# 02\_Classification\_using\_Bayes\_Theory

# 2.1 Bayes Decision Theory 贝叶斯决策理论

#### **Basic Assumptions**

- The decision problem is posed in probabilistic terms.
- ALL relevant probability values are known.

#### 2.1.1 Process

- Given:
  - 1. A test sample x.
    - Contains features  $x = [x_1, x_2, \dots x_l]^T$ .
    - Often reduced, removed some non-discriminative (un-useful) features.
  - 2. A list of classes/patterns  $\omega = \{\omega_1, \omega_2, \dots \omega_c\}$ .
    - Defined by human-being.
  - 3. A classification method M.
    - A **database** storing multiple samples with the same type of x.
    - Each sample is assigned to an arbitrary class  $\omega_{any} \in \{\omega_1, \omega_2, \dots \omega_c\}$ .
- Do:
  - $\{P(\omega_1|x), \ldots, P(\omega_c|x)\} \leftarrow classify(M, x, \omega)$
  - That is, for all the possible classes, find:
    - The probability that the given x belongs to that class.
- Get:
  - $\omega_{target}(x) = argmax_i[P(\omega_i|x)], i \in [1, c].$
  - That is, assign x a class/pattern from  $\omega$  with the **most probable** one.

#### **Example**

MNIST database.

- Test sample:
  - $x = A 28 \times 28$  grayscale image of a hand-written number.
- · Set of classes:
  - $\omega = \{0, 1, 2, 3, 4, 5, 6, 7, 8, 9\}.$
- Classification Method:
  - Derived from 10,000 of  $28 \times 28$  similar gray-scale images.
- Process:

- Given an image, using the classification method, get a list of probabilities  $P(\omega) = \{P(\omega_1), P(\omega_2), \dots, P(\omega_c)\}.$
- Select the  $\omega_i$  with the largest probability  $P(\omega_i)$ , that is  $selected = argmax[P(\omega_i)]$ .

## 2.1.2 Properties of Variables.

- The set of all classes  $\omega$  :
  - c available classes:  $\omega = \{\omega_1, \omega_2, \dots, \omega_c\}$
- Prior Probabilities  $P(\omega) = \{P(\omega_1), P(\omega_2), \dots, P(\omega_c)\}$ :
  - Probability Distribution of random variable  $\omega_j$  in the database.
    - The fraction of samples in the database that belongs to class  $\omega_j$ .
    - $P(\omega)$  is the prior knowledge on  $\omega = \{\omega_1, \omega_2, \dots, \omega_c\}$ .
  - It is Non-Negative.
    - $\forall i \in [1, c], P(\omega_i) \geq 0$ .
    - The probabilities of all classes are greater-or-equal to 0.
  - It is Normalized.
    - $\sum_{i=1}^{c} P(\omega_i) = 1$ .
    - The sum of the prior probabilities of all classes is 1.

# 2.2 Prior & Posterior Probabilities 先验与后验概率

# 2.2.1 Definition of Prior Probability 先验概率

- Decision BEFORE Observation (Naïve Decision Rule).
  - Don't care about test sample x.
  - Given x, always choose the class that:
    - has the most member in the database.
    - i.e., has the highest prior probability.
- Classification Process:
  - 1.  $\omega = \{\omega_1, \omega_2, \dots, \omega_c\}$ .
  - 2. By counting the number of members  $Num(\omega_i)$  for each class  $\omega_i \in \omega, i \in [1, c]$ , we get the prior probabilities  $P(\omega) = \{P(\omega_1), P(\omega_2), \dots, P(\omega_c)\}$ .
  - 3. Then, classify x directly into  $argmax_i[P(\omega_i)]$ .
- The decision is the same all the time obviously, and the prob. of a right guess is  $\frac{1}{c}$ .

# 2.2.2 Definition of Posterior Probability 后验概率

Decision WITH Observation.

- Cares about test sample x.
- Considering x, as well as the prior probabilities  $P(\omega) = \{P(\omega_1), P(\omega_2), \dots, P(\omega_c)\}$ ,
  - and give x the class with the biggest posterior probability.

#### Posterior Probability:

- [DEF] Posterior Probability of a class  $\omega_i$  on test sample x:
  - Given test sample x, how possible does x could be classified into class  $\omega_i$ .

$$ullet P(\omega_j|x) = rac{p(x|\omega_j)P(\omega_j)}{p(x)}, \, Posterior = rac{Likelihood imes Prior}{Evidence}.$$

- $p(x|\omega_i)$ : Likelihood (KNOWN)
  - The fraction of samples stored in the database that
    - is same to x, and
    - belongs to class  $\omega_i$ .
- $P(\omega_j)$ : Prior probability of class  $\omega_j$  (KNOWN)
  - The fraction of samples stored in the database that
    - belongs to class  $\omega_i$ .
- p(x): Evidence (IRRELEVANT)
  - Unconditional density of x.
  - That is,  $p(x) = \sum_{j=1}^{c} p(x|\omega_j) P(\omega_j)$ .

#### Special Cases:

- 1. Equal Prior Probability.
  - $P(\omega_1) = P(\omega_2) = \ldots = P(\omega_c) = \frac{1}{c}$ .
  - The amount of members in each class are same.
  - Here, posterior probs.  $\forall j \in [1,c], P(\omega_j|x)$  is dependent on the likelihoods  $P(x|\omega_j)$  only.
- 2. Equal Likelihood.
  - $P(x|\omega_1) = P(x|\omega_2) = \ldots = P(x|\omega_c)$ .
  - The amount of members that's same to x in each class are the same.
  - Here, posterior probs.  $\forall j \in [1, c], P(\omega_j | x)$  is dependent on the prior probabilities  $P(\omega_j)$  only.
  - Back to Naïve Decision Rule.

## 2.2.3 Classification Examples

#### Given:

- 1. Test sample  $x \in \{+, -\}$ .
- 2. A list of classes  $\omega = \{\omega_1 = cancer, \omega_2 = no\_cancer\}$ .
- 3. Classification Method M, with known probabilities:
  - Prior Probabilities:
  - $P(\omega_1) = 0.008$

- $P(\omega_2) = 1 P(\omega_1) = 0.992$
- Likelihoods:
- For class  $\omega_1=cancer$ :  $P(+|\omega_1)=0.98,\,P(-|\omega_1)=0.02$
- For class  $\omega_2=no\_cancer$ :  $P(+|\omega_2)=0.03$ ,  $P(-|\omega_2)=0.97$ .

