Basics of Machine Learning

Likelihood Ratio Test

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What is Machine Learning (ML)?

- **Components of Machine Learning (ML)**
  - Computer Program learning experience **(E)**
  - Class of task (T) corresponding to E
  - Performance Measure (P) of Task

  ➔ Machine Learning Algorithm : Program (or algorithm) improving performance (P) of task (T) using the experience (E)

- ML finds a target function f between data $X = (x_1, x_2, \dots, x_3)$ and states $Y = (y_1, y_2, \dots, y_n)$

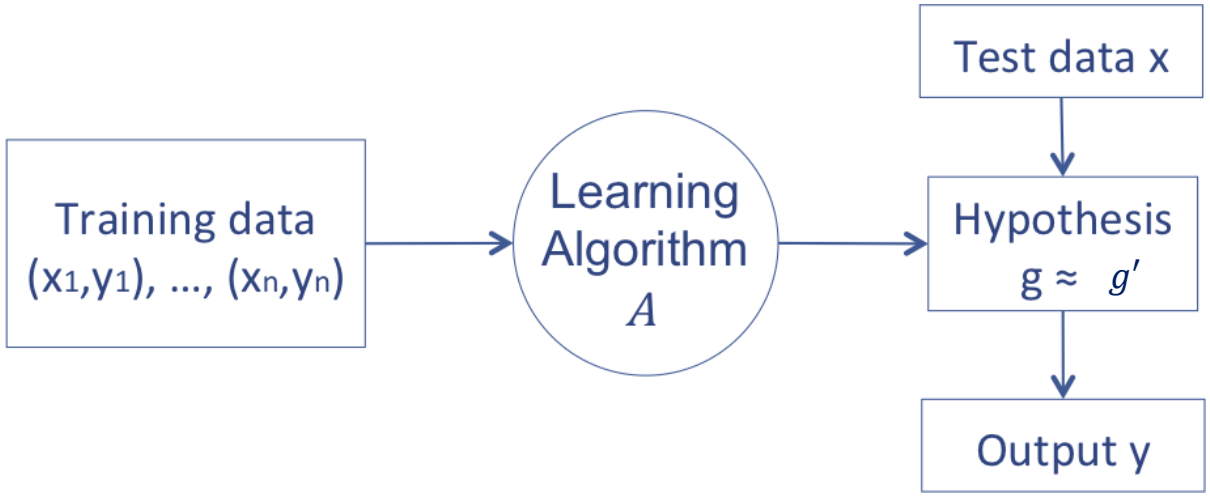
- ML sets a hypothesis function, f', which best approximates target function f with some performance measure

- Problem Setting
  - Set of possible instance(domain): X
  - Output: Y
  - Unknown target function $f: X \rightarrow Y$
  - Set of hypothesis function space $H \subset \{g | g: X \rightarrow Y\}$
  - **Input**: Training example $\{\langle x_i, y_i \rangle\}$
  - **Output**: $g' \in H$ that best approximates target function f with some performance measure

It is impossible to check all functions when setting hypothesis function space. Thus limit it into a set to find

What is Machine Learning (ML)?

- Learning using input data (training data)
  - Supervised learning : with label y $\{\langle x_i, y_i \rangle\}$
  - Unsupervised learning : without label y
- Return hypothesis, g′ among $g \in H$, best approximating target function g'



Probability Theory

- ML– Probabilistic Perspective
  - ML sets a probability density function (PDF), rather than a deterministic function of hypothesis, and find the parameters of the PDF

  Ex) Assume the data has a Gaussian PDF, and then mean and covariance need to be found
  - function parameter → PDF parameter

Estimation

- In most case, the information of real probability density distribution can’t be gotten
- This must be determined by the test data
- Parameter Estimation
  - Estimate parameter about density by MLE (maximum likelihood estimation) method
- Non-parametric Density Estimation
  - k-NNR

Maximum Likelihood Estimation

- Maximum Likelihood Estimation (MLE)
  - Estimate random variable's parameter using observation or data

Ex) when flipping coin, we can get the p (probability of the front) by counting the number of the front among all trials

  - PDF $f = \{f(\cdot\,|\theta)\}$ and observation $X = (x_1, x_2, \dots, x_n)$

If f is a Gaussian function, θ includes mean μ and covariance Σ.

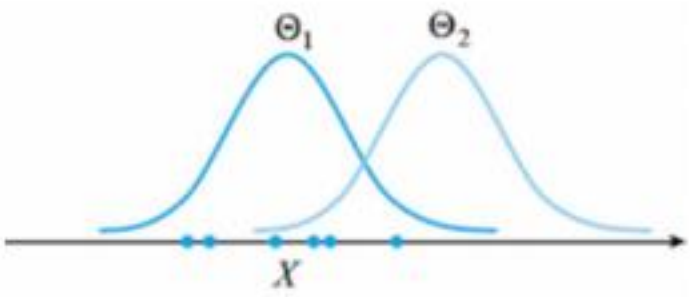
If f is a Bernoulli function, θ includes $0 \leq p \leq 1$

$$L(\theta; x_1, x_2, \dots, x_n) = L(\theta; X) = f(X|\theta) = f(x_1, x_2, \dots, x_n|\theta)$$
$$\hat{\theta} = \underset{\theta}{argmax}\, L(\theta; X) = \underset{\theta}{argmax}\, f(X|\theta)$$

Maximum Likelihood Estimation

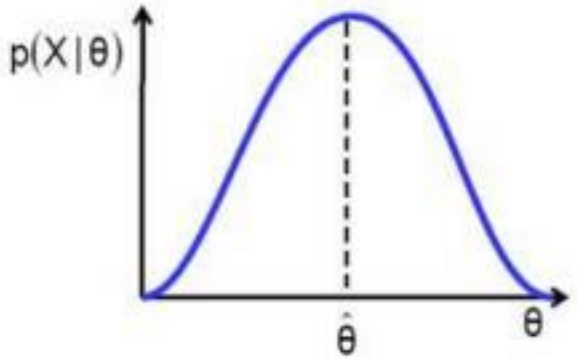
- Find the Θ that has maximum likelihood about given X

- P(X| Θ1) > P(X| Θ2)



$$\hat{\theta} = \arg\max[p(X \mid \theta)]$$

MAXIMUM LIKELIHOOD



Maximum Likelihood Estimation

- Estimate parameter θ=[θ1, θ2, …, θN] using sample data X={x1,x2,…,xN} observed at probability density function
  - The entire sample set is expressed by the joint probability density

$$p(X \mid \theta) = p(x^{(1} \mid \theta)\, p(x^{(2} \mid \theta) \ldots p(x^{(N} \mid \theta) = \prod_{k=1}^{N} p(x^{(k} \mid \theta)$$

