Artificial Intelligence III:
Artificial Intelligence and Deep Learning

Lecture 4

Classifiers

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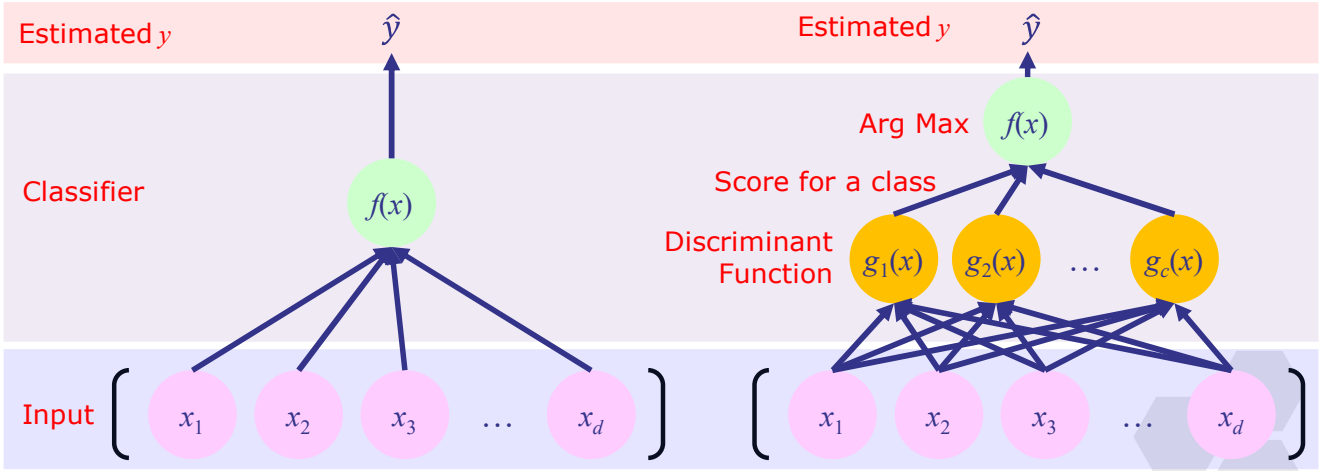
Agenda

- Linear Discriminant Function (LDF)
- Decision Tree (DT)
- K nearest neighbour (k-NN)
- Support Vector Machine (SVM)

Classifier

- Generally, a classifier f(x) return a class label
- Some classifiers estimate the probability of x belongs to a class
  - Contains a set of discriminant functions $g_i(\boldsymbol{x}), i = 1, ..., c$ indicates how likely $\boldsymbol{x}$ belongs to y_i
  - $\boldsymbol{x}$ is assigned to class y_i if $g_i(\mathrm{x})$ is max for $i = 1 \ldots c$



Linear Discriminant Function

- LDF: a linear combination of x

$$g(x) = \theta^T x$$

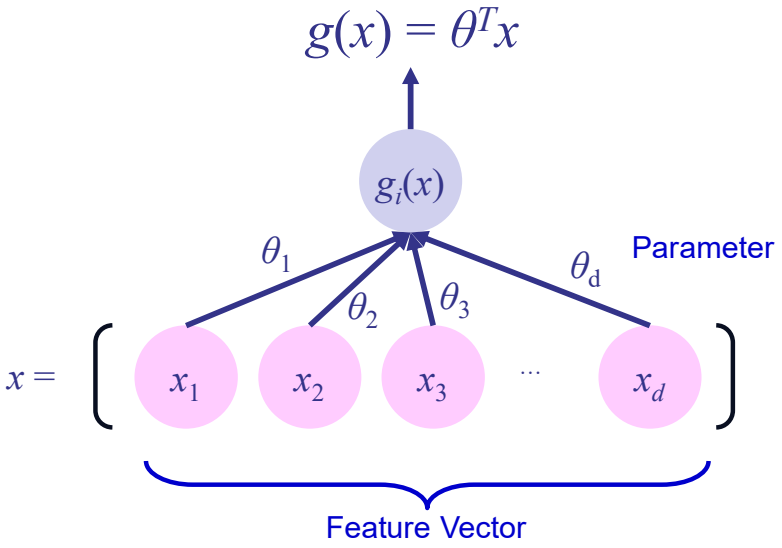
w : is the weight vector

* *the last feature of x can be set as 1 if bias term is needed*

  - One feature value in x can be fixed when a constant term is needed
    - $x = [1, x_1, x_2, \ldots, x_d]^T$
    - $g(x) = \theta^T x + \theta_0$

Linear Discriminant Function

- For each class



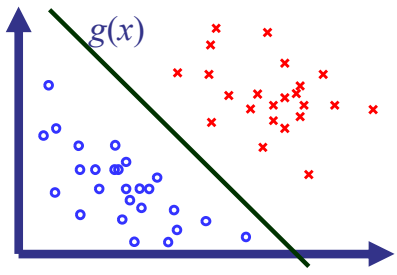
Linear Discriminant Function

- For a 2-class problem
  - Only one classifier is needed
  - $g(x) = g_1(x) - g_2(x)$

$$= \left(\left(\theta^{(1)}\right)^T - \left(\theta^{(2)}\right)^T \right) x$$

$$= \theta^T x$$

    - If $g(x) > 0$, decide y_1
    - If $g(x) < 0$, decide y_2
    - If $g(x) = 0$, ambiguity
  - All training samples are used, y = {1, -1}



Original Dataset

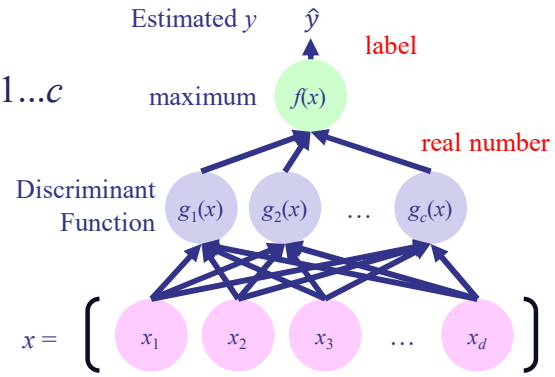
x	y
23	1
42	1
52	2
12	2

$g(x)$

x	y
23	1
42	1
52	-1
12	-1

Linear Discriminant Function

- For a multi-class problem
  - x is y_i if $g_i(x)$ is maximum for $i = 1...c$
  - c classifiers are required
  - $g_i(x)$ represents the probability that x belongs to class i
    - We will discuss this later
  - For $g_i(x)$, class i = 1, the rest = 0



Original Dataset

x	y
23	1
42	2
52	3
12	4

$g_1(x)$

x	$y^{(1)}$
23	1
42	0
52	0
12	0

$g_2(x)$

x	$y^{(2)}$
23	0
42	1
52	0
12	0

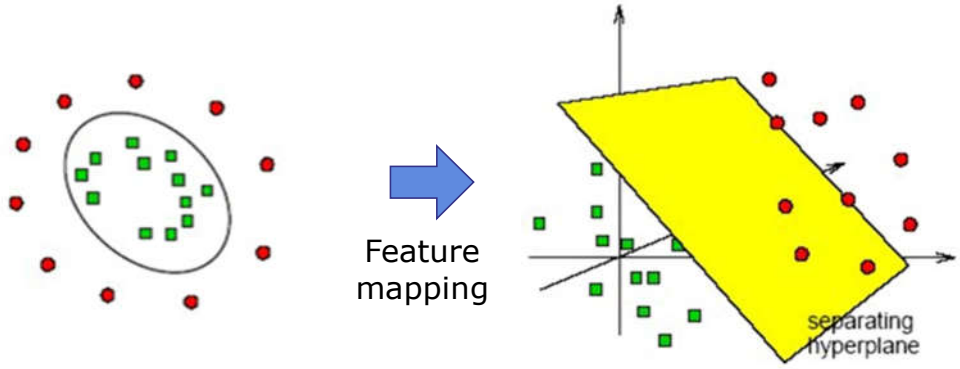
…

Linear Discriminant Function

- How to train g(x)?
  - LMS discussed in Regression previously can be used
  - Cost Function: $J(\theta) = \frac{1}{2n}\sum_{i=1}^{n}\left(h_\theta\left(x^{(i)}\right) - y^{(i)}\right)^2$
  - Minimize by
    - Pseudoinverse
    - Gradient descent

Mapping

- Practically, a problem is seldom linearly separable
- How can LDF handle a non-linearly separable problem?
  - Map nonlinearly to linearly separable problem
  - Usually high-dimensional space is required



nonlinearly separable
(a low-dimensional space)

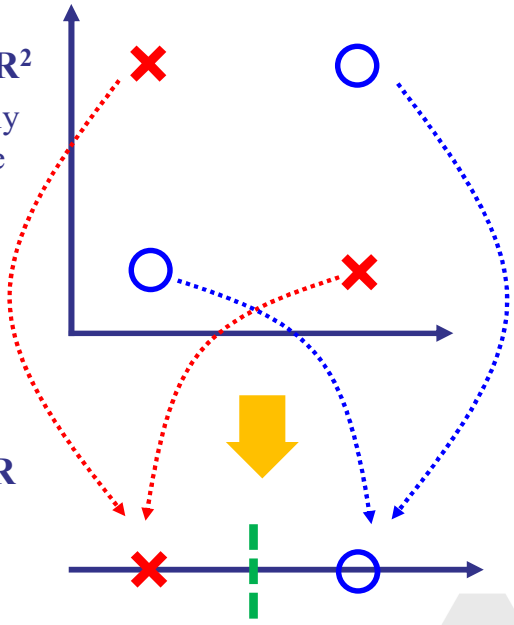
linearly separable
(a high-dimensional space)

