

机器学习

Machine learning

第二章 贝叶斯学习

Bayesian Learning

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第二章 贝叶斯学习

2.1 概述

2.2 贝叶斯决策论

2.3 贝叶斯分类器

2.4 贝叶斯学习与参数估计问题

贝叶斯分类器

预备知识

贝叶斯分类器：基于 Bayesian 决策的分类器

变量和参数：

类别 C : $C = \{c_1, c_2, \dots, c_M\}$,

数据 D 和样本 x : $D = \{x_i\}$

贝叶斯学习

$$P(c_i | x) \propto P(x | c_i)P(c_i)$$

核心是估计

$$P(c_i | x) \propto P(x | c_i)P(c_i)$$

贝叶斯分类器

预备知识

贝叶斯决策

类别相似性函数:

$$g_i(\mathbf{x}) = p(c_i | \mathbf{x}) = \frac{p(\mathbf{x} | c_i) p(c_i)}{\sum_{j=1}^c p(\mathbf{x} | c_j) p(c_j)}$$

$$g_i(\mathbf{x}) = p(\mathbf{x} | c_i) p(c_i)$$

$$g_i(\mathbf{x}) = \ln p(\mathbf{x} | c_i) + \ln p(c_i)$$

决策函数:

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

$$g(\mathbf{x}) = p(c_1 | \mathbf{x}) - p(c_2 | \mathbf{x})$$

$$g(\mathbf{x}) = \ln \frac{p(\mathbf{x} | c_1)}{p(\mathbf{x} | c_2)} + \ln \frac{p(c_1)}{p(c_2)}$$

贝叶斯分类器

预备知识

贝叶斯分类器

- 朴素贝叶斯分类器：假设 $P(x|c)$ 中 x 特征向量的各维属性独立；
- 半朴素贝叶斯分类器：假设 $P(x|c)$ 中 x 的各维属性存在依赖；
- 正态分布的贝叶斯分类器：假设 $P(x|c(\theta))$ 服从正态分布；

贝叶斯分类器

朴素贝叶斯分类器

采用了“属性条件独立性假设”

$$P(c|\mathbf{x}) = \frac{P(c)P(\mathbf{x}|c)}{P(\mathbf{x})} \propto P(c)P(\mathbf{x}|c) = P(c) \prod_{i=1}^d P(x_i|c)$$

关键问题：由训练样本学习类别条件概率和类别先验概率

$P(x_i|c)$ 和 $P(c)$

贝叶斯分类器

朴素贝叶斯分类器

采用了“属性条件独立性假设”

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关键问题：由训练样本学习类别条件概率和类别先验概率

$P(x_i|c)$ 和 $P(c)$

需要学习的概率分布？

k 个类别， d 个属性： $p(c)$ 和 $P(x_i|c_j)$, ($i=1, \dots, d$ 个属性, $j=1, \dots, k$)

共 $1 + d*k$ 个概率分布要统计.

贝叶斯分类器

朴素贝叶斯分类器

类别先验概率的估计 $P(c) = \frac{|D_c|}{|D|}$

类别概率密度估计

- x_i 离散情况:

$$P(x_i | c) = \frac{|D_{c,x_i}|}{|D_c|}$$

D_{c,x_i} 表示 D_c 中在第 i 个属性上取值为 x_i 的样本组成的集合;

- x_i 连续情况:

$$P(x_i | c) = \frac{1}{\sqrt{2\pi}\sigma_{c,i}} \exp\left(-\frac{(x_i - \mu_{c,i})^2}{2\sigma_{c,i}^2}\right) \quad (\text{由某一概率分布估计类别概率})$$

贝叶斯分类器

朴素贝叶斯分类器

学习过程

(1) 类别先验估计 $P(c) = \frac{|D_c|}{|D|}$

(2) 类别条件概率估计 $P(x_i | c) = \frac{|D_{c,x_i}|}{|D_c|}$

贝叶斯分类器

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决策过程

(1) 类别先验估计 $P(c) = \frac{|D_c|}{|D|}$

(2) 类别条件概率估计 $P(\mathbf{x} | c) = \prod_{i=1}^d P(x_i | c)$

(3) 贝叶斯决策 $h(\mathbf{x}) = \underset{c \in \mathcal{Y}}{\operatorname{argmax}} P(c) \prod_{i=1}^d P(x_i | c)$

贝叶斯分类器

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拉普拉斯平滑

避免因训练集样本不充分而导致概率估计值为零.

避免 $P(c|\mathbf{x}) \propto P(c) \prod_{i=1}^d P(x_i|c)$ 中, $P(c)$ 或 $P(x_i|c)$ 为 0 (即 $|D_c| = 0$ 或 $|D_{c,x_i}| = 0$)

进行拉普拉斯平滑

$$\hat{P}(c) = \frac{|D_c| + 1}{|D| + N}, \quad N \text{ 为类别数}$$

$$\hat{P}(x_i | c) = \frac{|D_{c,x_i}| + 1}{|D_c| + N_i}, \quad N_i \text{ 为 } x_i \text{ 的可能取值个数}$$

