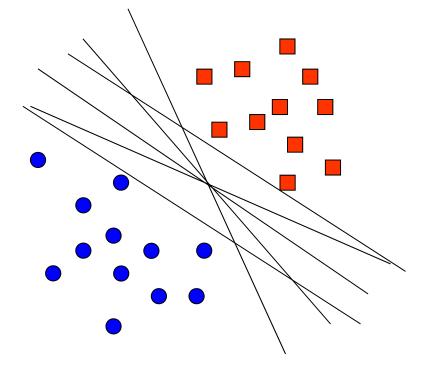
Linearly separable

Not linearly separable

## Linear SVM

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#### The linear separability



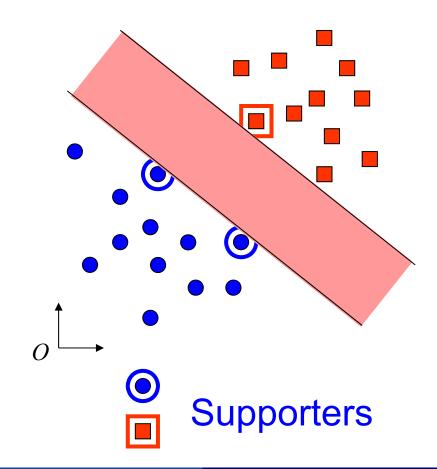
How would you classify these points using a linear discriminant function in order to minimize the error rate?

Linearly separable

## **Maximum Margin Classifier**

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#### $y_i(\mathbf{w}\mathbf{x}_i+b)-1 \ge 0 \quad \forall i$



*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

□Why is it the best?

Intuitively robust to outliners and thus strong generalization ability

#### Relation Between VC Dimension and Margin

- 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:

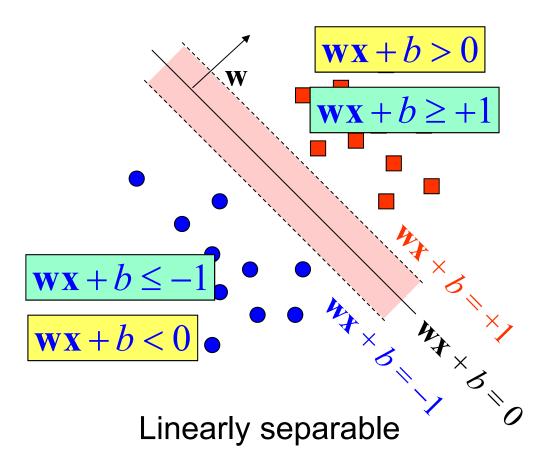
$$h \leq \min\left(\left(\frac{R}{\gamma}\right)^2, d\right) + 1$$

d is the dimension of x,

What does this mean?



The linear separability



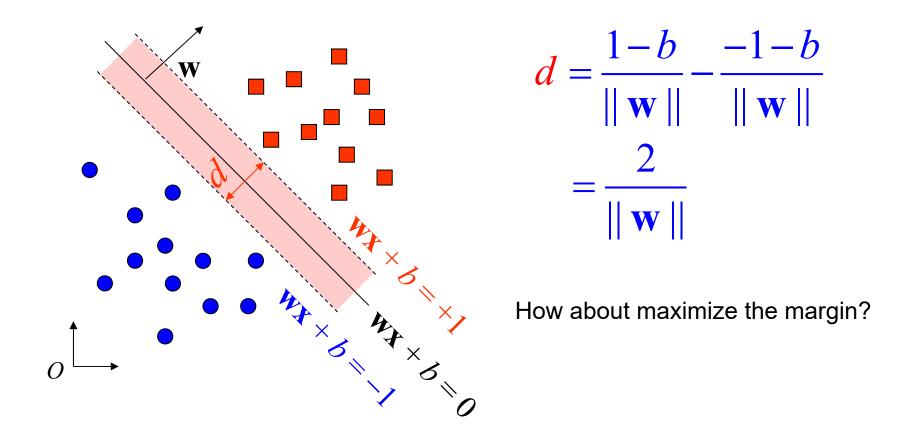
Linearly Separable

- $\implies \exists \mathbf{w}, b \text{ such that}$ 
  - $\mathbf{w}\mathbf{x}_i + b \ge +1 \text{ for } y_i = +1$
  - $\mathbf{w}\mathbf{x}_i + b \le -1 \text{ for } y_i = -1$

 $= y_i(\mathbf{w}\mathbf{x}_i + b) - 1 \ge 0 \quad \forall i$ 

## **Margin Width**

#### $y_i(\mathbf{w}\mathbf{x}_i+b)-1\geq 0 \quad \forall i$



## **Building SVM**



$$\begin{aligned} \text{Minimize} \quad \frac{1}{2} \| \mathbf{w} \|^2 \\ \text{Subject to} \quad y_i (\mathbf{w}^T \mathbf{x}_i + b) - 1 \ge 0 \quad \forall i \end{aligned}$$

This requires the knowledge about Lagrange Multiplier.

## **The Method of Lagrange**

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Minimize 
$$\frac{1}{2} \|\mathbf{w}\|^2$$
  
Subject to  $y_i (\mathbf{w}^T \mathbf{x}_i + b) - 1 \ge 0 \quad \forall i$ 

The Lagrangian:

$$L(\mathbf{w},b;\Lambda) = \frac{1}{2} ||\mathbf{w}||^2 - \sum_{i=1}^l \lambda_i \left[ y_i(\mathbf{w}^T \mathbf{x}_i + b) - 1 \right] \qquad \lambda_i \ge 0$$

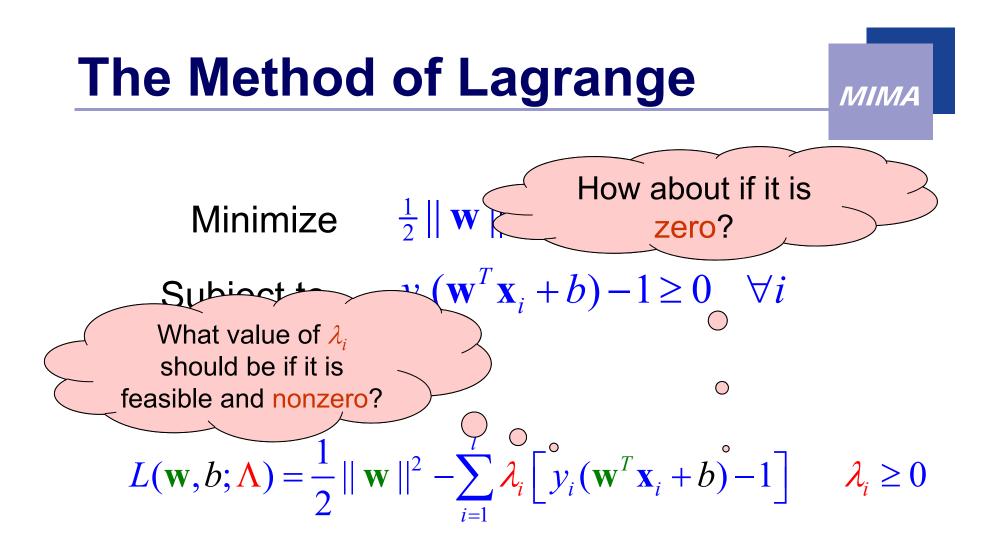
*Minimize* it w.r.t w & b, while *maximize* it w.r.t.  $\Lambda$ .

## The Method of Lagrange

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#### 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.