Mapping

- XOR Example

x_1	x_2	y
1	1	1
-1	1	-1
1	-1	-1
-1	-1	1

$(x_1, x_2) \in \mathbf{R}^2$
nonlinearly
separable



x_1	x_2	x_1x_2	y
1	1	1	1
-1	1	-1	-1
1	-1	-1	-1
-1	-1	1	1

$(x_1x_2) \in \mathbf{R}$
linearly
separable

Mapping

- Another Example

x	y
-2	1
-1	-1
0	-1
1	1
2	1

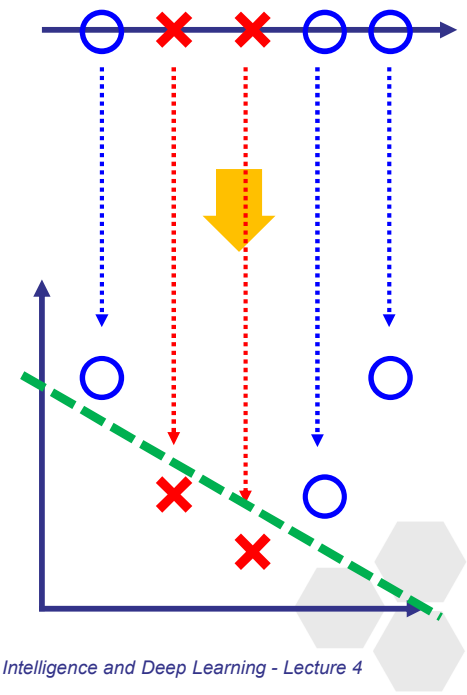
$(x) \in R$

nonlinearly separable

x	x	x^2	y
-2	-2	4	1
-1	-1	1	-1
0	0	0	-1
1	1	1	1
2	2	4	1

$(x, x^2) \in R^2$

linearly separable



Mapping

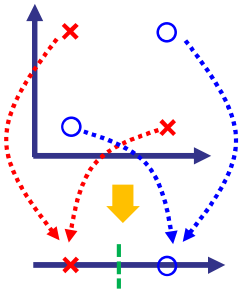
- Generalized Linear Discriminant Function

$$g(x) = w^t z(x)$$

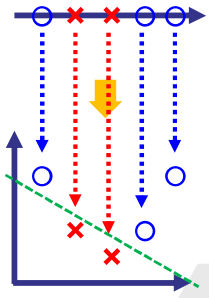
  - z is a mapping from x to $z(x)$
  - g is not linear in x, but linear in z

- For example

$z(x_1, x_2) = (x_1 x_2)$



$z(x) = \begin{pmatrix} x \\ x^2 \end{pmatrix}$

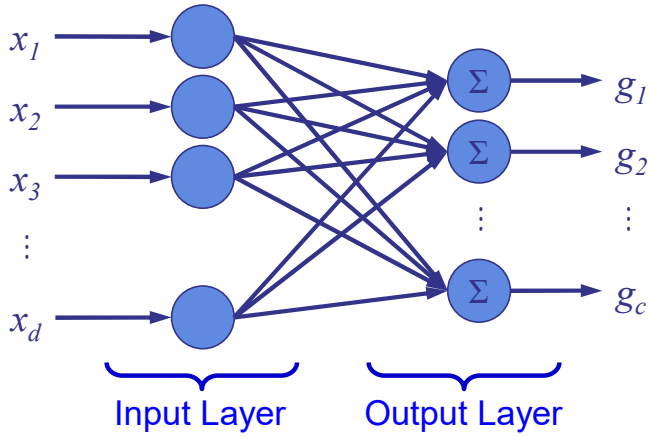


Mapping

- How to determine the feature space?
  - How to design a proper high dimensional space automatically by learning?
    - ANN, SVM…

Introduction

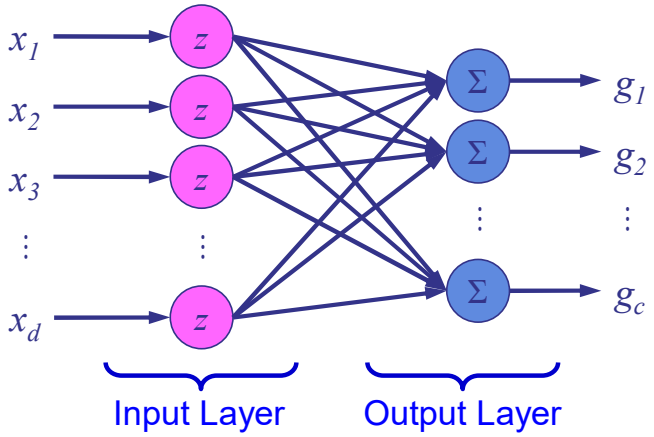
- Recall, **Linear Discriminant Functions**:



  - **Limited** generalization capability
  - Cannot handle the non-linearly separable problem

Introduction

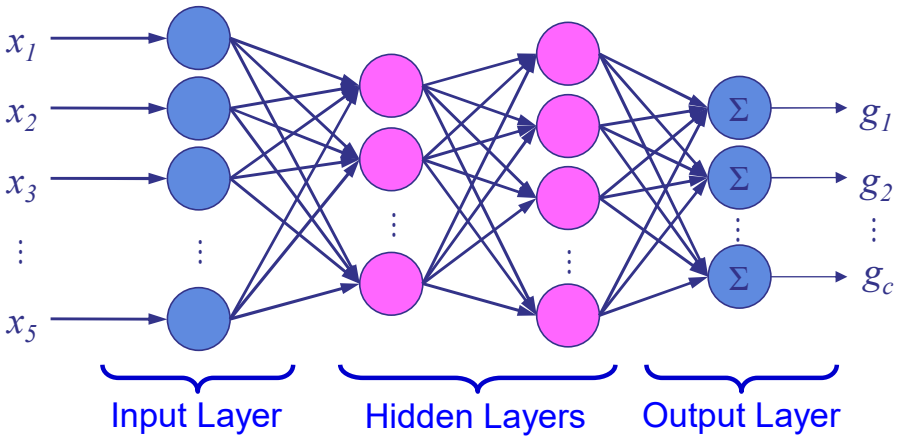
- Solution 1: **Mapping Function $\varphi(x)$**



  - Pro: Simple structure (still using LDF)
  - Cons: Selection of $z(x)$ and its parameters

Introduction

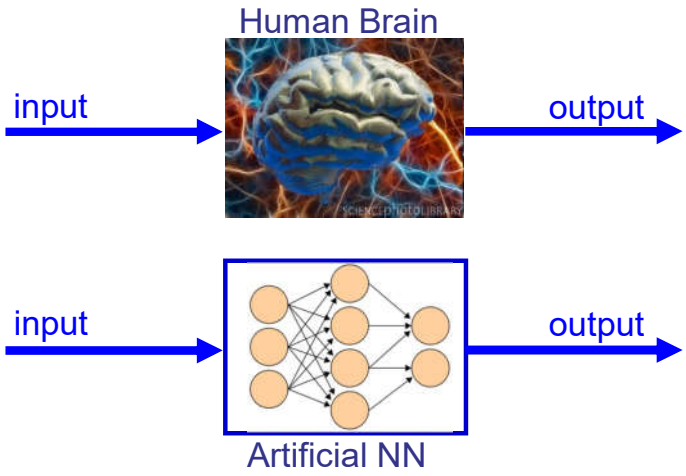
- Solution 2: **Multi-Layer Neural Network**



  - Standard structure
    - Hidden layers serve as mapping
  - No prior knowledge is required (no need to choose $z(x)$)

Artificial Neural Network

- ANN is inspired biologically by human brain



Decision Tree (DT)

- Most classifiers are black-box
- DT provides explanation on decisions
- One of the most widely used and practical methods for inductive inference
- Approximates discrete-valued functions (including disjunctions)

DT: Example

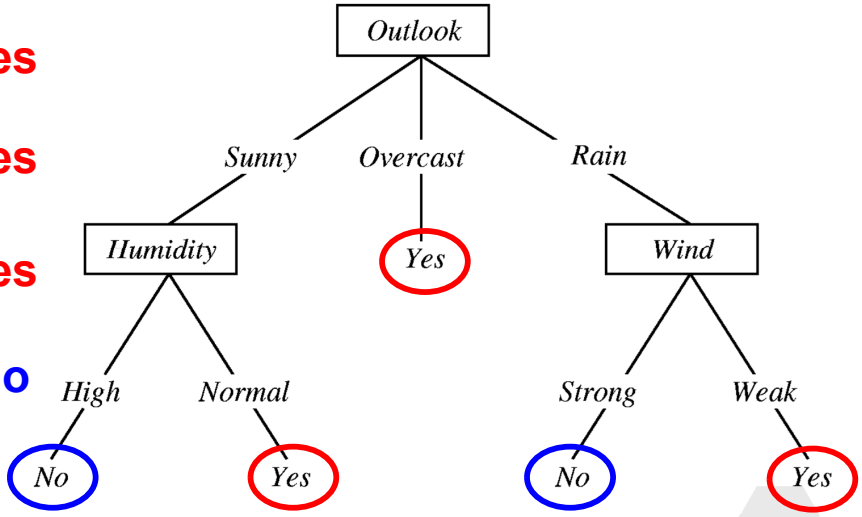
- Do we go to play tennis today?

