Spring 2019

# CSEN1083: Data Mining

## *Classification (1)*

Seif Eldawlatly

# Classification (1)

- Reference for this Lecture:

"Pattern Recognition and Machine Learning," Christopher M. Bishop, Springer, 2006

# Supervised Learning

- Definition

  *The task of inferring a function from labeled data*

- Typically involves two phases
  - Training phase: Infer the function from provided input vectors and their corresponding labels
  - Test phase: Use the inferred function to predict the label of a new input vector (different from input vectors used during training)

- Formally

  Given a training dataset of $N$ observations $\{x_n\}$, where $n$ = 1, 2, …, $N$ together with the corresponding target values $\{t_n\}$, the goal is to predict the value of $t$ for a new value of $x$

# Examples of Classification Tasks

| Task | Attribute set, $\mathbf{x}$ | Class label, $t$ |
|---|---|---|
| Categorizing email messages | Features extracted from email message header and content | spam or non-spam |
| Identifying tumor cells | Features extracted from MRI scans | malignant or benign cells |
| Cataloging galaxies | Features extracted from telescope images | Elliptical, spiral, or irregular-shaped galaxies |

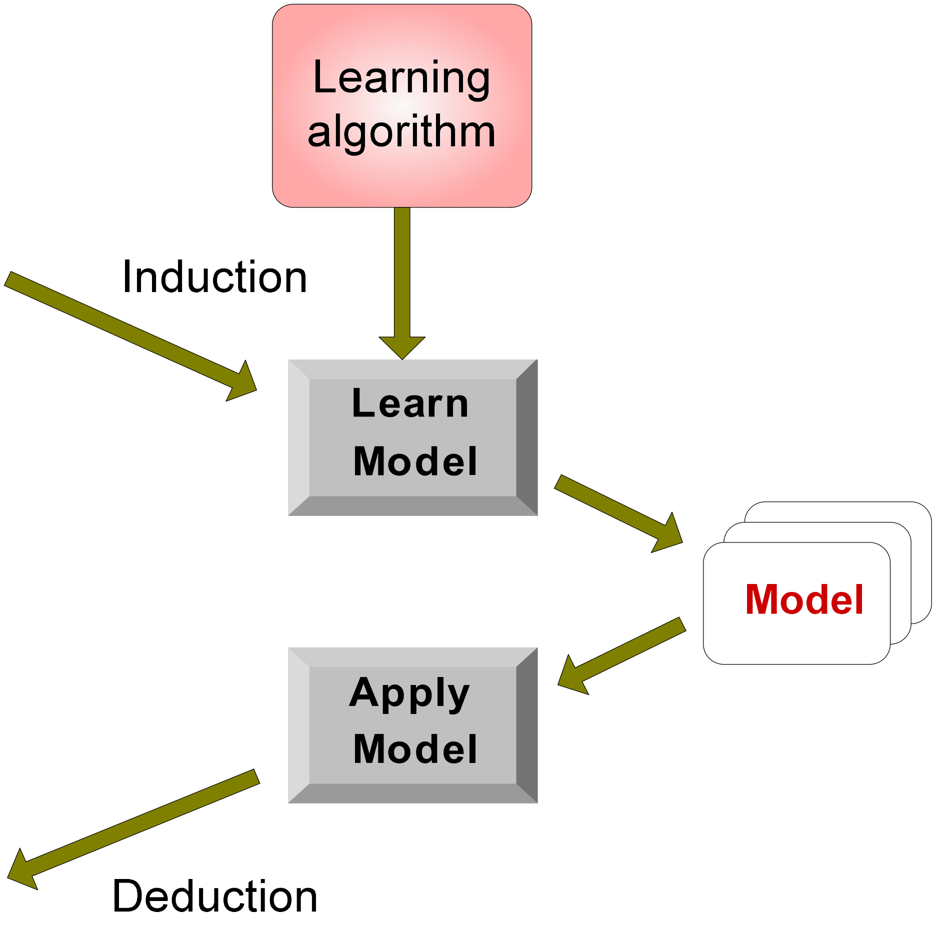
# General Approach

| *Tid* | Attrib1 | Attrib2 | Attrib3 | Class |
|---|---|---|---|---|
| 1 | Yes | Large | 125K | **No** |
| 2 | No | Medium | 100K | **No** |
| 3 | No | Small | 70K | **No** |
| 4 | Yes | Medium | 120K | **No** |
| 5 | No | Large | 95K | **Yes** |
| 6 | No | Medium | 60K | **No** |
| 7 | Yes | Large | 220K | **No** |
| 8 | No | Small | 85K | **Yes** |
| 9 | No | Medium | 75K | **No** |
| 10 | No | Small | 90K | **Yes** |

Training Set

| *Tid* | Attrib1 | Attrib2 | Attrib3 | Class |
|---|---|---|---|---|
| 11 | No | Small | 55K | **?** |
| 12 | Yes | Medium | 80K | **?** |
| 13 | Yes | Large | 110K | **?** |
| 14 | No | Small | 95K | **?** |
| 15 | No | Large | 67K | **?** |