#### Classification:

- Given a test sample x = +.
  - The prob. that this person gets cancer is:

$$P(\omega_1|+) = rac{P(+|\omega_1) imes P(\omega_1)}{P(+)} = rac{0.98 imes 0.008}{P(+)} = rac{0.00784}{P(+)}.$$

• The prob. that this person doesn't gets cancer is:

$$ullet P(\omega_2|+) = rac{P(+|\omega_2) imes P(\omega_2)}{P(+)} = rac{0.03 imes 0.992}{P(+)} = rac{0.02976}{P(+)}$$

- Therefore, the classification result would be:
  - $egin{aligned} \bullet & \omega_{target} = argmax_i[P(\omega_i|+)] \ &= argmax_i[rac{P(+|\omega_i) imes P(\omega_i)}{P(x)}] \ &= argmax_i[P(+|\omega_i) imes P(\omega_i)] \ &= \omega_2, ext{ for } 0.00784 < 0.02976 \end{aligned}$
  - That is, *no\_cancer*.

# 2.3 Loss Functions 决策成本函数

## 2.3.0 Why do we use loss functions?

- Different selection errors may have differently significant consequences, i.e., "losses" or "costs". 不同决策的成本、后果不同。
  - In pure Naïve Bayes classification, we only consider probability.
  - However.
    - we can tolerate "non-cancer" being classified into "cancer",
    - while it's more lossy to classify "cancer" into "non-cancer".
  - There is a need to consider this kind of "loss" into our decision method.
- We want to know if the Bayes decision rule is optimal.
  - Need a evaluation method
  - calc how many error you make, sum together

## 2.3.1 Probability of Error

For only two classes:

- If  $P(\omega_1|x) > P(\omega_2|x)$ ,  $x \leftarrow \omega_1$ . Prob. of error:  $P(\omega_2|x)$ .
- If  $P(\omega_1|x) < P(\omega_2|x)$ ,  $x \leftarrow \omega_2$ . Prob. of error:  $P(\omega_1|x)$ .

## 2.3.2 Loss Function (i.e., "Cost Function")

#### **Problem**

- Take action  $\alpha_i$  for a given x.
  - The action  $\alpha_i$ : To assign the test pattern x the class  $\omega_i$ .
- Introduce the loss/cost  $\lambda(\alpha_i|\omega_i)$ , for the true class  $\omega_i$  and action  $\alpha_i$  on x.
  - That is,  $\lambda(\alpha_i|\omega_j)$  is the cost of classifying **any** sample into class  $\omega_i$  when the true class of that sample is  $\omega_j$ .
  - For instance,  $\lambda(\alpha_{cancer}|\omega_{no\_cancer})$  is the cost of diagnosing a patient that actually doesn't have cancer as "having cancer".
    - (Which by intuition is not as serious as its reverse, therefore the value of this  $\lambda$  should also be lower than its reverse.)
- We don't actually know the true class  $\omega_j$  for a random sample x, so we use the Expected Loss.
  - That is, we consider the "average loss" of classifying x into  $\omega_i$  by considering:
    - The loss of classifying x into  $\omega_j$  for all  $\omega_j \in \omega$ .
    - The probability that  $x \in \omega_i$ , i.e.,  $P(\omega_i|x)$ .

#### [DEF]Expected Loss (Average Loss, Conditional Risk) 期望成本:

- The expected loss of classifying x into  $\omega_i$ .
- ullet  $R(lpha_i|x) = \sum_{j=1}^c \lambda(lpha_i|\omega_j) imes P(\omega_j|x)$  , where
  - $\lambda(\alpha_i|\omega_j)$ : The cost of classifying x into  $\omega_i$  under the true class  $\omega_j$ .
  - $P(\omega_j|x)$ : The posterior probability that x belongs to class  $\omega_j$ .
    - Computed during the Naïve Bayes Classification with  $P(\omega_j)$  and  $P(x|\omega_j)$ .

## [DEF]Bayes Risk 贝叶斯风险:

- The modified measurement of the original Bayes Rule.
  - Consider the importance of each error.
  - Consider minimum loss, instead of maximum probability.
- Bayes Risk finds the action that gives the minimum expected loss of x.
  - $egin{aligned} ullet & lpha(x) = argmin_{lpha_i \in A} R(lpha_i | x) \ & ullet = argmin_{lpha_i \in A} \sum_{j=1}^c \lambda(lpha_i | \omega_j) P(\omega_j | x) \end{aligned}$

#### **Derivation: For a 2-class problem**

- Known:
  - Test sample x.
  - Classes  $\omega = \{\omega_1, \omega_2\}$ .
  - The calculated posterior probabilities:
    - $P(\omega_1|x)$ ,  $P(\omega_2|x)$ .

• Loss Matrix: 
$$egin{bmatrix} \lambda_{11} & \lambda_{12} \ \lambda_{21} & \lambda_{22} \end{bmatrix}$$
 , where  $\lambda_{ij} = \lambda(lpha_i | \omega_j)$  .

•  $\lambda_{ij}$ : The cost of classifying x into  $\omega_i$  when the true class of x is  $\omega_j$ .

$$ullet \ \omega_{target} = argmin_{lpha_i \in A} R(lpha_i | x)$$

• If we choose  $\omega_1$ , we have:

• 
$$R(\alpha_1|x) < R(\alpha_2|x)$$

$$ullet$$
  $\iff \lambda_{11}P(\omega_1|x) + \lambda_{12}P(\omega_2|x) < \lambda_{21}P(\omega_1|x) + \lambda_{22}P(\omega_2|x)$ 

$$ullet$$
  $\iff (\lambda_{21}-\lambda_{11})P(\omega_1|x)>(\lambda_{12}-\lambda_{22})P(\omega_2|x)$ 

$$ullet \iff rac{P(\omega_1|x)}{P(\omega_2|x)} > rac{\lambda_{12} - \lambda_{22}}{\lambda_{21} - \lambda_{11}}$$

$$ullet \iff rac{P(x|\omega_1)P(\omega_1)}{P(x|\omega_2)P(\omega_2)} > rac{\lambda_{12}-\lambda_{22}}{\lambda_{21}-\lambda_{11}}$$

$$ullet \iff rac{P(x|\omega_1)}{P(x|\omega_2)} > rac{(\lambda_{12}-\lambda_{22})P(\omega_2)}{(\lambda_{21}-\lambda_{11})P(\omega_1)}$$

$$ullet \ \iff rac{P(x|\omega_1)}{P(x|\omega_2)} > heta_t$$

## 2.3.3 Examples

#### Minimum Prob. Error and Minimum Risk

Remark: Gaussian Distribution

• 
$$GD(x) = \frac{1}{\sigma\sqrt{2\pi}}e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

Given:

• Two probability distributions of evidence  $P(x|\omega_j)$  regarding  $j \in \{1, 2\}$ .

$$oldsymbol{P}(x|\omega_1)=rac{1}{\sqrt{\pi}}e^{-x^2}, ext{ where } \mu=0, \sigma=rac{1}{\sqrt{2}}.$$

$$ullet P(x|\omega_2)=rac{1}{\sqrt{\pi}}e^{-(x-1)^2},$$
 where  $\mu=1,\sigma=rac{1}{\sqrt{2}}.$ 

Loss matrix

$$-\begin{bmatrix} \lambda_{11} & \lambda_{12} \\ \lambda_{21} & \lambda_{22} \end{bmatrix} = \begin{bmatrix} 0 & 1.0 \\ 0.5 & 0 \end{bmatrix}$$

• The threshold  $x_0$  for minimum  $P_e$ .

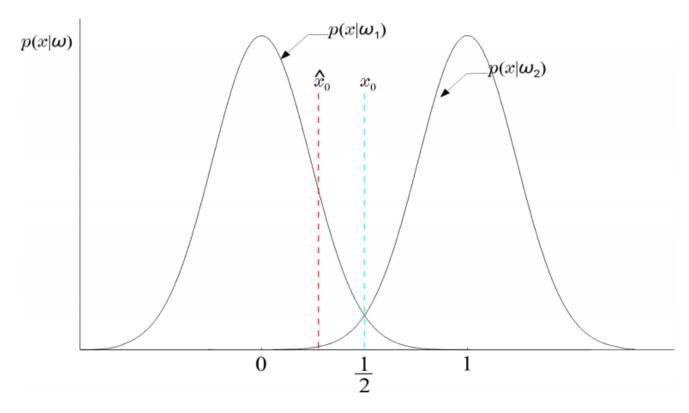
$$\begin{array}{ll} \bullet & P(x_0|\omega_1) = P(x_0|\omega_2) \\ \bullet & \Longrightarrow & \frac{1}{\sqrt{\pi}}e^{-x_0^2} = \frac{1}{\sqrt{\pi}}e^{-(x_0-1)^2} \\ \bullet & \Longrightarrow & x_0 = -x_0+1 \text{, omitting } x_0 = x_0-1 \text{ which is impossible;} \end{array}$$

$$x_0 = -x_0 + 1$$
, offilting  $x_0 = x_0 - 1$  which is impossible

$$\bullet \implies x_0 = \frac{1}{2}$$

• The threshold  $\hat{x_0}$  for minimum  $R(\alpha_i|x)$ .

$$\begin{array}{c} \bullet \ \ R(\alpha_{1}|x) = R(\alpha_{2}|x) \\ \bullet \ \ \Longrightarrow \ \frac{P(\hat{x_{0}}|\omega_{1})}{P(\hat{x_{0}}|\omega_{2})} = \frac{(\lambda_{12} - \lambda_{22})P(\omega_{2})}{(\lambda_{21} - \lambda_{11})P(\omega_{1})} \\ \bullet \ \ \Longrightarrow \ \frac{P(\hat{x_{0}}|\omega_{1})}{P(\hat{x_{0}}|\omega_{2})} = \frac{(1 - 0) \times \frac{1}{2}}{(0.5 - 0) \times \frac{1}{2}} \\ \bullet \ \ \Longrightarrow \ P(\hat{x_{0}}|\omega_{1}) = 2P(\hat{x_{0}}|\omega_{2}) \\ \bullet \ \ \Longrightarrow \ \frac{1}{\sqrt{\pi}}e^{-\hat{x_{0}}^{2}} = 2\frac{1}{\sqrt{\pi}}e^{-(\hat{x_{0}}-1)^{2}} \\ \bullet \ \ \Longrightarrow \ -\hat{x_{0}}^{2} = \ln 2 - \hat{x_{0}}^{2} + 2\hat{x_{0}} - 1 \\ \bullet \ \ \Longrightarrow \ \hat{x_{0}} = \frac{1 - \ln 2}{2} < \frac{1}{2} \end{array}$$



### **Minimum Error Rate Classification**

- A zero-one loss function
  - $\bullet \quad \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
  - All errors are equally costly.
- Conditional Risk:

$$ullet R(lpha_i|x) = \sum_{j=1}^c \lambda(lpha_i|x) P(\omega_j|x)$$

$$ullet = \lambda(lpha_i|\omega_i)P(\omega_i|x) + \sum_{j
eq i}\lambda(lpha_i|\omega_j)P(\omega_j|x)$$

$$ullet = 0 + \sum_{j 
eq i} 1 imes P(\omega_j|x)$$

$$ullet = \sum_{j 
eq i} P(\omega_j|x)$$

$$\bullet = 1 - P(\omega_i|x)$$

# 2.4 Discriminant Functions 判别函数

### 2.4.1 Definition of Discriminant Function

- If a function *f* satisfies:
  - If  $f(\cdot)$  monotonically increases, and
  - $\forall i \neq j, f(P(\omega_i|x)) > f(P(\omega_i|x))$ , then
  - $ullet x 
    ightarrow \omega_i$
- Then,  $g_i(x) = f(P(\omega_i|x))$  is a discriminant function.
- That is, this function is able to "tell" a certain one  $\omega_i$  from others on any input x. 给定一个测试样本x,判别函数能够从所有其它分类中挑选一个最可能的 $\omega_i$ 。
  - i.e., it separates  $\omega_i$  and  $\neg \omega_i$ .