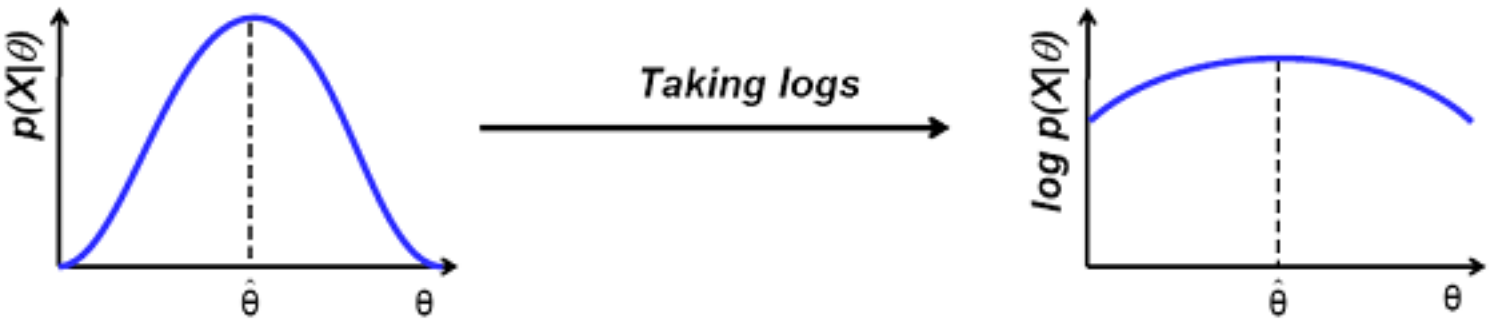
  - Θ , having the highest probability, becomes the estimated parameter
  - Take the log

$$\hat{\theta} = \text{argmax}\left[\log \prod_{k=1}^{N} p\left(x^{(k} \mid \theta\right) \right] = \text{argmax}\left[\sum_{k=1}^{N} \log p\left(x^{(k} \mid \theta\right) \right]$$

Maximum Likelihood Estimation

- The log function is convenient to calculate
  - Maximize ∑(sum) is easier than ∏(product)
  - If distribution is similar to gaussian, increase the efficiency

$$\hat{\theta} = \text{argmax}[p(X \mid \theta)] = \text{argmax}[\log p(X \mid \theta)]$$



Maximum Likelihood Estimation

- Probability density function p(x) = N(μ, σ).
  If X={x1,x2,…,xN} and σ is fixed. Get the MLE of μ.

$$\theta = \mu \Rightarrow \hat{\theta} = \operatorname{argmax} \sum_{k=1}^{N} \log p\left(x^{(k} \mid \theta\right)$$

$$= \operatorname{argmax} \sum_{k=1}^{N} \log\left(\frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2} \left(x^{(k} - \mu\right)^2 \right) \right)$$

$$= \operatorname{argmax} \sum_{k=1}^{N} \left\{ \log\left(\frac{1}{\sqrt{2\pi}\sigma} \right) - \frac{1}{2\sigma^2} \left(x^{(k} - \mu\right)^2 \right\}$$

Maximum Likelihood Estimation

- Maximum point

$$\frac{\partial}{\partial \mu}\sum_{k=1}^{N}\left\{\log\left(\frac{1}{\sqrt{2\pi}\sigma}\right)-\frac{1}{2\sigma^2}\left(x^{(k}-\mu\right)^2\right\}=-\frac{1}{2\sigma^2}\frac{\partial}{\partial \mu}\sum_{k=1}^{N}\left(x^{2(k}-2x^{(k}\mu+\mu^2\right)$$

$$=\frac{1}{2\sigma^2}\frac{\partial}{\partial \mu}\sum_{k=1}^{N}\left(2x^{(k}\mu-\mu^2\right)=\sum_{k=1}^{N}\left(x^{(k}-\mu\right)=\sum_{k=1}^{N}x^{(k}-N\mu=0\Rightarrow\mu=\frac{1}{N}\sum_{k=1}^{N}x^{(k}$$

- MLE of μ is average of X.

Maximum Likelihood Estimation

- Probability density function p(x) = N(μ, σ).
  If X={x1,x2,…,xN} and σ is fixed. Get the MLE of μ and σ.

$$\hat{\theta} = \begin{bmatrix} \theta_1 = \mu \\ \theta_2 = \sigma^2 \end{bmatrix} \Rightarrow \nabla_\theta = \begin{bmatrix} \frac{\partial}{\partial \theta_1} \sum_{k=1}^{N} \log p(x^{(k} \mid \theta) \\ \frac{\partial}{\partial \theta_2} \sum_{k=1}^{N} \log p(x^{(k} \mid \theta) \end{bmatrix} = \sum_{k=1}^{N} \begin{bmatrix} \frac{1}{\theta_2}(x^{(k} - \theta_1) \\ -\frac{1}{2\theta_2} + \frac{(x^{(k} - \theta_1)^2}{2\theta_2^2} \end{bmatrix} = 0$$

- Simplify them with respect to θ_1 and θ_2

$$\hat{\theta}_1 = \frac{1}{N} \sum_{k=1}^{N} x^{(k}; \quad \hat{\theta}_2 = \frac{1}{N} \sum_{k=1}^{N} (x^{(k} - \hat{\theta}_1)^2$$

Maximum Likelihood Estimation

- Disadvantage of MLE
  - Too sensitive to the observation

EX) when we only get the front of coin during flipping coin trials, then $p = 1$ by MLE

Solution ➔ Maximum a Posteriori Estimation (MAP)

Maximum a Posteriori Estimation (MAP)

- MLE : $\hat{\theta} = \underset{\theta}{argmax}\, f(X|Y,\theta)$
- MAP : $\hat{\theta} = \underset{\theta}{argmax}\, f(Y|X,\theta)$
- While MLE produces parameters based on the current observation, MAP uses general knowledge about the data as well as the observation (prior knowledge)
- EX) Flipping coin example
- ➔ MAP uses Bayes' Theorem

$$\hat{\theta} = \underset{\theta}{argmax}\, f(Y|X,\theta) = \underset{\theta}{argmax}\, \frac{f(X|Y,\theta)f(Y)}{f(X|\theta)}$$

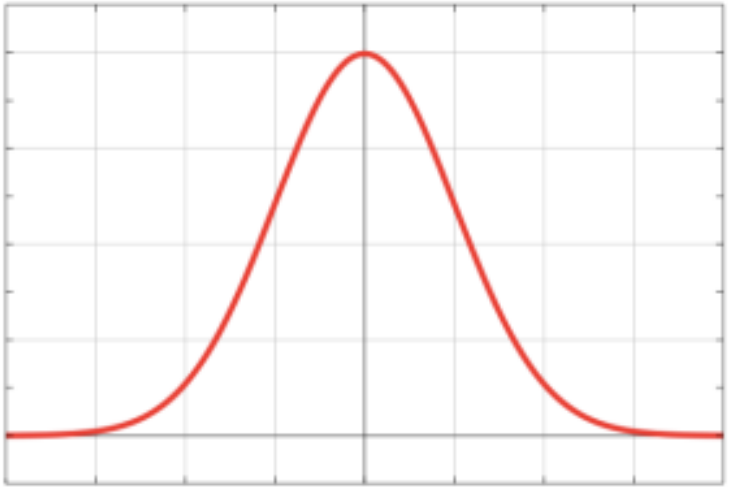
$$\rightarrow \hat{\theta} = \underset{\theta}{argmax}\, f(X|Y,\theta)f(Y)$$