Test Set



# Classification

- Classification

  Take an input $\mathbf{x}$ and assign it to one of $K$ discrete classes

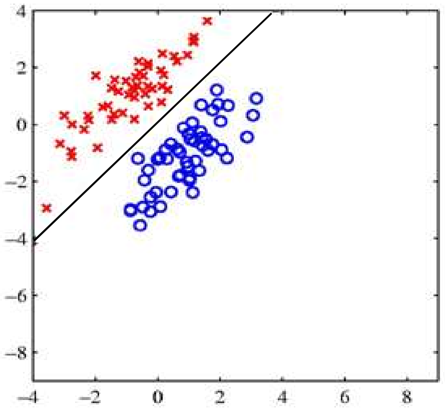
- Decision Boundary

  *A boundary (could be linear or non-linear) between two decision regions*

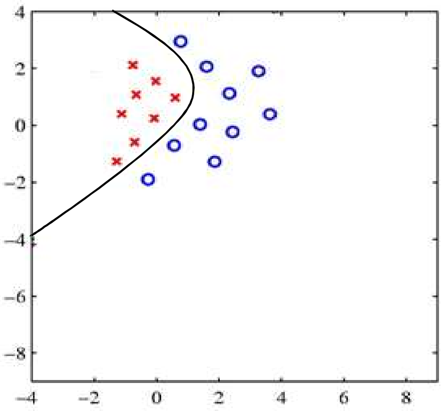
- Decision Regions:

  - Red or Blue, 1 or -1, Friend or Enemy

*Linearly Separable*



*Non-linearly Separable*



# Probabilistic Models for Classification

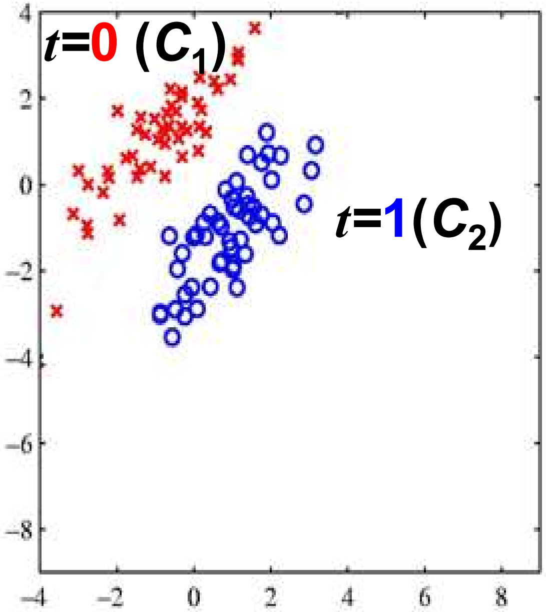
- Bayes' Theorem

$$p(C_k|\mathbf{x}) = \frac{p(\mathbf{x}|C_k)p(C_k)}{p(\mathbf{x})}$$

$p(C_k)$ : Prior probability

$p(\mathbf{x}|C_k)$ : Likelihood

$p(C_k|\mathbf{x})$ : Posterior probability (Knowing $\mathbf{x}$, what is the probability of $C_k$?)



# Probabilistic Models for Classification

- Example

$$p(C_k|\mathbf{x}) = \frac{p(\mathbf{x}|C_k)p(C_k)}{p(\mathbf{x})}$$

$$\overbrace{\phantom{\text{Non-smoker} \quad \text{Smoker}}}^{\mathbf{x}}$$

$C_k$

| | Non-smoker | Smoker | Total |
|---|---|---|---|
| Not cancer | 40 | 3 | 43 |
| Cancer | 7 | 10 | 17 |
| Total | 47 | 13 | 60 |

- If a patient is a smoker, would he have cancer?

$p$(Smoker|Cancer)=10/17, $p$(Cancer)=17/60, $p$(Smoker)=13/60

$$\left.\begin{array}{l} p(\text{Cancer|Smoker})=(10/17).(17/60)/(13/60)=10/13 \\ \\ p(\text{Not cancer|Smoker})=3/13 \end{array}\right\} \xrightarrow{max} C = \text{Cancer}$$

# Probabilistic Models for Classification

$$p(C_k|\mathbf{x}) = \frac{p(\mathbf{x}|C_k)p(C_k)}{p(\mathbf{x})}$$

- Inference Stage: Find $p(C_k|\mathbf{x})$
- Decision Stage: $k^* = \arg\max_k p(C_k|\mathbf{x})$

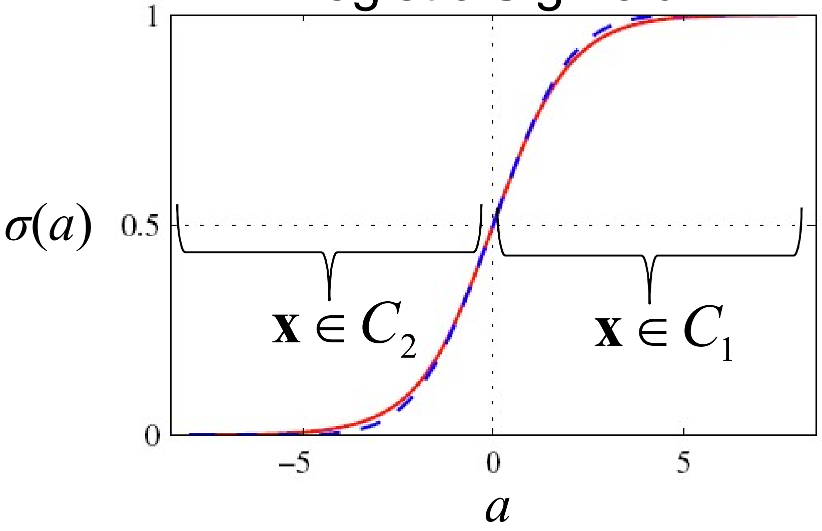
- Probabilistic Generative Model: Learns $p(\mathbf{x}|C_k)$ and $p(C_k)$
- Probabilistic Discriminative Model: Learns $p(C_k|\mathbf{x})$ directly