## 2.4.2 Property of Discriminant Function

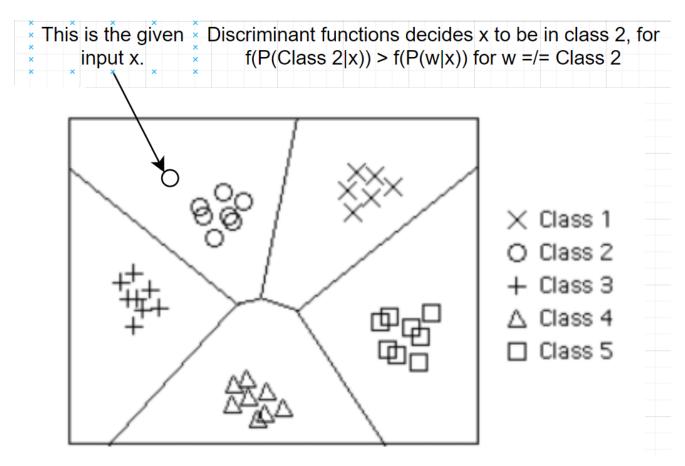
- 1. One function per class.
  - 1. A discriminant function is able to "tell" a certain one  $\omega_i$  specifically for any input x.
- 2. Various discriminant functions → Identical classification results. 样式各异, 结果相同。
  - 1. It is correct to say, the discriminant functions:
    - 1. **Preserves** the original monotonical-increase of its inputs.
    - 2. But changes the changing rate by **processing** the inputs.
  - 2. i.e.,
    - 1. " $\forall i \neq j, f(g_i(x)) > f(g_j(x)) \land f \nearrow$  "and " $\forall i \neq j, g_i(x) > g_j(x)$ " are equivalent in decision.
    - 2. Changing growth rate of input:
      - 1.  $f(g_i(x)) = k \cdot g_i(x)$ , a linear change.
      - 2.  $f(g_i(x)) = \ln g_i(x)$ , a log change, i.e., it grows, but slower as it proceed.
    - Therefore, the discriminant function may vary, but the output is always the same.
- 3. Examples of discriminant functions:
  - 1. Minimum Risk:  $g_i(x) = -R(\alpha_i|x) = -\lambda(\alpha_i|x) \times P(\omega_i|x)$ , for  $i \in [1,c]$
  - 2. Minimum Error Rate:  $g_i(x) = P(\omega_i|x)$ , for  $i \in [1, c]$

# 2.4.3 Decision Region 决策区域

- c discriminant functions  $\implies c$  decision regions
  - $\bullet \ g_i(x) \implies R_i \subset R^d, i \in [1,c]$
- One function per decision region that is distinct and mutual-exclusive.
  - ullet  $R_i=\{x|x\in R^d: orall i
    eq j, g_i(x)>g_i(x)\},$  where

# 2.4.4 Decision Boundaries 决策边界

- "Surface" in feature space, where ties occur among 2 or more largest discriminant functions.
- x<sub>0</sub> is on the decision boundary/surface if and only if
  - $ullet \ \exists \omega_i, \omega_j \in \omega, g_i(x_0) = g_j(x_0).$



# 2.5 Bayesian Classification for Normal Distributions

# 2.5.1 Multi-Dimensional Normal Distribution 高维正态分布

## 1-D Case 多类别,一维数据

- There are several classes:
  - Each class has its own distribution of data samples, i.e., each class has its own  $\mu$  and  $\sigma$ .
- For a specific class, there are plenty of data samples:

- Each sample is a **scalar**, that is a  $1 \times 1$  "matrix", which is a "plain number".
- The samples follows a Normal Distribution.

For a specific class  $\omega_i$ , suppose the data conforms a normal distribution. Here:

• 
$$x\sim N(\mu_i,\sigma_i):P(x|\omega_i)=rac{1}{\sigma_i\sqrt{2\pi}}e^{-rac{(x-\mu_i)^2}{2\sigma_i^2}}$$
 , where

μ is the mean value.

• 
$$\mu_i = E(x)$$

•  $\sigma^2$  is the variance.

• 
$$\sigma_i = E[(x-\mu)^2]$$

## Multivariate Case 多类别,高维数据

- There are several classes:
  - Each class has its own distribution of data samples, i.e., each class has its own  $\mu$ and  $\sigma$ .
- For a specific class, there are plenty of data samples:
  - Each sample is a **vector**, that is a  $d \times 1$  matrix, where d is the dimension of data.
  - The samples follow a *d*-dimensional Normal Distribution.

Here, for a specific class  $\omega_i$ , suppose the multi-dimensional data X conforms a normal distribution.

$$oldsymbol{X} \sim N(\mu_i, \Sigma_i) : P(X|\omega_i) = rac{1}{|\Sigma_i|^{rac{1}{2}} imes (2\pi)^{rac{1}{2}}} e^{-rac{1}{2}(X-\mu_i)^ op \Sigma_i^{-1}(X-\mu_i)}$$

$$* X \sim N(\mu_i, \Sigma_i) : P(X|\omega_i) = \frac{1}{\frac{1}{|\Sigma_i|}} \frac{d}{2} e^{-\frac{1}{2}(X - \mu_i)^\top \Sigma_i^{-1}(X - \mu_i)}$$

$$* Regular \ Variables:$$

$$* d\text{-dimensional random variables: } X = \begin{bmatrix} x_1 \\ x_2 \\ \dots \\ x_d \end{bmatrix};$$

$$* d\text{-dimensional mean vector: } \mu_i = \begin{bmatrix} \mu_{i1} \\ \mu_{i2} \\ \dots \\ \mu_{id} \end{bmatrix} = \begin{bmatrix} E(x_{i1}) \\ E(x_{i2}) \\ \dots \\ E(x_{id}) \end{bmatrix}, \text{ specifically for class } \omega_i;$$

$$\Sigma_i = egin{pmatrix} \sigma_{i11} & \sigma_{i12} & \cdots & \sigma_{i1d} \ \sigma_{i21} & \sigma_{i22} & \cdots & \sigma_{i2d} \ dots & dots & \ddots & dots \ \sigma_{id1} & \sigma_{id2} & \cdots & \sigma_{idd} \end{pmatrix} = E[(X-\mu_i)(X-\mu_i)^ op], ext{ specifically for class}$$