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

# The Method of Lagrange $L(\mathbf{w},b;\Lambda) = \frac{1}{2} ||\mathbf{w}||^2 - \sum_{i=1}^{l} \lambda_i y_i (\mathbf{w}^T \mathbf{x}_i + b) + \sum_{i=1}^{l} \lambda_i$ Minimize $\frac{1}{2} ||\mathbf{w}||^2$ Subject to $y_i (\mathbf{w}^T \mathbf{x}_i + b) - 1 \ge 0 \quad \forall i$

The Lagrangian:

$$L(\mathbf{w}, b; \mathbf{\Lambda}) = \frac{1}{2} ||\mathbf{w}||^2 - \sum_{i=1}^l \lambda_i \Big[ y_i(\mathbf{w}^T \mathbf{x}_i + b) - 1 \Big] \qquad \lambda_i \ge 0$$
$$= \frac{1}{2} ||\mathbf{w}||^2 - \sum_{i=1}^l \lambda_i y_i(\mathbf{w}^T \mathbf{x}_i + b) + \sum_{i=1}^l \lambda_i$$

#### Duality MIMA $L(\mathbf{w},b;\mathbf{\Lambda}) = \frac{1}{2} ||\mathbf{w}||^2 - \sum_{i=1}^{l} \lambda_i y_i (\mathbf{w}^T \mathbf{x}_i + b) + \sum_{i=1}^{l} \lambda_i$ Minimize $\frac{1}{2} \|\mathbf{w}\|^2$ $y_i(\mathbf{w}^T\mathbf{x}_i+b)-1\geq 0$ $\forall i$ Subject to $L(\mathbf{w}^*, b^*; \Lambda)$ Maximize Subject to $\nabla_{\mathbf{w}\,b} L(\mathbf{w},b;\Lambda) = \mathbf{0}$

 $\lambda_i \geq 0, \quad i=1, K, l$ 

## Duality

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$$L(\mathbf{w},b;\Lambda) = \frac{1}{2} ||\mathbf{w}||^2 - \sum_{i=1}^l \lambda_i y_i (\mathbf{w}^T \mathbf{x}_i + b) + \sum_{i=1}^l \lambda_i$$
$$\nabla_{\mathbf{w}} L(\mathbf{w},b;\Lambda) = \mathbf{w} - \sum_{i=1}^l \lambda_i y_i \mathbf{x}_i = \mathbf{0} \qquad \qquad \mathbf{w}^* = \sum_{i=1}^l \lambda_i y_i \mathbf{x}_i$$
$$\nabla_b L(\mathbf{w},b;\Lambda) = \sum_{i=1}^l \lambda_i y_i = \mathbf{0} \qquad \qquad \qquad \sum_{i=1}^l \lambda_i y_i = \mathbf{0}$$

Maximize  $L(\mathbf{w}^*, b^*; \Lambda)$ Subject to  $\nabla_{\mathbf{w}, b} L(\mathbf{w}, b; \Lambda) = \mathbf{0}$  $\lambda_i \ge 0, \quad i = 1, K, l$ 

# Duality MIMA $L(\mathbf{w},b;\Lambda) = \frac{1}{2} ||\mathbf{w}||^2 - \sum_{i=1}^{i} \lambda_i y_i (\mathbf{w}^T \mathbf{x}_i + b) + \sum_{i=1}^{i} \lambda_i$ $\nabla_{\mathbf{w}} L(\mathbf{w}, b; \Lambda) = \mathbf{w} - \sum_{i=1}^{l} \lambda_{i} y_{i} \mathbf{x}_{i} = \mathbf{0} \quad \mathbf{w}^{*} = \sum_{i=1}^{l} \lambda_{i} y_{i} \mathbf{x}_{i}$ $L(\mathbf{w}^*, b^*; \mathbf{\Lambda}) = \frac{1}{2} \left( \sum_{i=1}^l \lambda_i y_i \mathbf{x}_i \right)^l \sum_{i=1}^l \lambda_i y_i \mathbf{x}_i - \left( \sum_{i=1}^l \lambda_i y_i \mathbf{x}_i \right)^l \sum_{i=1}^l \lambda_i y_i \mathbf{x}_i - b \sum_{i=1}^l \lambda_i y_i + \sum_{i=1}^l \lambda_i y_i \mathbf{x}_i \right)^l$ $=\sum_{i=1}^{l}\lambda_{i}-\frac{1}{2}\left(\sum_{i=1}^{l}\lambda_{i}y_{i}\mathbf{x}_{i}\right)^{T}\sum_{i=1}^{l}\lambda_{i}y_{i}\mathbf{x}_{i}$ $=\sum_{i=1}^{l} \lambda_{i} - \frac{1}{2} \sum_{i=1}^{l} \sum_{j=1}^{l} \lambda_{i} \lambda_{j} y_{i} y_{j} < \mathbf{x}_{i}, \mathbf{x}_{j} >$ Maximize

# Duality MIMA $L(\mathbf{w},b;\Lambda) = \frac{1}{2} ||\mathbf{w}||^2 - \sum_{i=1}^{i} \lambda_i y_i (\mathbf{w}^T \mathbf{x}_i + b) + \sum_{i=1}^{i} \lambda_i$ $\nabla_{\mathbf{w}} L(\mathbf{w}, b; \mathbf{\Lambda}) = \mathbf{w} - \sum_{i=1}^{l} \lambda_{i} y_{i} \mathbf{x}_{i} = \mathbf{0} \quad \mathbf{w}^{*} = \sum_{i=1}^{l} \lambda_{i} y_{i} \mathbf{x}_{i}$ $L(\mathbf{w}^*, b^*; \mathbf{\Lambda}) = \frac{1}{2} \left( \sum_{i=1}^l \lambda_i y_i \mathbf{x}_i \right)^l \sum_{i=1}^l \lambda_i y_i \mathbf{x}_i - \left( \sum_{i=1}^l \lambda_i y_i \mathbf{x}_i \right)^l \sum_{i=1}^l \lambda_i y_i \mathbf{x}_i - b \sum_{i=1}^l \lambda_i y_i + \sum_{i=1}^l \lambda_i y_i \mathbf{x}_i \right)^l$ $=\sum_{i=1}^{l}\lambda_{i}-\frac{1}{2}\left(\sum_{i=1}^{l}\lambda_{i}y_{i}\mathbf{x}_{i}\right)^{T}\sum_{i=1}^{l}\lambda_{i}y_{i}\mathbf{x}_{i} \qquad F(\Lambda)=\Lambda\cdot\mathbf{1}-\frac{1}{2}\Lambda^{T}D\Lambda$ $=\sum_{i=1}^{l} \lambda_{i} - \frac{1}{2} \sum_{i=1}^{l} \sum_{j=1}^{l} \lambda_{i} \lambda_{j} y_{i} y_{j} < \mathbf{x}_{i}, \mathbf{x}_{j} >$ Maximize

## Duality

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Minimize
$$\frac{1}{2} || \mathbf{w} ||^2$$
The PrimalSubject to $y_i (\mathbf{w}^T \mathbf{x}_i + b) - 1 \ge 0 \quad \forall i$ The DualMaximize $F(\Lambda) = \Lambda \cdot 1 - \frac{1}{2} \Lambda^T D \Lambda$ Subject to $\Lambda^T \mathbf{y} = 0$  $\Lambda \ge \mathbf{0}$ 