# Probabilistic Generative Models

- We first represent the posterior probability as

$$
\begin{aligned}
p(\mathcal{C}_1|\mathrm{x}) &= \frac{p(\mathrm{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\mathrm{x}|\mathcal{C}_1)p(\mathcal{C}_1)+p(\mathrm{x}|\mathcal{C}_2)p(\mathcal{C}_2)} \\
&= \frac{1}{1+\exp(-a)} = \sigma(a)
\end{aligned}
$$

Logistic Sigmoid



where

$$a = \ln \frac{p(\mathrm{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\mathrm{x}|\mathcal{C}_2)p(\mathcal{C}_2)}$$

If $a$ > 0 → $\frac{p(\mathrm{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\mathrm{x}|\mathcal{C}_2)p(\mathcal{C}_2)}$ >1 → $p(C_1|\mathbf{x}) > p(C_2|\mathbf{x})$ → $\mathbf{x} \in C_1$

If $a$ < 0 → $\frac{p(\mathrm{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\mathrm{x}|\mathcal{C}_2)p(\mathcal{C}_2)}$ <1 → $p(C_1|\mathbf{x}) < p(C_2|\mathbf{x})$ → $\mathbf{x} \in C_2$

# Probabilistic Generative Models

- Assume Gaussian distribution for class-conditional densities $p(\mathbf{x}|\mathcal{C}_k)$

$$p(\mathbf{x}|\mathcal{C}_k) = \frac{1}{(2\pi)^{D/2}}\frac{1}{|\boldsymbol{\Sigma}|^{1/2}}\exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_k)^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_k)\right\}$$

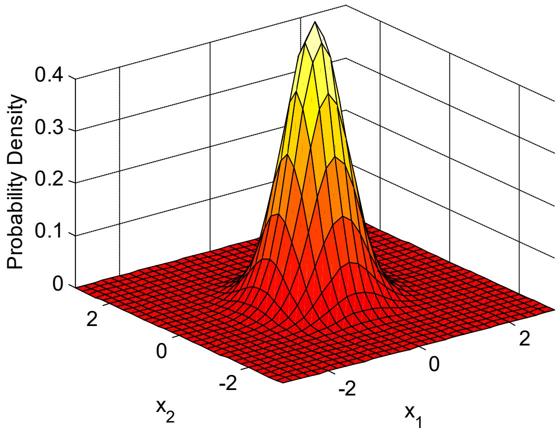
$\boldsymbol{\mu}_k$ : Mean

$\boldsymbol{\Sigma}$ : Covariance Matrix

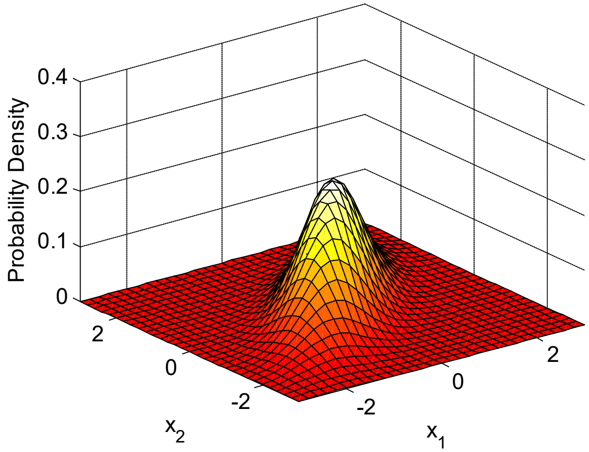
(Common for both classes)