• Explanations on 
$$-\frac{1}{2}(X-\mu_i)^{ op}\Sigma_i^{-1}(X-\mu_i)$$

Parts:

$$\bullet \quad (X-\mu_i)^\top = \begin{bmatrix} x_1-\mu_{i1} \\ x_2-\mu_{i2} \\ \dots \\ x_d-\mu_{id} \end{bmatrix}^\top = [(x_1-\mu_{i1}) \quad (x_2-\mu_{i2}) \quad \cdots \quad (x_d-\mu_{id})]$$

$$\bullet \quad \Sigma_i^{-1} = \begin{pmatrix} \sigma'_{i11} & \sigma'_{i12} & \cdots & \sigma'_{i1d} \\ \sigma'_{i21} & \sigma'_{i22} & \cdots & \sigma'_{i2d} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma'_{id1} & \sigma'_{id2} & \cdots & \sigma'_{idd} \end{pmatrix}, \text{ the inverse of the covariance matrix.}$$

$$\bullet \quad (X-\mu_i) = \begin{bmatrix} x_1-\mu_{i1} \\ x_2-\mu_{i2} \\ \dots \\ x_d-\mu_{id} \end{bmatrix}$$

Whole:

$$\begin{array}{l} \bullet \quad -\frac{1}{2}(X-\mu_i)^\top \Sigma_i^{-1}(X-\mu_i) \\ \bullet \quad = -\frac{1}{2}[(x_1-\mu_{i1}) \quad (x_2-\mu_{i2}) \quad \cdots \quad (x_d-\mu_{id})] \begin{pmatrix} \sigma'_{i11} & \sigma'_{i12} & \cdots & \sigma'_{i1d} \\ \sigma'_{i21} & \sigma'_{i22} & \cdots & \sigma'_{i2d} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma'_{id1} & \sigma'_{id2} & \cdots & \sigma'_{idd} \end{pmatrix} \begin{bmatrix} x_1-x_2-x_2 \\ x_2-x_3-x_4 \\ x_4-x_4-x_4 \end{bmatrix} \\ \bullet \quad = -\frac{1}{2}[a_1 \quad a_2 \quad \cdots a_d] \begin{bmatrix} x_1-\mu_{i1} \\ x_2-\mu_{i2} \\ \dots \\ x_d-\mu_{id} \end{bmatrix}$$

#### **Example: 2-D Case**

$$ullet X \sim N(\mu, \Sigma) : P(X) = rac{1}{|\Sigma_i|} e^{-rac{1}{2}[(x_1 - \mu_{i1}) \quad (x_2 - \mu_{i2})]\Sigma_i^{-1}igg[ rac{(x_1 - \mu_{i1})}{(x_2 - \mu_2)} igg]}$$

• 
$$2$$
 - dimensional random variable  $X$ :  $X = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$ 

• 
$$2$$
 - dimensional mean vector:  $\mu_i = egin{bmatrix} \mu_{i1} \\ \mu_{i2} \end{bmatrix} = egin{bmatrix} E(x_{i1}) \\ E(x_{i2}) \end{bmatrix}$ 

•  $2 \times 2$  covariant matrix  $\Sigma_i$ :

$$egin{aligned} ullet & \Sigma_i = E[(X - \mu_i)(X - \mu_i)^ op] \ ullet & = E(egin{bmatrix} x_1 - \mu_{i1} \ x_2 - \mu_{i2} \end{bmatrix} [x_1 - \mu_{i1} & x_2 - \mu_{i2}]) \ ullet & = egin{bmatrix} (x_1 - \mu_{i1})^2 & (x_1 - \mu_{i1})(x_2 - \mu_{i2}) \ (x_2 - \mu_{i2})(x_1 - \mu_{i1}) & (x_2 - \mu_{i2})^2 \end{bmatrix} \ ullet & = egin{bmatrix} \sigma_1^2 & \sigma \ \sigma & \sigma_2^2 \end{bmatrix} \end{aligned}$$

### 2.5.2 Minimum-error-rate classification

#### Recall:

- Minimum-error-rate means that we ignore the "cost" of each decision.
- In other words, we only select the classes based on probabilities.

#### **Pattern of Discriminant Function**

- Discriminant Function:  $g_i(x) = \ln P(\omega_i|x), \forall i \in [1,c] \cap \mathbb{N}^+$ 
  - $g_i(x) = \ln[P(\omega_i|x)]$
  - $\implies g_i(x) = \ln[P(X|\omega_i) \times P(\omega_i)]$

$$egin{aligned} ullet &\implies g_i(x) = \ln[rac{1}{2} rac{1}{2} \left( 2\pi 
ight)^{rac{d}{2}} e^{-rac{1}{2}(X-\mu)^T \Sigma^{-1}(X-\mu)}] + \ln[P(\omega_i)] \end{aligned}$$

$$egin{align} ullet &\Longrightarrow g_i(x) = \ &ullet -rac{d}{2} \mathrm{ln}(2\pi) \ &ullet -rac{1}{2} |\Sigma_i| \ &ullet -rac{1}{2} (X-\mu_i)^T \Sigma_i^{-1} (X-\mu_i) \ &ullet + \mathrm{ln}[P(\omega_i)] \ \end{pmatrix}$$

• Here,  $-\frac{d}{2}\ln(2\pi)$  is a constant, which can be ignored. The discriminant function is then updated as:

$$egin{aligned} \bullet & g_i(x) = \ & \bullet & -rac{1}{2} \mathrm{ln} \left| \Sigma_i 
ight| \ & \bullet & -rac{1}{2} (X - \mu_i)^ op \Sigma_i^{-1} (X - \mu_i) \ & \bullet & + \mathrm{ln} [P(\omega_i)] \end{aligned}$$

## Case I: $\Sigma_i = \sigma^2 I$

• That is, 
$$\Sigma_1=\Sigma_2=\cdots=\Sigma_{|\omega|}=\sigma^2I=egin{bmatrix}\sigma^2&0&\cdots&0\\0&\sigma^2&\cdots&0\\ \vdots&\vdots&\ddots&\vdots\\0&0&\cdots&\sigma^2\end{bmatrix}$$

- All the classes have a common covariance matrix  $\sigma^2 I$ .
- A diagonal matrix suggests that the distribution of data in is isotropic (各向同性的), with respect to any specific class.
  - That is, the variance or spread is the same in all directions.