If Outlook is Sunny AND Humidity is Normal — **Yes**

If Outlook is Overcast — **Yes**

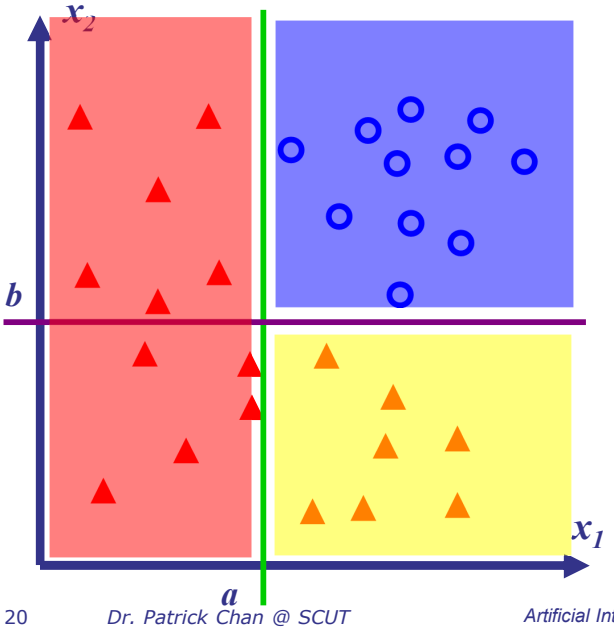
If Outlook is Rain AND Wind is Weak — **Yes**

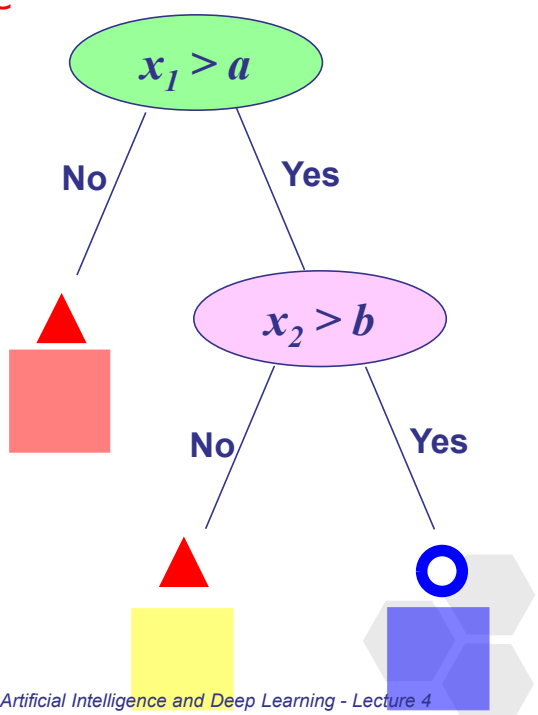
Other situation? — **No**



DT: Classification

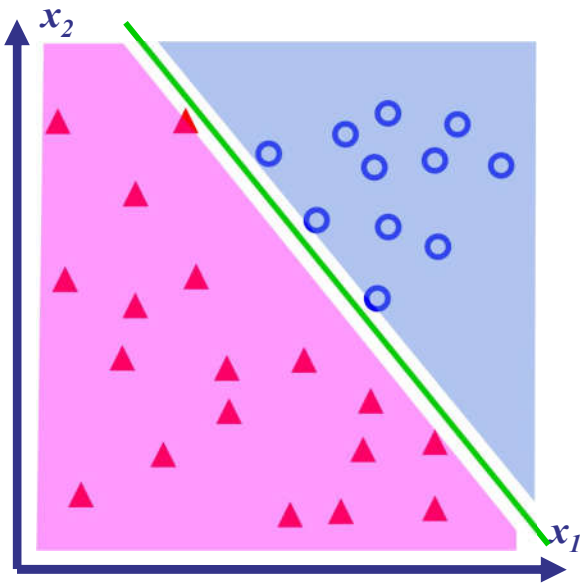
- Decision Region:
  - Internal nodes can be univariate
  - (Only one feature is used)

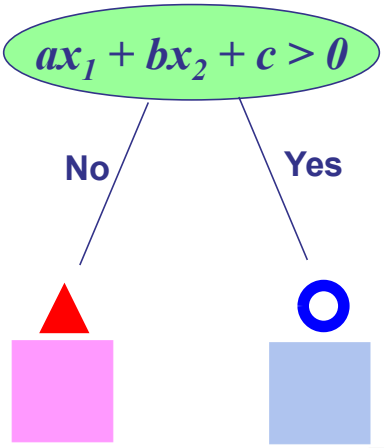




DT: Classification

- Internal nodes can be multivariate
  - More than one features are used
  - Shape of Decision Region is irregular

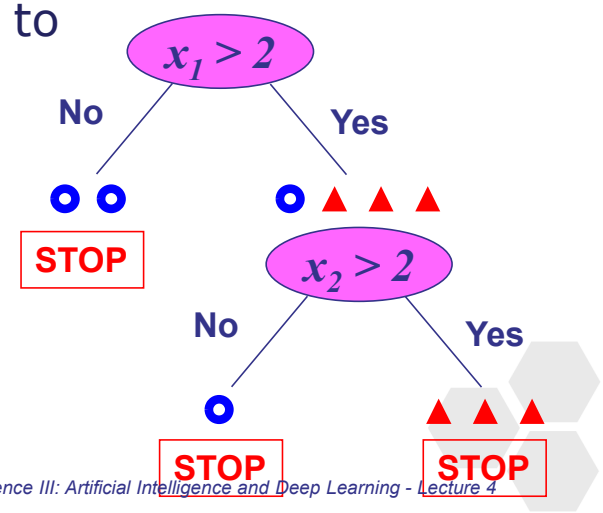




DT: Learning Algorithm

- LOOP:
  1. Select the best feature (A)
  2. For each value of A, create new descendant of node
  3. Sort training samples to leaf nodes
- STOP when training samples perfectly classified

#	x_1	x_2	x_3	
1	1	3	5	○
2	1	4	2	○
3	3	1	5	○
4	3	5	6	△
5	3	3	4	△
6	4	5	7	△



DT: Learning Algorithm

- Observation
  - Many trees may code a training set without any error
  - Finding the smallest tree is a NP-hard problem
- Local search algorithm to find reasonable solutions
  - What is the best feature?

DT: Feature Measurement

- Entropy is used to evaluate features
  - Measure of uncertainty
  - Range: 0 - 1
  - Smaller value, less uncertainty

$$H(X) = -\sum_{i=1}^{n} p(x_i)\log(p(x_i))$$

where

X: a random variable with n outcomes, $X = \{x_i \mid i = 1,2,\ldots,n\}$

$p(x)$: the probability mass function of outcome x.

  - If all samples belongs to x_i, then $p(x_i) = 1$, and other $p(x_j) = 0$, $i \neq j$
    - Thus, $H(X) = 0$ (no uncertainty)

DT: Feature Measurement

- Information Gain
  - Reduction in entropy (reduce uncertainty) due to sorting on a feature A

$$Gain(X, A) = H(X) - H(X|A)$$

Current entropy — **Entropy after using feature A**

DT: Example

- Which feature is the best?

Day	Outlook	Temperature	Humidity	Wind	PlayTennis
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

$$H(X) = -\sum_{i=1}^{n} p(x_i) \log_2 p(x_i)$$

x_1 = yes x_2 = No

$$H(X) = -\sum_{i=1}^{2} p(x_i) \log_2 p(x_i)$$

$$= -\frac{9}{14}\log_2\left(\frac{9}{14}\right) - \frac{5}{14}\log_2\left(\frac{5}{14}\right)$$

$$= 0.410 + 0.531$$

$$= 0.941$$

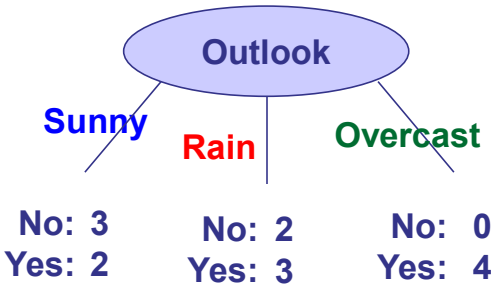
Current: $H(X) = 0.941$

Uncertainty is high without considering any feature

DT: Example

Day	Outlook	Temperature	Humidity	Wind	PlayTennis
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

Let A = Outlook



Recall:

$$Gain(X, A) = H(X) - H(X \mid A)$$

$$\begin{aligned} H(X \mid A) = \; & H(X \mid A = sunny)P(A = sunny) + \\ & H(X \mid A = Rain)P(A = Rain) + \\ & H(X \mid A = overcast)P(A = overcast) \end{aligned}$$