- $f(\theta)$ is a prior knowledge or prior assumption

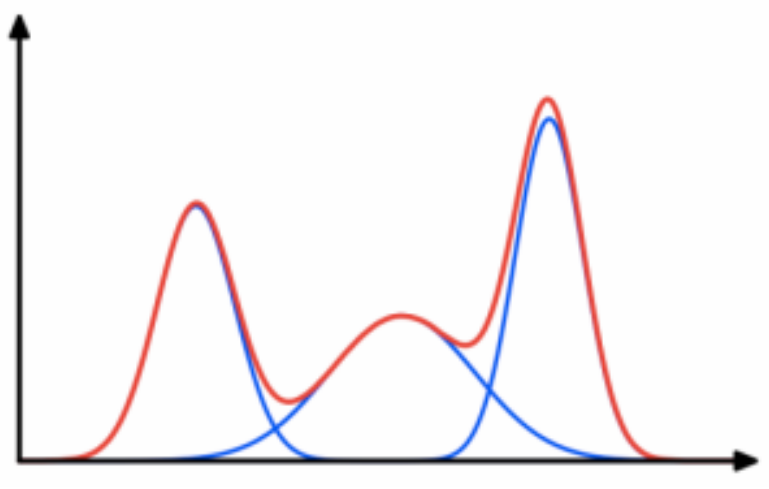
Maximum a Posteriori Estimation (MAP)

- Prior knowledge could be prejudice
- The results are depending on the prior, and thus it is very important to set the prior probability function carefully

Likelihood Ratio Test



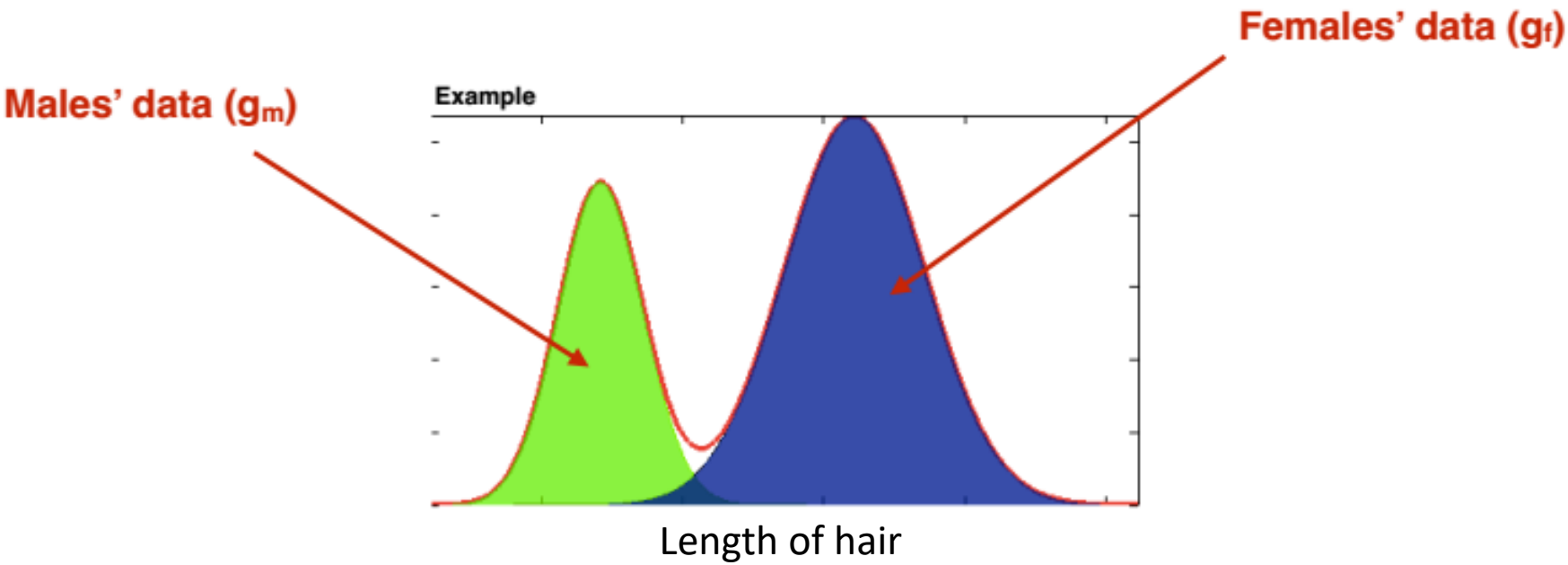
Gaussian Distribution



Gaussian Mixture Model

Likelihood Ratio Test

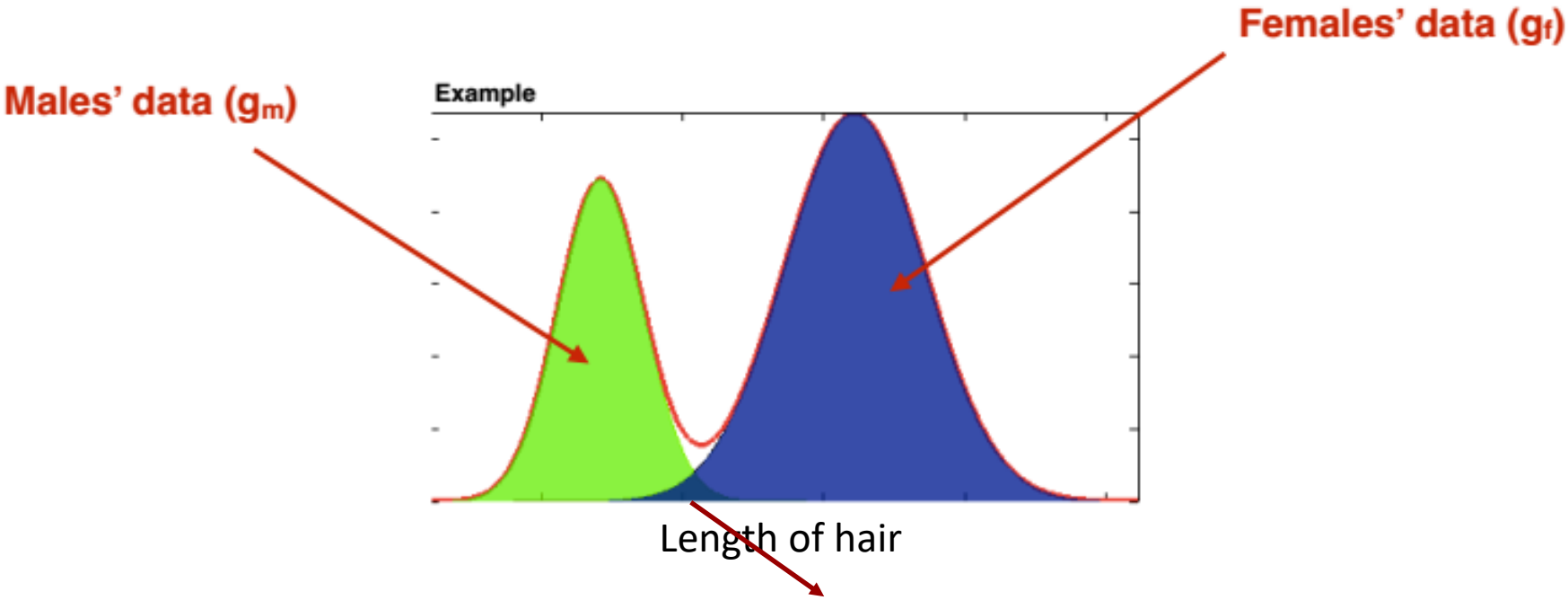
* PDF of hair length of the students in our class