- In other words, there is no directional preference in the spread of the distribution.
- Therefore, we have:

$$ullet |\Sigma_i| = \sigma^{2d}$$
 $ullet \Sigma_i^{-1} = rac{1}{r^2}I$ 

• And the discriminant function  $g_i(x)$  is:

• Here, as  $|\Sigma_i| = \sigma^{2d}$  is a constant, it is ignored. Therefore,

$$\begin{split} \bullet & g_i(x) = \\ & \bullet - \frac{1}{2}(X - \mu_i)^\top \Sigma_i^{-1}(X - \mu_i) \\ & \bullet + \ln[P(\omega_i)] \\ \bullet & = -\frac{1}{2}(X - \mu_i)^\top \times \left[\frac{1}{\sigma^2}I\right] \times (X - \mu_i) \ + \ \ln[P(\omega_i)], \\ \bullet & = -\frac{(X - \mu_i)^\top (X - \mu_i)}{2\sigma^2} + \ln[P(\omega_i)], \\ \bullet & = -\frac{(X^\top - \mu_i^\top)(X - \mu_i)}{2\sigma^2} + \ln[P(\omega_i)], \\ \bullet & = -\frac{X^\top X - X^\top \mu_i - \mu_i^\top X + \mu_i^\top \mu_i}{2\sigma^2} + \ln[P(\omega_i)], \\ \bullet & = -\frac{X^\top X - 2\mu_i^\top X + \mu_i^\top \mu_i}{2\sigma^2} + \ln[P(\omega_i)], \text{ known that } a^\top b = b^\top a \\ \bullet & = -\frac{||X - \mu_i||^2}{2\sigma^2} + \ln[P(\omega_i)], \text{ where } ||\cdot|| \text{ is the Euclidean Distance}. \end{split}$$

• Here, we ignore  $X^{\top}X$  because it is the same for any class. (Remember X is just the random variable that needs us to classify.)

$$\begin{split} \bullet & \ g_i(x) = -\frac{-2\mu_i^\top X + \mu_i^\top \mu_i}{2\sigma^2} + \ln[P(\omega_i)], \text{ with } X^\top X \text{ ignored.} \\ \bullet & = \frac{\mu_i^\top X}{\sigma^2} - \frac{\mu_i^\top \mu_i}{2\sigma^2} + \ln[P(\omega_i)] \\ \bullet & = (\frac{\mu_i}{\sigma^2})^\top X + (-\frac{\mu_i^\top \mu_i}{2\sigma^2} + \ln[P(\omega_i)]) \\ \bullet & = w_i^T X + w_{i0}, \text{ where} \\ \bullet & w_i = \frac{\mu_i}{\sigma^2} = \begin{bmatrix} \frac{\mu_{i1}}{\sigma^2} \\ \frac{\mu_{i2}}{\sigma^2} \\ \vdots \\ \frac{\mu_{id}}{\sigma^2} \end{bmatrix} \text{ is the weight vector, and} \\ \bullet & w_{i0} = (-\frac{\mu_i^\top \mu_i}{2\sigma^2} + \ln[P(\omega_i)]) \text{ is the threshold/bias scalar.} \end{split}$$

- We have got a Linear Discriminant Function.
- Having the discriminant functions defined, we get the decision surface by:

• 
$$g_i(X) - g_j(X) = 0$$
  
•  $\implies w_i X + w_{i0} - (w_j X + w_{j0}) = 0$   
•  $\implies \frac{\mu_i}{\sigma^2} X + w_{i0} - (\frac{\mu_j}{\sigma^2} X + w_{jo}) = 0$   
•  $\implies (\frac{\mu_i - \mu_j}{\sigma^2}) X + (w_{i0} - w_{j0}) = 0$   
•  $\implies (\mu_i - \mu_j) X + \sigma^2(w_{i0} - w_{j0}) = 0$ 

### Case II: $\Sigma_i = \Sigma$

- That is,  $\Sigma_1 = \Sigma_2 = \dots = \Sigma_{|\omega|} = \Sigma$ 
  - All the classes have a common covariance matrix  $\Sigma$ .
  - · More general than Case I.
- And the discriminant function  $g_i(x)$  is:

• Here, as  $|\Sigma_i| = |\Sigma|$  is a constant, it is ignored. Therefore,

$$ullet g_i(x) = -rac{1}{2}(X-\mu_i)^ op \Sigma^{-1}(X-\mu_i) + \ln P(\omega_i)$$

- where  $(X \mu_i)^{\top} \Sigma^{-1} (X \mu_i)$  is the **Squared Mahalanobis Distance**.
- When  $\Sigma = I$ , it reduces to **Euclidean Distance**.

$$\begin{split} \bullet &= -\frac{1}{2} (X - \mu_i)^\top (\Sigma^{-1} X - \Sigma^{-1} \mu_i) + \ln P(\omega_i) \\ \bullet &= -\frac{1}{2} (X^\top - \mu_i^\top) (\Sigma^{-1} X - \Sigma^{-1} \mu_i) + \ln P(\omega_i) \\ \bullet &= -\frac{1}{2} (X^\top \Sigma^{-1} X - X^\top \Sigma^{-1} \mu_i - \mu_i^\top \Sigma^{-1} X + \mu_i^\top \Sigma^{-1} \mu_i) + \ln P(\omega_i) \\ \bullet &= -\frac{1}{2} (X^\top \Sigma^{-1} X - 2\mu_i^\top \Sigma^{-1} X + \mu_i^\top \Sigma^{-1} \mu_i) + \ln P(\omega_i) \end{split}$$

• Here,  $X^{\top}\Sigma^{-1}X$  is the same for all class, thus can be ignored.

$$ullet g_i(x) = (\mu_i^ op \Sigma^{-1}) X + (-rac{\mu_i^ op \Sigma^{-1} \mu_i}{2} + \ln P(\omega_i))$$