- Example

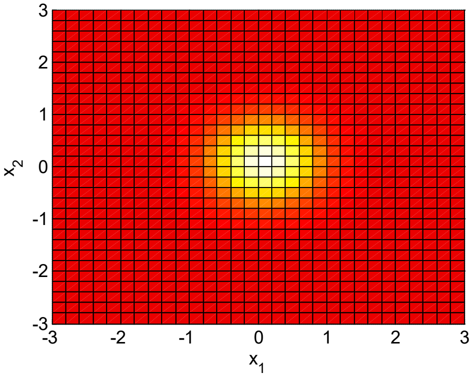
$p(\mathbf{x}|C_k)$



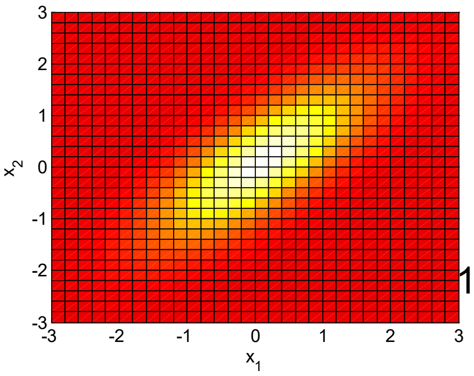
$p(\mathbf{x}|C_k)$



$$\Sigma = \begin{bmatrix} 0.3 & 0 \\ 0 & 0.3 \end{bmatrix}$$



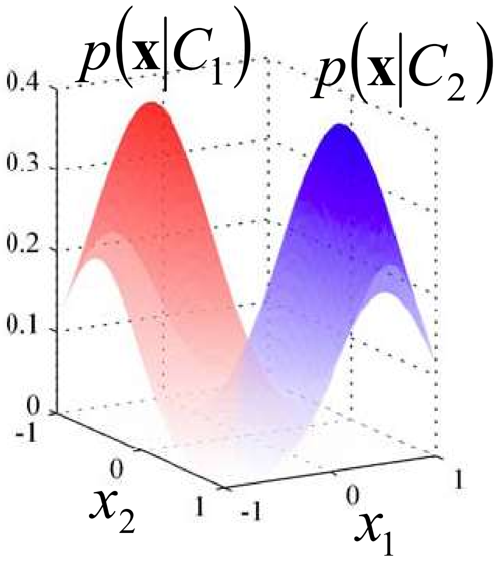
$$\Sigma = \begin{bmatrix} 1 & 0.75 \\ 0.75 & 1 \end{bmatrix}$$

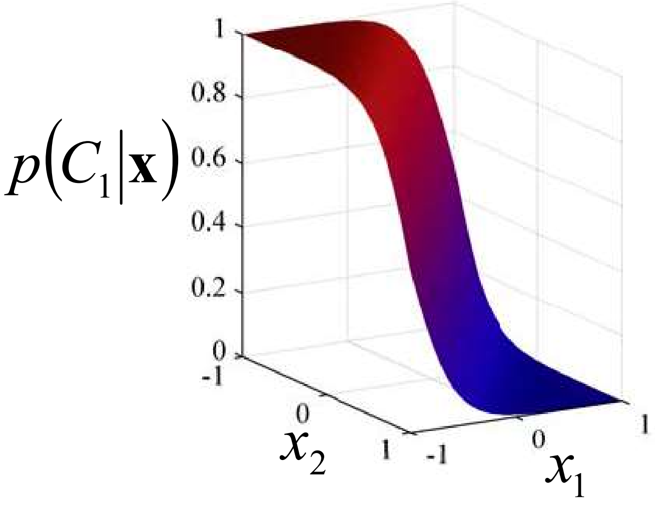


# Probabilistic Generative Models

- Using Gaussian assumption and logistic sigmoid representation, we can show that

$$p(\mathcal{C}_1|\mathbf{x}) = \sigma(\mathbf{w}^{\mathrm{T}}\mathbf{x} + w_0)$$





# Probabilistic Generative Models

- Using the previous assumptions and a training dataset $\{\mathbf{x}_n, t_n\}$, we can estimate the values of the parameters

$$\boldsymbol{\mu}_k \quad \boldsymbol{\Sigma} \quad p(\mathcal{C}_k)$$

- Maximum Likelihood Estimation (MLE)
    - Let $t_n$ = 1 denote class $C_1$ and $t_n$ = 0 denote class $C_2$
    - Let $p(\mathcal{C}_1) = \pi$ → $p(\mathcal{C}_2) = 1 - \pi$
    - For $\mathbf{x}_n \in C_1$

$$p(\mathbf{x}_n, \mathcal{C}_1) = p(\mathcal{C}_1)p(\mathbf{x}_n|\mathcal{C}_1) = \pi\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_1, \boldsymbol{\Sigma})$$

- For $\mathbf{x}_n \in C_2$

$$p(\mathbf{x}_n, \mathcal{C}_2) = p(\mathcal{C}_2)p(\mathbf{x}_n|\mathcal{C}_2) = (1 - \pi)\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_2, \boldsymbol{\Sigma})$$

# Probabilistic Generative Models

- Maximum Likelihood Estimation (MLE)
  - We define the likelihood of the data as the probability of observing the available data
  - Let $\mathbf{D}$ denote the available data, where $\mathbf{D} = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N\}$
  - The probability of observing the data $p(\mathbf{D})$ (Given the parameters)

$$p(\mathbf{D}) = p(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N)$$

  - Assuming independence between the input vectors

$$p(\mathbf{D}) = p(\mathbf{x}_1)p(\mathbf{x}_2) \ldots p(\mathbf{x}_N) = \prod_{n=1}^{N} p(\mathbf{x}_n) = \prod_{i=1}^{N_1} p(\mathbf{x}_i, C_1) \prod_{j=1}^{N_2} p(\mathbf{x}_j, C_2)$$

  - Given the assumption of the previous slide, the likelihood can be modeled as

$$p(\mathbf{t}|\pi, \boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \boldsymbol{\Sigma}) = \prod_{n=1}^{N} [\pi \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_1, \boldsymbol{\Sigma})]^{t_n} [(1-\pi)\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_2, \boldsymbol{\Sigma})]^{1-t_n}$$

# Maximum Likelihood Estimation

- MLE Solution:
  - Find the parameters that maximize the likelihood of the data
  - Given that the maximum of this function is achieved at the same value that maximizes the log of the function, we use the Log-likelihood of the function for convenience
  - Remember that $\ln(\mathrm{AB}) = \ln(\mathrm{A}) + \ln(\mathrm{B}), \ln(\mathrm{A}^m) = m \ln(\mathrm{A})$

$$\ln p(\mathbf{t}|\pi, \boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \Sigma) = \ln \prod_{n=1}^{N} \left[\pi \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_1, \Sigma)\right]^{t_n} \left[(1-\pi)\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_2, \Sigma)\right]^{1-t_n}$$

$$= \sum_{n=1}^{N} \ln\left(\left[\pi \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_1, \Sigma)\right]^{t_n} \left[(1-\pi)\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_2, \Sigma)\right]^{1-t_n}\right)$$

$$= \sum_{n=1}^{N} t_n \ln\left(\pi \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_1, \Sigma)\right) + (1-t_n)\ln\left((1-\pi)\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_2, \Sigma)\right)$$

$$= \sum_{n=1}^{N} t_n \ln(\pi) + t_n \ln\left(\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_1, \Sigma)\right) + (1-t_n)\ln((1-\pi)) + (1-t_n)\ln\left(\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_2, \Sigma)\right)$$

