第2章：贝叶斯决策理论

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2015年9月13日

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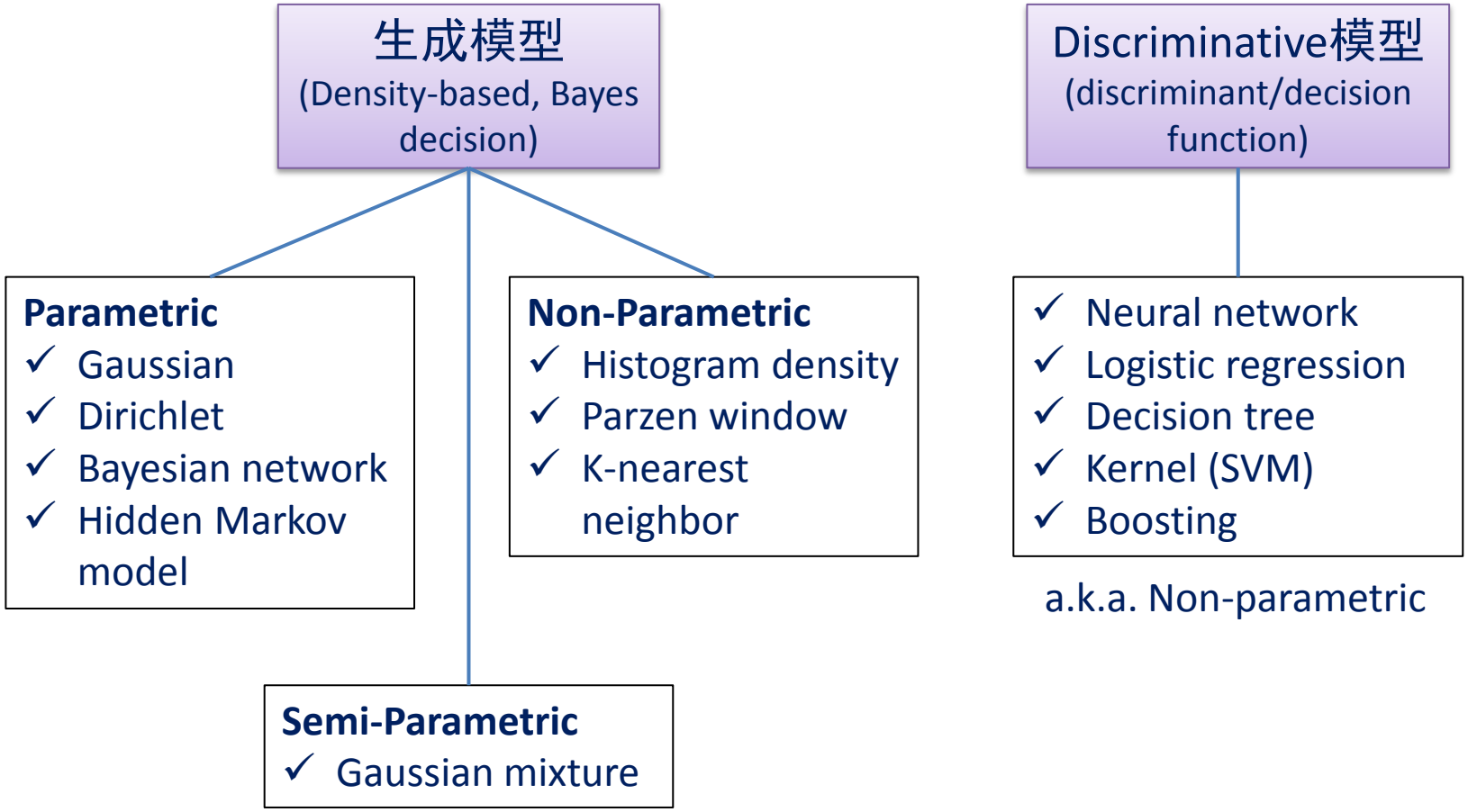
统计模式识别方法


生成模型
(Density-based, Bayes decision)
Discriminative模型
(discriminant/decision function)
Parametric
✓ Gaussian
✓ Dirichlet
✓ Bayesian network
✓ Hidden Markov model
Non-Parametric
✓ Histogram density
✓ Parzen window
✓ K-nearest neighbor
Semi-Parametric
✓ Gaussian mixture
✓ Neural network
✓ Logistic regression
✓ Decision tree
✓ Kernel (SVM)
✓ Boosting
a.k.a. Non-parametric

提纲

- 导论：2类的例子
- 最小风险决策
- 判别函数和决策面
- 高斯概率密度
- 高斯密度下的判别函数
- 分类错误率

导论：问题表示

- 类别： $\omega_i, i = 1, \ldots, c$
- 特征矢量 $\mathbf{x} = [x_1, \ldots, x_d] \in R^d$
- 先验概率 $P(\omega_i)$ $\sum_{i=1}^{c} P(\omega_i) = 1$
- 概率密度函数(条件概率) $p(\mathbf{x} \mid \omega_i)$
- 后验概率

$$P(\omega_i \mid \mathbf{x}) = \frac{p(\mathbf{x} \mid \omega_i) P(\omega_i)}{p(\mathbf{x})} = \frac{p(\mathbf{x} \mid \omega_i) P(\omega_i)}{\sum_{j=1}^{c} p(\mathbf{x} \mid \omega_j) P(\omega_j)}$$

$$\sum_{i=1}^{c} P(\omega_i \mid \mathbf{x}) = 1$$

2类的例子

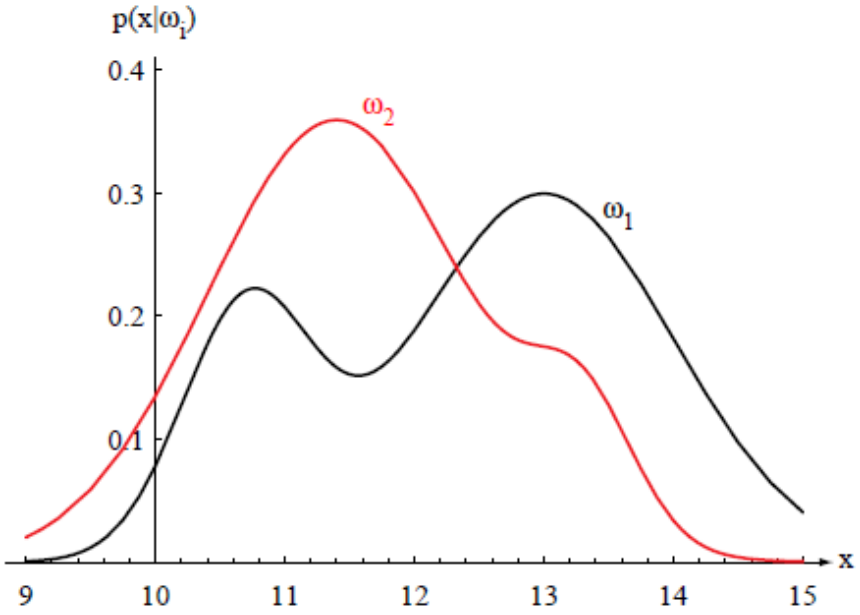
- Salmon (ω_1) and sea bass (ω_2)
- If we have only prior probability
  - 例如，教室门口判断进来的是男生还是女生，没有任何传感器
  - Decide ω_1 if $P(\omega_1) > P(\omega_2)$, otherwise ω_2
  - Minimum error decision

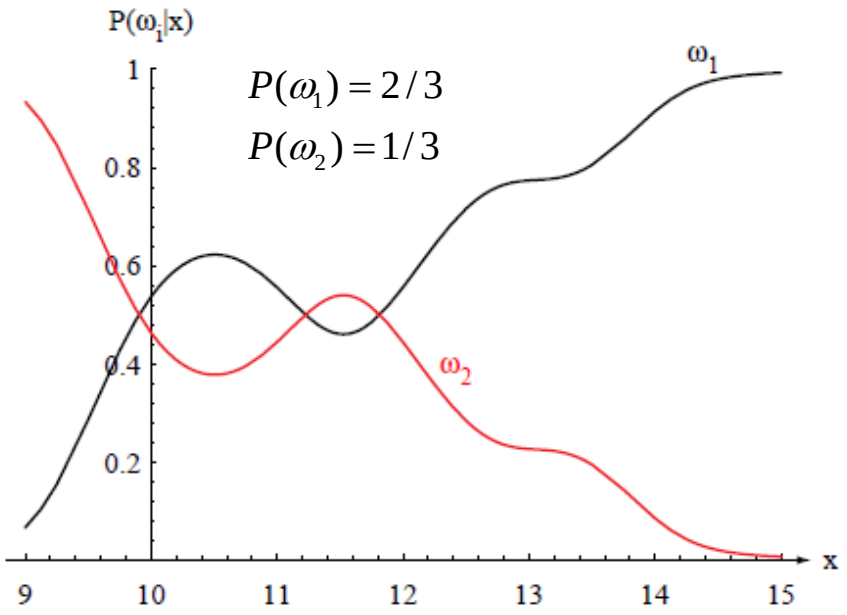
$$P(error) = \begin{cases} P(\omega_2) & \text{if we decide } \omega_1 \\ P(\omega_1) & \text{if we decide } \omega_2 \end{cases}$$