DT: Example

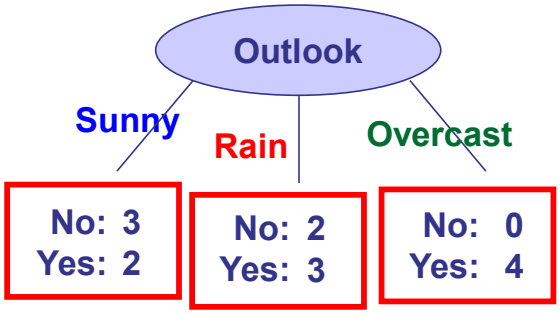
$$\begin{aligned} H(X \mid A) = \; & H(X \mid A = sunny)P(A = sunny) + \\ & H(X \mid A = Rain)P(A = Rain) + \\ & H(X \mid A = overcast)P(A = overcast) \end{aligned}$$

Let A = Outlook

$$H(X \mid sunny) = -\frac{3}{5}\log_2(\frac{3}{5}) - \frac{2}{5}\log_2(\frac{2}{5}) = 0.971$$

$$H(X \mid Rain) = -\frac{2}{5}\log_2(\frac{2}{5}) - \frac{3}{5}\log_2(\frac{3}{5}) = 0.971$$

$$H(X \mid overcast) = -\frac{0}{4}\log_2(\frac{0}{4}) - \frac{4}{4}\log_2(\frac{4}{4}) = 0$$



$$\begin{aligned} H(X \mid A) &= 0.971 \times \left(\frac{5}{14}\right) + 0.971 \times \left(\frac{5}{14}\right) + 0 \times \left(\frac{4}{14}\right) \\ &= 0.694 \end{aligned}$$

DT: Example

Outlook is the best feature and Should be used as the first node

Day	Outlook	Temperature	Humidity	Wind	PlayTennis
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

Current: $H(X) = 0.941$

Similarly, for each feature

$$H(X \mid Outlook) = 0.694$$
$$H(X \mid Temperature) = 0.911$$
$$H(X \mid Humidity) = 0.789$$
$$H(X \mid Wind) = 0.892$$

Information Gain is:

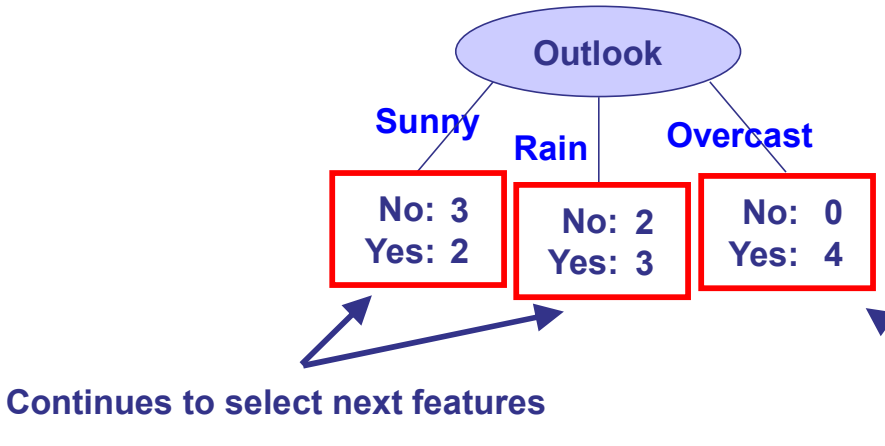
$$Gain(X, Outlook) = 0.247$$
$$Gain(X, Temperature) = 0.030$$
$$Gain(X, Humidity) = 0.152$$
$$Gain(X, Wind) = 0.049$$

Recall:

$$Gain(X, A) = H(X) - H(X \mid A)$$

DT: Example

- Next Step
  - Repeat the steps for each sub-branch
  - Until there is no ambiguity
    (all samples are of the same class)



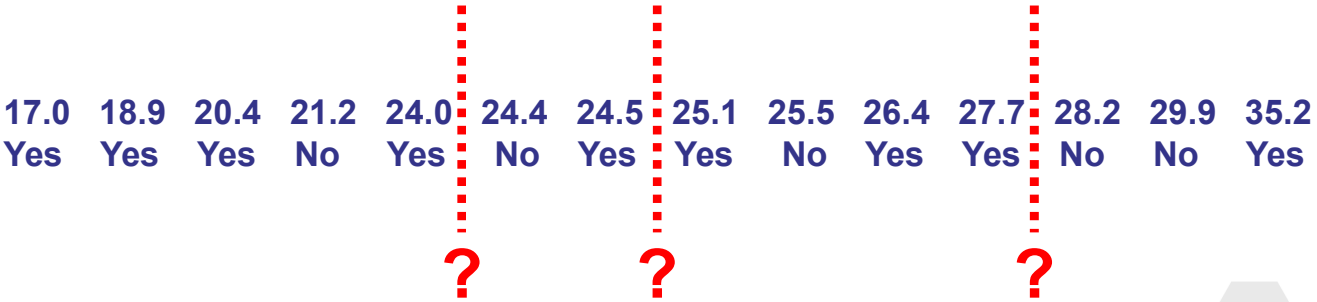
DT: Continuous-Valued Feature

- So far, we handle features with categorial values
- How to build a decision tree whose features are numerical?

Day	Outlook	Temperature	Humidity	Wind	PlayTennis
D1	Sunny	29.9	High	Weak	No
D2	Sunny	28.2	High	Strong	No
D3	Overcast	35.2	High	Weak	Yes
D4	Rain	26.4	High	Weak	Yes
D5	Rain	18.9	Normal	Weak	Yes
D6	Rain	21.2	Normal	Strong	No
D7	Overcast	20.4	Normal	Strong	Yes
D8	Sunny	24.4	High	Weak	No
D9	Sunny	17.0	Normal	Weak	Yes
D10	Rain	25.1	Normal	Weak	Yes
D11	Sunny	24.0	Normal	Strong	Yes
D12	Overcast	24.5	High	Strong	Yes
D13	Overcast	27.7	Normal	Weak	Yes
D14	Rain	25.5	High	Strong	No

DT: Continuous-Valued Feature

- Accomplished by partitioning the continuous attribute value into a discrete set of intervals
- A new Boolean feature A_c ($A < c$) can be created, c is the threshold
- How to select the best value for c?



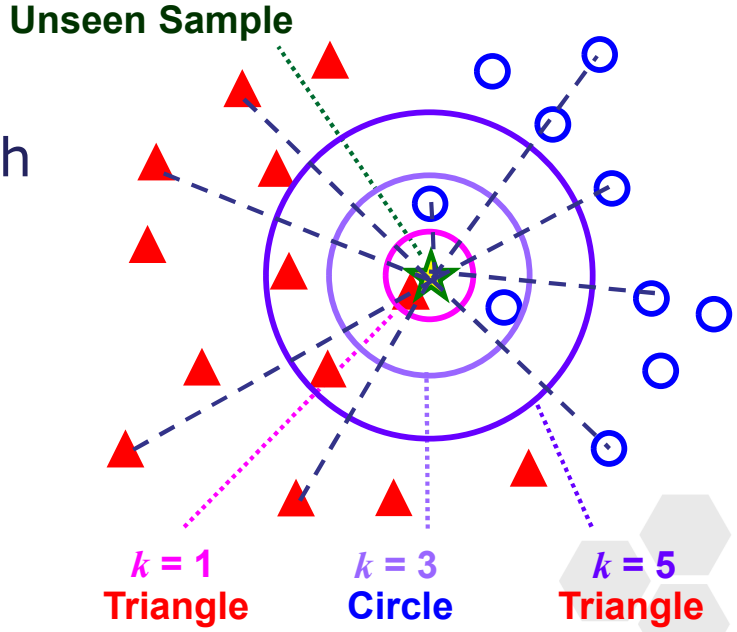
DT: Continuous-Valued Feature

- Objective is to minimize the entropy (or maximize the information gain)
- Entropy only needs to be evaluated between points of different classes

- Best c is: $c^* = \arg\max_c Gain(X, A_c)$

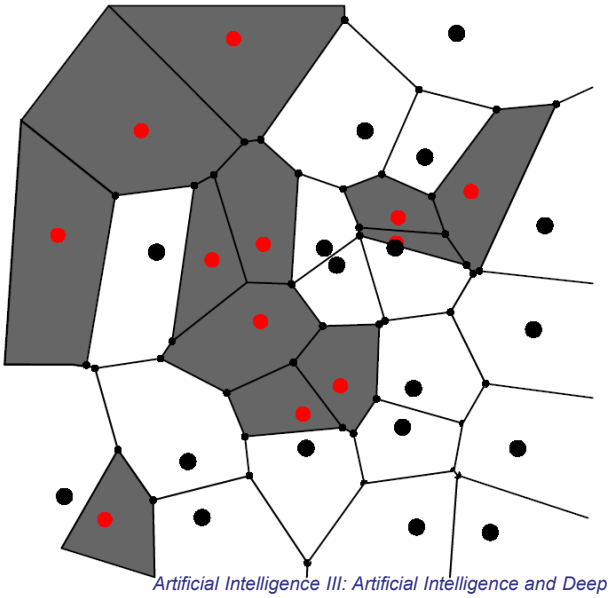
K-Nearest Neighbor (K-NN)