https://www.youtube.com/watch?v=U8mjbpqsOTI

Likelihood Ratio Test

- PDF of hair length of the students in our class



- Assume we are going to classify an object into classes based on the evidence provided by a measurement (or feature vector) **x**

Likelihood Ratio Test

- Choose a class most ‘probable’ given the observed feature vector **x**
- In formal

  Evaluate the posterior probability of each class $P(w_i|x)$ and choose a class with the largest $P(w_i|x)$

Likelihood Ratio Test

- 2 class classification example
- The decision rule

$$if\ P(w_1|x) > P(w_2|x), choose\ w_1$$
$$else, \qquad choose\ w_2$$

- Or

$$P(w_1|x) \underset{w_2}{\overset{w_1}{\gtrless}} P(w_2|x)$$

- Using Bayes theorem

Likelihood ratio test

$$\frac{P(x|w_1)P(w_1)}{P(x)} \underset{w_2}{\overset{w_1}{\gtrless}} \frac{P(x|w_2)P(w_2)}{P(x)} \Rightarrow \Lambda(x) = \frac{P(x|w_1)}{P(x|w_2)} \underset{w_2}{\overset{w_1}{\gtrless}} \frac{P(w_2)}{P(w_1)}$$

Likelihood ratio

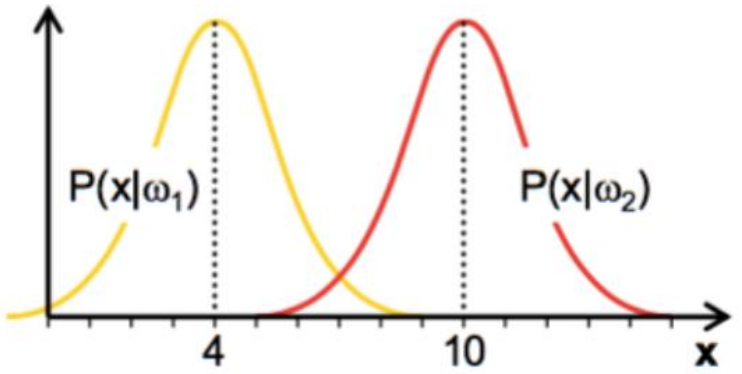
Likelihood Ratio Test

- Example

Derive a classification rule using the likelihood ratio test with assuming the priors of two classes are equal

$$P(x|w_1) = \frac{1}{\sqrt{2\pi}} exp\{-\frac{1}{2}(x-4)^2\}$$

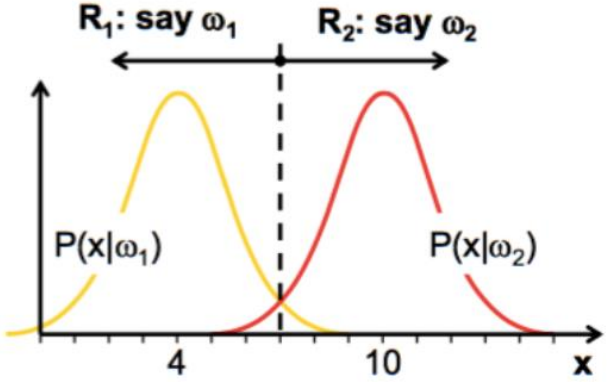
$$P(x|w_2) = \frac{1}{\sqrt{2\pi}} exp\{-\frac{1}{2}(x-10)^2\}$$



$$\Lambda(x) = \frac{1/\sqrt{2\pi}\ exp\{-\frac{1}{2}(x-4)^2\}}{1/\sqrt{2\pi}\ exp\{-\frac{1}{2}(x-10)^2\}} \underset{w_2}{\overset{w_1}{\gtrless}} \frac{1}{1}$$

$$(x-4)^2 - (x-10)^2 \underset{w_2}{\overset{w_1}{\gtrless}} 0 \Rightarrow x \underset{w_2}{\overset{w_1}{\lessgtr}} 7 \Rightarrow$$

Comput



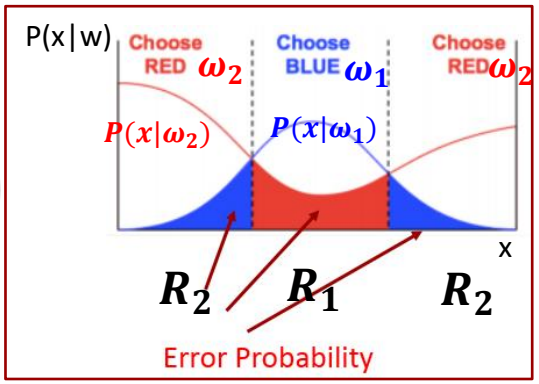
Error Probability

Decided by the borders

$$P(error) = P(x \in R_2, \omega_1) + P(x \in R_1, \omega_2)$$

$$= P(x \in R_2 \mid \omega_1)P(\omega_1) + P(x \in R_1 \mid \omega_2)P(\omega_2)$$

$$= \int_{R_2} p(x \mid \omega_1)P(\omega_1)dx + \int_{R_1} p(x \mid \omega_2)P(\omega_2)dx$$