  - 教室门口判断性别的例子：错误率？

2类的例子

- Decision based on posterior probabilities





$$P(\omega_i \mid \mathbf{x}) = \frac{p(\mathbf{x} \mid \omega_i)P(\omega_i)}{p(\mathbf{x})} = \frac{p(\mathbf{x} \mid \omega_i)P(\omega_i)}{\sum_{j=1}^{c} p(\mathbf{x} \mid \omega_j)P(\omega_j)}$$

- Decision based on posterior probabilities

$$P(error|x) = \begin{cases} P(\omega_1|x) & \text{if we decide } \omega_2 \\ P(\omega_2|x) & \text{if we decide } \omega_1. \end{cases}$$

$$\text{Decide } \omega_1 \text{ if } P(\omega_1|x) > P(\omega_2|x); \text{ otherwise decide } \omega_2$$

$$P(error|x) = \min\,[P(\omega_1|x), P(\omega_2|x)].$$

- Evidence (a.k.a. likelihood)

$$\text{Decide } \omega_1 \text{ if } p(x|\omega_1)P(\omega_1) > p(x|\omega_2)P(\omega_2); \quad \text{otherwise decide } \omega_2$$

  - see $$P(\omega_i \,|\, \mathbf{x}) = \frac{p(\mathbf{x} \,|\, \omega_i)P(\omega_i)}{p(\mathbf{x})}$$

最小风险决策

- 决策代价(loss)
  - True class ω_j, decided as α_i $\quad \lambda_{ij} = \lambda(\alpha_i \mid \omega_j)$
    - 有时2类代价相差很大，比如医疗诊断的场合、工业检测、自动商店判断性别
- Condition risk

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

- Overall (expected) risk

$$R = \int R(\alpha(\mathbf{x})|\mathbf{x}) p(\mathbf{x})\ d\mathbf{x}$$

- Minimum risk decision (Bayes decision)

$$\arg\min_i R(\alpha_i \mid x)$$

- Minimum risk decision: 2-class case
  - Condition risk

$$R(\alpha_1|\mathbf{x}) = \lambda_{11}P(\omega_1|\mathbf{x}) + \lambda_{12}P(\omega_2|\mathbf{x})$$
$$R(\alpha_2|\mathbf{x}) = \lambda_{21}P(\omega_1|\mathbf{x}) + \lambda_{22}P(\omega_2|\mathbf{x})$$

  - Decision rule

$$R(\alpha_1 \mid x) < R(\alpha_2 \mid x) \leftrightarrow (\lambda_{21} - \lambda_{11})P(\omega_1|\mathbf{x}) > (\lambda_{12} - \lambda_{22})P(\omega_2|\mathbf{x})$$

    - Equivalently, decide ω_1 if

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

$$\frac{p(\mathbf{x}|\omega_1)}{p(\mathbf{x}|\omega_2)} > \frac{\lambda_{12} - \lambda_{22}}{\lambda_{21} - \lambda_{11}} \frac{P(\omega_2)}{P(\omega_1)}$$

最小错误率分类

- Zero-one loss

$$\lambda(\alpha_i|\omega_j) = \begin{cases} 0 & i = j \\ 1 & i \neq j \end{cases} \qquad i, j = 1, ..., c$$

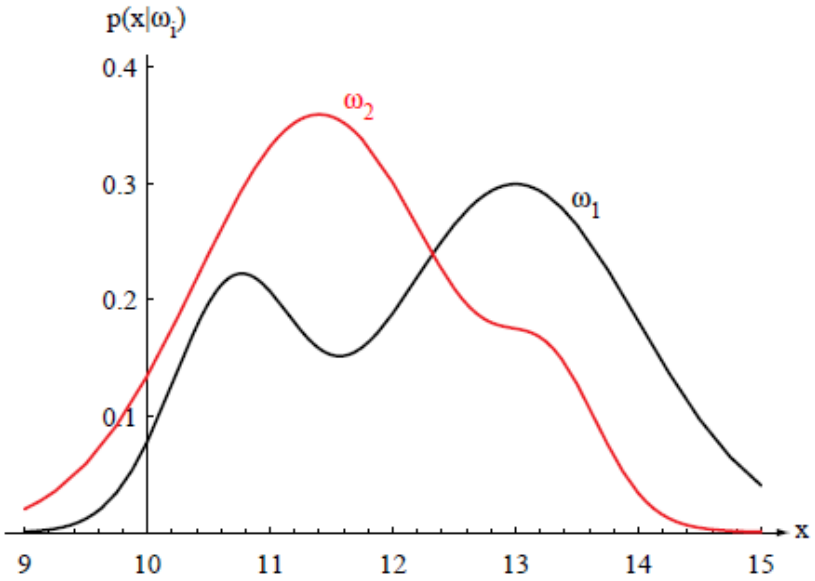
$$\begin{aligned} R(\alpha_i|\mathbf{x}) &= \sum_{j=1}^{c} \lambda(\alpha_i|\omega_j) P(\omega_j|\mathbf{x}) \\ &= \sum_{j \neq i} P(\omega_j|\mathbf{x}) \\ &= 1 - P(\omega_i|\mathbf{x}) \end{aligned}$$

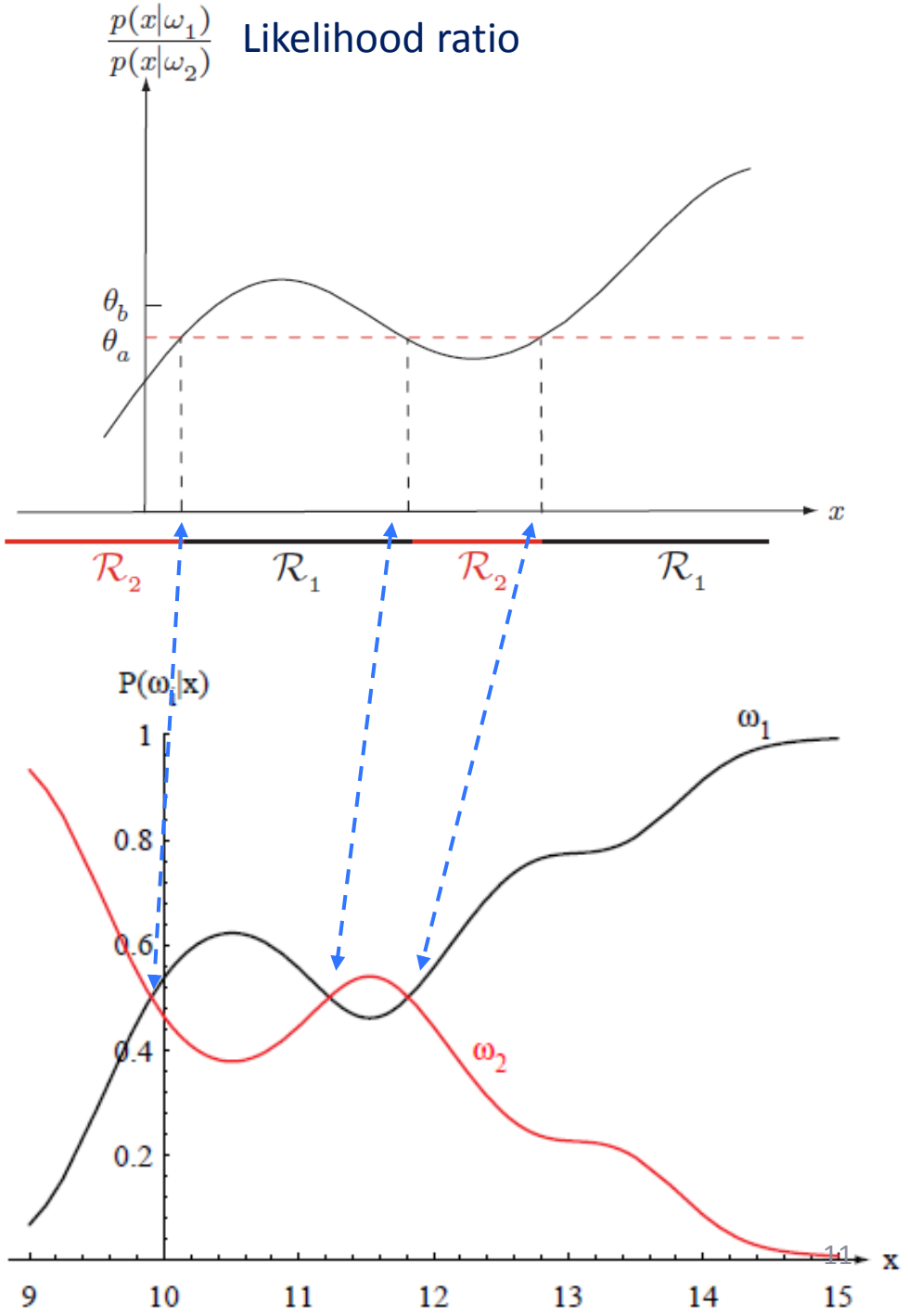
- Minimum error decision: Maximum a posteriori (MAP)

$$\text{Decide } \omega_i \text{ if } P(\omega_i|\mathbf{x}) > P(\omega_j|\mathbf{x}) \qquad \text{for all } j \neq i$$