贝叶斯分类器

朴素贝叶斯分类器

例子：《机器学习》教材 p.151

- 数据： pp.84
- 离散属性：色泽、根蒂、敲声、纹理、脐部、触感；
连续属性：密度、含糖绿
类别属性：好瓜？（是与否）

贝叶斯分类器

朴素贝叶斯分类器

- 训练数据

| 编号 | 色泽 | 根蒂 | 敲声 | 纹理 | 脐部 | 触感 | 密度 | 含糖率 | 好瓜 |
|----|----|----|----|----|----|----|-------|-------|----|
| 1 | 青绿 | 蜷缩 | 浊响 | 清晰 | 凹陷 | 硬滑 | 0.697 | 0.460 | 是 |
| 2 | 乌黑 | 蜷缩 | 沉闷 | 清晰 | 凹陷 | 硬滑 | 0.774 | 0.376 | 是 |
| 3 | 乌黑 | 蜷缩 | 浊响 | 清晰 | 凹陷 | 硬滑 | 0.634 | 0.264 | 是 |
| 4 | 青绿 | 蜷缩 | 沉闷 | 清晰 | 凹陷 | 硬滑 | 0.608 | 0.318 | 是 |
| 5 | 浅白 | 蜷缩 | 浊响 | 清晰 | 凹陷 | 硬滑 | 0.556 | 0.215 | 是 |
| 6 | 青绿 | 稍蜷 | 浊响 | 清晰 | 稍凹 | 软粘 | 0.403 | 0.237 | 是 |
| 7 | 乌黑 | 稍蜷 | 浊响 | 稍糊 | 稍凹 | 软粘 | 0.481 | 0.149 | 是 |
| 8 | 乌黑 | 稍蜷 | 浊响 | 清晰 | 稍凹 | 硬滑 | 0.437 | 0.211 | 是 |
| 9 | 乌黑 | 稍蜷 | 沉闷 | 稍糊 | 稍凹 | 硬滑 | 0.666 | 0.091 | 否 |
| 10 | 青绿 | 硬挺 | 清脆 | 清晰 | 平坦 | 软粘 | 0.243 | 0.267 | 否 |
| 11 | 浅白 | 硬挺 | 清脆 | 模糊 | 平坦 | 硬滑 | 0.245 | 0.057 | 否 |
| 12 | 浅白 | 蜷缩 | 浊响 | 模糊 | 平坦 | 软粘 | 0.343 | 0.099 | 否 |
| 13 | 青绿 | 稍蜷 | 浊响 | 稍糊 | 凹陷 | 硬滑 | 0.639 | 0.161 | 否 |
| 14 | 浅白 | 稍蜷 | 沉闷 | 稍糊 | 凹陷 | 硬滑 | 0.657 | 0.198 | 否 |
| 15 | 乌黑 | 稍蜷 | 浊响 | 清晰 | 稍凹 | 软粘 | 0.360 | 0.370 | 否 |
| 16 | 浅白 | 蜷缩 | 浊响 | 模糊 | 平坦 | 硬滑 | 0.593 | 0.042 | 否 |
| 17 | 青绿 | 蜷缩 | 沉闷 | 稍糊 | 稍凹 | 硬滑 | 0.719 | 0.103 | 否 |

测试数据

| 编号 | 色泽 | 根蒂 | 敲声 | 纹理 | 脐部 | 触感 | 密度 | 含糖率 | 好瓜 |
|-----|----|----|----|----|----|----|-------|-------|----|
| 测 1 | 青绿 | 蜷缩 | 浊响 | 清晰 | 凹陷 | 硬滑 | 0.697 | 0.460 | ? |

贝叶斯分类器

朴素贝叶斯分类器

学习过程：

(1) 类别先验估计

$$P(c) = \frac{|D_c|}{|D|} \Rightarrow \begin{cases} P(\text{好瓜} = \text{是}) = \frac{|D_{\text{好瓜}=\text{是}}|}{|D|} \\ P(\text{好瓜} = \text{否}) = \frac{|D_{\text{好瓜}=\text{否}}|}{|D|} \end{cases}$$

首先估计类别先验概率 $P(c)$ ，显然有

$$P(\text{好瓜} = \text{是}) = \frac{8}{17} \approx 0.471,$$

$$P(\text{好瓜} = \text{否}) = \frac{9}{17} \approx 0.529.$$

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(2) 类别条件概率估计

对于离散值属性: $P(x_i | c) = \frac{|D_{c,xi}|}{|D_c|} \Rightarrow \begin{cases} P(x_i | \text{好瓜} = \text{是}) = \frac{|D_{\text{好瓜}=\text{是},xi}|}{|D_c|} \\ P(x_i | \text{好瓜} = \text{否}) = \frac{|D_{\text{好瓜}=\text{否},xi}|}{|D_c|} \end{cases}$

对于连续值属性:

$$P(x_i | c) = \frac{1}{\sqrt{2\pi}\sigma_{c,i}} \exp\left(-\frac{(x_i - \mu_{c,i})^2}{2\sigma_{c,i}^2}\right) \Rightarrow \begin{cases} P(x_i | \text{好瓜} = \text{是}) = \frac{1}{\sqrt{2\pi}\sigma_{\text{好瓜}=\text{是},i}} \exp\left(-\frac{(x_i - \mu_{\text{好瓜}=\text{是},i})^2}{2\sigma_{\text{好瓜}=\text{是},i}^2}\right) \\ P(x_i | \text{好瓜} = \text{否}) = \frac{1}{\sqrt{2\pi}\sigma_{\text{好瓜}=\text{否},i}} \exp\left(-\frac{(x_i - \mu_{\text{好瓜}=\text{否},i})^2}{2\sigma_{\text{好瓜}=\text{否},i}^2}\right) \end{cases}$$

均值、方差作为参数, 可用 ML 估计,

$$P_{\text{青绿}|\text{是}} = P(\text{色泽} = \text{青绿} | \text{好瓜} = \text{是}) = \frac{3}{8} = 0.375$$

$$P_{\text{青绿}|\text{否}} = P(\text{色泽} = \text{青绿} | \text{好瓜} = \text{否}) = \frac{3}{9} = 0.333$$

$$P_{\text{蜷缩}|\text{是}} = P(\text{根蒂} = \text{蜷缩} | \text{好瓜} = \text{是}) = \frac{5}{8} = 0.625$$

$$P_{\text{蜷缩}|\text{否}} = P(\text{根蒂} = \text{蜷缩} | \text{好瓜} = \text{否}) = \frac{3}{9} = 0.333$$

$$P_{\text{浊响}|\text{是}} = P(\text{敲声} = \text{浊响} | \text{好瓜} = \text{是}) = \frac{6}{8} = 0.750$$

$$P_{\text{浊响}|\text{否}} = P(\text{敲声} = \text{浊响} | \text{好瓜} = \text{否}) = \frac{4}{9} = 0.444$$

$$P_{\text{清晰}|\text{是}} = P(\text{纹理} = \text{清晰} | \text{好瓜} = \text{是}) = \frac{7}{8} = 0.875$$

$$P_{\text{清晰}|\text{否}} = P(\text{纹理} = \text{清晰} | \text{好瓜} = \text{否}) = \frac{2}{9} = 0.222$$

$$P_{\text{凹陷}|\text{是}} = P(\text{脐部} = \text{凹陷} | \text{好瓜} = \text{是}) = \frac{6}{8} = 0.750$$

$$P_{\text{凹陷}|\text{否}} = P(\text{脐部} = \text{凹陷} | \text{好瓜} = \text{否}) = \frac{2}{9} = 0.222$$

$$P_{\text{硬滑}|\text{是}} = P(\text{触感} = \text{硬滑} | \text{好瓜} = \text{是}) = \frac{6}{8} = 0.750$$

$$P_{\text{硬滑}|\text{否}} = P(\text{触感} = \text{硬滑} | \text{好瓜} = \text{否}) = \frac{6}{9} = 0.667$$