## Case III: $\Sigma_i = arbitrary$

In most cases, for each class  $\omega_i$ ,  $\Sigma_i$ , the covariance/spread of data in this class is arbitrary.

$$ullet g_i(x) = -rac{1}{2}(X-\mu_i)^ op \Sigma_i^{-1}(X-\mu_i) - rac{1}{2} ext{ln}\,|\Sigma_i| + ext{ln}\,P(\omega_i)$$

$$\begin{split} \bullet &= -\frac{1}{2}(X - \mu_i)^\top (\Sigma_i^{-1} X - \Sigma_i^{-1} \mu_i) - \frac{1}{2} \ln |\Sigma_i| + \ln P(\omega_i) \\ \bullet &= -\frac{1}{2}(X^\top - \mu_i^\top) (\Sigma_i^{-1} X - \Sigma_i^{-1} \mu_i) - \frac{1}{2} \ln |\Sigma_i| + \ln P(\omega_i) \\ \bullet &= -\frac{1}{2}(X^\top \Sigma_i^{-1} X - X^\top \Sigma_i^{-1} \mu_i - \mu_i^\top \Sigma_i^{-1} X + \mu_i^\top \Sigma_i^{-1} \mu_i) - \frac{1}{2} \ln |\Sigma_i| + \ln P(\omega_i) \\ \bullet &= -\frac{1}{2}(X^\top \Sigma_i^{-1} X - 2\mu_i^\top \Sigma_i^{-1} X + \mu_i^\top \Sigma_i^{-1} \mu_i) - \frac{1}{2} \ln |\Sigma_i| + \ln P(\omega_i) \\ \bullet &= X^\top (-\frac{1}{2} \Sigma_i^{-1}) X + (\mu_i^\top \Sigma_i^{-1}) X + (-\frac{\mu_i^\top \Sigma^{-1} \mu_i}{2} - \frac{\ln |\Sigma_i|}{2} + \ln P(\omega_i)) \\ \text{Thus,} \end{split}$$

$$ullet g_i(X) = X^ op W_i X + w_i^ op X + w_{i0},$$
 where

• 
$$W_i = -rac{1}{2}\Sigma_i^{-1}$$
 is the Quadratic matrix.

$$ullet w_i = \mu_i^ op \Sigma_i^{-1}$$
 is the Weight Vector

• 
$$w_{i0} = -rac{\mu_i^ op \Sigma^{-1} \mu_i}{2} - rac{\ln |\Sigma_i|}{2} + \ln P(\omega_i)$$
 is the Threshold/Bias.

Again, for special covariance matrices:

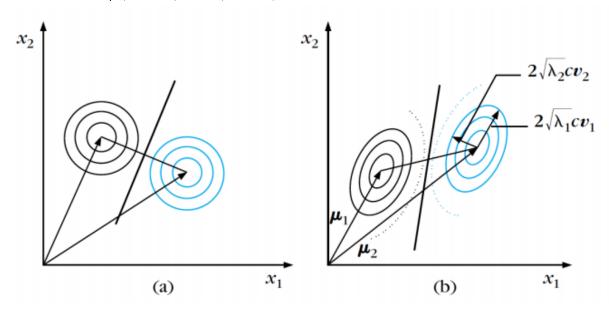
• 
$$\Sigma_i = \sigma^2 I$$
:

• Assign 
$$x$$
 to  $\omega_i$  if there is a smaller **Euclidean Distance**:  $d_{Euclidean} = \|X - \mu_i\|$ 

• 
$$\Sigma_i = \Sigma$$
:

- Assign x to  $\omega_i$  if there is a smaller **Mahalanobis Distance**:

$$d_{Mahalanobis} = \sqrt{(X - \mu_i)^{ op} \Sigma^{-1} (X - \mu_i)}$$



# 2.6 (Additional) Geometric Description of Covariance Matrix

## 2.6.1 Meta Matrices

Take the 2-D case as an example. Geometrically, the covariance matrix tells how the original Euclidean Space could be transformed into a Mahalanobis space.

The transformation info of a 2-D covariance matrix could be described as:

Scale factor: Multiplication

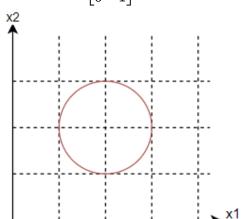
Skew factor: Addition

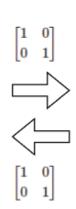
$$egin{bmatrix} x_1 \ scale \ factor & x_1 \ skew \ factor \ x_2 \ skew \ factor & x_2 \ scale \ factor \end{bmatrix}$$

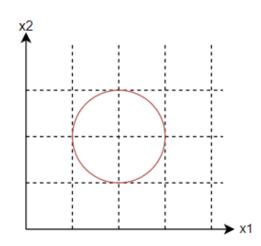
## 1. Identity Matrix

In the trivial case,  $I^2$  as the covariance matrix does no effect on the original Euclidean space. The inverse of the identity matrix is itself.

$$\Sigma = \Sigma^{-1} = egin{bmatrix} 1 & 0 \ 0 & 1 \end{bmatrix}$$





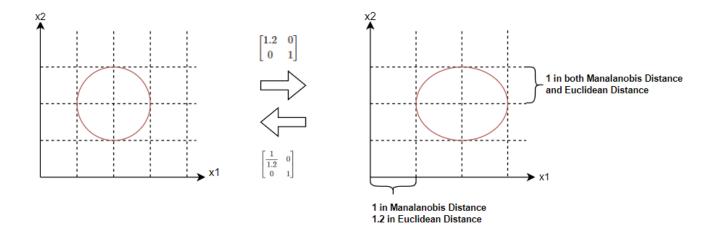


## 2. Scales $x_1$

By setting the  $x_1$  scale factor non-1, the matrix scales the Euclidean space on the  $x_1$  axis. The inverse of covariance matrix does the opposite, that is to scale a coordinate back.

$$\Sigma = egin{bmatrix} 1.2 & 0 \ 0 & 1 \end{bmatrix} \Sigma^{-1} = egin{bmatrix} rac{1}{1.2} & 0 \ 0 & 1 \end{bmatrix}$$