- 2-class case
  - decide ω_1 if

$$\frac{p(\mathbf{x}|\omega_1)}{p(\mathbf{x}|\omega_2)} > \boxed{} \frac{P(\omega_2)}{P(\omega_1)}$$





带拒识的决策

- (Problem 13, Chapter 2)
  - C+1 classes

$$\lambda(\alpha_i \mid \omega_j) = \begin{cases} 0, & i = j \\ \lambda_s, & i \neq j \\ \lambda_r, & \text{reject} \end{cases} \qquad \lambda_r < \lambda_s$$

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

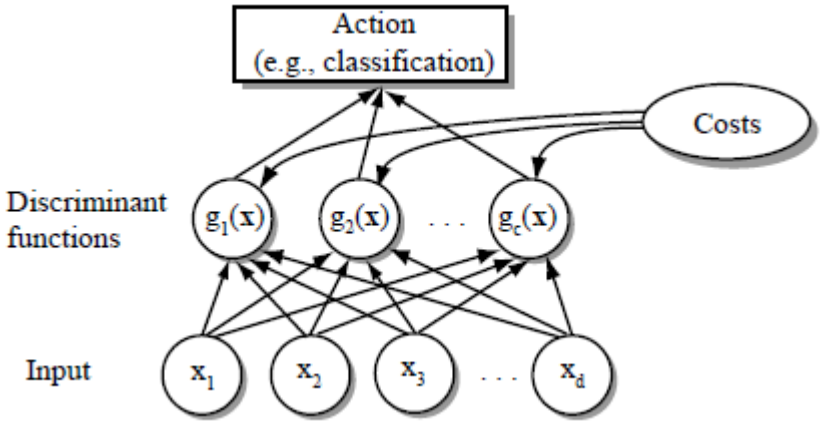
$$\Rightarrow \quad R_i(\mathbf{x}) = \begin{cases} \lambda_s[1 - P(\omega_i \mid \mathbf{x})], & i = 1, \ldots, c \\ \lambda_r, & \text{reject} \end{cases}$$

$$\arg\min_i R_i(\mathbf{x}) = \begin{cases} \arg\max_i P(\omega_i \mid \mathbf{x}), & \text{if } \max_i P(\omega_i \mid \mathbf{x}) > 1 - \lambda_r / \lambda_s \\ \text{reject}, & \text{otherwise} \end{cases}$$

判别函数、决策面

- 判别函数(Discriminant Function)
  - 表征模式属于每一类的广义似然度$g_i(\mathbf{x})$, i=1,…,c
  - 分类决策 $\arg\max_i g_i(\mathbf{x})$
  - E.g., conditional risk $g_i(\mathbf{x}) = -R(\alpha_i \mid \mathbf{x})$
  - Posterior probability $g_i(\mathbf{x}) = P(\omega_i \mid \mathbf{x})$
  - Likelihood $g_i(\mathbf{x}) = p(\mathbf{x} \mid \omega_i)P(\omega_i)$

$$g_i(\mathbf{x}) = \log p(\mathbf{x} \mid \omega_i) + \log P(\omega_i)$$

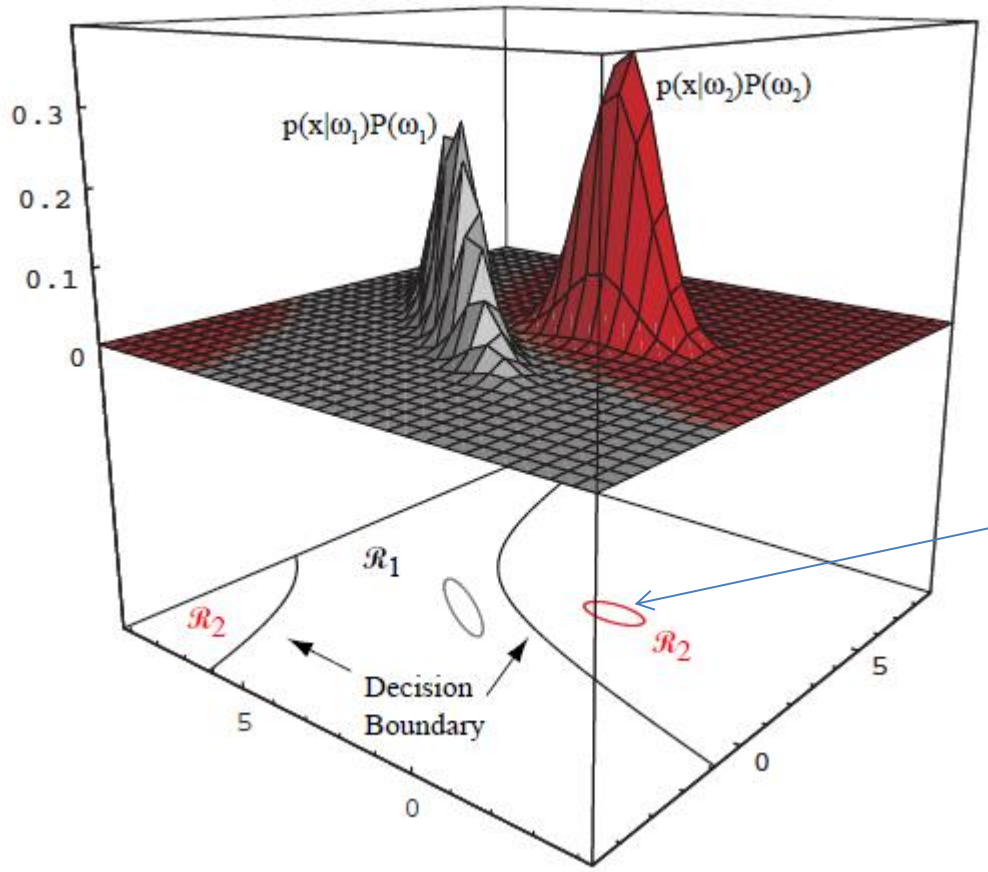


- 决策面(Decision surface)
  - 特征空间中二类判别函数相等的点的集合

$$g(\mathbf{x}) \equiv g_1(\mathbf{x}) - g_2(\mathbf{x}) \qquad g(\mathbf{x}) = P(\omega_1|\mathbf{x}) - P(\omega_2|\mathbf{x})$$

$$g(\mathbf{x}) = \ln\frac{p(\mathbf{x}|\omega_1)}{p(\mathbf{x}|\omega_2)} + \ln\frac{P(\omega_1)}{P(\omega_2)}$$

正态分布下的一个例子



Break

高斯密度函数

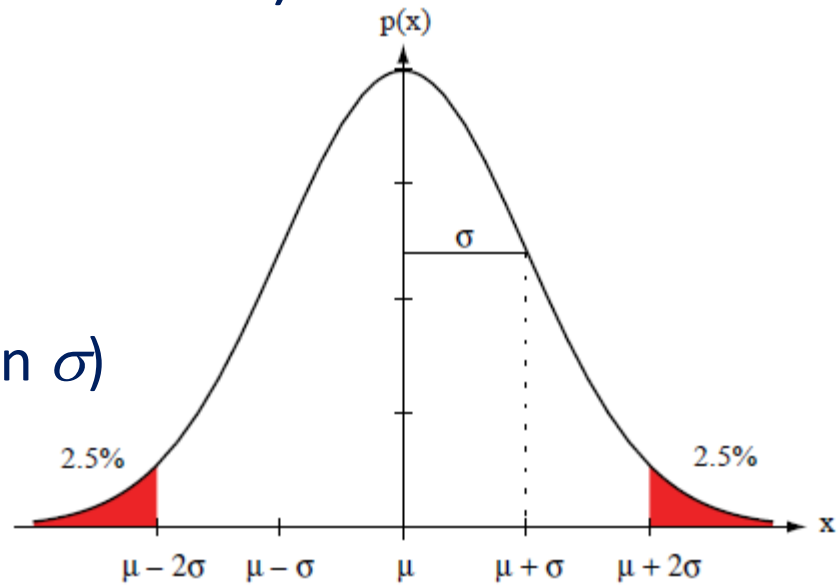
- Gaussian density (normal distribution)

$$p(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right]$$

  - Mean μ
  - Variance σ^2 (standard deviation σ)

$$\mu \equiv \mathcal{E}[x] = \int_{-\infty}^{\infty} x p(x)\, dx$$

$$\sigma^2 \equiv \mathcal{E}[(x-\mu)^2] = \int_{-\infty}^{\infty} (x-\mu)^2 p(x)\, dx$$



$$H(p(x)) = -\int p(x) \ln p(x)\, dx$$

- 在给定均值和方差的所有分布中，正态分布的熵最大(Problem 20, Chapter 2)
- 根据Central Limit Theorem，大量独立随机变量之和趋近正态分布
- 实际环境中，很多类别的特征分布趋近正态分布