为每个属性估计条件概率 $P(x_i | c)$

$$P_{\text{密度:0.697}|\text{是}} = p(\text{密度} = 0.697 | \text{好瓜} = \text{是})$$

$$= \frac{1}{\sqrt{2\pi} \cdot 0.129} \exp\left(-\frac{(0.697 - 0.574)^2}{2 \cdot 0.129^2}\right) \approx 1.959$$

$$P_{\text{密度:0.697}|\text{否}} = p(\text{密度} = 0.697 | \text{好瓜} = \text{否})$$

$$= \frac{1}{\sqrt{2\pi} \cdot 0.195} \exp\left(-\frac{(0.697 - 0.496)^2}{2 \cdot 0.195^2}\right) \approx 1.203$$

$$P_{\text{含糖:0.460}|\text{是}} = p(\text{含糖率} = 0.460 | \text{好瓜} = \text{是})$$

$$= \frac{1}{\sqrt{2\pi} \cdot 0.101} \exp\left(-\frac{(0.460 - 0.279)^2}{2 \cdot 0.101^2}\right) \approx 0.788$$

$$P_{\text{含糖:0.460}|\text{否}} = p(\text{含糖率} = 0.460 | \text{好瓜} = \text{否})$$

$$= \frac{1}{\sqrt{2\pi} \cdot 0.108} \exp\left(-\frac{(0.460 - 0.154)^2}{2 \cdot 0.108^2}\right) \approx 0.066$$

贝叶斯分类器

朴素贝叶斯分类器

(3) 贝叶斯决策

$$\begin{aligned} &P(\text{好瓜} = \text{是}) \times P_{\text{青绿}|\text{是}} \times P_{\text{蜷缩}|\text{是}} \times P_{\text{浊响}|\text{是}} \times P_{\text{清晰}|\text{是}} \times P_{\text{凹陷}|\text{是}} \\ &\quad \times P_{\text{硬滑}|\text{是}} \times p_{\text{密度}:0.697|\text{是}} \times p_{\text{含糖}:0.460|\text{是}} \approx 0.038, \\ &P(\text{好瓜} = \text{否}) \times P_{\text{青绿}|\text{否}} \times P_{\text{蜷缩}|\text{否}} \times P_{\text{浊响}|\text{否}} \times P_{\text{清晰}|\text{否}} \times P_{\text{凹陷}|\text{否}} \\ &\quad \times P_{\text{硬滑}|\text{否}} \times p_{\text{密度}:0.697|\text{否}} \times p_{\text{含糖}:0.460|\text{否}} \approx 6.80 \times 10^{-5}. \end{aligned}$$

由于 $0.038 > 6.80 \times 10^{-5}$ ，因此，朴素贝叶斯分类器将测试样本“测 1”判别为“好瓜”。

Have a break !

贝叶斯分类器

正态密度的贝叶斯分类器

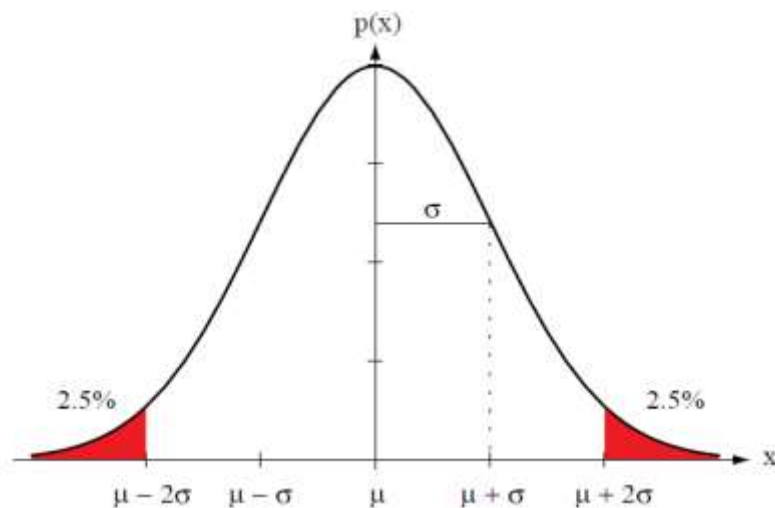
类别条件概率为正态分布

$$h(\mathbf{x}) = \operatorname{argmax}_{c \in \mathcal{Y}} P(c) \underbrace{P(\mathbf{x}|c)}_{\text{正态分布}}$$

正态分布

- 正态分布的概率密度 $N(\mu, \sigma^2)$:

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



贝叶斯分类器

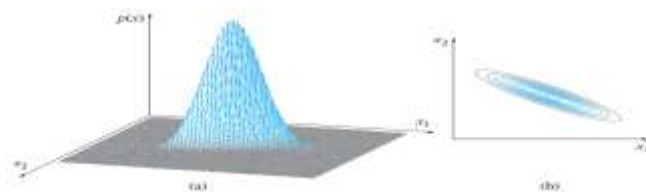
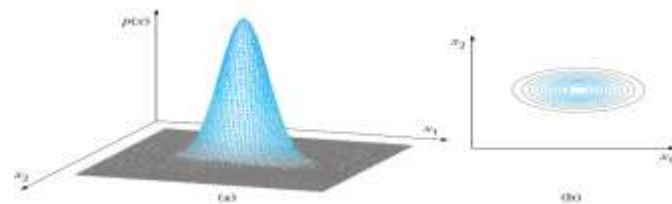
正态密度的贝叶斯分类器

- 多维正态分布的概率密度 $N(\mu, \Sigma)$:

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

$$\mu \equiv \mathcal{E}[\mathbf{x}] = \int \mathbf{x} p(\mathbf{x}) d\mathbf{x}$$

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



每个维度上都是正态分布 $\mu_i = \mathcal{E}[x_i]$; $\sigma_{ij} = \mathcal{E}[(x_i - \mu_i)(x_j - \mu_j)]$

贝叶斯分类器

正态密度的贝叶斯分类器

贝叶斯分类：

- 贝叶斯学习（结果取对数）：

$$g_i(\mathbf{x}) = \ln(p(\mathbf{x} | \omega_i) p(\omega_i)) = \ln p(\mathbf{x} | \omega_i) + \ln p(\omega_i)$$

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

$$g_i(\mathbf{x}) = -\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_i)^T \Sigma_i^{-1}(\mathbf{x} - \boldsymbol{\mu}_i) - \frac{d}{2} \ln 2\pi - \frac{1}{2} \ln |\Sigma_i| + \ln p(\omega_i) \quad (1)$$

贝叶斯分类器

正态密度的贝叶斯分类器

- 决策函数:

$$g_{ij}(x) \equiv g_i(x) - g_j(x)$$

$g_{ij}(x)=0$ 为决策界

如果 $g_{ij}(x) \geq 0$, 则归为 i 类

如果 $g_{ij}(x) < 0$, 则归为 j 类

贝叶斯分类器

正态密度的贝叶斯分类器

不同高斯参数情况讨论

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

$$g_i(x) = -\frac{1}{2}(x - \mu_i)^T \Sigma_i^{-1} (x - \mu_i) + \ln p(\omega_i) + c_i$$

$$g_i(x) = -\frac{\|x - \mu_i\|^2}{2\sigma^2} + \ln p(\omega_i)$$

$$g_i(x) = -\frac{1}{2\sigma^2} [x^T x - 2\mu_i^T x + \mu_i^T \mu_i] + \ln p(\omega_i) \rightarrow \text{与类别无关, 可忽略}$$

$$\Rightarrow g_i(x) = w_i^T x + w_{i0}, \quad w_i = \frac{1}{\sigma^2} \mu_i, \quad w_{i0} = \frac{-1}{2\sigma^2} \mu_i^T \mu_i + \ln p(\omega_i)$$