# Maximum Likelihood Estimation

$$\ln p\left(\mathbf{t}\middle|\pi,\boldsymbol{\mu}_1,\boldsymbol{\mu}_2,\Sigma\right)$$

$$=\sum_{n=1}^{N} t_n \ln(\pi\ ) + t_n \ln\left(\mathcal{N}\left(\mathbf{x}_n\middle|\boldsymbol{\mu}_1,\Sigma\right)\right) + (1-t_n)\ln\left((1-\pi)\ \right) + (1-t_n)\ln\left(\mathcal{N}\left(\mathbf{x}_n\middle|\boldsymbol{\mu}_2,\Sigma\right)\right)$$

- Derivative w.r.t. parameters and equate with zero

$\pi$

$$\pi = \frac{1}{N}\sum_{n=1}^{N} t_n = \frac{N_1}{N} = \frac{N_1}{N_1+N_2}$$

$\boldsymbol{\mu}_1$

$$\boldsymbol{\mu}_1 = \frac{1}{N_1}\sum_{n=1}^{N} t_n \mathbf{x}_n$$

$\boldsymbol{\mu}_2$

$$\boldsymbol{\mu}_2 = \frac{1}{N_2}\sum_{n=1}^{N} (1-t_n)\mathbf{x}_n$$

$\boldsymbol{\Sigma}$

$$\boldsymbol{\Sigma} = \frac{N_1}{N}\mathbf{S}_1 + \frac{N_2}{N}\mathbf{S}_2$$

$$\mathbf{S}_1 = \frac{1}{N_1}\sum_{n\in\mathcal{C}_1}(\mathbf{x}_n-\boldsymbol{\mu}_1)(\mathbf{x}_n-\boldsymbol{\mu}_1)^{\mathrm{T}}$$

$$\mathbf{S}_2 = \frac{1}{N_2}\sum_{n\in\mathcal{C}_2}(\mathbf{x}_n-\boldsymbol{\mu}_2)(\mathbf{x}_n-\boldsymbol{\mu}_2)^{\mathrm{T}}$$

- Using the expression in slide 8, $p(\mathcal{C}_1|\mathbf{x}) = \sigma(\mathbf{w}^{\mathrm{T}}\mathbf{x} + w_0)$ can be obtained

# Naïve Bayes Classifier

- Sometimes it’s difficult to estimate $p(\mathbf{x}|C_k)$ for high dimensional data
- Naïve Bayes approximation

$$p(\mathbf{x}|C_k) \approx \prod_{j=1}^{D} p(x_j|C_k)$$

where $D$ is the dimensionality of the input data

- For Gaussian conditional density

$$p(\mathbf{x}|C_k) = N(\mathbf{x}|\mu, \Sigma) \approx \prod_{j=1}^{D} p(x_j|C_k) = \prod_{j=1}^{D} N(x_j|\mu_j, \sigma_j^2)$$

# Naïve Bayes Classifier

- Example:

Consider the data about car theft given in the table below

| Example No. | Color | Type | Origin | **Stolen?** |
|---|---|---|---|---|
| 1 | Red | Sports | Domestic | **Yes** |
| 2 | Red | Sports | Domestic | **No** |
| 3 | Red | Sports | Domestic | **Yes** |
| 4 | Black | Sports | Domestic | **No** |
| 5 | Black | Sports | Imported | **Yes** |
| 6 | Black | SUV | Imported | **No** |
| 7 | Black | SUV | Imported | **Yes** |
| 8 | Black | SUV | Domestic | **No** |
| 9 | Red | SUV | Imported | **No** |
| 10 | Red | Sports | Imported | **Yes** |

Using Naïve Bayes classifier, predict whether a Red Domestic SUV is stolen or not. Note that since the data is discrete, you can use the frequentist statistics to compute the needed probabilities.

# Naïve Bayes Classifier

- Solution:

Since the goal is to classify a Red Domestic SUV as stolen or not, we first define two classes $C_1$ and $C_2$, corresponding to Stolen = Yes and Stolen = No, respectively.

To classify the given car with attributes $\mathbf{x}$, we need to compute $p(C_1|\mathbf{x})$:

*p*(Stolen = Yes | Color = Red, Type = SUV, Origin = Domestic)

and $p(C_2|\mathbf{x})$:

*p*(Stolen = No | Color = Red, Type = SUV, Origin = Domestic)

and find which conditional probability is larger. If the first one is larger, then our prediction is Stolen = Yes. If the second one is larger, then our prediction is Stolen = No. Note that $\mathbf{x}$ here is 3 dimensional corresponding to Color, Type and Origin.

# Naïve Bayes Classifier

Since $p(C_1|\mathbf{x}) = \dfrac{p(\mathbf{x}|C_1)p(C_1)}{p(\mathbf{x})}$

We need to compute $p(\mathbf{x}|C_1)$ = *p*(Color = Red, Type = SUV, Origin = Domestic | Stolen = Yes).