- A new pattern is classified by a majority vote of its k nearest neighbors (training samples)
- n distances are calculated for each new sample
  - n: the number of training samples



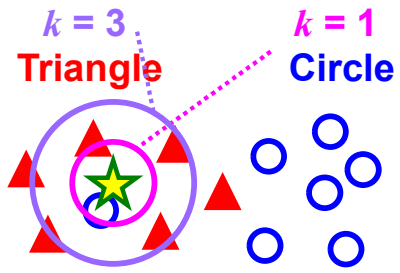
K-Nearest Neighbor (K-NN)

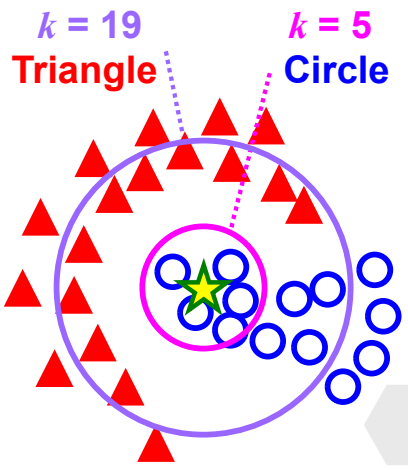
- Target function for the entire space may be described as a combination of less complex local approximations



K-Nearest Neighbor (K-NN)

- How to determine k?
  - Small k
    - Noise Sensitive
  - Large k
    - Neighbours may be too far away from the unseen sample
      - Less representative





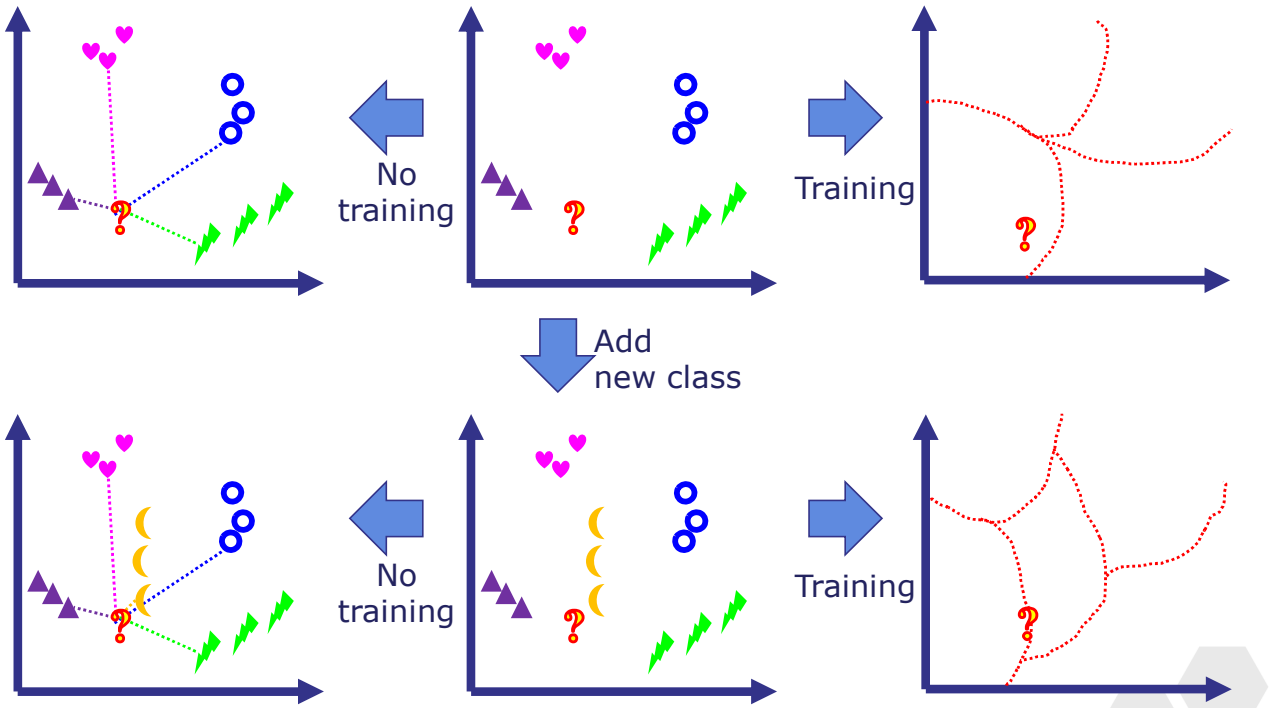
K-NN: Characteristic

- Advantages:
  - Very simple
  - No training is needed
    - All computations deferred until classification
- Disadvantages:
  - Difficult to determine k
  - Affected by noisy training data
  - Classification is time consuming
    - Need to calculate the distance between the unseen sample and each training sample

K-NN: Advanced Discussion

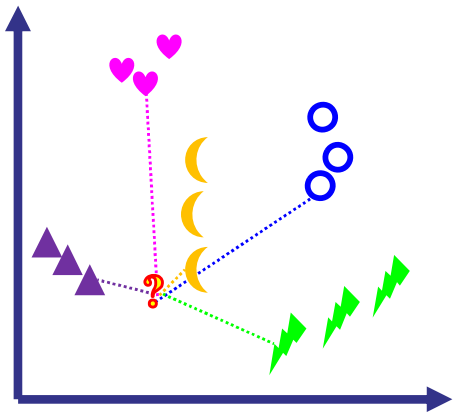
- No need for training is a significant advantage
- Which applications need it?
- Classes update frequently
- E.g. Face Recognition
  - When face images of a new user is added, will the system be re-trained?
  - How can adding a new class without retraining be possible?

K-NN: Advanced Discussion



Query-based Framework

- **Query-based framework**
  - K-nn mechanism

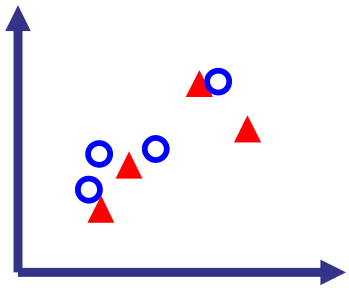


Gallery: reference samples, which are few good quality samples representing a class

Query: unseen sample

Space

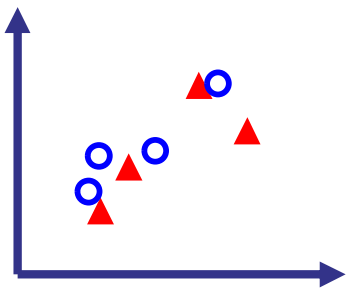
- However, in the original feature space, are samples that are more similar to each other more likely to belong to the same class?



- K-NN may not be useful in the original feature space

Metric Learning

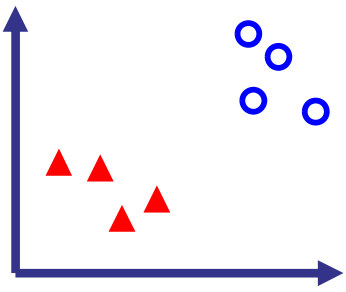
- **Metric Learning**: Aim to obtain a space which fulfills a certain measure
  - E.g. get closer > higher change to be the same class