贝叶斯分类器

正态密度的贝叶斯分类器

不同高斯参数情况讨论

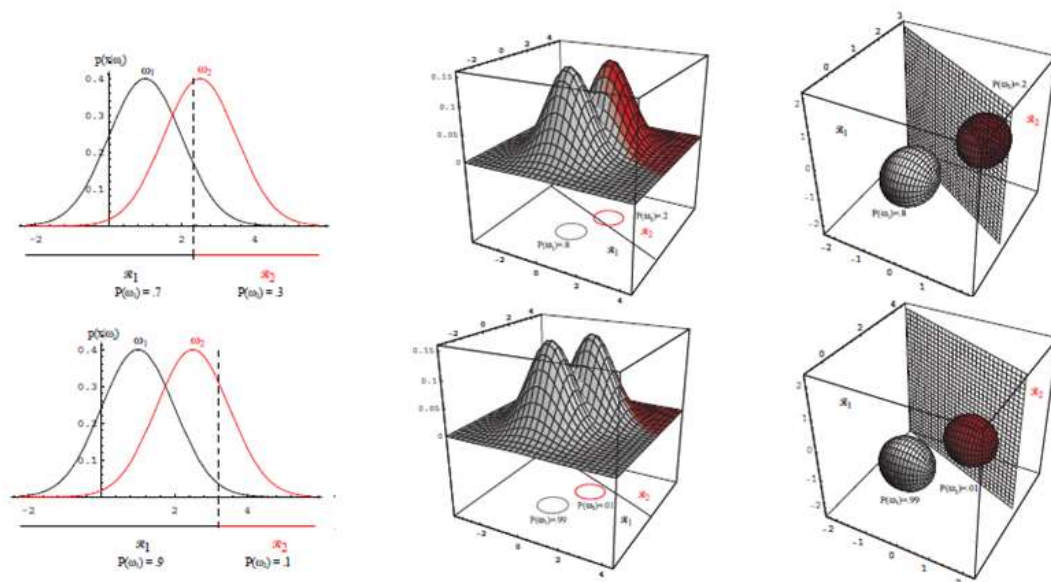
Case 1: $\Sigma_i = \sigma^2 I$

决策界: $g_i(x) - g_j(x) = 0$

$$w^T (x - x_0) = 0$$

$$w = \mu_i - \mu_j$$

$$x_0 = \frac{1}{2}(\mu_i + \mu_j) - \frac{\sigma^2}{\|\mu_i - \mu_j\|^2} \ln \frac{p(\omega_i)}{p(\omega_j)} (\mu_i - \mu_j)$$



贝叶斯分类器

正态密度的贝叶斯分类器

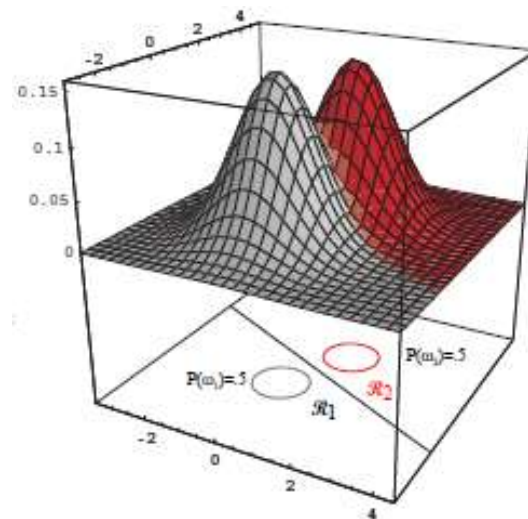
不同高斯参数情况讨论

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

特殊情况，当各个类别先验相等时，退化为最小距离分类器。

$$W = \mu_i - \mu_j$$

$$x_0 = \frac{1}{2}(\mu_i + \mu_j)$$



贝叶斯分类器

正态密度的贝叶斯分类器

不同高斯参数情况讨论

Case 2: $\Sigma_i = \Sigma$

$$g_i(x) = -\frac{1}{2}(x - \mu_i)^T \Sigma_i^{-1}(x - \mu_i) + \ln p(\omega_i)$$

该式分解后: $x^T \Sigma_i^{-1} x$ 各类都相等, 可以忽略

$$g_i(x) = w_i^T x + w_{i0}, \quad w_i = \Sigma^{-1} \mu_i, \quad w_{i0} = -\frac{1}{2} \mu_i^T \Sigma^{-1} \mu_i + \ln p(\omega_i)$$

贝叶斯分类器

正态密度的贝叶斯分类器

不同高斯参数情况讨论

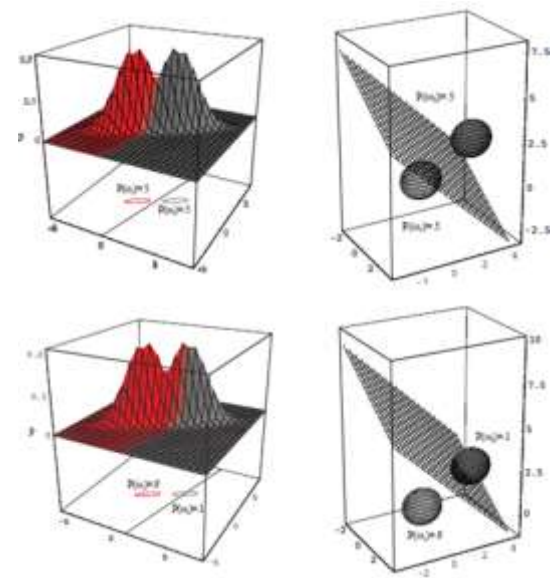
Case 2: $\Sigma_i = \Sigma$

决策界: $g_i(\mathbf{x}) - g_j(\mathbf{x}) = 0$

$$\mathbf{w}^T (\mathbf{x} - \mathbf{x}_0) = 0$$

$$\mathbf{w} = \Sigma^{-1}(\mu_i - \mu_j)$$

$$\mathbf{x}_0 = \frac{1}{2}(\mu_i + \mu_j) - \frac{\ln[p(\omega_i)/p(\omega_j)]}{(\mu_i - \mu_j)^T \Sigma^{-1}(\mu_i - \mu_j)}(\mu_i - \mu_j)$$