## **The Solution**

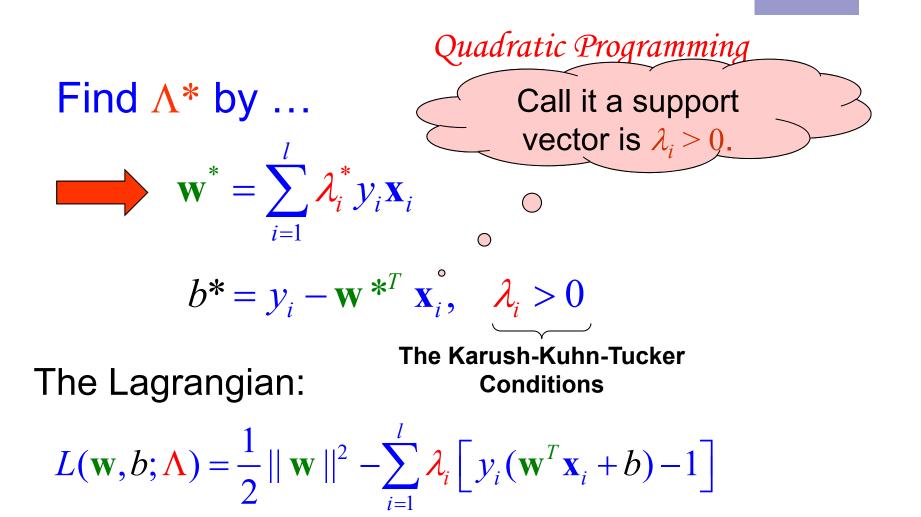
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#### Quadratic Programming

Find  $\Lambda^*$  by ...  $\mathbf{w}^* = \sum_{i=1}^{l} \lambda_i^* y_i \mathbf{x}_i \qquad b^* = ?$ Maximize  $F(\Lambda) = \Lambda \cdot \mathbf{1} - \frac{1}{2} \Lambda^T D \Lambda$ The Dual Subject to  $\Lambda^T \mathbf{y} = \mathbf{0}$  $\Lambda \geq 0$ 

## **The Solution**

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## The Karush-Kuhn-Tucker Conditions

$$L(\mathbf{w}, b; \mathbf{\Lambda}) = \frac{1}{2} \| \mathbf{w} \|^{2} - \sum_{i=1}^{l} \lambda_{i} \Big[ y_{i} (\mathbf{w}^{T} \mathbf{x}_{i} + b) - 1 \\ \nabla_{\mathbf{w}} L(\mathbf{w}, b; \mathbf{\Lambda}) = \mathbf{w} - \sum_{i=1}^{l} \lambda_{i} y_{i} \mathbf{x}_{i} = \mathbf{0} \\ \nabla_{b} L(\mathbf{w}, b; \mathbf{\Lambda}) = \sum_{i=1}^{l} \lambda_{i} y_{i} = 0 \\ y_{i} (\mathbf{w}^{T} \mathbf{x}_{i} + b) - 1 \ge 0, \quad i = 1, \mathbf{K}, l \\ \lambda_{i} \ge 0, \quad i = 1, \mathbf{K}, l \\ \lambda_{i} \ge 0, \quad i = 1, \mathbf{K}, l \end{bmatrix}$$

## Classification

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$$\mathbf{w}^* = \sum_{i=1}^l \lambda_i^* y_i \mathbf{x}_i$$
$$f(\mathbf{x}) = \operatorname{sgn}\left(\mathbf{w}^{*T} \mathbf{x} + b^*\right)$$
$$= \operatorname{sgn}\left(\sum_{i=1}^l \lambda_i^* y_i < \mathbf{x}_i, \mathbf{x} > b^*\right)$$
$$= \operatorname{sgn}\left(\sum_{\lambda_i^* \neq 0} \lambda_i^* y_i < \mathbf{x}_i, \mathbf{x} > b^*\right)$$

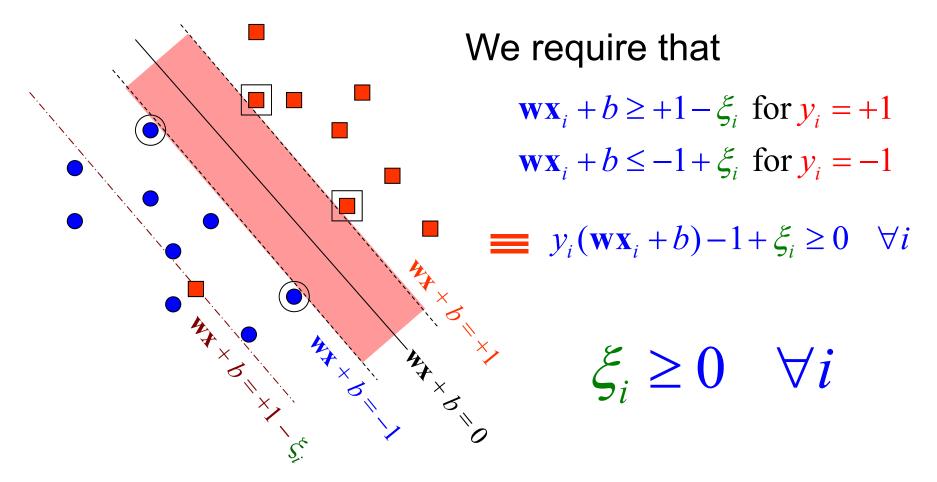
#### **Classification Using Supporters**

The weight for the *i*<sup>th</sup> support vector. Bias  $\int (\mathbf{X}) = \operatorname{sgn}\left(\sum_{\lambda_i^* \neq 0} \lambda_i^* y_i < \mathbf{X}_i, \mathbf{X} > + b^*\right)$ The similarity measure btw. input and the *i*<sup>th</sup> support vector.

### Linear SVM



#### Then non-separable case



### **Mathematic Formulation**

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For simplicity, we consider k = 1.

 $\begin{array}{ll} \text{Minimize} & \frac{1}{2} \| \mathbf{w} \|^2 + C \left( \sum_i \xi_i \right)^k \\ \text{Subject to} & y_i (\mathbf{w}^T \mathbf{x}_i + b) - 1 + \xi_i \geq 0 \quad \forall i \\ & \xi_i \geq 0 \quad \forall i \end{array}$ 

### **Mathematic Formulation**

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For simplicity, we consider k = 1.

 $\begin{array}{ll} \text{Minimize} & \frac{1}{2} \| \mathbf{w} \|^2 + C \left( \sum_i \xi_i \right)^k \\ \text{Subject to} & y_i (\mathbf{w}^T \mathbf{x}_i + b) - 1 + \xi_i \geq 0 \quad \forall i \\ & \xi_i \geq 0 \quad \forall i \end{array}$ 