Using the Naïve Bayes assumption which assumes that the dimensions of the input data (the attributes of the car) are independent, we can re-write $p(\mathbf{x}|C_1)$ as

$$p(\mathbf{x}|C_1) = \prod_{i=1}^{D} p(x_i|C_1)$$

= *p*(Color = Red | Stolen = Yes) *p*(Type = SUV | Stolen = Yes) *p*(Origin = Domestic | Stolen = Yes)

Similarly, $p(\mathbf{x}|C_2)$ can be re-written as $p(\mathbf{x}|C_2) = \prod_{i=1}^{D} p(x_i|C_2)$

= *p*(Color = Red | Stolen = No) *p*(Type = SUV | Stolen = No) *p*(Origin = Domestic | Stolen = No)

# Naïve Bayes Classifier

- From the available data in the table and using frequentist statistics:

*p*(Color = Red | Stolen = Yes) = 3/5 (out of the 5 stolen cars, 3 were red)
*p*(Color = Red | Stolen = No) = 2/5 (out of the 5 non-stolen cars, 2 were red)
*p*(Type = SUV | Stolen = Yes) = 1/5 (out of the 5 stolen cars, 1 was SUV)
*p*(Type = SUV | Stolen = No) = 3/5
*p*(Origin = Domestic | Stolen = Yes) = 2/5
*p*(Origin = Domestic | Stolen = No) = 3/5

Therefore,
*p*(Color = Red | Stolen = Yes) *p*(Type = SUV | Stolen = Yes) *p*(Origin = Domestic | Stolen = Yes) = (3/5) x (1/5) x (2/5) = 0.048

And
*p*(Color = Red | Stolen = No) *p*(Type = SUV | Stolen = No) *p*(Origin = Domestic | Stolen = No) = (2/5) x (3/5) x (3/5) = 0.144

Also *p*(Stolen = Yes) = 5/10 and *p*(Stolen = No) = 5/10

# Naïve Bayes Classifier

To classify the given car, we need to compare $p(C_1|\mathbf{x})$ to $p(C_2|\mathbf{x})$ such that

If $\frac{p(C_1|\mathbf{x})}{p(C_2|\mathbf{x})} > 1$ then $\mathbf{x} \in C_1$ , otherwise $\mathbf{x} \in C_2$

$$\because \frac{p(C_1|\mathbf{x})}{p(C_2|\mathbf{x})} = \frac{p(\mathbf{x}|C_1)p(C_1)}{p(\mathbf{x}|C_2)p(C_2)}$$

Therefore, for the this problem

$$\frac{p(C_1|\mathbf{x})}{p(C_2|\mathbf{x})} = \frac{p(\mathbf{x}|C_1)p(C_1)}{p(\mathbf{x}|C_2)p(C_2)} = \frac{0.048 \times 0.5}{0.144 \times 0.5} = 0.333$$

Therefore, our prediction is $C_2$ which is that the car is not stolen.

# Probabilistic Discriminative Models

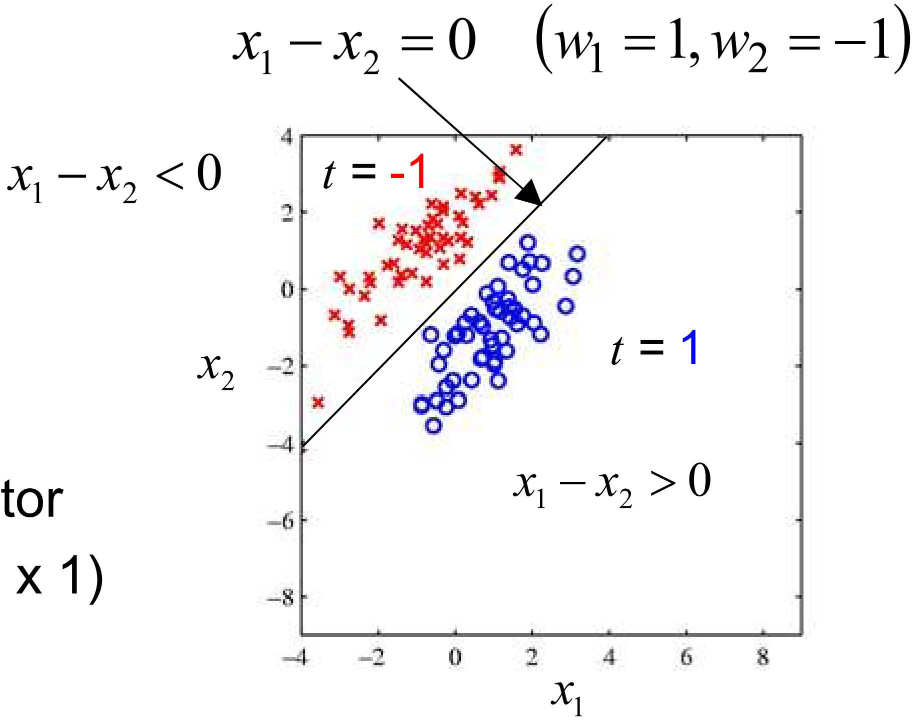
- For the case of two classes

$$y(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + w_0$$

$\mathbf{x}$ : Input vector

$\mathbf{w}$: Weight vector

$w_\mathbf{0}$: bias



- For this example, $\mathbf{w}$ is a (2 x 1) vector and each input vector $\mathbf{x}$ is also a (2 x 1) vector