$$P(error) = \sum_{i=1}^{C} P(error \mid \omega_i)P(\omega_i)$$

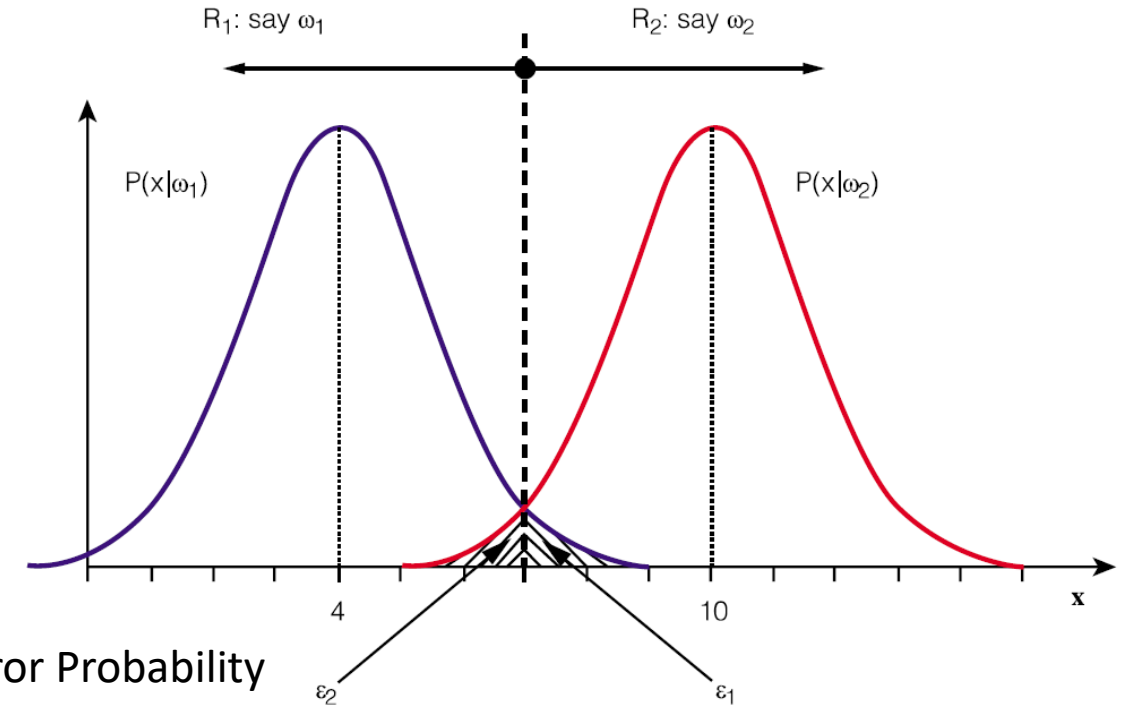
, where

$$P(error \mid \omega_i) = P(choose\ \ \omega_j \mid \omega_i) = \int_{R_j} P(x \mid \omega_i)dx$$

Error Probability

$$P[\text{error}] = P[\omega_1] \underbrace{\int_{R_2} P(x \mid \omega_1)dx}_{\varepsilon_1} + P[\omega_2] \underbrace{\int_{R_1} p(x \mid \omega_2)dx}_{\varepsilon_2}$$

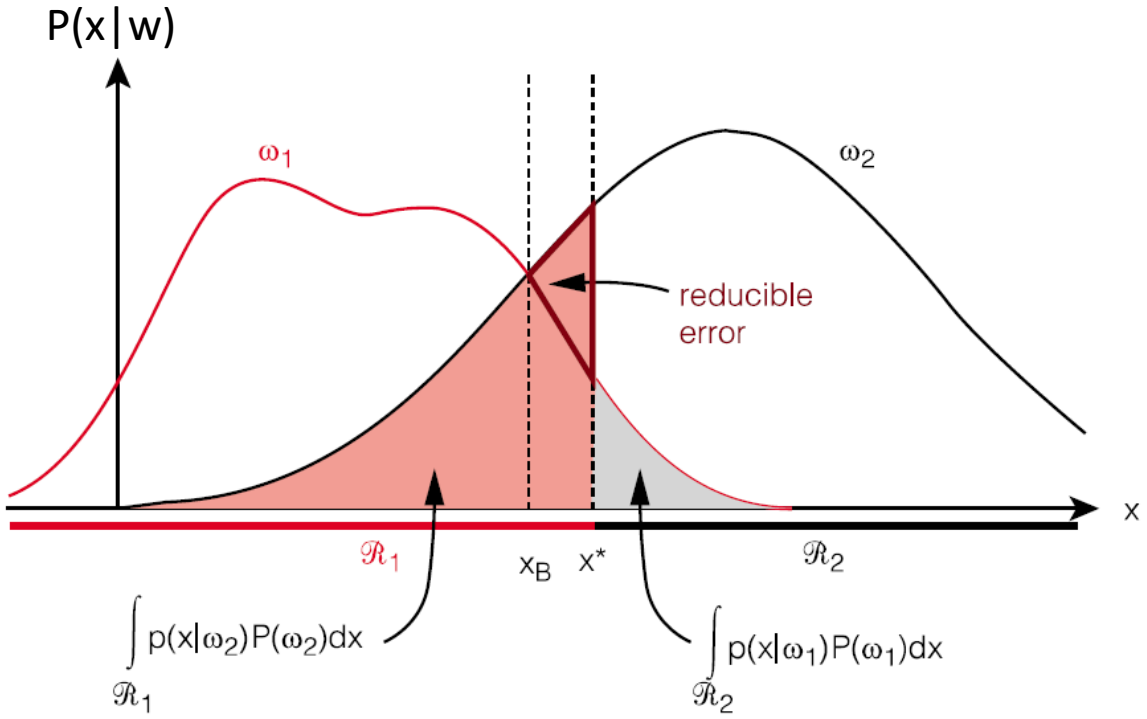
$P(\text{error}) = (\varepsilon_1 + \varepsilon_2)/2$, given $P(w_1) = P(w_2) = \frac{1}{2}$



Error Probability

Error Probability

- The optimal border = minimum error probability



[그림 5-3] 오류확률에 의한 결정 경계의 결정 [Duda, Hart, Stock, 2001]

Loss (or Cost) function

- In the previous slides, the error was 0 or 1 (misclassification number) when the classification was correct or wrong.
- However, the number of error can be a summation of squared difference between target data and estimated data. (This is one example)

  ➔ Cost function or Lost function

- For example, let's think about buying a wrong plane ticket to find a person in the world
- While true value is constant, the estimated value can be changed depending on the updated parameters

$$L(\theta, \hat{\theta}) : Loss\ function$$

(θ : true parameter, $\hat{\theta}$: estimated parameter)