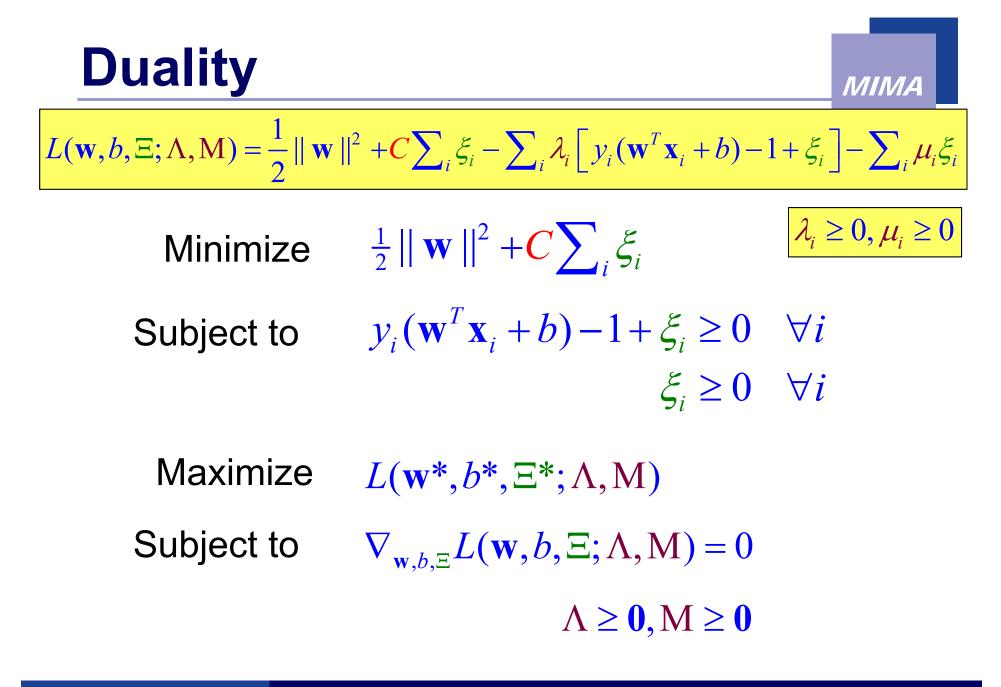
# The Lagrangian



$$\begin{array}{ll} \text{Minimize} & \frac{1}{2} \| \mathbf{w} \|^2 + C \sum_i \xi_i \\\\ \text{Subject to} & y_i (\mathbf{w}^T \mathbf{x}_i + b) - 1 + \xi_i \geq 0 \quad \forall i \\\\ & \xi_i \geq 0 \quad \forall i \end{array}$$

$$L(\mathbf{w}, b, \Xi; \Lambda, \mathbf{M})$$
  
=  $\frac{1}{2} \| \mathbf{w} \|^{2} + C \sum_{i} \xi_{i} - \sum_{i} \lambda_{i} \Big[ y_{i} (\mathbf{w}^{T} \mathbf{x}_{i} + b) - 1 + \xi_{i} \Big] - \sum_{i} \mu_{i} \xi_{i}$   
 $\lambda_{i} \ge 0, \mu_{i} \ge 0$ 

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**Duality**  

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

$$\mu_{i} \ge 0$$

$$\mu_{i} \ge 0$$

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

$$\mu_{i} \ge 0$$

$$\mu_{i} \ge 0$$

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

$$\mu_{i} \ge 0, \mu_{i} \le 0$$

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

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

$$\sum_{i} \lambda_{i} y_{i} = 0$$

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

$$\mu_{i} = C - \lambda_{i}$$

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

$$F(\Lambda, \mathbf{M}) = L(\mathbf{w}^{*}, b^{*}, \Xi^{*}; \Lambda, \mathbf{M}) = \sum_{i} \lambda_{i} - \frac{1}{2} \sum_{i} \sum_{j} \lambda_{i} \lambda_{j} y_{i} y_{j} < \mathbf{x}_{i}, \mathbf{x}_{j} > 0$$
Maximize this

**Duality**  

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

$$\mu_{i} \ge 0$$

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

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$$\lambda_{i} \ge 0 \ge \lambda_{i} \le 0$$

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$$\lambda_{i} \ge 0 \le \lambda_{i} \le 0$$

$$\lambda_{i} \ge 0$$

$$\lambda_{$$

# **Duality**

Minimize
$$\frac{1}{2} || \mathbf{w} ||^2 + C \left( \sum_i \xi_i \right)^k$$
Subject to $y_i (\mathbf{w}^T \mathbf{x}_i + b) - 1 + \xi_i \ge 0 \quad \forall i$  $\xi_i \ge 0 \quad \forall i$ The DualMaximize $F(\Lambda) = \Lambda \cdot 1 - \frac{1}{2} \Lambda^T D \Lambda$ Subject to $\Lambda^T \mathbf{y} = 0$  $\mathbf{0} \le \Lambda \le C \mathbf{1}$ 

# The Karush-Kuhn-Tucker Conditions

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

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

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

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

$$y_{i} (\mathbf{w}^{T} \mathbf{x}_{i} + b) - 1 + \xi_{i} \ge 0$$

$$\mu_{i} \ge 0$$

$$\lambda_{i} \ge 0$$

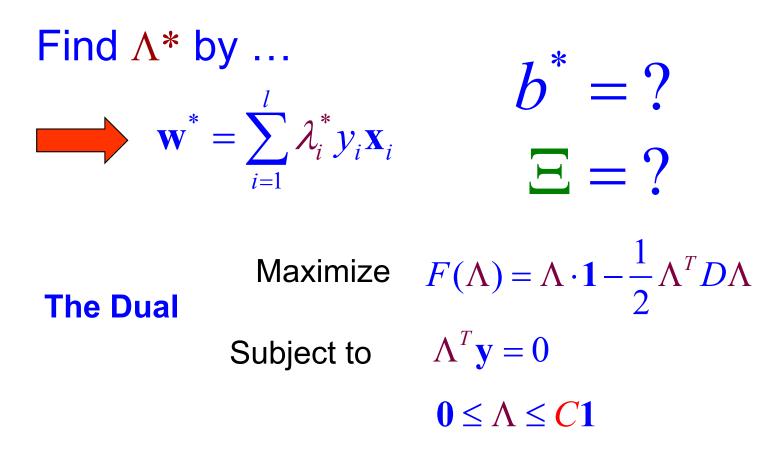
$$\lambda_{i} \left[ y_{i} (\mathbf{w}^{T} \mathbf{x}_{i} + b) - 1 + \xi_{i} \right] = 0$$