贝叶斯分类器

正态密度的贝叶斯分类器

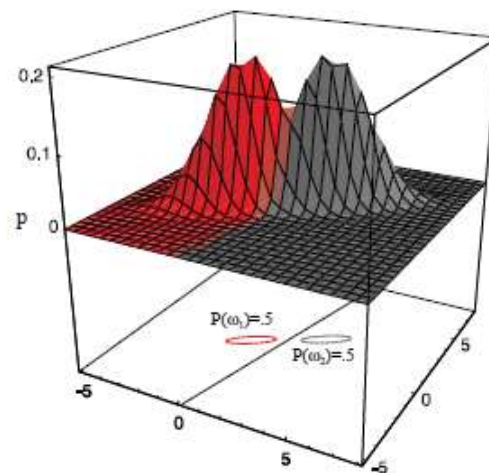
不同高斯参数情况讨论

Case 2: $\Sigma_i = \Sigma$

当各个类别先验相等时,

$$w = \Sigma^{-1}(\mu_i - \mu_j)$$

$$x_0 = \frac{1}{2}(\mu_i + \mu_j)$$



贝叶斯分类器

正态密度的贝叶斯分类器

不同高斯参数情况讨论

Case 3: $\Sigma_i = \text{arbitrary}$

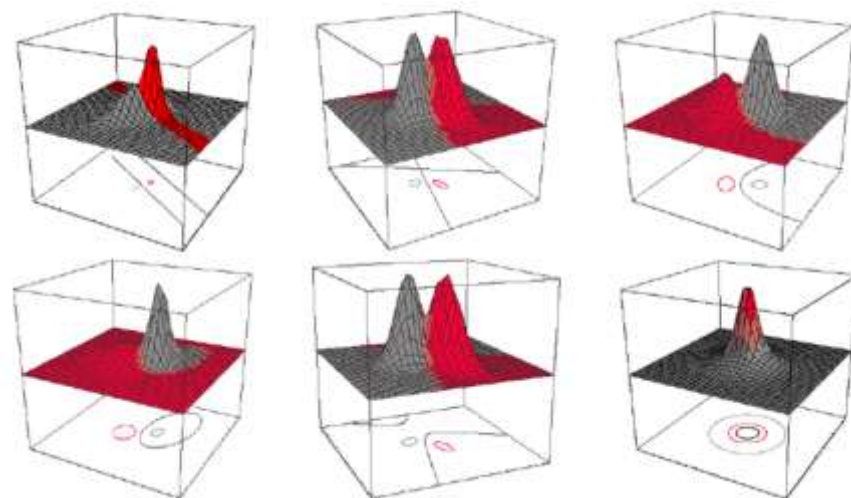
$$g_i(x) = x^T W_i x + w_i^T x + w_{i0}$$

$$W_i = -\frac{1}{2} \Sigma_i^{-1}$$

$$w_i = \Sigma_i^{-1} \mu_i$$

$$w_{i0} = -\frac{1}{2} \mu_i^T \Sigma_i^{-1} \mu_i - \frac{1}{2} \ln |\Sigma_i| + \ln p(\omega_i)$$

决策界: $g_i(x) - g_j(x) = 0$, 情况比较复杂, 可能非线性。



贝叶斯分类器

正态密度的贝叶斯分类器

例子：

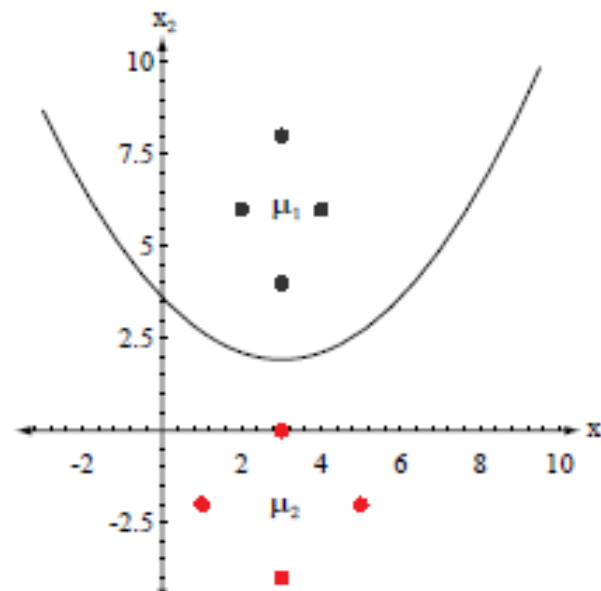
$$\mu_1 = \begin{bmatrix} 3 \\ 6 \end{bmatrix}; \quad \Sigma_1 = \begin{pmatrix} 1/2 & 0 \\ 0 & 2 \end{pmatrix} \text{ and } \mu_2 = \begin{bmatrix} 3 \\ -2 \end{bmatrix}; \quad \Sigma_2 = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$$

$$\Sigma_1^{-1} = \begin{pmatrix} 2 & 0 \\ 0 & 1/2 \end{pmatrix} \quad \text{and} \quad \Sigma_2^{-1} = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$$

$$p(\omega_1) = p(\omega_2) = 0.5$$

决策界： $g_1(x) \equiv g_2(x)$

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



Have a break !

第二章 贝叶斯学习

2.1 概述

2.2 贝叶斯决策论

2.3 贝叶斯分类器

2.4 贝叶斯学习与参数估计问题

贝叶斯学习与参数估计问题

问题描述

\mathcal{D} — data set

\mathcal{M} — models (or parameters)

The probability of a model \mathcal{M} given data set \mathcal{D} is:

$$P(\mathcal{M}|\mathcal{D}) = \frac{P(\mathcal{D}|\mathcal{M})P(\mathcal{M})}{P(\mathcal{D})}$$

$P(\mathcal{D}|\mathcal{M})$ is the *evidence* (or *likelihood*)

$P(\mathcal{M})$ is the *prior* probability of \mathcal{M}

$P(\mathcal{M}|\mathcal{D})$ is the *posterior probability* of \mathcal{M}

$$P(\mathcal{D}) = \int P(\mathcal{D}|\mathcal{M})P(\mathcal{M}) d\mathcal{M}$$

三个基本问题: **Bayes, MAP and ML**

Bayesian Learning:



Assumes a prior over the model parameters. Computes the posterior distribution of the parameters: $P(\theta|\mathcal{D})$.

Maximum a Posteriori (MAP) Learning:



Assumes a prior over the model parameters $P(\theta)$. Finds a parameter setting that maximises the posterior: $P(\theta|\mathcal{D}) \propto P(\theta) P(\mathcal{D}|\theta)$.

Maximum Likelihood (ML) Learning:



Does not assume a prior over the model parameters. Finds a parameter setting that maximises the likelihood of the data: $P(\mathcal{D}|\theta)$.