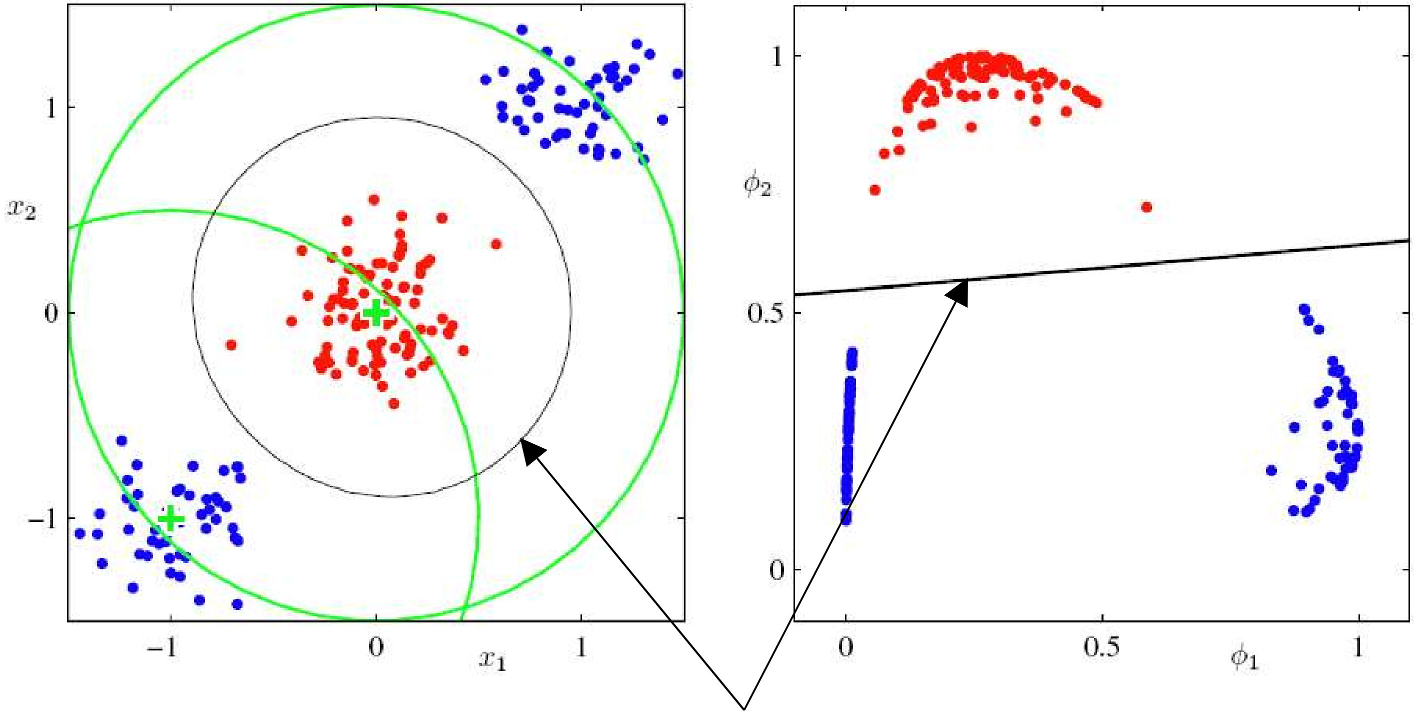
$$y(\mathbf{x}) = \begin{bmatrix} w_1 & w_2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + w_0$$

If the total number of input vectors is 100, then the input dataset consists of $\mathbf{x}_1$, $\mathbf{x}_2$, $\mathbf{x}_3$, …, $\mathbf{x}_{100}$, where $\mathbf{x}_i = [x_{i1}, x_{i2}]$ , $i = 1{:}100$

- Decision Surface is a hyperplane

# Probabilistic Discriminative Models

- Learn $p(C_k|\mathbf{x})$ directly
- Using a nonlinear transformation of the data $\phi(\mathbf{x})$ (basis function)



Decision Boundary

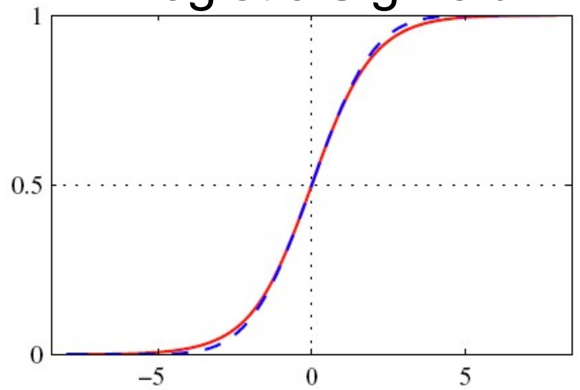
# Logistic Regression

- Assumption

$$p(\mathcal{C}_1|\phi) = y(\phi) = \sigma\left(\mathrm{w}^{\mathrm{T}}\phi\right)$$

where $\sigma(a) = \dfrac{1}{1+\exp(-a)}$

Logistic Sigmoid



- Logistic Regression vs. MLE for Gaussian Generative Model (For 2 classes)
  - No. of Parameters for Logistic Regression: $D$ parameters
  - No. of Parameters for MLE: $D(D+5)/2 + 1$ parameters

$$\begin{tikzcd} \mu_k \arrow[d] & \Sigma \arrow[d] & p(\mathcal{C}_k) \arrow[d] \\ 2D & D(D+1)/2 & 1 \end{tikzcd}$$