- Multivariate normal density $p(\mathbf{x}) \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$
  - 公式要牢记

$$p(\mathbf{x}) = \frac{1}{(2\pi)^{d/2}|\boldsymbol{\Sigma}|^{1/2}} \exp\left[-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^t \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right]$$

  - Mean $\boldsymbol{\mu} \equiv \mathcal{E}[\mathbf{x}] = \int \mathbf{x} p(\mathbf{x})\, d\mathbf{x}$ $\mu_i = \mathcal{E}[x_i]$
  - Covariance matrix

$$\boldsymbol{\Sigma} \equiv \mathcal{E}[(\mathbf{x}-\boldsymbol{\mu})(\mathbf{x}-\boldsymbol{\mu})^t] = \int (\mathbf{x}-\boldsymbol{\mu})(\mathbf{x}-\boldsymbol{\mu})^t p(\mathbf{x})\, d\mathbf{x}$$

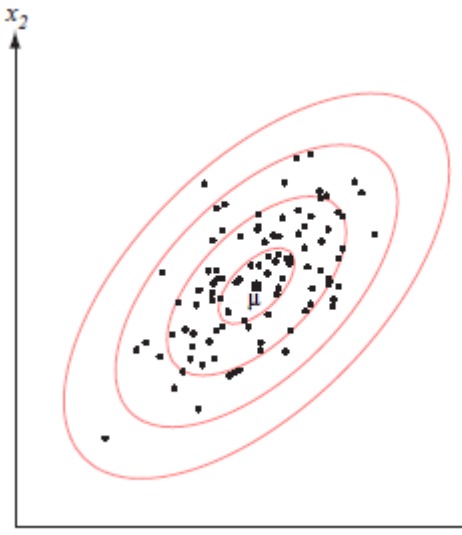
$$\sigma_{ij} = \mathcal{E}[(x_i-\mu_i)(x_j-\mu_j)]$$

If x_i and x_j are *statistically independent*, $\sigma_{ij} = 0$

$$\begin{bmatrix} \sigma_{11} & \sigma_{12} & \cdots & \sigma_{1d} \\ \sigma_{21} & \sigma_{22} & \cdots & \sigma_{2d} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{d1} & \sigma_{d2} & \cdots & \sigma_{dd} \end{bmatrix}$$

  - 等密度点轨迹：hyperellipsoid
  - Mahalanobis distance

$$r^2 = (\mathbf{x}-\boldsymbol{\mu})^t \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})$$



- Covariance matrix eigenvalues & eigenvecters

$$\Sigma = \Phi \Lambda \Phi^t \qquad \Phi = [\phi_1 \phi_2 \cdots \phi_d] \qquad \Lambda = diag[\lambda_1, \lambda_2, \cdots, \lambda_d]$$

  - Orthonormal $\Phi^t \Phi = I \qquad \Phi^t = \Phi^{-1}$

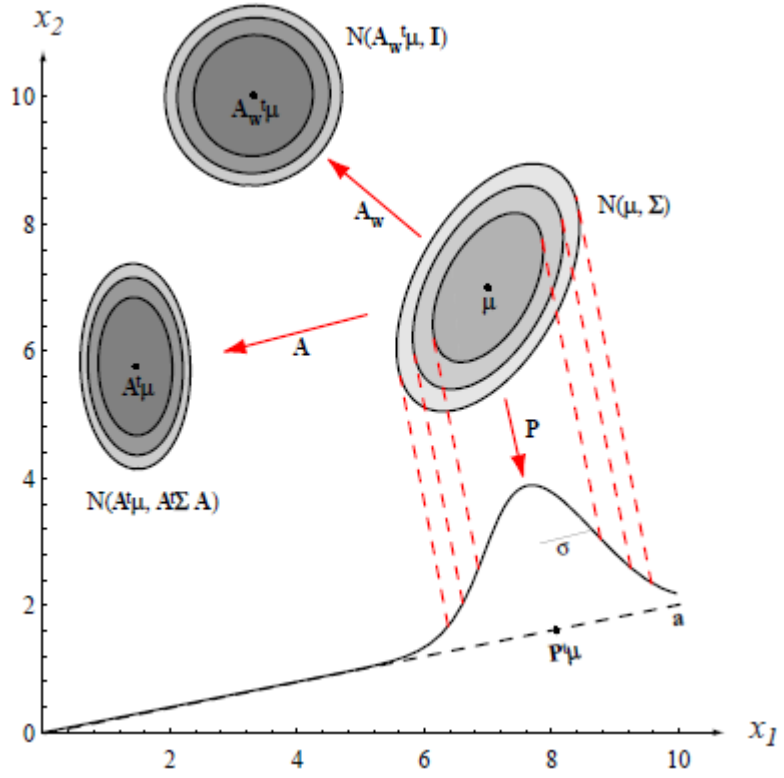
- 线性变换 $\mathbf{y} = \mathbf{A}^t \mathbf{x}$
  - $A^tA=1$: 正交变换(坐标轴旋转)
  - 变换后的分布仍为正态分布

$$p(\mathbf{y}) \sim N(\mathbf{A}^t \boldsymbol{\mu}, \mathbf{A}^t \boldsymbol{\Sigma} \mathbf{A})$$

  - Whitening transform

$$\mathbf{A}_w = \Phi \Lambda^{-1/2}$$

$$A_w^t \Sigma A_w = \Lambda^{-1/2} \Phi^t \Sigma \Phi \Lambda^{-1/2}$$
$$= \Lambda^{-1/2} \Lambda \Lambda^{-1/2} = I$$



高斯密度下的判别函数

- 判别函数 $g_i(\mathbf{x}) = \ln p(\mathbf{x}|\omega_i) + \ln P(\omega_i)$

$$p(\mathbf{x}) = \frac{1}{(2\pi)^{d/2}|\boldsymbol{\Sigma}|^{1/2}} \exp\left[-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^t \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right]$$

$$g_i(\mathbf{x}) = -\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_i)^t \boldsymbol{\Sigma}_i^{-1}(\mathbf{x}-\boldsymbol{\mu}_i) - \frac{d}{2}\ln 2\pi - \frac{1}{2}\ln|\boldsymbol{\Sigma}_i| + \ln P(\omega_i)$$

  - Quadratic discriminant function (QDF)

  - 在不同covariance假设条件下得到一些特殊形式

- Case 1: $\Sigma_i=\sigma^2 I$

$$g_i(\mathbf{x}) = -\frac{\|\mathbf{x}-\boldsymbol{\mu}_i\|^2}{2\sigma^2} + \ln P(\omega_i)$$

  - Euclidean distance $\|\mathbf{x}-\boldsymbol{\mu}_i\|^2 = (\mathbf{x}-\boldsymbol{\mu}_i)^t(\mathbf{x}-\boldsymbol{\mu}_i)$
  - 展开二次式 $(\mathbf{x}-\boldsymbol{\mu}_i)^t(\mathbf{x}-\boldsymbol{\mu}_i)$

$$g_i(\mathbf{x}) = -\frac{1}{2\sigma^2}[\mathbf{x}^t\mathbf{x} - 2\boldsymbol{\mu}_i^t\mathbf{x} + \boldsymbol{\mu}_i^t\boldsymbol{\mu}_i] + \ln P(\omega_i)$$

  - 忽略与类别无关项，得到线性判别函数

$$g_i(\mathbf{x}) = \mathbf{w}_i^t\mathbf{x} + w_{i0}$$

$$\mathbf{w}_i = \frac{1}{\sigma^2}\boldsymbol{\mu}_i \qquad w_{i0} = \frac{-1}{2\sigma^2}\boldsymbol{\mu}_i^t\boldsymbol{\mu}_i + \ln P(\omega_i)$$