贝叶斯学习与参数估计问题

贝叶斯学习

通过观测数据 likelihood 修正模型的先验，得到后验概率分布：

$$p(\theta|\mathcal{D}, \alpha) \propto p(\mathcal{D}|\theta)p(\theta|\alpha)$$

其中， α 是超参数，不是估计的参数。

例子 1: Beta 先验分布

贝叶斯学习与参数估计问题

贝叶斯学习

例子 1: Beta 先验分布

- 观察数据

Coin example: we have a coin that can be biased

H H T T H H T H T H T T T H T H H H H T H H H H T
1 1 0 0 1 1 0 1 0 1 0 0 0 1 0 1 1 1 1 0 1 1 1 0

Data: D a sequence of outcomes x_i such that

- **head** $x_i = 1$
- **tail** $x_i = 0$

Model: probability of a head θ
probability of a tail $(1 - \theta)$

贝叶斯学习与参数估计问题

贝叶斯学习

例子 1: Beta 先验分布

Binary Variables

$$x \in \{0, 1\}$$

$$p(x = 1 | \theta) = \theta$$

$$p(x = 0 | \theta) = 1 - \theta$$

- 贝努力分布(**Bernoulli**):

$$\text{Bern}(x | \theta) = \theta^x (1 - \theta)^{1-x}$$

贝叶斯学习与参数估计问题

贝叶斯学习

例子 1: Beta 先验分布

Binary Variables

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- 贝努力分布(**Bernoulli**):

$$\text{Bern}(x | \theta) = \theta^x (1 - \theta)^{1-x}$$

- **Likelihood** (观察似然) :

H H T T H H T H T H T T T H T H H H H T H H H H T
1 1 0 0 1 1 0 1 0 1 0 0 0 1 0 1 1 1 1 0 1 1 1 0

$$P(D | \theta) = \prod_{i=1}^n \theta^{x_i} (1 - \theta)^{(1-x_i)}$$

$$P(D | \theta) = \theta^{N_1} (1 - \theta)^{N_2} \quad (N_1 + N_2 = N)$$

贝叶斯学习与参数估计问题

贝叶斯学习

例子 1: Beta 先验分布

- Binary Variables

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H H T T H H T H T H T T T H T H H H H T H H H H T
1 1 0 0 1 1 0 1 0 1 0 0 0 1 0 1 1 1 1 0 1 1 1 0

$$P(D | \theta) = \prod_{i=1}^n \theta^{x_i} (1 - \theta)^{(1-x_i)}$$

$$P(D | \theta) = \theta^{N_1} (1 - \theta)^{N_2} \quad (N_1 + N_2 = N)$$

(对比)二项式分布:

$$\text{Bin}(m | N, \theta) = \binom{N}{m} \theta^m (1 - \theta)^{N-m}$$

贝叶斯学习与参数估计问题

贝叶斯学习

例子 1: Beta 先验分布

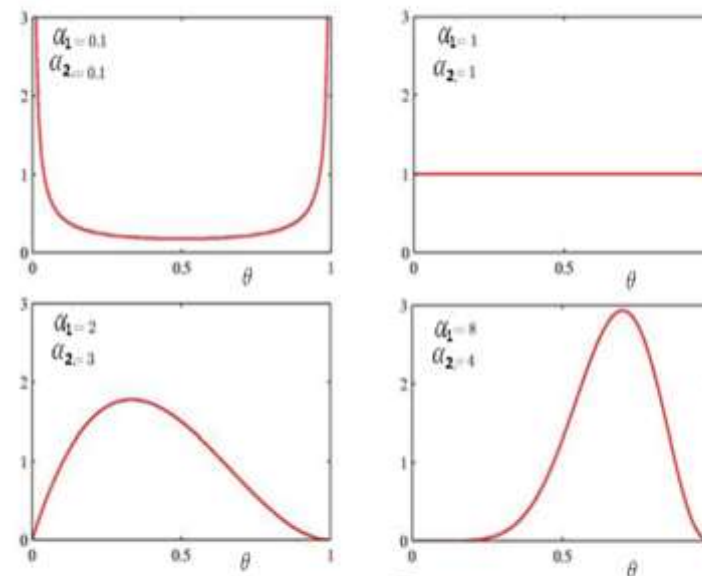
- **Prior**

Choice of prior: **Beta distribution**

$$p(\theta | \alpha) = \text{Beta}(\theta | \alpha_1, \alpha_2) = \frac{\Gamma(\alpha_1 + \alpha_2)}{\Gamma(\alpha_1)\Gamma(\alpha_2)} \theta^{\alpha_1-1} (1-\theta)^{\alpha_2-1}$$

$\Gamma(x)$ - a Gamma function $\Gamma(x) = (x-1)\Gamma(x-1)$
For integer values of x $\Gamma(n) = (n-1)!$

Beta distribution



$$p(\theta | \alpha) = \text{Beta}(\theta | \alpha_1, \alpha_2) = \frac{\Gamma(\alpha_1 + \alpha_2)}{\Gamma(\alpha_1)\Gamma(\alpha_2)} \theta^{\alpha_1-1} (1-\theta)^{\alpha_2-1}$$

贝叶斯学习与参数估计问题

贝叶斯学习

例子 1: Beta 先验分布

- **Prior**

Choice of prior: **Beta distribution**

$$p(\theta | \alpha) = \text{Beta}(\theta | \alpha_1, \alpha_2) = \frac{\Gamma(\alpha_1 + \alpha_2)}{\Gamma(\alpha_1)\Gamma(\alpha_2)} \theta^{\alpha_1-1} (1-\theta)^{\alpha_2-1}$$

$\Gamma(x)$ - a Gamma function $\Gamma(x) = (x-1)\Gamma(x-1)$
For integer values of x $\Gamma(n) = (n-1)!$

Why to use Beta distribution?