$$\mu_{i} \xi_{i} = 0$$

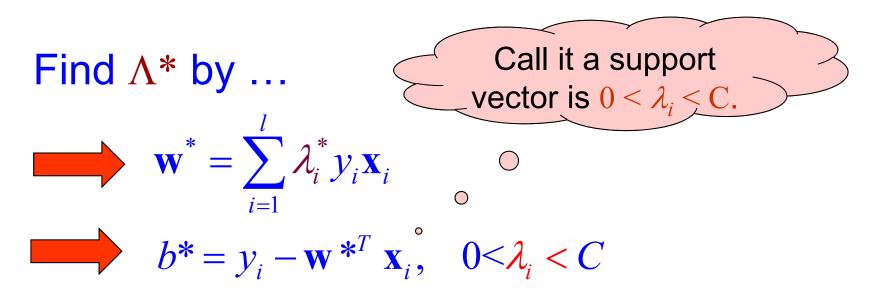
#### **The Solution**



#### Quadratic Programming



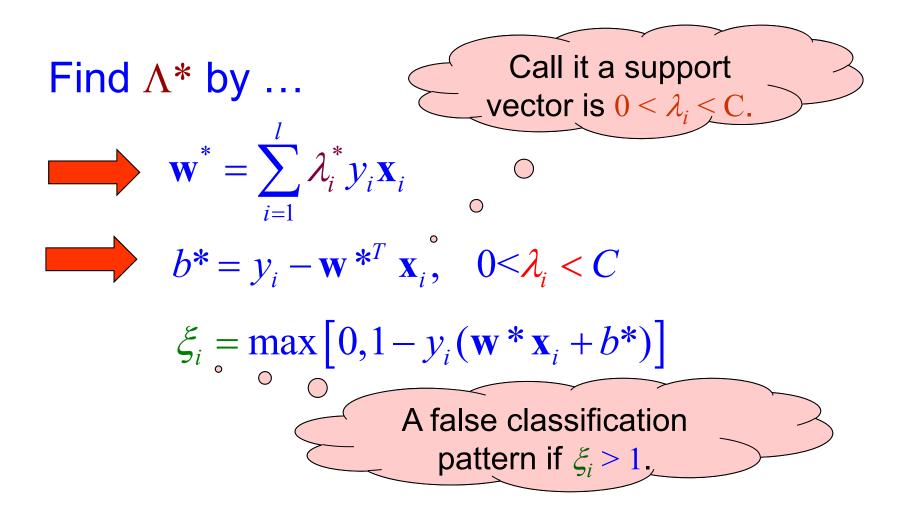
### **The Solution**



#### The Lagrangian:

 $L(\mathbf{w}, b, \Xi; \Lambda, \mathbf{M})$ =  $\frac{1}{2} ||\mathbf{w}||^2 + C \sum_i \xi_i - \sum_i \lambda_i [y_i(\mathbf{w}^T \mathbf{x}_i + b) - 1 + \xi_i] - \sum_i \mu_i \xi_i$ 

#### **The Solution**



#### Classification

$$\mathbf{w}^* = \sum_{i=1}^l \lambda_i^* y_i \mathbf{x}_i$$
$$f(\mathbf{x}) = \operatorname{sgn}\left(\mathbf{w}^{*T} \mathbf{x} + b^*\right)$$
$$= \operatorname{sgn}\left(\sum_{i=1}^l \lambda_i^* y_i < \mathbf{x}_i, \mathbf{x} > b^*\right)$$
$$= \operatorname{sgn}\left(\sum_{\lambda_i^* \neq 0} \lambda_i^* y_i < \mathbf{x}_i, \mathbf{x} > b^*\right)$$

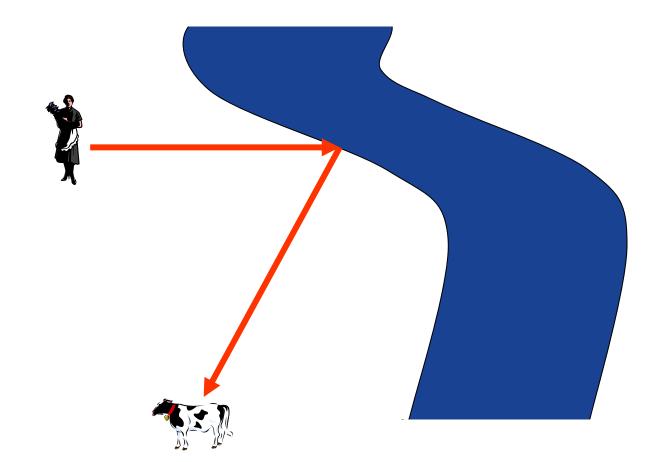
#### **Classification Using Supporters**

The weight for the *i*<sup>th</sup> support vector. Bias  $\int (\mathbf{X}) = \operatorname{sgn}\left(\sum_{\lambda_i^* \neq 0} \lambda_i^* y_i < \mathbf{X}_i, \mathbf{X} > + b^*\right)$ The similarity measure btw. input and the *i*<sup>th</sup> support vector.

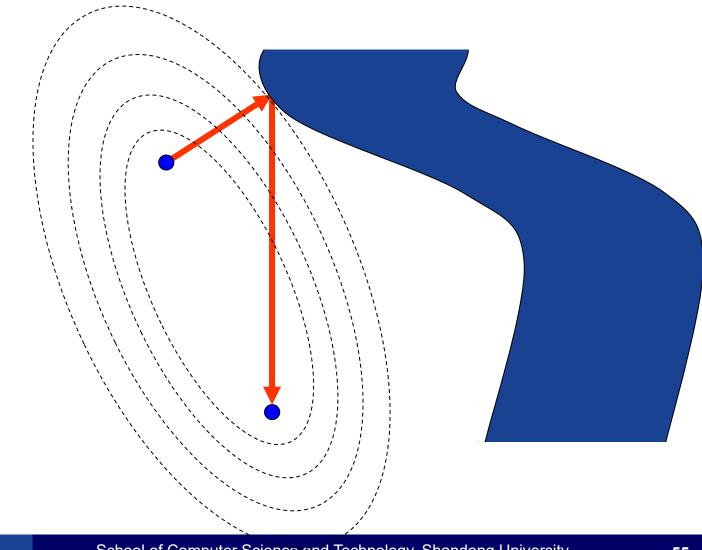
# Lagrange Multiplier

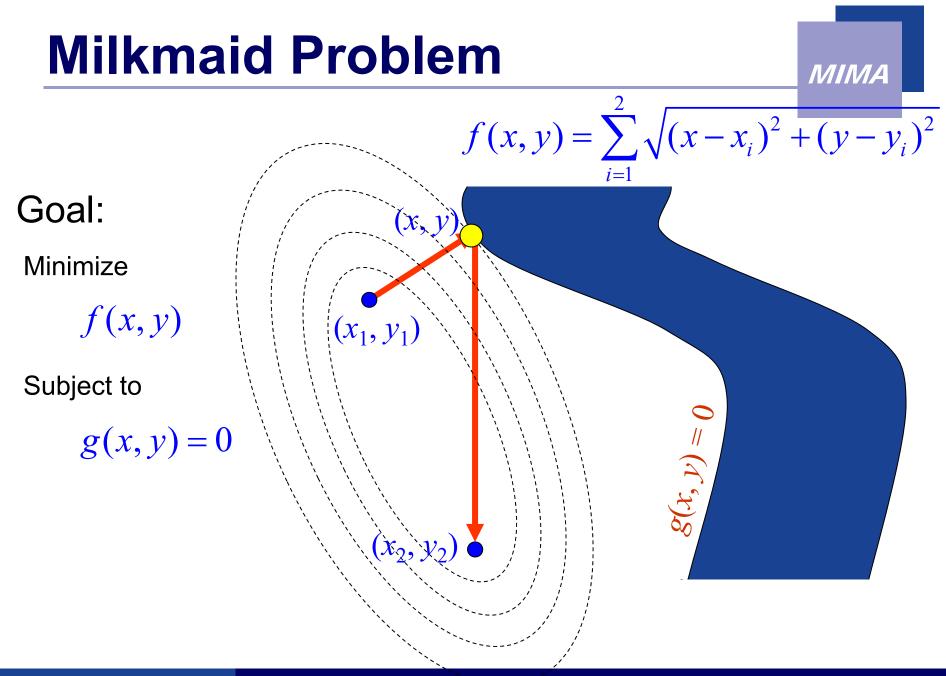
- "Lagrange Multiplier Method" is a powerful tool for constraint optimization.
- Contributed by Riemann.