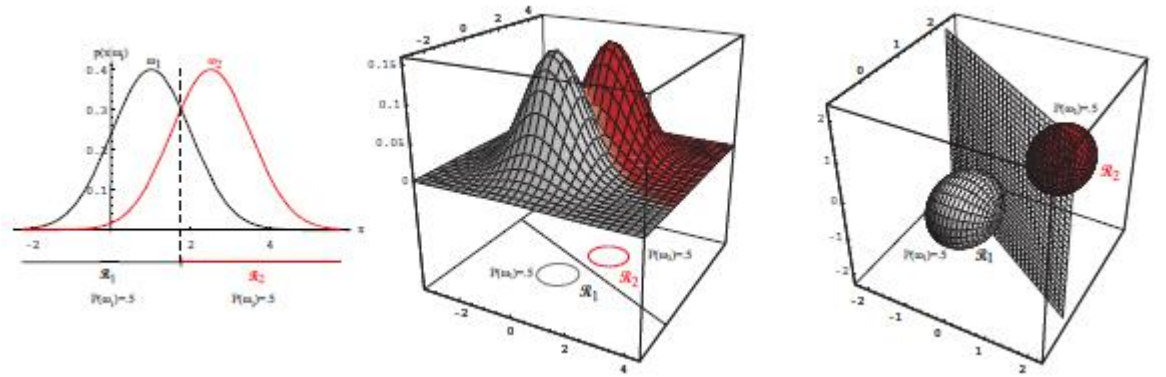
  - 二类决策面 $g_i(\mathbf{x}) = g_j(\mathbf{x})$

$$\mathbf{w}^t(\mathbf{x}-\mathbf{x}_0) = 0 \qquad \mathbf{w} = \boldsymbol{\mu}_i - \boldsymbol{\mu}_j$$

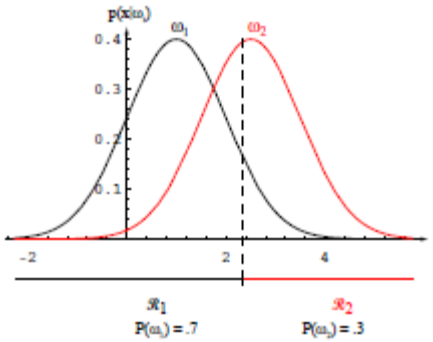
$$\mathbf{x}_0 = \frac{1}{2}(\boldsymbol{\mu}_i + \boldsymbol{\mu}_j) - \frac{\sigma^2}{\|\boldsymbol{\mu}_i - \boldsymbol{\mu}_j\|^2}\ln\frac{P(\omega_i)}{P(\omega_j)}(\boldsymbol{\mu}_i - \boldsymbol{\mu}_j)$$

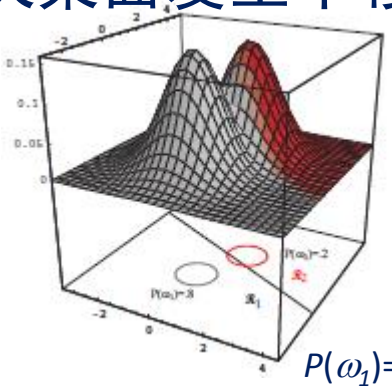
– 1D, 2D, 3D的情况

- 当$P(\omega_1)= P(\omega_2)$，决策面为二类均值的等分面

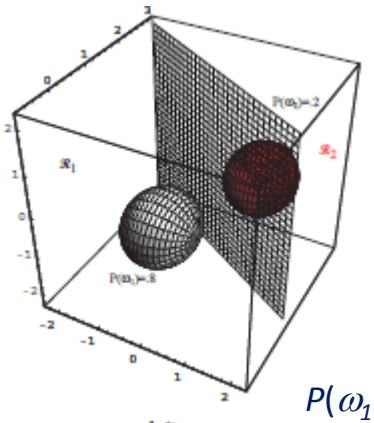


– 当先验概率变化，决策面发生平移

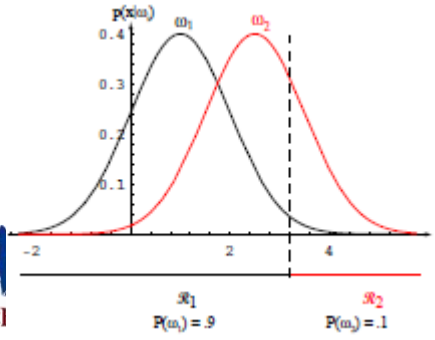


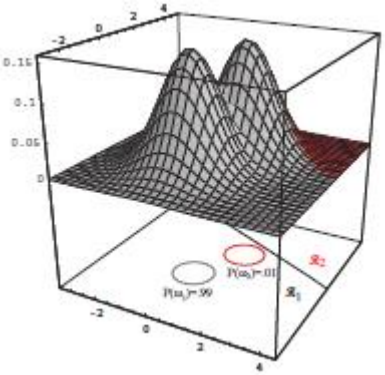


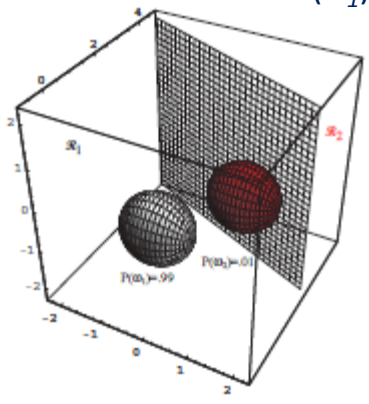
$P(\omega_1)$=0.8



$P(\omega_1)$=0.99







- Case 1: $\Sigma_i = \Sigma$

$$g_i(\mathbf{x}) = -\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_i)^t\boldsymbol{\Sigma}_i^{-1}(\mathbf{x}-\boldsymbol{\mu}_i) - \frac{d}{2}\ln 2\pi - \frac{1}{2}\ln|\boldsymbol{\Sigma}_i| + \ln P(\omega_i)$$

$$\Rightarrow \quad g_i(\mathbf{x}) = -\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_i)^t\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_i) + \ln P(\omega_i)$$

– 展开二次式 $(\mathbf{x}-\boldsymbol{\mu}_i)^t\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_i)$

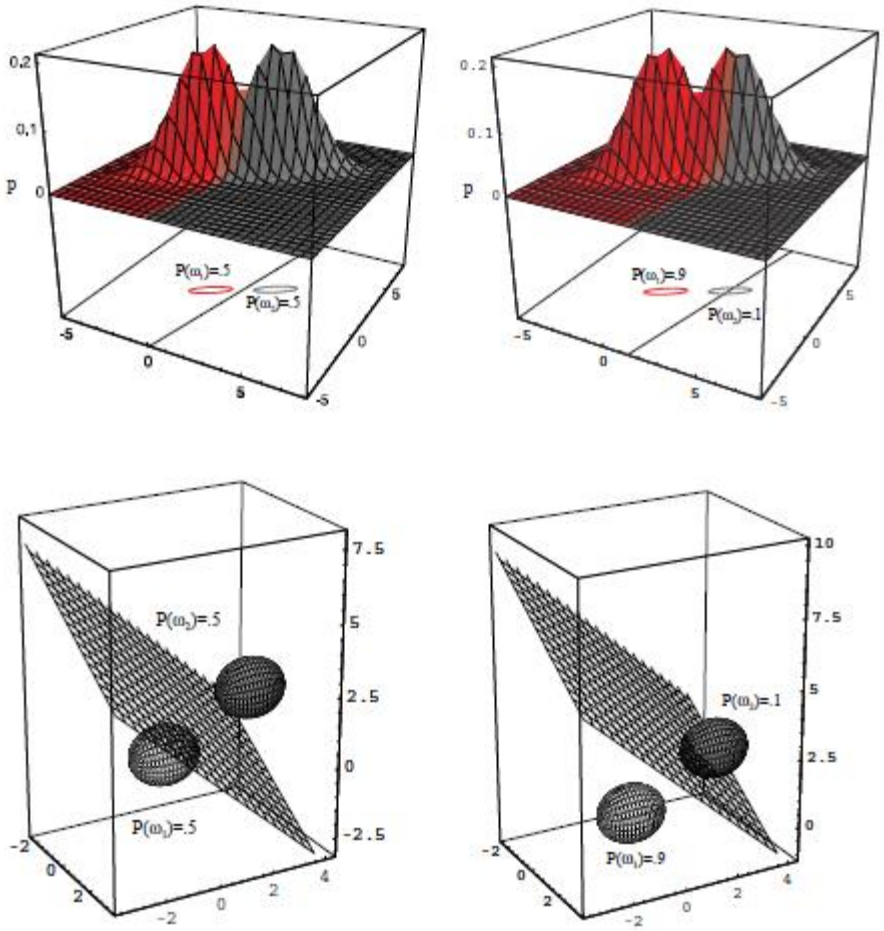
线性判别函数！ $g_i(\mathbf{x}) = \mathbf{w}_i^t\mathbf{x} + w_{i0}$

$$\mathbf{w}_i = \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_i \qquad w_{i0} = -\frac{1}{2}\boldsymbol{\mu}_i^t\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_i + \ln P(\omega_i)$$