For 
$$v=egin{bmatrix} v_1 \ v_2 \end{bmatrix}$$
 ,  $\Sigma imes v=egin{bmatrix} 1.2 & 0 \ 0 & 1 \end{bmatrix} egin{bmatrix} v_1 \ v_2 \end{bmatrix} = egin{bmatrix} 1.2v_1 \ v_2 \end{bmatrix}$ 

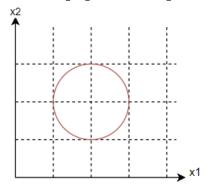


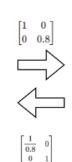
### 3. Scales $x_2$

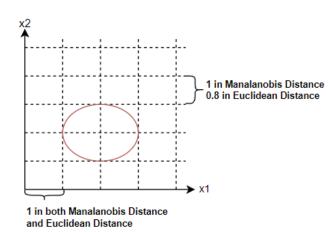
By setting the  $x_2$  scale factor non-1, the matrix scales the Euclidean space on the  $x_2$  axis. The inverse of covariance matrix does the opposite, that is to scale a coordinate back.

$$\Sigma = \begin{bmatrix} 1 & 0 \\ 0 & 0.8 \end{bmatrix} \, \Sigma^{-1} = \begin{bmatrix} \frac{1}{0.8} & 0 \\ 0 & 1 \end{bmatrix}$$

For 
$$v=egin{bmatrix} v_1 \ v_2 \end{bmatrix}$$
 ,  $\Sigma imes v=egin{bmatrix} 1 & 0 \ 0 & 0.8 \end{bmatrix} egin{bmatrix} v_1 \ v_2 \end{bmatrix} = egin{bmatrix} v_1 \ 0.8 v_2 \end{bmatrix}$ 







## 4. Skews $x_1$

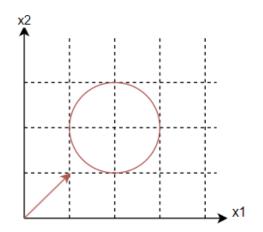
By setting the  $x_1$  skewing factor non-zero, the matrix pans (平移) the  $x_1$  coordinate of a vector by the multiplication of:

- The factor
- And the  $x_2$  coordinate of that vector.

Therefore, the larger  $x_2$  coordinate the vector has, the more it is panned.

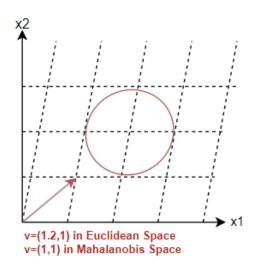
$$\Sigma = egin{bmatrix} 1 & 0.2 \ 0 & 1 \end{bmatrix} \Sigma^{-1} = egin{bmatrix} 1 & -0.2 \ 0 & 1 \end{bmatrix}$$

For 
$$v=egin{bmatrix} v_1 \ v_2 \end{bmatrix}$$
 ,  $\Sigma imes v=egin{bmatrix} 1 & 0.2 \ 0 & 1 \end{bmatrix} egin{bmatrix} v_1 \ v_2 \end{bmatrix} = egin{bmatrix} v_1+0.2v_2 \ v_2 \end{bmatrix}$ 





$$\begin{bmatrix} 1 & -0.2 \\ 0 & 1 \end{bmatrix}$$



## 5. Skews $x_2$

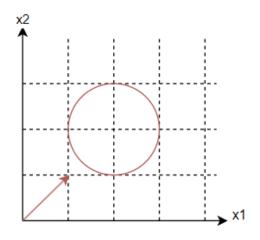
By setting the  $x_2$  skewing factor non-zero, the matrix pans (平移) the  $x_2$  coordinate of a vector by the multiplication of:

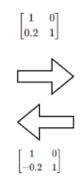
- The factor
- And the  $x_1$  coordinate of that vector.

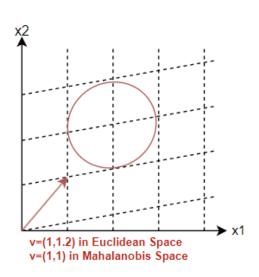
Therefore, the larger  $x_1$  coordinate the vector has, the more it is panned.

$$\Sigma = egin{bmatrix} 1 & 0 \ 0.2 & 1 \end{bmatrix} \Sigma^{-1} = egin{bmatrix} 1 & 0 \ -0.2 & 1 \end{bmatrix}$$

For 
$$v = \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}$$
,  $\Sigma imes v = \begin{bmatrix} 1 & 0 \\ 0.2 & 1 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} = \begin{bmatrix} v_1 \\ 0.2v_1 + v_2 \end{bmatrix}$ 







## 2.6.2 Combined Matrices

Several meta matrices could be combined to a single covariance matrix, performing batch operations.

$$\begin{bmatrix} 1.2 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 0.8 \end{bmatrix} \begin{bmatrix} 1 & 0.2 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0.2 & 1 \end{bmatrix}$$

$$=\begin{bmatrix}1.2 & 0\\0 & 0.8\end{bmatrix}\begin{bmatrix}1 & 0.2\\0 & 1\end{bmatrix}\begin{bmatrix}1 & 0\\0.2 & 1\end{bmatrix}$$

$$=\begin{bmatrix}1.2 & 0.24\\0 & 0.8\end{bmatrix}\begin{bmatrix}1 & 0\\0.2 & 1\end{bmatrix}$$

$$=\begin{bmatrix}1.2 & 0.24\\0 & 0.8\end{bmatrix}\begin{bmatrix}1 & 0\\0.2 & 1\end{bmatrix}$$

$$=\begin{bmatrix}1.248 & 0.24\\0.16 & 0.8\end{bmatrix}$$

#### **Calculation of Squared Mahalanobis Distance**

$$d_M^2 = (X - \mu_i)^{ op} \Sigma^{-1} (X - \mu_i) = (X - \mu_i)^{ op} [\Sigma^{-1} (X - \mu_i)]$$

 $d_M^2 = (X - \mu_i)^\top \Sigma^{-1} (X - \mu_i) = (X - \mu_i)^\top [\Sigma^{-1} (X - \mu_i)]$  The inverse of the covariance matrix  $\Sigma^{-1}$  reverses the transformed space back to its original Euclidean Space to compute the Mahalanobis distance.