# Logistic Regression

$$p(\mathcal{C}_1|\phi) = y(\phi) = \sigma\left(\mathbf{w}^{\mathrm{T}}\phi\right)$$

- Using maximum likelihood to estimate $\mathbf{w}$ from the training dataset $\{\boldsymbol{\varphi}_n, t_n\}$. Likelihood function

$$p(\mathbf{t}|\mathbf{w}) = \prod_{n=1}^{N} y_n^{t_n} \left\{1 - y_n\right\}^{1-t_n}$$

- Minimizing the negative of the log-likelihood is equivalent to maximizing the log-likelihood

$$E(\mathbf{w}) = -\ln p(\mathbf{t}|\mathbf{w}) = -\sum_{n=1}^{N} \left\{t_n \ln y_n + (1 - t_n)\ln(1 - y_n)\right\}$$

# Logistic Regression

- We make use of the property

$$\frac{d\sigma}{da} = \sigma(1-\sigma)$$

- Take the derivative of $E(\mathbf{w})$ w.r.t. $\mathbf{w}$

$$\begin{aligned}\nabla E(\mathbf{w}) &= -\sum_{n=1}^{N}\left\{t_n \frac{1}{\sigma_n}\sigma_n(1-\sigma_n)\phi_n + (1-t_n)\frac{1}{1-\sigma_n}(-\sigma_n(1-\sigma_n))\phi_n\right\} \\ &= -\sum_{n=1}^{N}\{t_n(1-\sigma_n)\phi_n - (1-t_n)\sigma_n\phi_n\} \\ &= \sum_{n=1}^{N}(y_n - t_n)\phi_n\end{aligned}$$

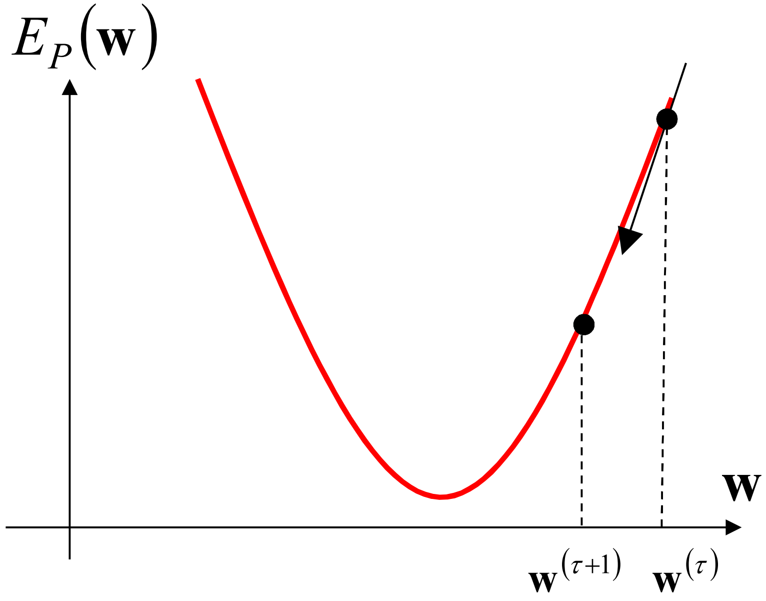
- Optimal $\mathbf{w}$ can be found using gradient descent

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta\frac{\partial E}{\partial \mathbf{w}^{(\tau)}}$$

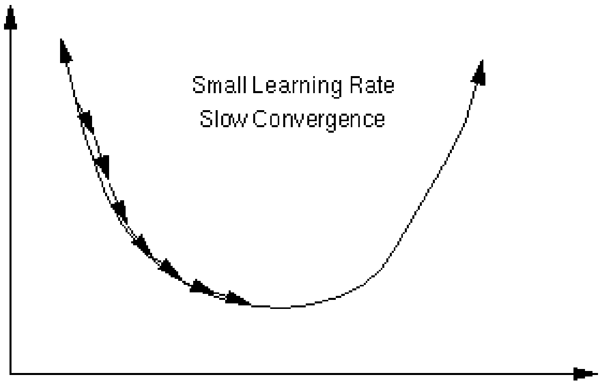
where $\eta$ is the learning rate parameter

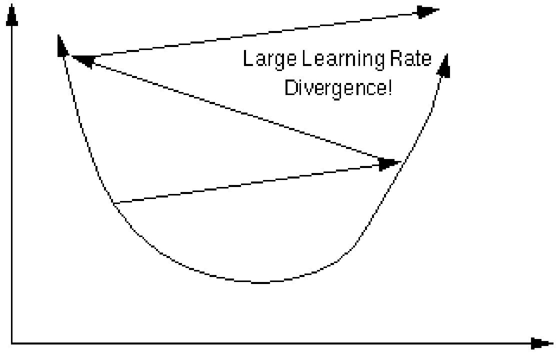
# Logistic Regression

- Consider a 1-dimension $\mathbf{w}$:



$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta \frac{\partial E_P}{\partial \mathbf{w}^{(\tau)}} = \mathbf{w}^{(\tau)} - \eta \sum_{n=1}^{N} \left( y_n - t_n \right) \varphi_n$$


Small Learning Rate
Slow Convergence


Large Learning Rate
Divergence!