Original (input) Space

- K-NN may not work well here

Mapping by Metric Learning model

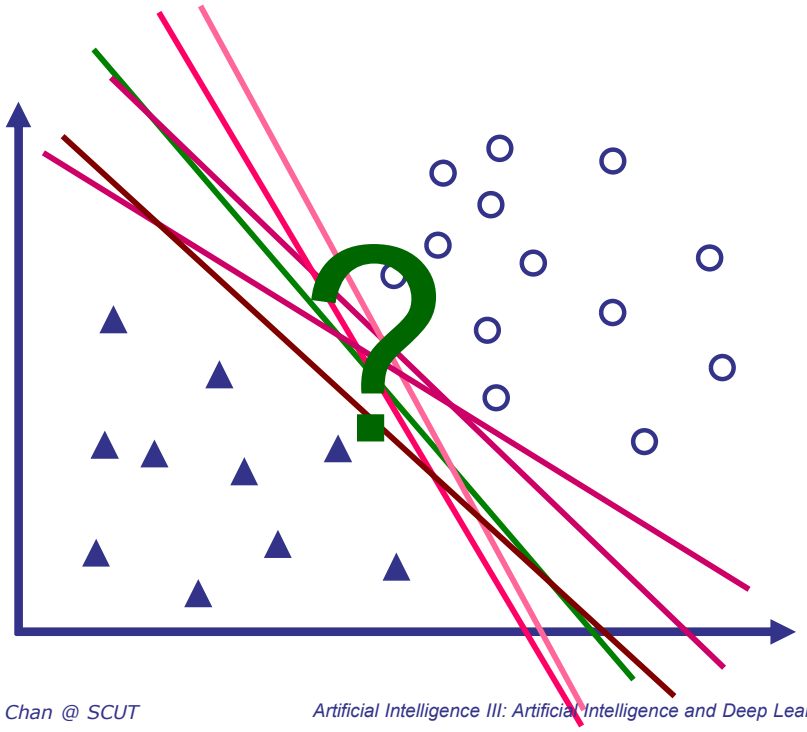


Feature Space

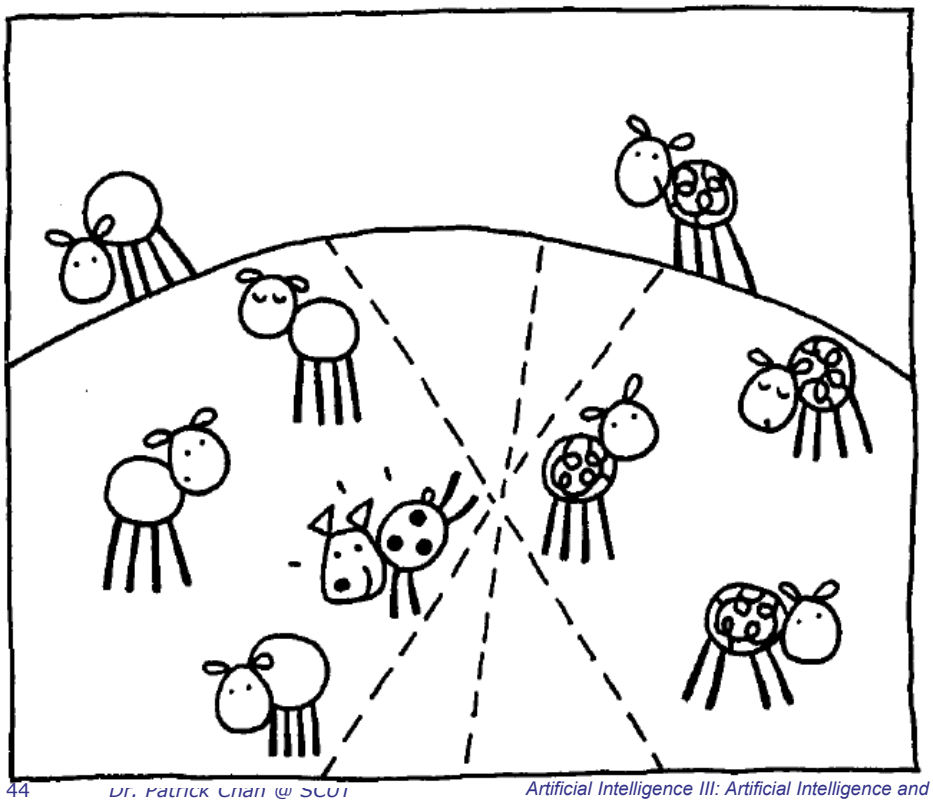
- Good for K-NN

Support Vector Machine (SVM)

- Which one is the **best** linear separator?



Support Vector Machine (SVM)



A clever sheep dog who was herding his sheep…

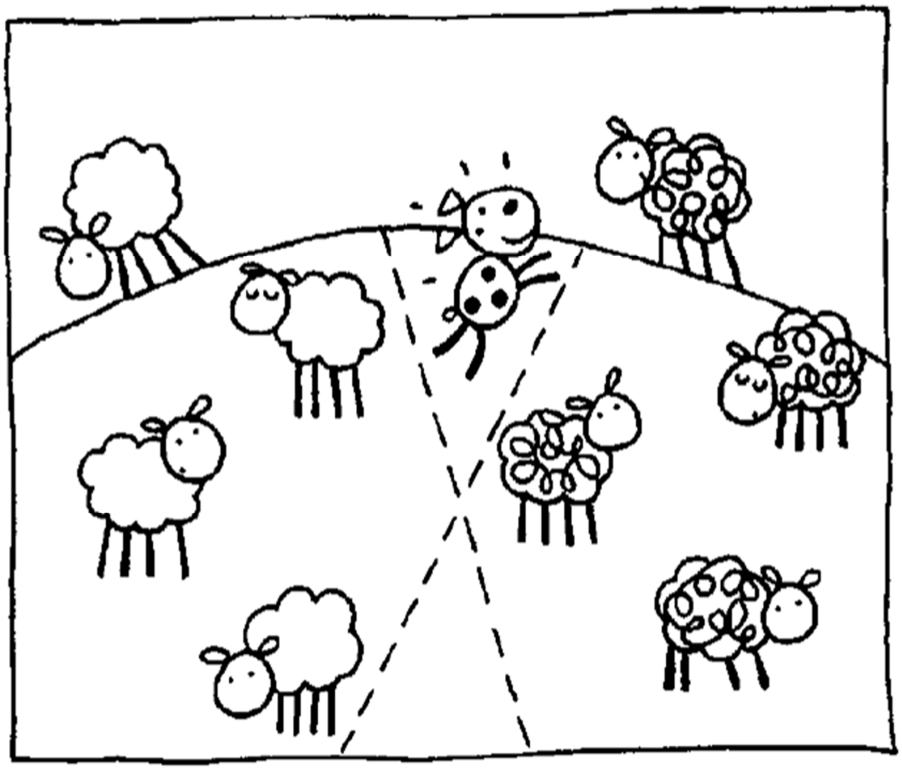
It runs between the sheep and tries to separate the black sheep and white sheep

Clever Sheep dog

White Sheep

Black Sheep

Support Vector Machine (SVM)

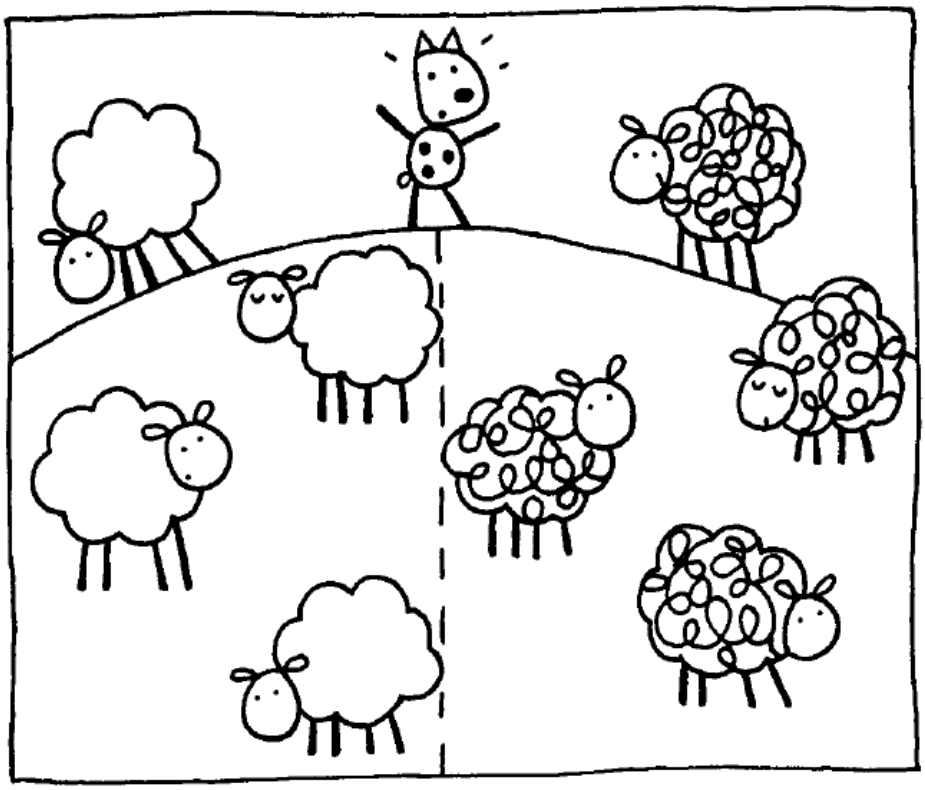


The sheep dog keeps running…

The sheep start to grow wools…

The dog feel the gap between black sheep and white sheep is narrower…

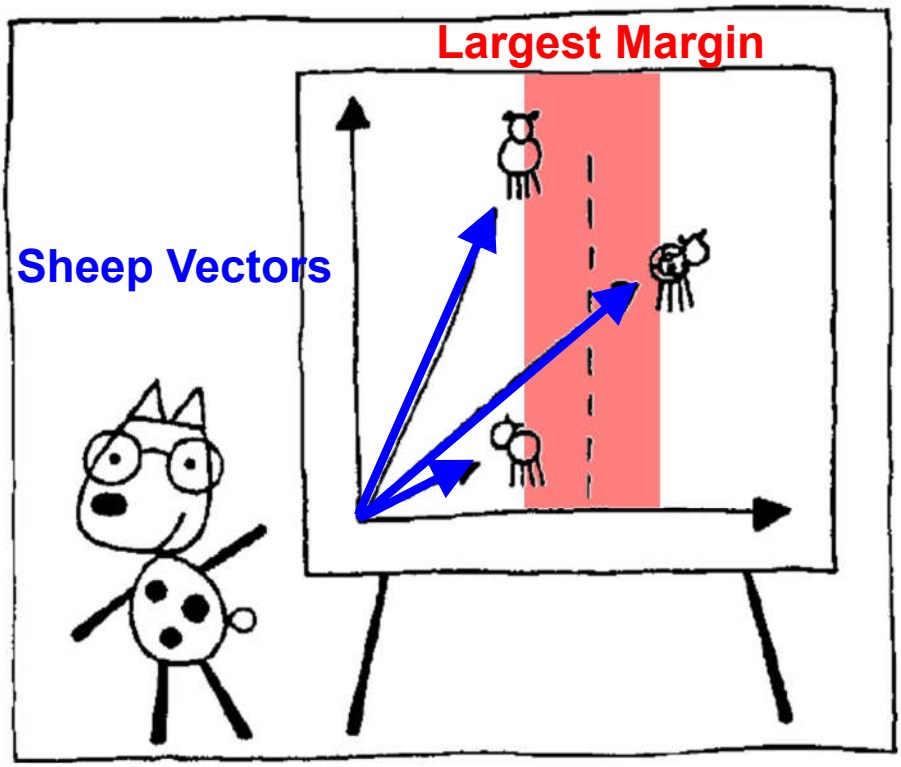
Support Vector Machine (SVM)



The wools become bigger and bigger…

Finally, only one path is left..