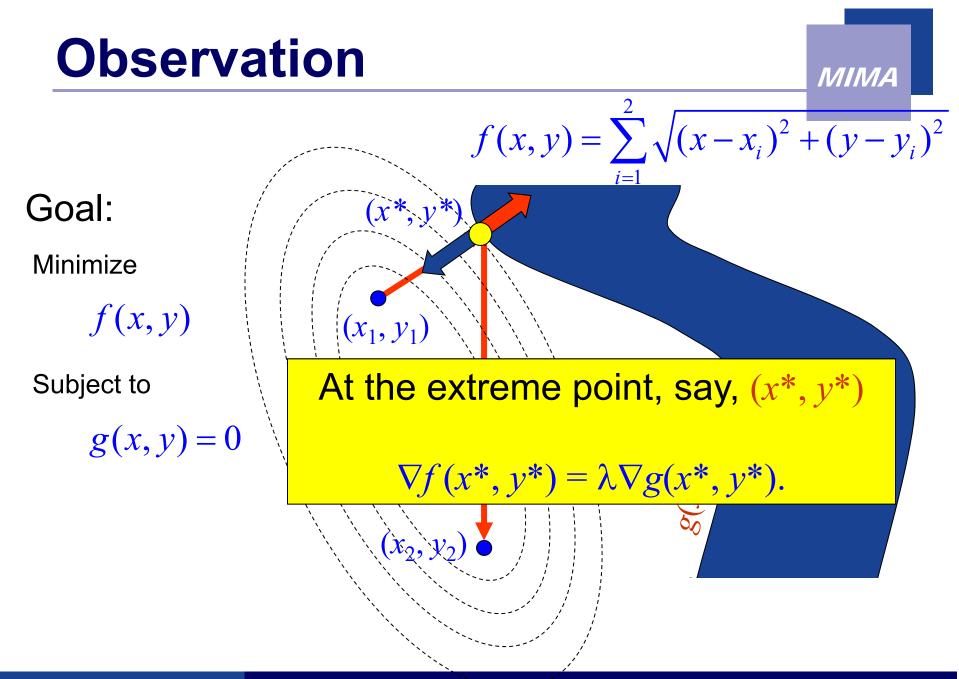
#### **Milkmaid Problem**



### **Milkmaid Problem**







#### **Optimization with Equality Constraints**

Goal: Min/Max  $f(\mathbf{x})$ Subject to  $g(\mathbf{x}) = 0$ 

Lemma:

At an extreme point, say, x\*, we have

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

# Proof

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

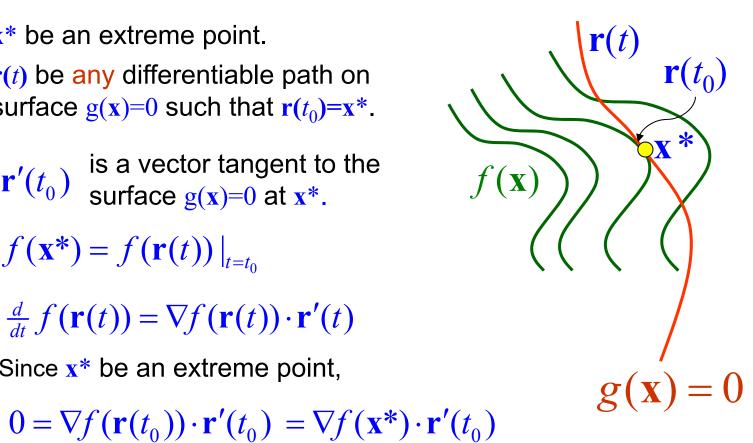
**x**\* be an extreme point.

- Let **r**(*t*) be any differentiable path on surface g(x)=0 such that  $r(t_0)=x^*$ .
  - $\mathbf{r}'(t_0)$  is a vector tangent to the surface  $\mathbf{g}(\mathbf{x})=0$  at  $\mathbf{x}^*$ .

 $f(\mathbf{x}^*) = f(\mathbf{r}(t))|_{t=t_0}$ 

 $\frac{d}{dt} f(\mathbf{r}(t)) = \nabla f(\mathbf{r}(t)) \cdot \mathbf{r}'(t)$ 

Since **x**<sup>\*</sup> be an extreme point,



# Proof

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

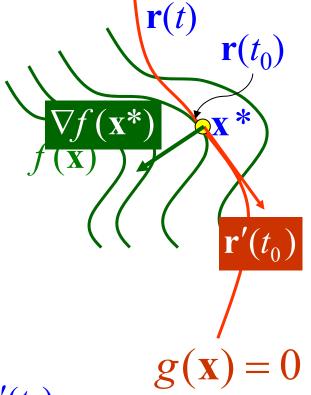
$$\nabla f(\mathbf{x}^*) \perp \mathbf{r}'(t_0)$$

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

It implies that

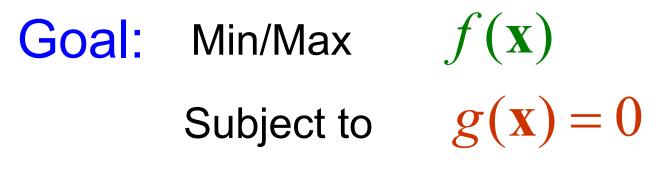
 $\nabla f(\mathbf{x}^*) \perp \Gamma$ ,

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



 $0 = \nabla f(\mathbf{r}(t_0)) \cdot \mathbf{r}'(t_0) = \nabla f(\mathbf{x}^*) \cdot \mathbf{r}'(t_0)$ 

#### **Optimization with Equality Constraints**



Lemma:

At an extreme point, say,  $\mathbf{x}^*$ , we have  $\nabla f(\mathbf{x}^*) = \lambda \nabla g(\mathbf{x}^*) \text{ if } \nabla g(\mathbf{x}^*) \neq 0$ Lagrange Multiplier

# **The Method of Lagrange**

**x**: dimension *n*.

Goal: Min/Max  $f(\mathbf{x})$ Subject to  $g(\mathbf{x}) = 0$ 

Find the extreme points by solving the following equations.

$$\nabla f(\mathbf{x}) = \lambda \nabla g(\mathbf{x})$$
  

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

$$\begin{cases} n+1 \text{ equations} \\ \text{with } n+1 \text{ variables} \end{cases}$$



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Goal: Min/Max 
$$f(\mathbf{x})$$
  
Subject to  $g(\mathbf{x}) = 0$ 

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

Solve  $\begin{array}{c} \nabla_{\mathbf{x}} L(\mathbf{x}; \lambda) = \mathbf{0} \\ \nabla_{\lambda} L(\mathbf{x}; \lambda) = \mathbf{0} \end{array} \right\} \begin{array}{c} \text{Unconstraint} \\ \text{Optimization} \end{array}$ 

Optimization with  
Multiple Equality Constraints  

$$\Lambda = (\lambda_1, K, \lambda_m)^T$$

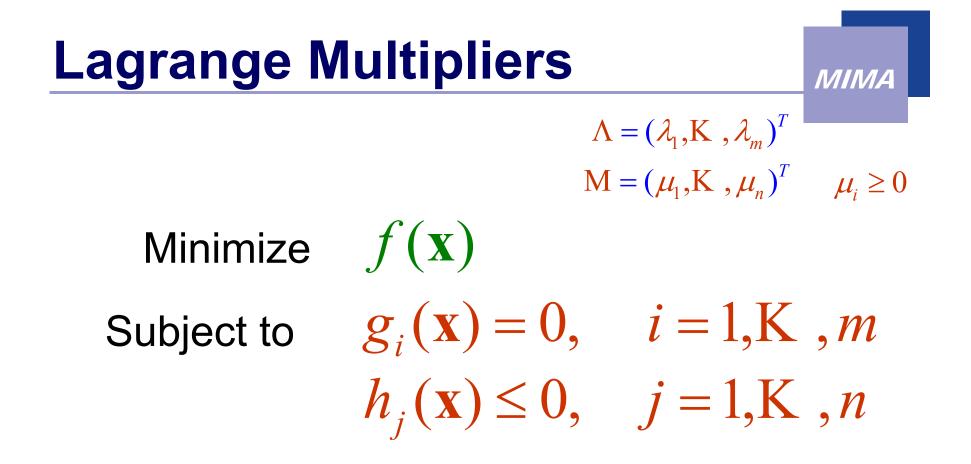
$$Min/Max \qquad f(\mathbf{x})$$
Subject to 
$$g_i(\mathbf{x}) = 0, \quad i = 1, K, m$$
Define 
$$L(\mathbf{x}; \Lambda) = f(\mathbf{x}) + \sum_{i=1}^m \lambda_i g_i(\mathbf{x}) - \text{Lagrangian}$$
Solve 
$$\nabla_{\mathbf{x}, \Lambda} L(\mathbf{x}; \Lambda) = \mathbf{0}$$