– 二类决策面 $\mathbf{w}^t(\mathbf{x}-\mathbf{x}_0) = 0 \qquad \mathbf{w} = \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_i - \boldsymbol{\mu}_j)$

$$\mathbf{x}_0 = \frac{1}{2}(\boldsymbol{\mu}_i + \boldsymbol{\mu}_j) - \frac{\ln\left[P(\omega_i)/P(\omega_j)\right]}{(\boldsymbol{\mu}_i - \boldsymbol{\mu}_j)^t\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_i - \boldsymbol{\mu}_j)}(\boldsymbol{\mu}_i - \boldsymbol{\mu}_j)$$

- 注意跟μ_1-μ_2的关系，决策面不一定与之垂直
- 当$P(\omega_1) = P(\omega_2)$，决策面经过$(\mu_1+\mu_2)/2$


0.2
0.1
p
0
P(ω1)=.5
P(ω2)=.5
-5
0
5
P(ω1)=.9
P(ω2)=.1
7.5
5
2.5
0
-2.5
P(ω2)=.5
P(ω1)=.5
10
7.5
5
2.5
0
P(ω2)=.1
P(ω1)=.9
-2
0
2
4

- Case 3: Σ_i= arbitrary

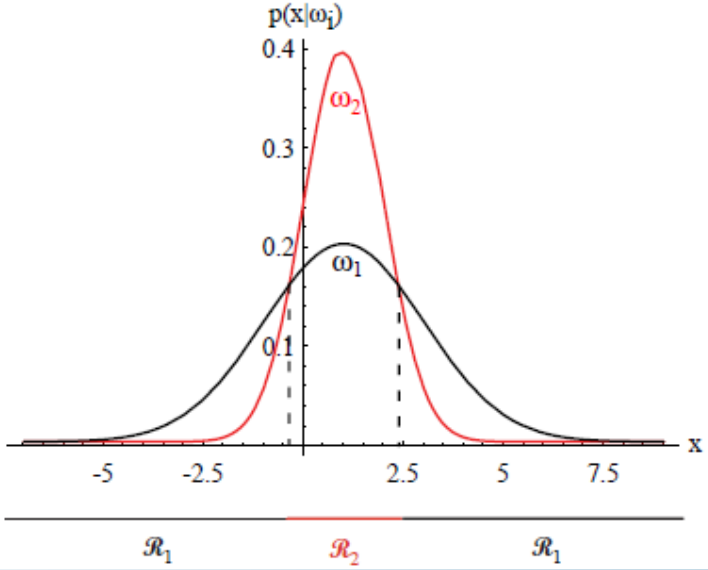
$$g_i(\mathbf{x}) = -\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_i)^t\boldsymbol{\Sigma}_i^{-1}(\mathbf{x}-\boldsymbol{\mu}_i) - \frac{d}{2}\ln 2\pi - \frac{1}{2}\ln|\boldsymbol{\Sigma}_i| + \ln P(\omega_i)$$

$$g_i(\mathbf{x}) = \mathbf{x}^t\mathbf{W}_i\mathbf{x} + \mathbf{w}_i^t\mathbf{x} + w_{i0}$$

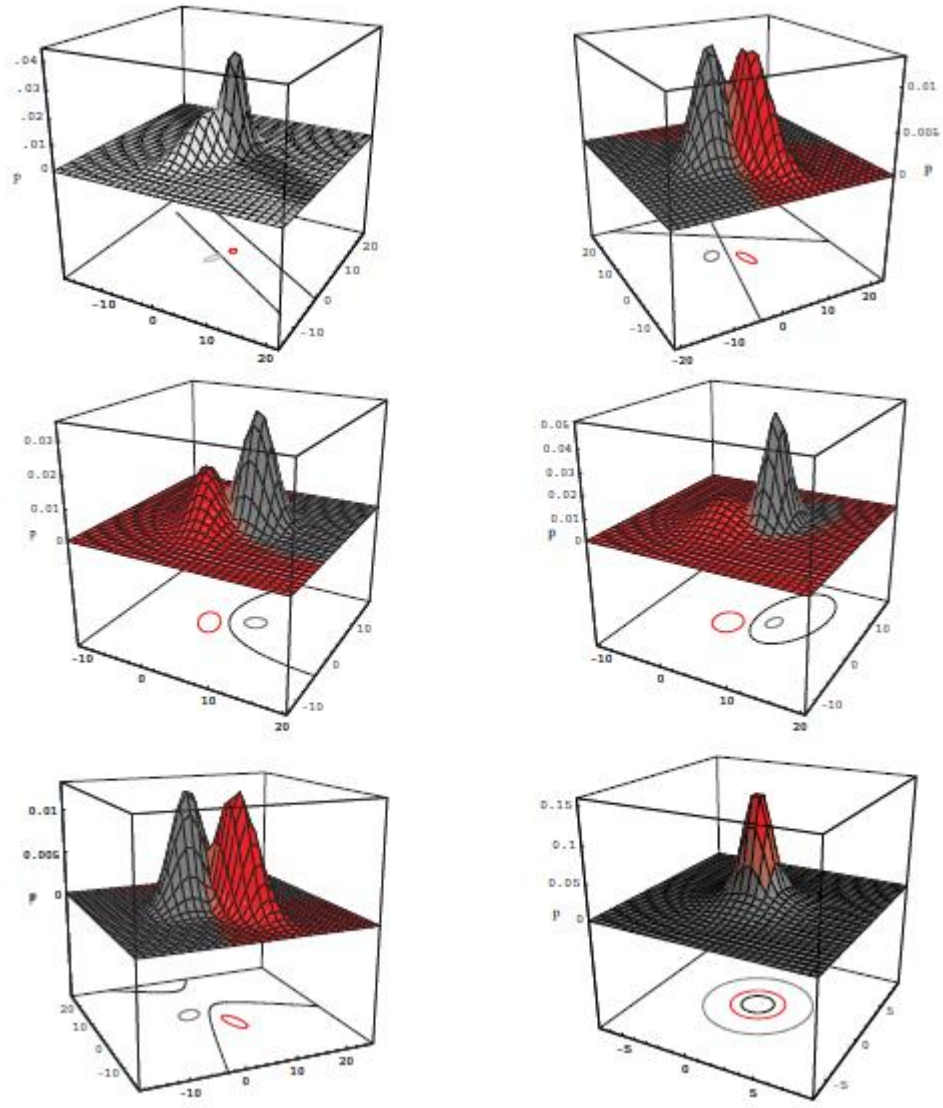
$$\mathbf{W}_i = -\frac{1}{2}\boldsymbol{\Sigma}_i^{-1} \qquad \mathbf{w}_i = \boldsymbol{\Sigma}_i^{-1}\boldsymbol{\mu}_i$$

$$w_{i0} = -\frac{1}{2}\boldsymbol{\mu}_i^t\boldsymbol{\Sigma}_i^{-1}\boldsymbol{\mu}_i - \frac{1}{2}\ln|\boldsymbol{\Sigma}_i| + \ln P(\omega_i)$$