Support Vector Machine (SVM)



The sheep found out that the single path relies only on the some sheep.

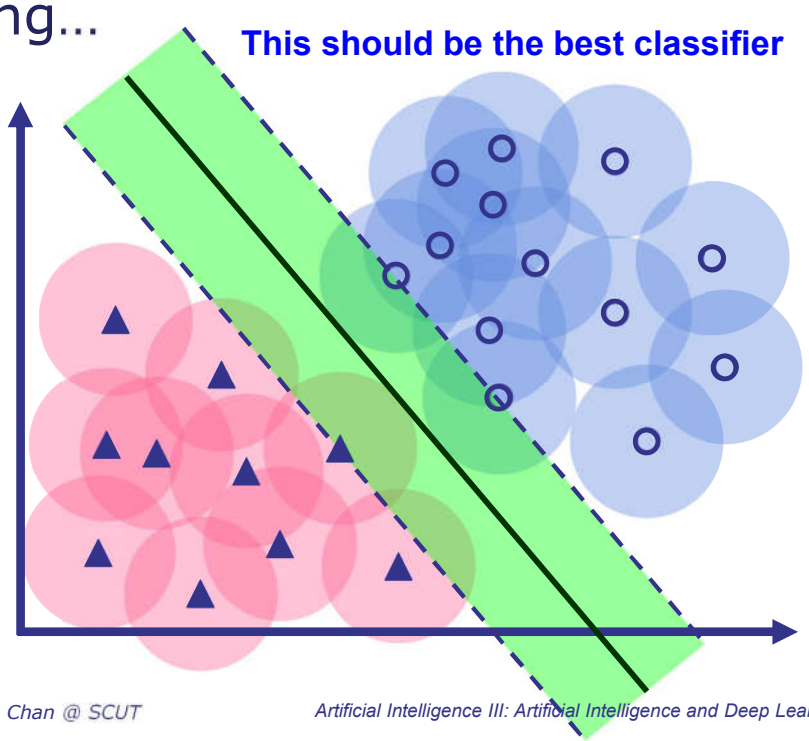
These sheep are "sheep vectors"

** "Support vector" in SVM*

From: Learning with Kernels, Scholkopf & Smola

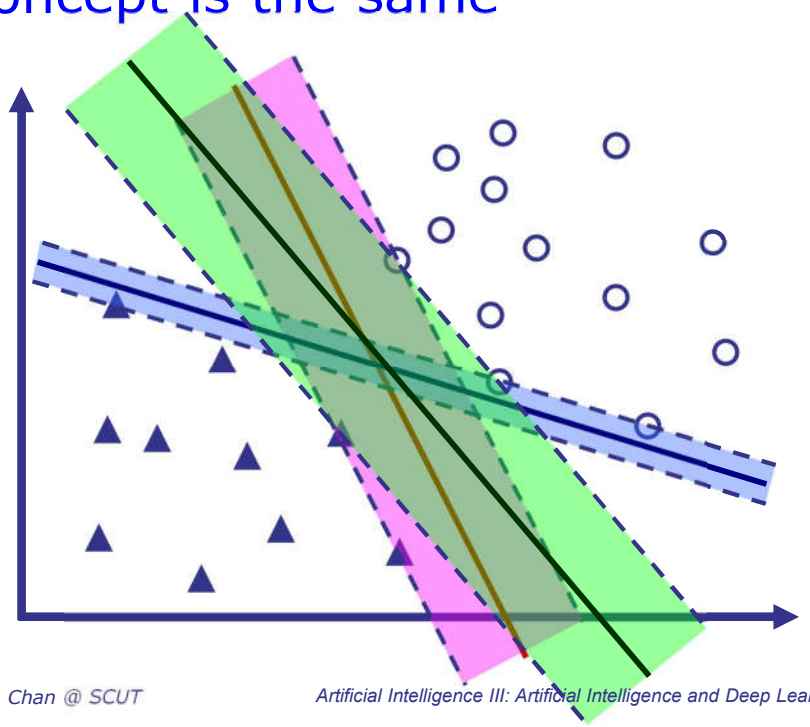
Support Vector Machine (SVM)

- Similar to the sheep, if a sample is growing…



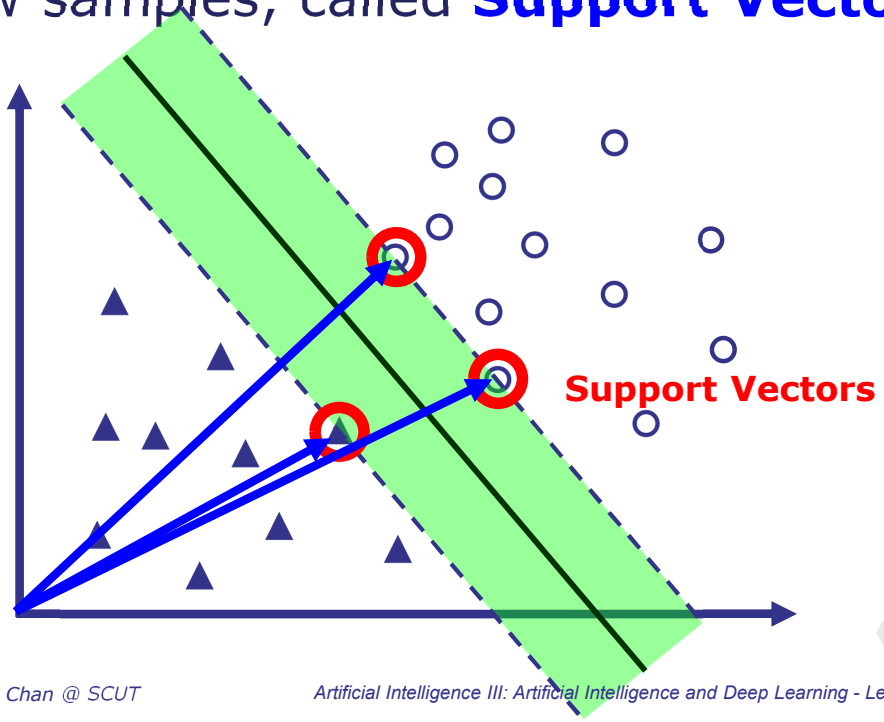
Support Vector Machine (SVM)

- A classifier with the largest margin
- The concept is the same



Support Vector Machine (SVM)

- Maximum Margin Classifier ONLY depends on few samples, called **Support Vectors**



Support Vector Machine (SVM)

- SVM has a solid and strong mathematics background
- Only the concept of SVM is focused in this course

SVM: Linearly Separable

- Problem can be formulated as Quadratic Optimization Problem and solve for w and b

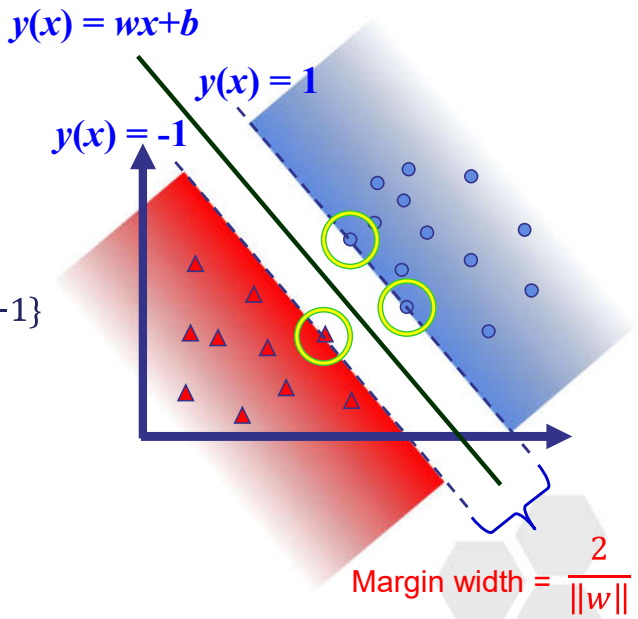
Margin Width

$$\underset{w,\ b}{\text{minimize}} \quad \frac{1}{2}\|w\|^2$$

$$\text{subject to} \quad y_i(w^T x_i + b) \geq 1$$

$$\text{where} \quad i = 1 \ldots n \quad \text{and} \quad y = \{1, -1\}$$

All samples should be behind the margin



SVM: Linearly Separable

- This optimization problem can be formulated as **Dual Problem** using Lagrangian method:

$$\begin{aligned} &\underset{w,\,b}{\text{minimize}} && \frac{1}{2}\|w\|^2 \\ &\text{subject to} && y_i(w^T x_i + b) \geq 1 \\ &\text{where} && i = 1 \ldots n \quad \text{and} \\ & && y = \{1, -1\} \end{aligned}$$

$$\underset{\alpha}{\text{Maximum}} \quad \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j x_i^T x_j$$