Bayes Risk

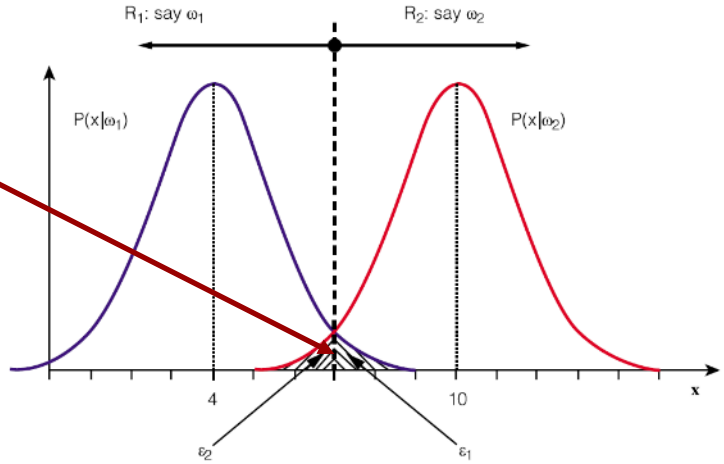
- So far we have assumed that the penalty of misclassifying a class w_1 as class w2 is the same as the opposite way $(w_2 \rightarrow w_1)$
- In general, this is not the case:
  - For example, misclassifying a cancer sufferer as a healthy patient is a much more serious problem than the other way around
- This concept can be also formalised in terms of a cost (or lost) function C_{ij}
  - C_{ij} represents the cost of choosing (wrong) class $w_i$when class w_j is the true class
- We define the Bayes Risk as the expected value of the cost

$$\Re = E[C] = \sum_{i=1}^{2}\sum_{j=1}^{2} C_{ij} \cdot P(\text{choose } w_i \text{ and } x \in w_j) = \sum_{i=1}^{2}\sum_{j=1}^{2} C_{ij} \cdot P(x \in R_i \mid w_j) \cdot P(w_j)$$

Bayes Risk

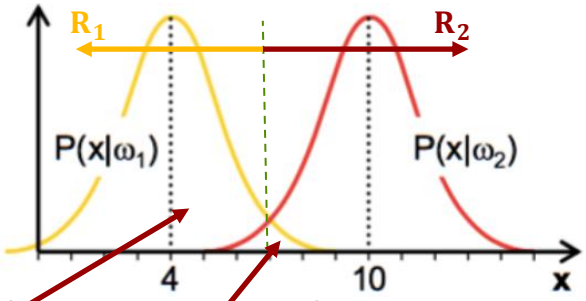
$$R = E[C] = \sum_{i=1}^{2}\sum_{j=1}^{2} C_{ij} \cdot P(\text{choose } \omega_i ,\ x \in \omega_j) = \sum_{i=1}^{2}\sum_{j=1}^{2} C_{ij} \cdot P(x \in R_i \mid \omega_j) \cdot P(\omega_j)$$

, where $P(x \in R_i \mid \omega_j) = \int_{R_i} P(x \mid \omega_j) dx$



$$R = \int_{R_1} [C_{11}P(\omega_1)P(x \mid \omega_1) + C_{12}P(\omega_2)P(x \mid \omega_2)]dx +$$
$$\int_{R_2} [C_{21}P(\omega_1)P(x \mid \omega_1) + C_{22}P(\omega_2)P(x \mid \omega_2)]dx$$

Bayes Risk



- Decision rule to reduce the Bayes risk

when i=1

$$\int_{R_1} P(x \mid \omega_i)dx + \int_{R_2} P(x \mid \omega_i)dx = \int_{R_1 \cup R_2} P(x \mid \omega_i)dx = 1$$

$$\begin{aligned} R = {} & C_{11}P(\omega_1)\int_{R_1} P(x \mid \omega_1)dx + C_{12}P(\omega_2)\int_{R_1} P(x \mid \omega_2)dx + \\ & + C_{21}P(\omega_1)\int_{R_2} P(x \mid \omega_1)dx + C_{22}P(\omega_2)\int_{R_2} P(x \mid \omega_2)dx + \\ & + C_{21}P(\omega_1)\int_{R_1} P(x \mid \omega_1)dx + C_{22}P(\omega_2)\int_{R_2} P(x \mid \omega_2)dx + \\ & - C_{21}P(\omega_1)\int_{R_1} P(x \mid \omega_1)dx - C_{22}P(\omega_2)\int_{R_1} P(x \mid \omega_2)dx \end{aligned}$$

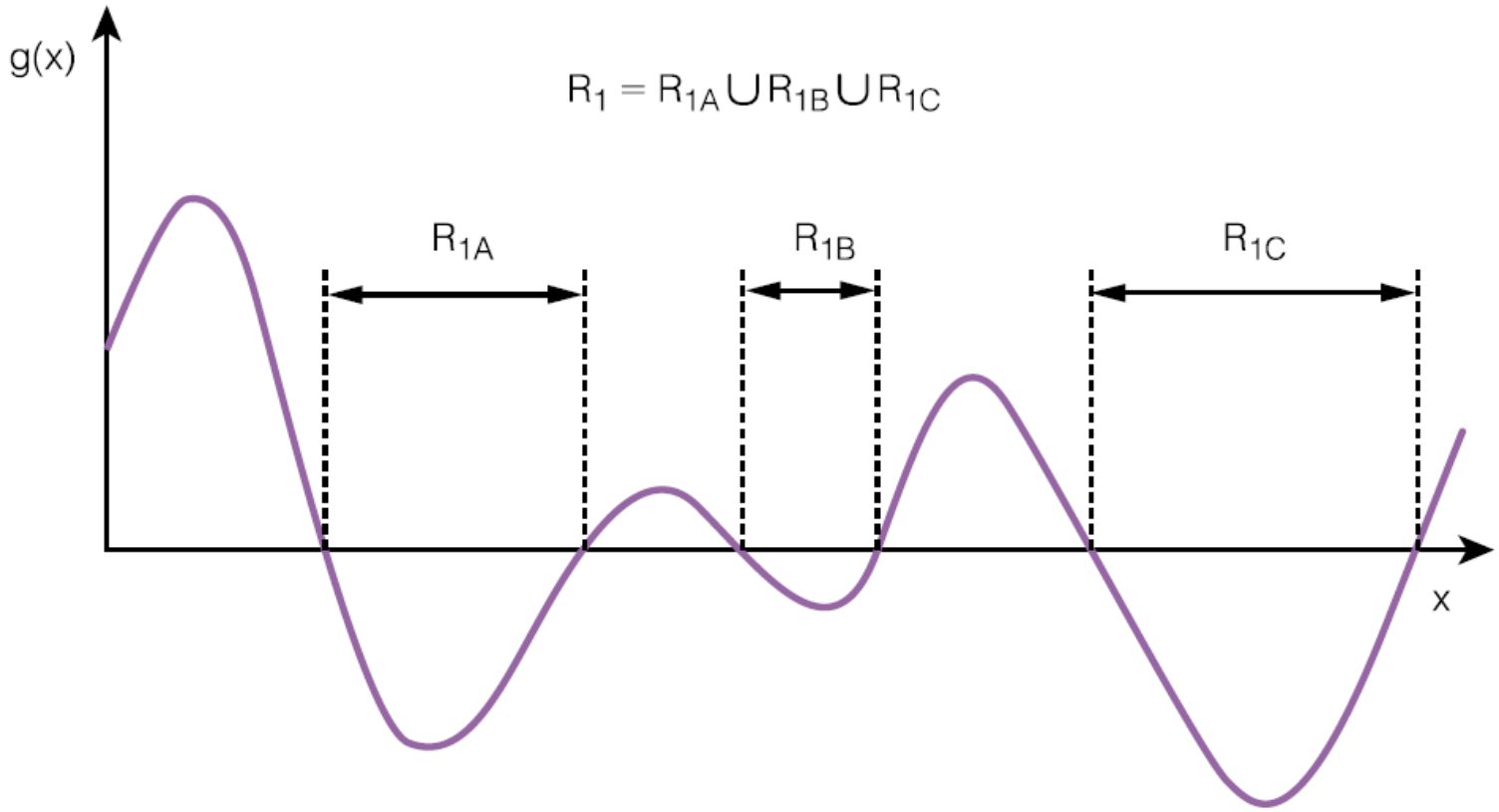
$$\begin{aligned} R = {} & C_{21}P(\omega_1) + C_{22}P(\omega_2) \\ & + (C_{12} - C_{22})P(\omega_2)\int_{R_1} P(x \mid \omega_2)dx - (C_{21} - C_{11})P(\omega_1)\int_{R_1} P(x \mid \omega_1)dx \end{aligned}$$