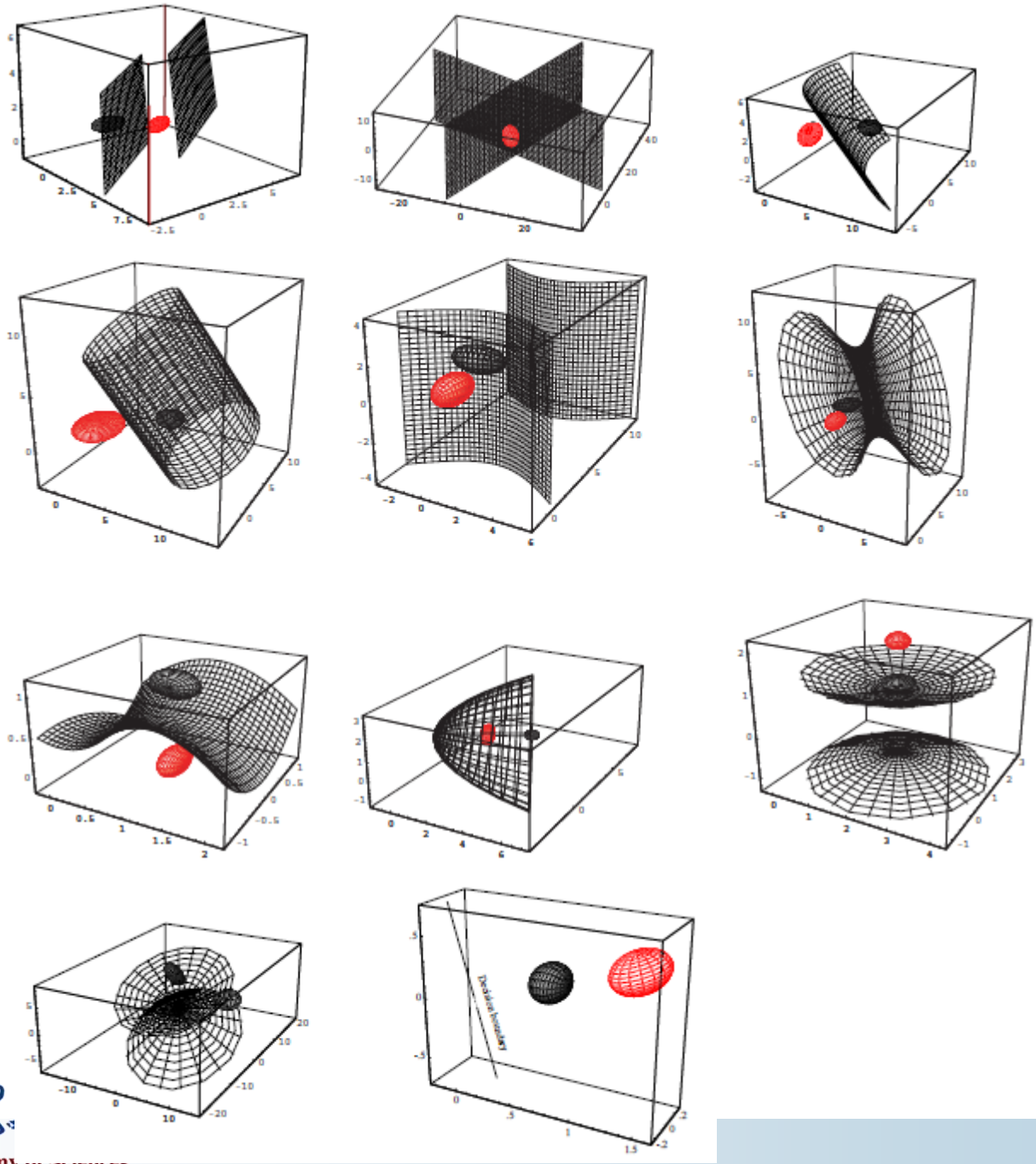
  - 二类决策面：$g_1(\mathbf{x})=g_2(\mathbf{x})$, hyperquadratics
    - 等均值的情况下，1D的例子



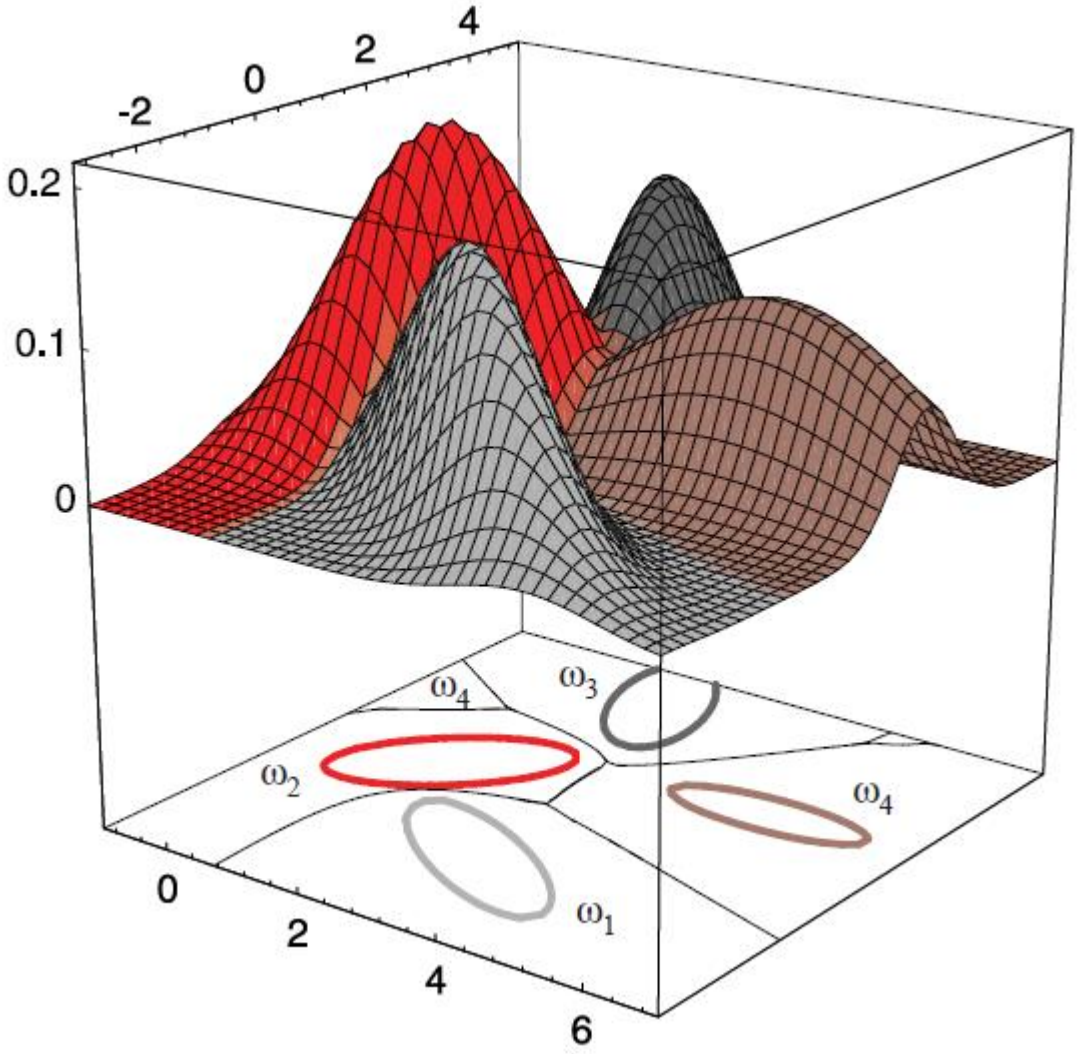
2D的例子



3D的例子



2D，4类的例子



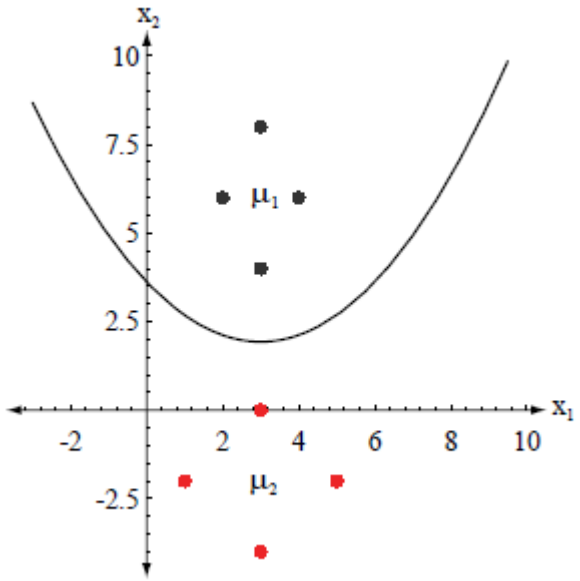
- 一个具体例子
  - 2类，2D $P(\omega_1) = P(\omega_2) = 0.5$

$$\mu_1 = \begin{bmatrix} 3 \\ 6 \end{bmatrix}; \quad \Sigma_1 = \begin{pmatrix} 1/2 & 0 \\ 0 & 2 \end{pmatrix} \qquad \Sigma_1^{-1} = \begin{pmatrix} 2 & 0 \\ 0 & 1/2 \end{pmatrix}$$

$$\mu_2 = \begin{bmatrix} 3 \\ -2 \end{bmatrix}; \quad \Sigma_2 = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix} \qquad \Sigma_2^{-1} = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$$