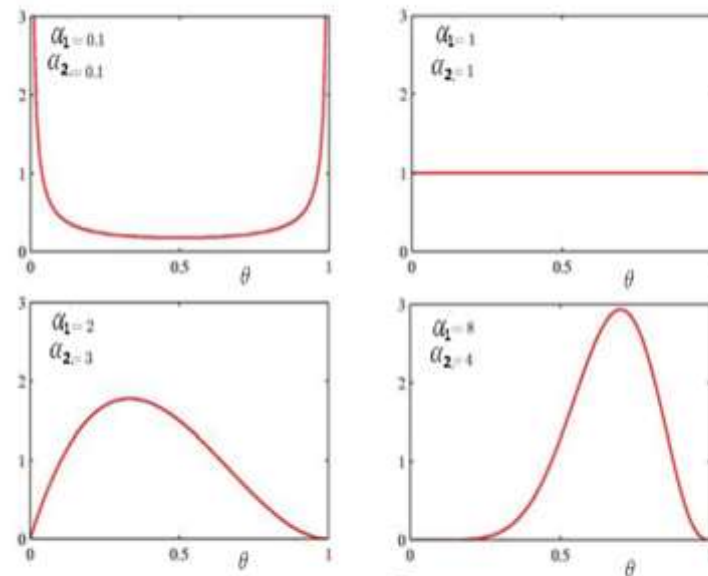
Beta distribution “fits” Bernoulli trials - **conjugate choices**

$$P(D | \theta) = \theta^{N_1} (1-\theta)^{N_2}$$

Posterior distribution is again a Beta distribution

$$p(\theta | D, \alpha) = \frac{P(D | \theta) \text{Beta}(\theta | \alpha_1, \alpha_2)}{P(D | \alpha)} = \text{Beta}(\theta | \alpha_1 + N_1, \alpha_2 + N_2)$$

Beta distribution



$$p(\theta | \alpha) = \text{Beta}(\theta | \alpha_1, \alpha_2) = \frac{\Gamma(\alpha_1 + \alpha_2)}{\Gamma(\alpha_1)\Gamma(\alpha_2)} \theta^{\alpha_1-1} (1-\theta)^{\alpha_2-1}$$

贝叶斯学习与参数估计问题

贝叶斯学习

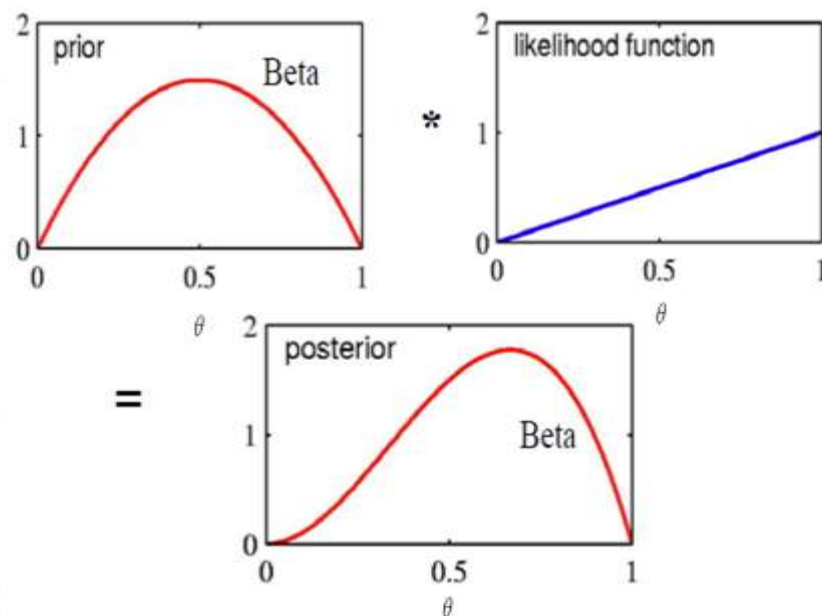
例子 1: Beta 先验分布

- **Posterior:**

$$p(\theta | D, \alpha) = \frac{P(D | \theta) \text{Beta}(\theta | \alpha_1, \alpha_2)}{P(D | \alpha)} = \text{Beta}(\theta | \alpha_1 + N_1, \alpha_2 + N_2)$$
$$= \frac{\Gamma(\alpha_1 + \alpha_2 + N_1 + N_2)}{\Gamma(\alpha_1 + N_1) \Gamma(\alpha_2 + N_2)} \theta^{N_1 + \alpha_1 - 1} (1 - \theta)^{N_2 + \alpha_2 - 1}$$

Notice that parameters of the prior
act like counts of heads and tails
(sometimes they are also referred to as **prior counts**)

Posterior distribution



$$p(\theta | D, \alpha) = \frac{P(D | \theta) \text{Beta}(\theta | \alpha_1, \alpha_2)}{P(D | \alpha)} = \text{Beta}(\theta | \alpha_1 + N_1, \alpha_2 + N_2)$$

贝叶斯学习与参数估计问题

极大似然估计

问题描述

- 最大化观察数据的概率

$$p(\theta|\mathcal{D}, \alpha) \propto p(\mathcal{D}|\theta)p(\theta|\alpha)$$

← 最大化

似然函数 likelihood:

$$p(\mathcal{D}|\theta) = p(\mathbf{x}_1, \dots, \mathbf{x}_n|\theta) = \prod_{i=1}^n p(\mathbf{x}_i|\theta)$$

Maximum Likelihood

$$\hat{\theta} = \arg \max_{\theta} p(\mathcal{D}|\theta)$$

转化为求 log-likelihood 极大的问题

$$\hat{\theta} = \arg \max_{\theta} \sum_{i=1}^n \log p(\mathbf{x}_i|\theta)$$

求解过程

$$\sum_{i=1}^n \nabla_{\theta} \log p(\mathbf{x}_i|\theta) = 0$$

贝叶斯学习与参数估计问题

极大似然估计

例子 1：二项式分布的 ML

- likelihood

$$p(\mathcal{D}|\theta) = \prod_{n=1}^N p(x_n|\theta) = \prod_{n=1}^N \theta^{x_n} (1 - \theta)^{1-x_n}.$$

- Log-likelihood

$$\ln p(\mathcal{D}|\theta) = \sum_{n=1}^N \ln p(x_n|\theta) = \sum_{n=1}^N \{x_n \ln \theta + (1 - x_n) \ln(1 - \theta)\}$$

- 最优的参数

$$\theta_{\text{ML}} = \frac{1}{N} \sum_{n=1}^N x_n \quad \theta_{\text{ML}} = \frac{m}{N}$$

贝叶斯学习与参数估计问题

极大似然估计

例子 1 : 二项式分布的 ML

- 实例:
 - Assume the unknown and possibly biased coin
 - Probability of the head is θ
 - Data:
H H T T H H T H T T T H T H H H H T H H H H T
– Heads: 15
– Tails: 10

What is the ML estimate of the probability of head and tail ?