$$R_1 = \arg\min_{R_1} \left\{ \int_{R_1} [(C_{12} - C_{22})P[\omega_2]P(x \mid \omega_2) - (C_{21} - C_{11})P[\omega_1]P(x \mid \omega_1)]dx \right\}$$

$$= \arg\min_{R_1} \left\{ \int_{R_1} g(x)dx \right\}$$

Bayes Risk

- Find the decision area based on the Bayes risk



Bayes Risk

$$\mathbf{R}_1 = \arg\min\left\{\int_{\mathbf{R}_1}[(\mathbf{C}_{12}-\mathbf{C}_{22})\mathbf{P}[\omega_2]\mathbf{P}(\mathbf{x}\,|\,\omega_2)-(\mathbf{C}_{21}-\mathbf{C}_{11})\mathbf{P}[\omega_1]\mathbf{P}(\mathbf{x}\,|\,\omega_1)]\mathbf{dx}\right\}$$

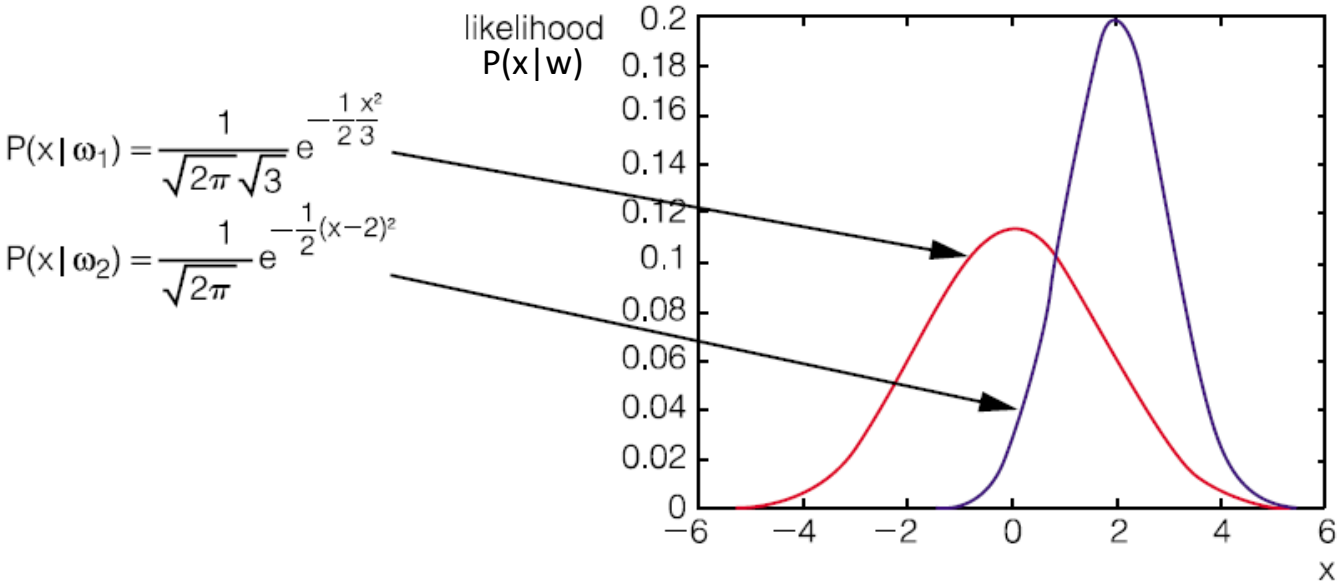
$$= \arg\min\left\{\int_{\mathbf{R}_1}\mathbf{g}(\mathbf{x})\mathbf{dx}\right\}$$

$$(\mathbf{C}_{12}-\mathbf{C}_{22})\mathbf{P}[\omega_2]\mathbf{P}(\mathbf{x}\,|\,\omega_2) \underset{\omega_1}{\overset{\omega_2}{\gtrless}} (\mathbf{C}_{21}-\mathbf{C}_{11})\mathbf{P}[\omega_1]\mathbf{P}(\mathbf{x}\,|\,\omega_1)$$

$$\frac{\mathbf{P}(\mathbf{x}\,|\,\omega_1)}{\mathbf{P}(\mathbf{x}\,|\,\omega_2)} \underset{\omega_2}{\overset{\omega_1}{\gtrless}} \frac{(\mathbf{C}_{12}-\mathbf{C}_{22})\mathbf{P}[\omega_2]}{(\mathbf{C}_{21}-\mathbf{C}_{11})\mathbf{P}[\omega_1]}$$

Bayes Risk

Ex) Given the likelihood functions below for two classes, their prior probabilities, $P(w_1) = P(w_2) = 0.5$, and costs $C_{11} = C_{22} = 0, C_{12} = 1, C_{21} = 3^{\frac{1}{2}}$, find the likelihood ratio based on the Bayes risk and decision boundary to minimize the error probability



Minimise Bayes Risk

Likelihood Ratio

$$\Lambda(x) = \frac{\frac{1}{\sqrt{2\pi}\sqrt{3}} e^{-\frac{1}{2}\frac{x^2}{3}}}{\frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}(x-2)^2}} \underset{\omega_2}{\overset{\omega_1}{\lessgtr}} \frac{1}{\sqrt{3}}$$

$$\frac{e^{-\frac{1}{2}\frac{x^2}{3}}}{e^{-\frac{1}{2}(x-2)^2}} \underset{\omega_2}{\overset{\omega_1}{\lessgtr}} 1$$