  - 决策面 $g_1(\mathbf{x})=g_2(\mathbf{x})$

$$x_2 = 3.514 - 1.125x_1 + 0.1875x_1^2$$



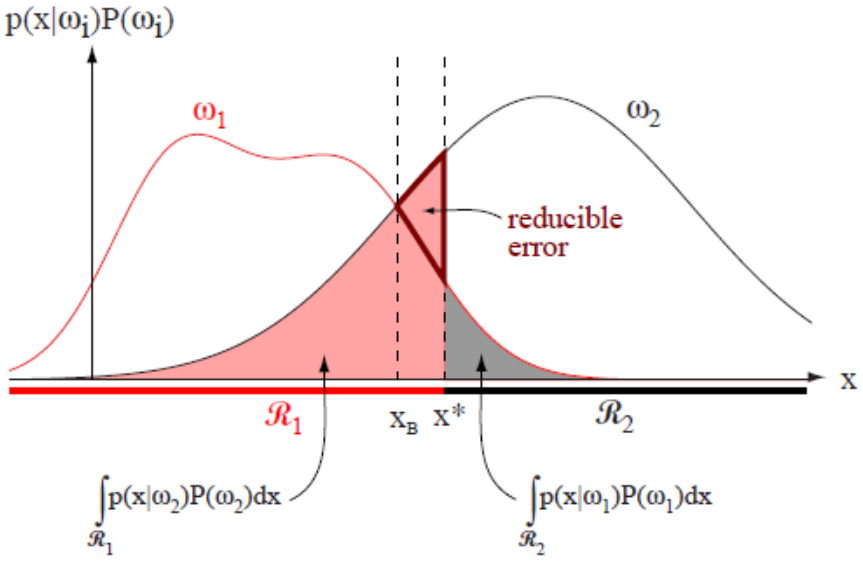
分类错误率

- 2类的情况

$$\begin{aligned} P(error) &= P(\mathbf{x} \in \mathcal{R}_2, \omega_1) + P(\mathbf{x} \in \mathcal{R}_1, \omega_2) \\ &= P(\mathbf{x} \in \mathcal{R}_2 | \omega_1) P(\omega_1) + P(\mathbf{x} \in \mathcal{R}_1 | \omega_2) P(\omega_2) \\ &= \int_{\mathcal{R}_2} p(\mathbf{x}|\omega_1) P(\omega_1)\ d\mathbf{x} + \int_{\mathcal{R}_1} p(\mathbf{x}|\omega_2) P(\omega_2)\ d\mathbf{x}. \end{aligned}$$

- 一般情况

$$\begin{aligned} P(correct) &= \sum_{i=1}^{c} P(\mathbf{x} \in \mathcal{R}_i, \omega_i) \\ &= \sum_{i=1}^{c} P(\mathbf{x} \in \mathcal{R}_i | \omega_i) P(\omega_i) \\ &= \sum_{i=1}^{c} \int_{\mathcal{R}_i} p(\mathbf{x}|\omega_i) P(\omega_i)\ d\mathbf{x} \end{aligned}$$

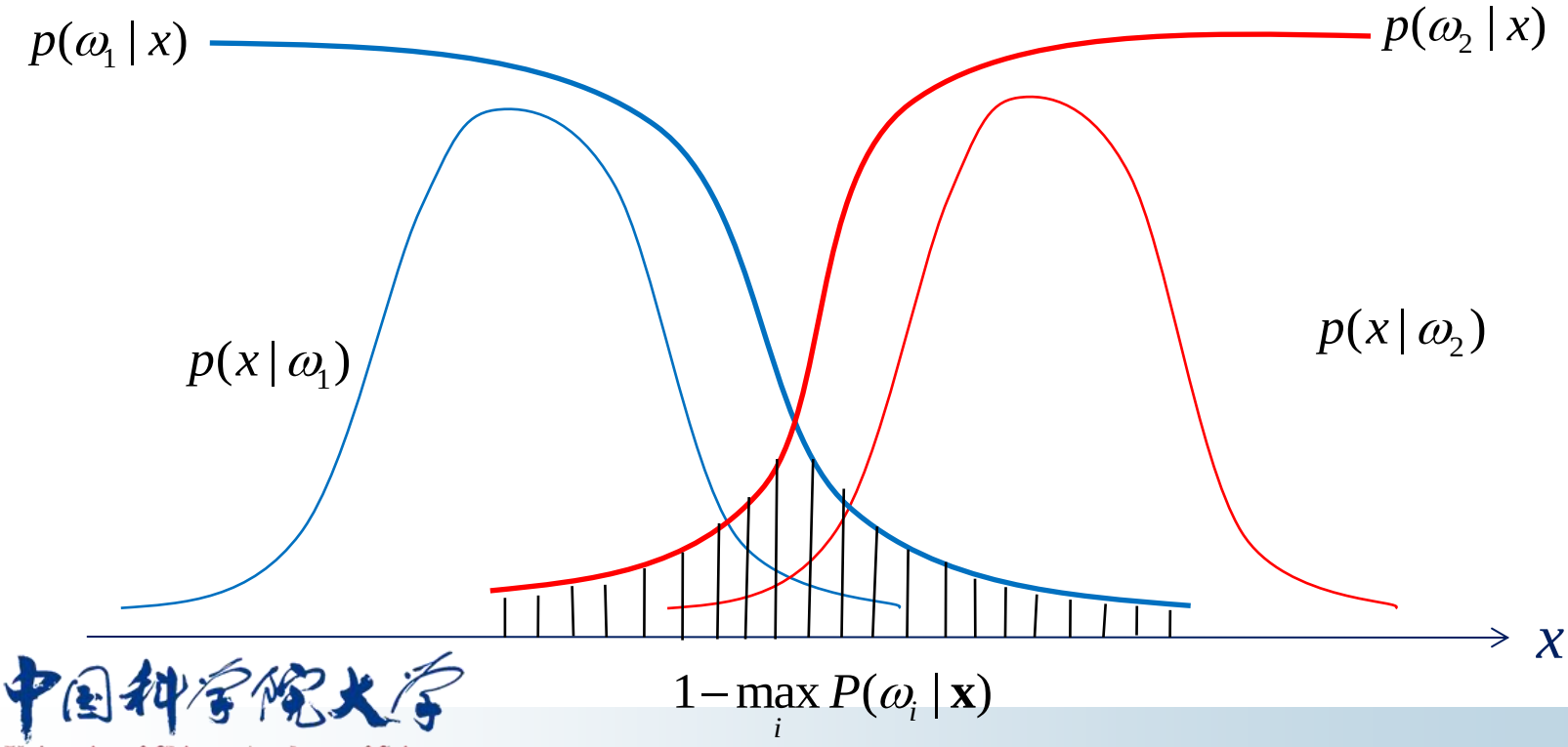


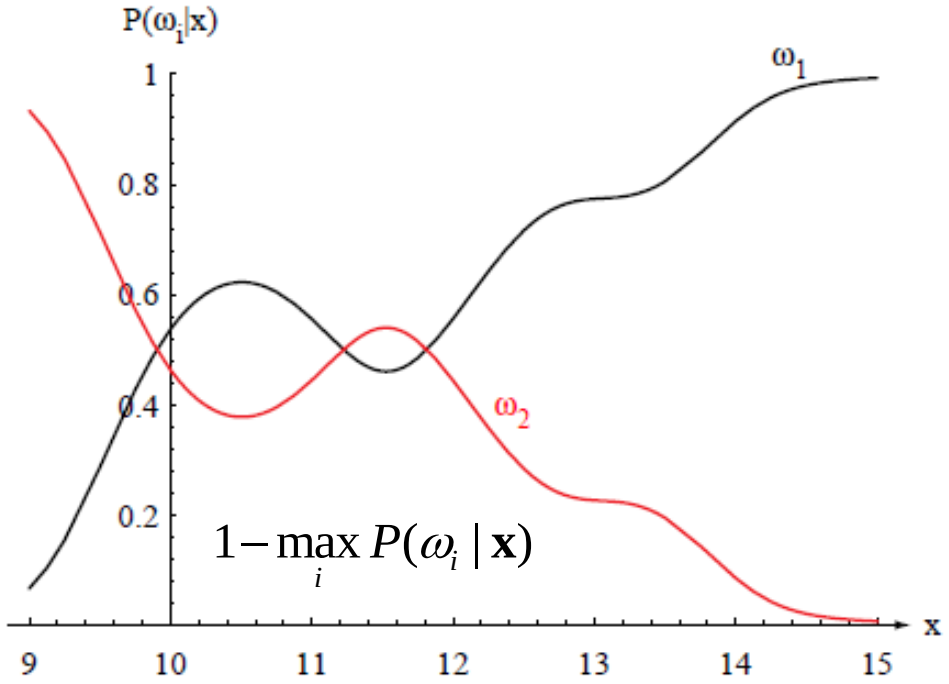
- 最大后验概率决策(0-1 loss)的情况

$$P(correct) = \int_{\mathbf{x}} \max_i P(\mathbf{x} \mid \omega_i) P(\omega_i) d\mathbf{x}$$

$$= \int_{\mathbf{x}} \max_i P(\omega_i \mid \mathbf{x}) P(\mathbf{x}) d\mathbf{x}$$

$$P(error) = \int_{\mathbf{x}} \left[1 - \max_i P(\omega_i \mid \mathbf{x}) \right] P(\mathbf{x}) d\mathbf{x}$$




P(ω_i|x)
1
0.8
0.6
0.4
0.2
ω_1
ω_2
1−max_i P(ω_i | x)
x
9
10
11
12
13
14
15

讨论

- 贝叶斯分类器是最优的吗？
  - 最小风险、最大后验概率决策
  - 最优的条件：概率密度、风险能准确估计
  - 判别模型：回避了概率密度估计，以较小复杂度估计后验概率或判别函数
  - 什么方法能胜过贝叶斯分类器：在不同的特征空间！

下次课内容

- 第2章
  - 离散变量的贝叶斯决策
  - 复合模式分类
- 第3章
  - 最大似然参数估计
  - 贝叶斯估计