#### Optimization with Inequality Constraints



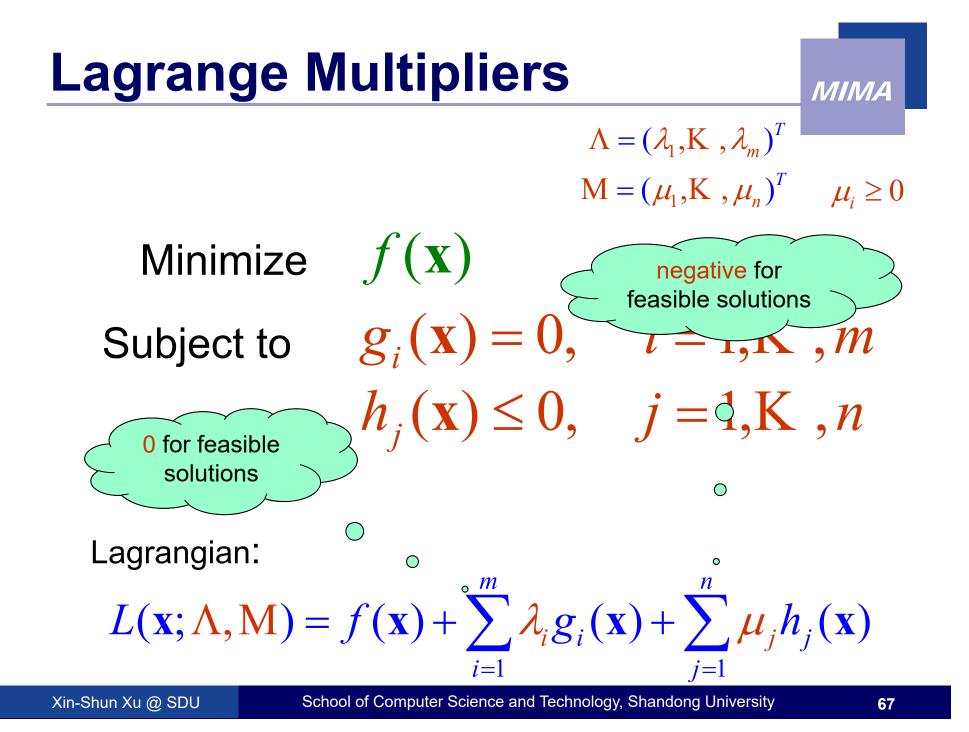
# 

You can always reformulate your problems into the about form.



Lagrangian:

$$L(\mathbf{x}; \mathbf{\Lambda}, \mathbf{M}) = f(\mathbf{x}) + \sum_{i=1}^{m} \lambda_i g_i(\mathbf{x}) + \sum_{j=1}^{n} \mu_j h_j(\mathbf{x})$$

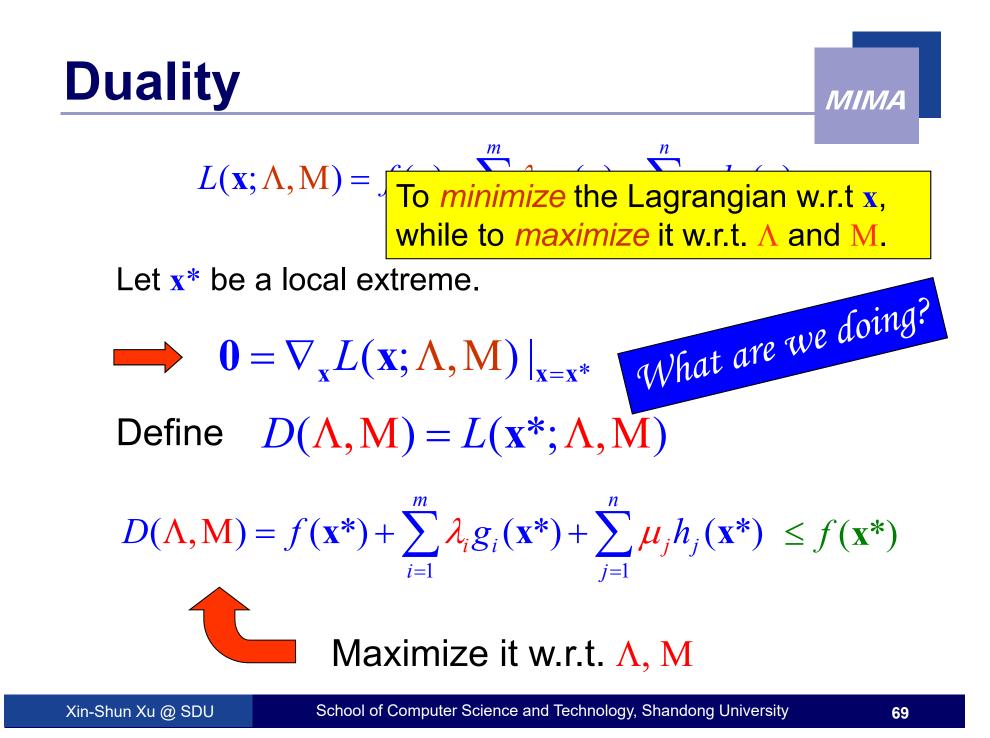


### **Duality**

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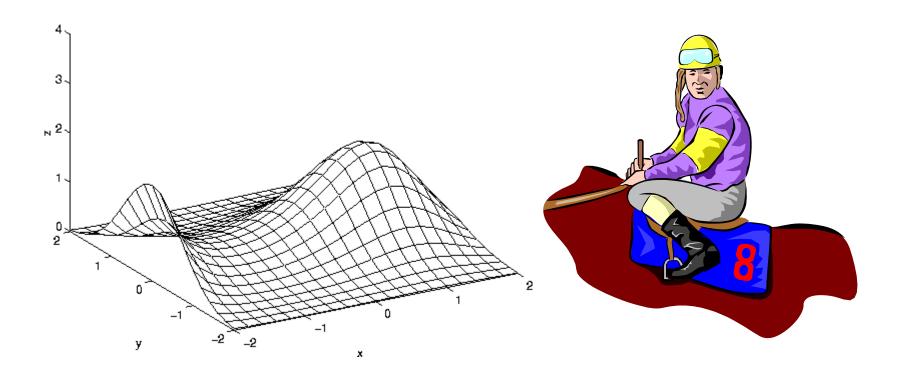
$$L(\mathbf{x}; \mathbf{\Lambda}, \mathbf{M}) = f(\mathbf{x}) + \sum_{i=1}^{m} \lambda_i g_i(\mathbf{x}) + \sum_{j=1}^{n} \mu_j h_j(\mathbf{x})$$

Let x\* be a local extreme.