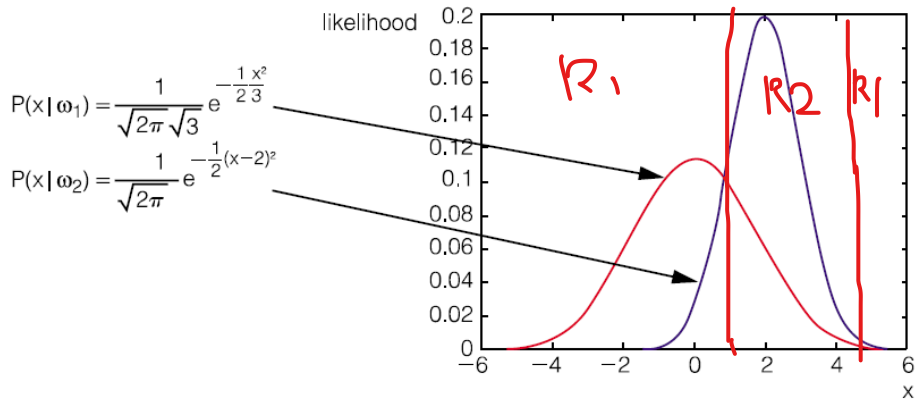
$$-\frac{1}{2}\frac{x^2}{3} + \frac{1}{2}(x-2)^2 \underset{\omega_2}{\overset{\omega_1}{\lessgtr}} 0$$

$$2x^2 - 12x + 12 \underset{\omega_2}{\overset{\omega_1}{\lessgtr}} 0 \Rightarrow x = 4.73, 1.27$$

$$\frac{P(x|\omega_1)}{P(x|\omega_2)} \underset{\omega_2}{\overset{\omega_1}{\lessgtr}} \frac{(C_{12}-C_{22})P[\omega_2]}{(C_{21}-C_{11})P[\omega_1]}$$

, $P(w_1) = P(w_2) = 0.5$, and

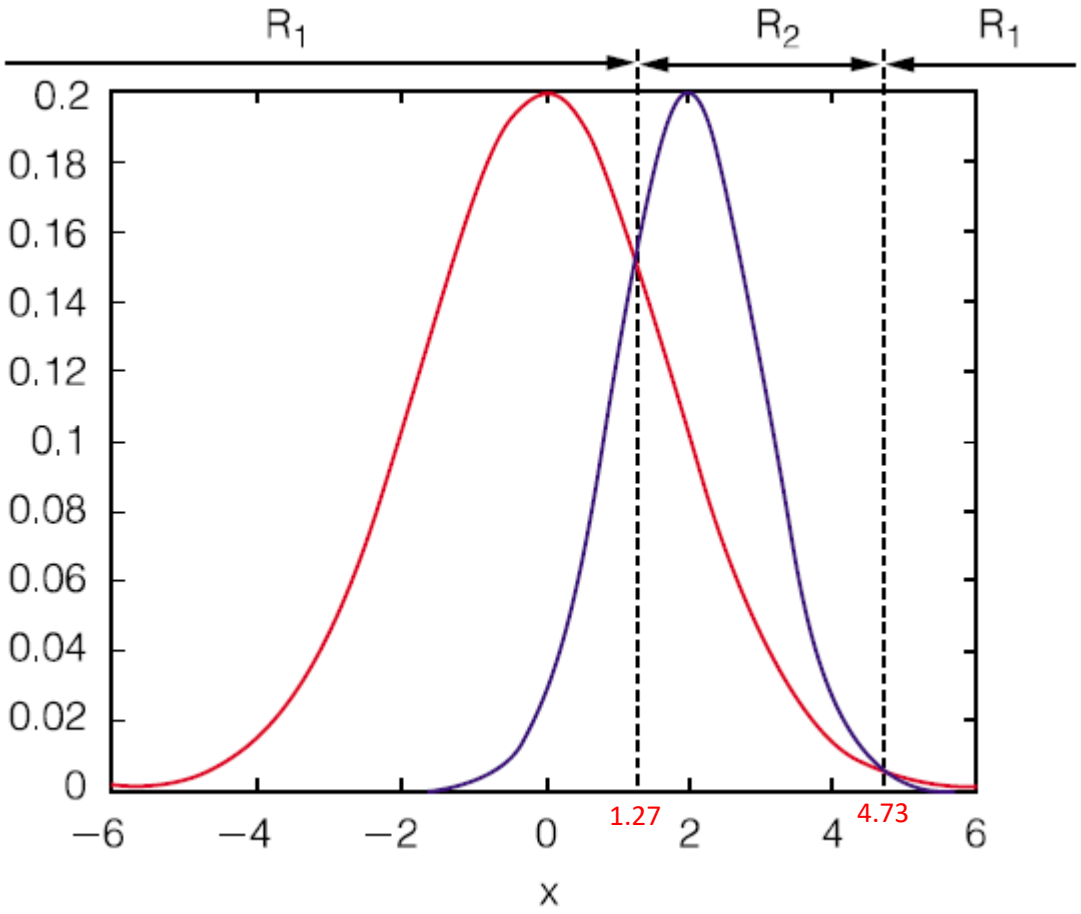
costs $C_{11} = C_{22} = 0, C_{12} = 1, C_{21} = 3^{\frac{1}{2}}$



$\therefore \omega_1 < 1.27, \omega_1 > 4.73$

$1.27 < \omega_2 < 4.73$

Minimise Bayes Risk



Variations of LRT Decision Rule

- Bayes' Criterion
  - LRT decision rule with reducing the Bayes' risk

$$\Lambda(\mathbf{x}) = \frac{P(\mathbf{x}\mid\omega_1)}{P(\mathbf{x}\mid\omega_2)} \underset{\omega_2}{\overset{\omega_1}{\gtrless}} \frac{(C_{12}-C_{22})P[\omega_2]}{(C_{21}-C_{11})P[\omega_1]}$$

- MAP Criterion
  - Symmetric or zero-one cost functions make Bayes' criterion a ratio of posteriori functions➔ called maximum a posteriori (MAP) criterion

$$C_{ij} = \begin{cases} 0 & i = j \\ 1 & i \neq j \end{cases} \Rightarrow \Lambda(\mathbf{x}) = \frac{P(\mathbf{x}\mid\omega_1)}{P(\mathbf{x}\mid\omega_2)} \underset{\omega_2}{\overset{\omega_1}{\gtrless}} \frac{P[\omega_2]}{P[\omega_1]} \Leftrightarrow \frac{P(\omega_1\mid\mathbf{x})}{P(\omega_2\mid\mathbf{x})} \underset{\omega_2}{\overset{\omega_1}{\gtrless}} 1$$

Variations of LRT Decision Rule

- ML Criterion
  - Equal prior probabilities and zero-one cost functions make Bayes' criterion a ratio of likelihood functions ➔ called maximum likelihood (ML) criterion

$$\left.\begin{aligned} C_{ij} &= \begin{cases} 0 & i = j \\ 1 & i \neq j \end{cases} \\ P(\omega_i) &= \frac{1}{C} \;\forall i \end{aligned}\right\} \Rightarrow \Lambda(x) = \frac{P(x \mid \omega_1)}{P(x \mid \omega_2)} \underset{\omega_2}{\overset{\omega_1}{\gtrless}} 1$$