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

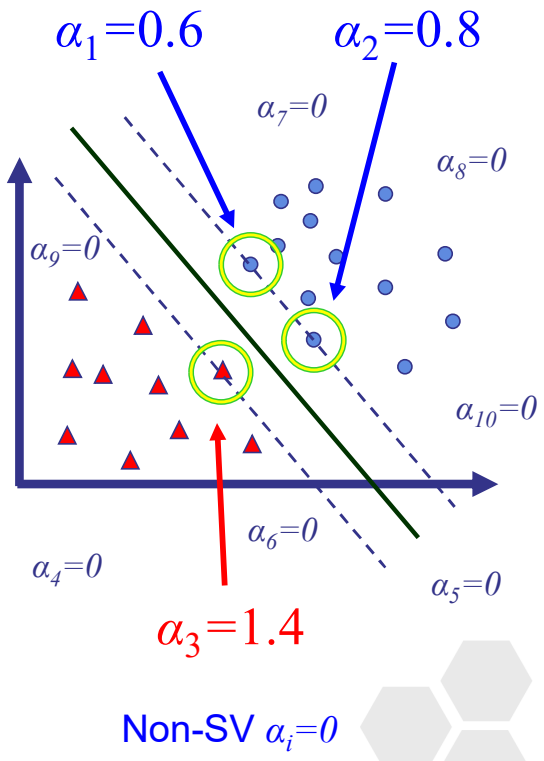
- Weight is determined by: $w = \sum_{i=1}^{n} \alpha_i y_i x_i$

SVM: Linearly Separable

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

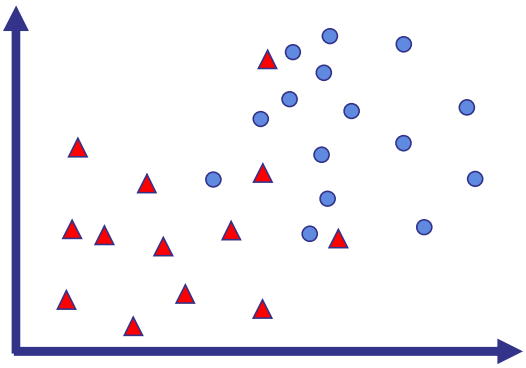
- Many α_i are zero
- x_i with non-zero α_i are **support vectors (SV)**
  - The decision boundary is determined only by the SV
- Let t_j (i = 1, ..., l) be the indices of the support vectors.

$$w = \sum_{j=1}^{l} \alpha_{t_j} y_{t_j} x_{t_j}$$



SVM: Non-Linearly Separable

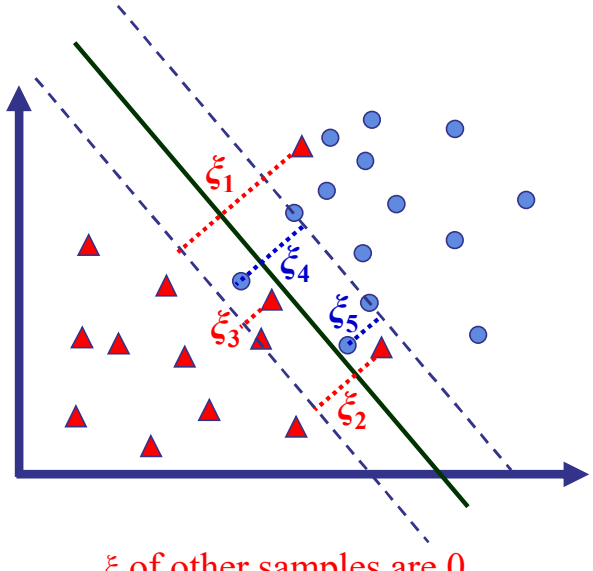
- How about Non-Linearly Separable Case?
  - The margin cannot be defined anymore



- Two approaches:
  - Add a slack variables
  - Use a kernel (Non-Linear SVM)

Slack Variable

$\xi_1 > 1$ **Error**
$\xi_2 > 1$ **Error**
$\xi_3 < 1$ **Correct**
$\xi_4 > 1$ **Error**
$\xi_5 < 1$ **Correct**



ξ of other samples are 0

- **Slack Variable (ξ)** is added as a punishment to allow a sample in / far away from the margin
- Optimalization:

Margin Width — Punishment

$$\underset{w,\,b}{\text{Minimize}} \quad \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{N}\xi_i$$

$$\text{subject to} \quad y_i(w^T x_i + b) \geq 1 - \xi_i \qquad i = 1 \ldots N$$

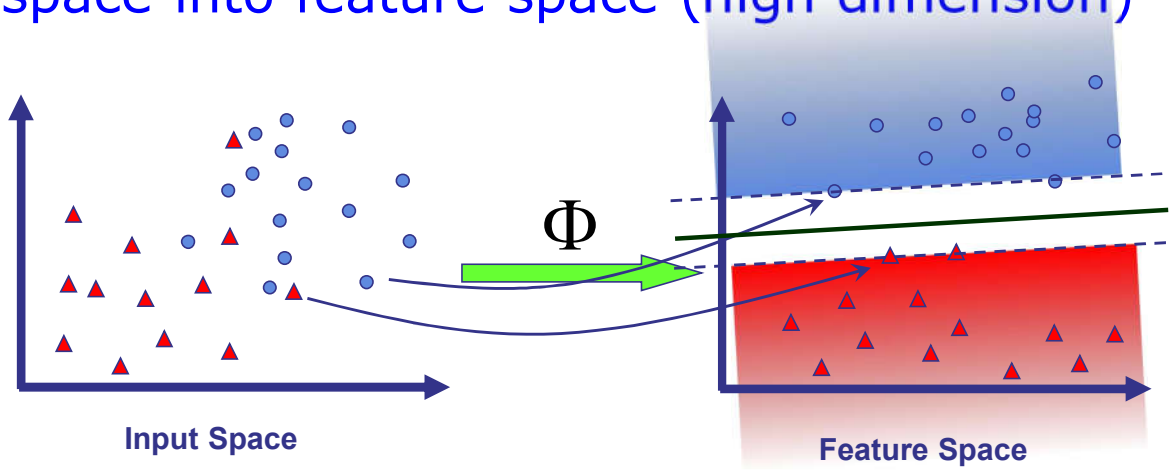
$$\xi_i \geq 0$$

Punishment allow a sample not behind the margin

where
C : tradeoff parameter between error and margin

SVM: Non-Linearly Separable
Kernel Method

- Kernel is a function which maps input space into feature space (high dimension)



- Construct linear SVM in feature space

SVM: Non-Linearly Separable
Kernel Method

- Similar to the linearly separable case but change all inner products to kernel functions

$$\begin{aligned} \underset{w,\, b}{\text{minimize}} \quad & \frac{1}{2}\|w\|^2 \\ \text{subject to} \quad & y_i(w^T\varphi(x_i) + b) \geq 1 \qquad i = 1 \ldots N \end{aligned}$$

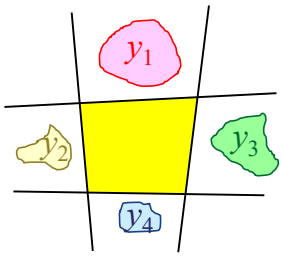
$$\begin{aligned} \underset{\alpha}{\text{maximum}} \quad & \sum_{i=1}^{n} \alpha_i - \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j K(x_i, x_j) \\ \text{subject to} \quad & \alpha_i \geq 0 \qquad i = 1 \ldots n \quad \text{and} \quad \sum_{i=1}^{n} \alpha_i y_i = 0 \end{aligned}$$

SVM: Multi-Class Problem

- SVM is a binary classifier
- How to handle multi-class problem?
  - g in LDF can be formulated as the estimation on posterior probability to a class
  - However, SVM must considers two classes
    - Do not estimate the probability of a class
    - Max method cannot be applied to SVM

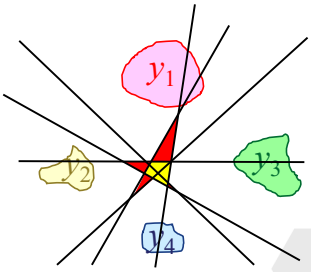
SVM: Multi-Class Problem

- How to handle multi-class problem?
  - **1-against-All**
    - 4-class example
      - C1 vs Non-C1, C2 vs Non-C2, C3 vs Non-C3, C4 vs Non-C4
    - c classifiers



1-against-All

  - **1-against-1**
    - 4-class example
      - C1 vs C2, C1 vs C3, C1 vs C4, C2 vs C3, C2 vs C4, C3 vs C4
    - c(c-1)/2 classifiers



1-against-1

SVM: Characteristic

- **Advantages**
  - Training is relatively easy
    - No local optimal
  - It scales relatively well to high dimensional data (inner product)
  - Tradeoff between classifier complexity and error can be controlled explicitly
- **Disadvantage**
  - Slow when the number of samples is large
  - Need to choose a "good" kernel function