#### **Saddle Point Determination**

$$L(\mathbf{x}; \mathbf{\Lambda}, \mathbf{M}) = f(\mathbf{x}) + \sum_{i=1}^{m} \lambda_i g_i(\mathbf{x}) + \sum_{j=1}^{n} \mu_j h_j(\mathbf{x})$$



# **Saddle Point Determination**

$$L(\mathbf{x}; \Lambda, \mathbf{M}) = f(\mathbf{x}) + \sum_{i=1}^{m} \lambda_i g_i(\mathbf{x}) + \sum_{j=1}^{n} \mu_j h_j(\mathbf{x})$$
  
**The primal**  
**The primal**  
**Subject to**  

$$g_i(\mathbf{x}) = 0, \quad i = 1, \mathbf{K}, m$$
  

$$h_j(\mathbf{x}) \le 0, \quad j = 1, \mathbf{K}, n$$
  
**Maximize**  

$$L(\mathbf{x}^*; \Lambda, \mathbf{M})$$
  
**Subject to**  

$$\nabla_{\mathbf{x}, \Lambda} L(\mathbf{x}; \Lambda, \mathbf{M}) = \mathbf{0}$$
  

$$\mathbf{M} \ge \mathbf{0}$$

# The Karush-Kuhn-Tucker Conditions

$$L(\mathbf{x}; \mathbf{\Lambda}, \mathbf{M}) = f(\mathbf{x}) + \sum_{i=1}^{m} \lambda_i g_i(\mathbf{x}) + \sum_{j=1}^{n} \mu_j h_j(\mathbf{x})$$

$$\nabla_{\mathbf{x}} L(\mathbf{x}; \mathbf{\Lambda}, \mathbf{M}) = \nabla_{\mathbf{x}} f(\mathbf{x}) + \sum_{i=1}^{m} \lambda_i \nabla_{\mathbf{x}} g_i(\mathbf{x}) + \sum_{j=1}^{n} \mu_j \nabla_{\mathbf{x}} h_j(\mathbf{x}) = \mathbf{0}$$

$$g_i(\mathbf{x}) = 0, \quad i = 1, \mathbf{K}, m$$

$$\mu_j \ge 0, \quad j = 1, \mathbf{K}, n$$

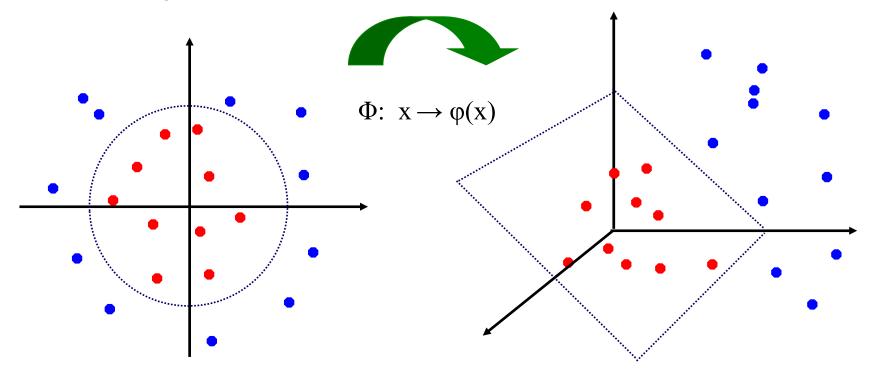
$$h_j(\mathbf{x}) \le 0, \quad j = 1, \mathbf{K}, n$$

$$\mu_j h_j(\mathbf{x}) = 0, \quad j = 1, \mathbf{K}, n$$

# **Non-linear SVMs** MIMA Datasets that are linearly separable with noise work out great: x But what are we going to do if the dataset is just too hard? х 0 How about... mapping data to a higher-dimensional space: X

#### Non-linear SVMs: Feature Space

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

With this mapping, our discriminant function is now:

$$g(x) = w^T \phi(x) + b = \sum_{x_i \in SV} \lambda_i y_i \phi(x_i) \phi(x) + b$$

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

$$K(\mathbf{x}_i, \mathbf{x}_j) \equiv \boldsymbol{\phi}(\mathbf{x}_i)^T \boldsymbol{\phi}(\mathbf{x}_j)$$

#### Nonlinear SVMs: The Kernel Trick

#### An example:

2-dimensional vectors  $x=[x_1 \ x_2]$ ; let  $K(x_i,x_j)=(1 + x_i^T x_j)^2$ . Need to show that  $K(x_i,x_j) = \varphi(x_i)^T \varphi(x_j)$ :

$$K(\mathbf{x}_{i},\mathbf{x}_{j}) = (1 + \mathbf{x}_{i}^{T}\mathbf{x}_{j})^{2},$$
  
=  $1 + x_{il}^{2}x_{jl}^{2} + 2 x_{il}x_{jl} x_{i2}x_{j2} + x_{i2}^{2}x_{j2}^{2} + 2x_{il}x_{jl} + 2x_{i2}x_{j2}$   
=  $[1 \ x_{il}^{2} \ \sqrt{2} x_{il}x_{i2} \ x_{i2}^{2} \ \sqrt{2}x_{il} \ \sqrt{2}x_{i2}] [1 \ x_{jl}^{2} \ \sqrt{2} \ x_{jl}x_{j2} \ x_{j2}^{2} \ \sqrt{2}x_{jl} \ \sqrt{2}x_{j2}]^{T}$ 

$$= \varphi(\mathbf{x}_i)^{\mathrm{T}} \varphi(\mathbf{x}_j), \text{ where } \varphi(\mathbf{x}) = \begin{bmatrix} 1 & x_1^2 & \sqrt{2} & x_1 x_2 & x_2^2 & \sqrt{2} x_1 & \sqrt{2} x_2 \end{bmatrix}^{\mathrm{T}}$$

## Nonlinear SVMs: The Kernel Trick

Examples of commonly-used kernel functions:

Linear kernel: 
$$K(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i^T \mathbf{x}_j$$

Polynomial kernel: 
$$K(\mathbf{x}_i, \mathbf{x}_j) = (1 + \mathbf{x}_i^T \mathbf{x}_j)^p$$

Gaussian (Radial-Basis Function (RBF))  
kernel:  
$$K(\mathbf{x}_i, \mathbf{x}_j) = \exp(-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{2\sigma^2})$$

Sigmoid:

$$K(\mathbf{x}_i, \mathbf{x}_j) = \tanh(\beta_0 \mathbf{x}_i^T \mathbf{x}_j + \beta_1)$$

In general, functions that satisfy *Mercer's condition* can be kernel functions.

## **Nonlinear SVM: Optimization**

Formulation: (Lagrangian Dual Problem)

$$\max \sum_{i} \lambda_{i} - \frac{1}{2} \sum_{i} \sum_{j} \lambda_{i} \lambda_{j} y_{i} y_{j} K(x_{i}, x_{j})$$
  
such that  $0 \le \lambda_{i} \le C$   
 $\sum_{i} \lambda_{i} y_{i} = 0$ 

The solution of the discriminant function is

$$g(x) = w^T \phi(x) + b = \sum_{x_i \in SV} \lambda_i y_i K(x, x_i) + b$$

The optimization technique is the same.

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#### Support Vector Machine: Algorithm

- 1. Choose a kernel function
- 2. Choose a value for C
- 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 Network

- 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

**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 Group

# **Thank You!**

**Any Question?** 

 Xin-Shun Xu @ SDU
 School of Computer Science and Technology, Shandong University