Likelihood: $P(D | \theta) = \theta^{N_1} (1 - \theta)^{N_2}$

最优的参数:

$$\text{Head: } \theta_{ML} = \frac{N_1}{N} = \frac{N_1}{N_1 + N_2} = \frac{15}{25} = 0.6$$

$$\text{Tail: } (1 - \theta_{ML}) = \frac{N_2}{N} = \frac{N_2}{N_1 + N_2} = \frac{10}{25} = 0.4$$

贝叶斯学习与参数估计问题

极大似然估计

例子 2 : 高斯分布的 ML-估计 μ

Let $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N$ be vectors stemmed from a normal distribution with known covariance matrix and unknown mean, that is,

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

- Log-likelihood:

$$L(\boldsymbol{\mu}) \equiv \ln \prod_{k=1}^N p(\mathbf{x}_k; \boldsymbol{\mu}) = -\frac{N}{2} \ln((2\pi)^I |\Sigma|) - \frac{1}{2} \sum_{k=1}^N (\mathbf{x}_k - \boldsymbol{\mu})^T \Sigma^{-1}(\mathbf{x}_k - \boldsymbol{\mu})$$

贝叶斯学习与参数估计问题

极大似然估计

例子 2 : 高斯分布的 ML-估计 μ

Taking the gradient with respect to μ , we obtain

$$\frac{\partial L(\mu)}{\partial \mu} \equiv \begin{bmatrix} \frac{\partial L}{\partial \mu_1} \\ \frac{\partial L}{\partial \mu_2} \\ \vdots \\ \frac{\partial L}{\partial \mu_l} \end{bmatrix} = \sum_{k=1}^N \Sigma^{-1}(\mathbf{x}_k - \mu) = 0$$

or

$$\hat{\mu}_{ML} = \frac{1}{N} \sum_{k=1}^N \mathbf{x}_k$$

贝叶斯学习与参数估计问题

极大似然估计

例子 3 : 高斯分布的 ML-估计方差

Assume that N data points, x_1, x_2, \dots, x_N , have been generated by a one-dimensional Gaussian pdf of known mean, μ , but of unknown variance. Derive the ML estimate of the variance.

The log-likelihood function for this case is given by

$$\begin{aligned} L(\sigma^2) &= \ln \prod_{k=1}^N p(x_k; \sigma^2) = \ln \prod_{k=1}^N \frac{1}{\sqrt{2\pi}\sqrt{\sigma^2}} \exp\left(-\frac{(x_k - \mu)^2}{2\sigma^2}\right) \\ &= -\frac{N}{2} \ln(2\pi\sigma^2) - \frac{1}{2\sigma^2} \sum_{k=1}^N (x_k - \mu)^2 \end{aligned}$$

Taking the derivative of the above with respect to σ^2 and equating to zero, we obtain

$$-\frac{N}{2\sigma^2} + \frac{1}{2\sigma^4} \sum_{k=1}^N (x_k - \mu)^2 = 0 \qquad \hat{\sigma}_{ML}^2 = \frac{1}{N} \sum_{k=1}^N (x_k - \mu)^2$$

贝叶斯学习与参数估计问题

最大后验估计

问题描述

求使后验概率最大的模型或参数(θ)。

$$p(\theta | \mathcal{D}, \alpha) \propto p(\mathcal{D} | \theta) p(\theta | \alpha)$$

贝叶斯公式中

最大化

$$p(\theta | D, \alpha) = \frac{P(D | \theta) p(\theta | \alpha)}{P(D | \alpha)}$$

$$\hat{\theta}_{MAP} : \frac{\partial}{\partial \theta} p(\theta | D, \alpha) = 0 \quad \text{or} \quad \frac{\partial}{\partial \theta} P(D | \theta) p(\theta | \alpha) = 0$$

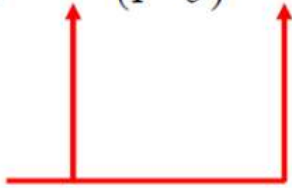
贝叶斯学习与参数估计问题

最大后验估计

例子 1 : Beta 先验分布的 MAP

Maximum a posteriori estimate

- Selects the mode of the **posterior distribution**

$$p(\theta | D, \alpha) = \frac{P(D | \theta) \text{Beta}(\theta | \alpha_1, \alpha_2)}{P(D | \alpha)} = \text{Beta}(\theta | \alpha_1 + N_1, \alpha_2 + N_2)$$
$$= \frac{\Gamma(\alpha_1 + \alpha_2 + N_1 + N_2)}{\Gamma(\alpha_1 + N_1) \Gamma(\alpha_2 + N_2)} \theta^{N_1 + \alpha_1 - 1} (1 - \theta)^{N_2 + \alpha_2 - 1}$$


Notice that parameters of the prior
act like counts of heads and tails
(sometimes they are also referred to as **prior counts**)

MAP Solution:

$$\theta_{MAP} = \frac{\alpha_1 + N_1 - 1}{\alpha_1 + \alpha_2 + N_1 + N_2 - 2}$$

贝叶斯学习与参数估计问题

最大后验估计

例子 1 : Beta 先验分布的 MAP

- 实例：
 - Assume the unknown and possibly biased coin
 - Probability of the head is θ
 - Data:**
H H T T H H T H T T T H T H H H H T H H H H T
 - Heads: 15
 - Tails: 10
 - Assume $p(\theta | \alpha) = \text{Beta}(\theta | 5, 5)$
- What is the MAP estimate ?

$$\theta_{MAP} = \frac{N_1 + \alpha_1 - 1}{N - 2} = \frac{N_1 + \alpha_1 - 1}{N_1 + N_2 + \alpha_1 + \alpha_2 - 2} = \frac{19}{33}$$

与 ML 比较: $\theta_{ML} = 15/25 = 0.6$, $\theta_{MAP} = 19/33 = 0.5758$

贝叶斯学习与参数估计问题

最大后验估计

例子 2 : 高斯分布的 MAP-估计 u

Let $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N$ be vectors stemmed from a normal distribution with known covariance matrix and unknown mean, that is,

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

$$p(\boldsymbol{\mu}) = \frac{1}{(2\pi)^{J/2} \sigma_\mu^J} \exp\left(-\frac{1}{2} \frac{\|\boldsymbol{\mu} - \boldsymbol{\mu}_0\|^2}{\sigma_\mu^2}\right)$$

The MAP estimate is given by the solution of

$$\frac{\partial}{\partial \boldsymbol{\mu}} \ln\left(\prod_{k=1}^N p(\mathbf{x}_k | \boldsymbol{\mu}) p(\boldsymbol{\mu})\right) = 0$$

or, for $\Sigma = \sigma^2 I$,

$$\sum_{k=1}^N \frac{1}{\sigma^2} (\mathbf{x}_k - \hat{\boldsymbol{\mu}}) - \frac{1}{\sigma_\mu^2} (\hat{\boldsymbol{\mu}} - \boldsymbol{\mu}_0)$$

$$\hat{\boldsymbol{\mu}}_{MAP} = \frac{\boldsymbol{\mu}_0 + \frac{\sigma_\mu^2}{\sigma^2} \sum_{k=1}^N \mathbf{x}_k}{1 + \frac{\sigma_\mu^2}{\sigma^2} N}$$

小 结

1. beyas 决策准则
2. 几种贝叶斯分类器
3. 贝叶斯学习与参数估计问题
 - Beyas Learning
 - M L 参数估计
 - M A P 参数估计

本讲参考文献

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