机器学习

Machine learning

第二章 贝叶斯学习

Bayesian Learning

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2023-9-22

课件放映 PDF-〉视图-〉全屏模式

第二章 贝叶斯学习

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： $C = \{c_1, c_2, \ldots c_M\}$，

数据 D 和样本 $\boldsymbol{x}$： $D=\{\boldsymbol{x}_i\}$

贝叶斯学习

$$P(c_i \mid \mathbf{x}) \propto P(\mathbf{x} \mid c_i) P(c_i)$$

核心是估计

$$P(c_i \mid \mathbf{x}) \propto P(\mathbf{x} \mid c_i) P(c_i)$$

预备知识

贝叶斯决策

类别相似性函数：

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

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

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

决策函数：

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

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

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

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

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

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”

$$P(c \mid \boldsymbol{x}) = \frac{P(c)P(\boldsymbol{x} \mid c)}{P(\boldsymbol{x})} \quad \propto \quad P(c)P(\boldsymbol{x} \mid c) = P(c)\prod_{i=1}^{d} P(x_i \mid c)$$

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$P(c)$

需要学习的概率分布?

***k* 个类别，*d* 个属性：** $p(\mathrm{c})$和$P(x_i|c_j)$,（$i=1,\ldots,d$ 个属性，$j=1,\ldots,k$）

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 $P(c)=\dfrac{|D_c|}{|D|}$

类别概率密度估计

- $\boldsymbol{x}_i$ 离散情况：

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

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

- $\boldsymbol{x}_i$ 连续情况：

$$P(x_i \mid c)=\frac{1}{\sqrt{2\pi}\sigma_{c,i}}\exp\left(-\frac{(x_i-\mu_{c,i})^2}{2\sigma^2_{c,i}}\right)$$

（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 $P(c)=\dfrac{|D_c|}{|D|}$

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

贝叶斯分类器

朴素贝叶斯分类器

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 $P(\boldsymbol{x}\mid c)=\prod_{i=1}^{d}P(x_i\mid c)$

(3) 贝叶斯决策 $h(\boldsymbol{x}) = \underset{c\in y}{\operatorname{argmax}}\, P(c)\prod_{i=1}^{d}P(x_i\mid c)$

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

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

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

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)

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	?

朴素贝叶斯分类器

学习过程：

(1) 类别先验估计

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

首先估计类别先验概率 $P(c)$ ，显然有

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

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

朴素贝叶斯分类器

(2) 类别条件概率估计

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

对于连续值属性：

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

均值、方差作为参数，可用 ML 估计，

为每个属性估计条件概率 $P(x_i \mid c)$

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

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

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

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

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

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

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

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

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

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

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

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

$$P_{\text{密度:0.697|是}} = p(\text{密度} = 0.697 \mid \text{好瓜} = \text{是}) = \frac{1}{\sqrt{2\pi} \cdot 0.129} \exp\left(-\frac{(0.697 - 0.574)^2}{2 \cdot 0.129^2} \right) \approx 1.959$$

$$P_{\text{密度:0.697|否}} = p(\text{密度} = 0.697 \mid \text{好瓜} = \text{否}) = \frac{1}{\sqrt{2\pi} \cdot 0.195} \exp\left(-\frac{(0.697 - 0.496)^2}{2 \cdot 0.195^2} \right) \approx 1.203$$

$$P_{\text{含糖:0.460|是}} = p(\text{含糖率} = 0.460 \mid \text{好瓜} = \text{是}) = \frac{1}{\sqrt{2\pi} \cdot 0.101} \exp\left(-\frac{(0.460 - 0.279)^2}{2 \cdot 0.101^2} \right) \approx 0.788$$

$$P_{\text{含糖:0.460|否}} = p(\text{含糖率} = 0.460 \mid \text{好瓜} = \text{否}) = \frac{1}{\sqrt{2\pi} \cdot 0.108} \exp\left(-\frac{(0.460 - 0.154)^2}{2 \cdot 0.108^2} \right) \approx 0.066$$

朴素贝叶斯分类器

(3) 贝叶斯决策

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

由于 $0.038>6.80\times10^{-5}$，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

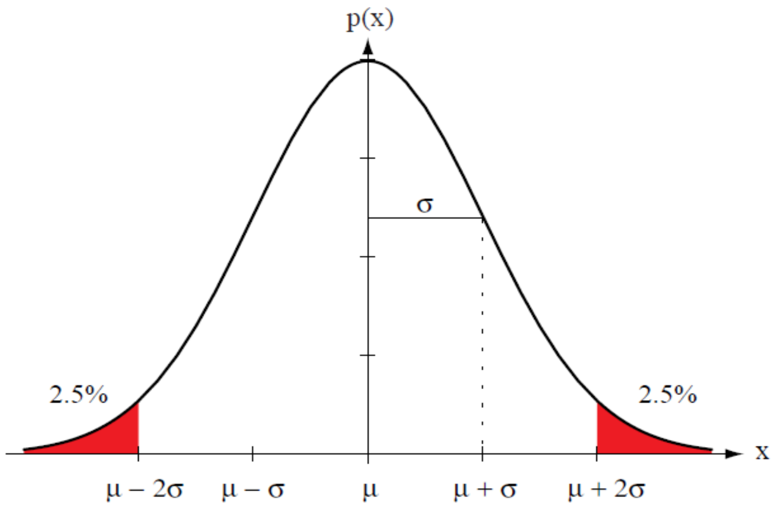
类别条件概率为正态分布

$$h(\boldsymbol{x}) = \underset{c \in y}{\operatorname{argmax}}\ P(c)\boxed{P(\boldsymbol{x}|c)}$$

正态分布

- 正态分布的概率密度 $N(\mu, \sigma^2)$：

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

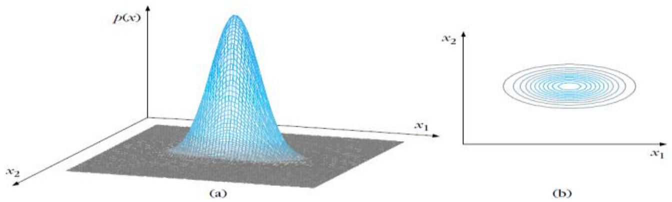


贝叶斯分类器

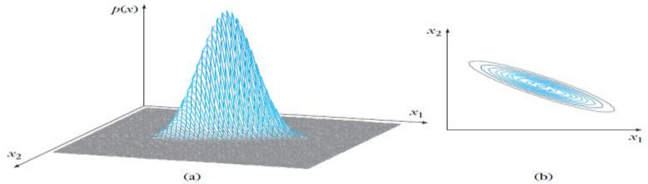
正态密度的贝叶斯分类器

- 多维正态分布的概率密度 $N(\boldsymbol{\mu},\Sigma)$：

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



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



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

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

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）：

$$g_i(\boldsymbol{x}) = \ln\left(p(\boldsymbol{x} \mid \omega_i)\, p(\omega_i)\right) = \ln p(\boldsymbol{x} \mid \omega_i) + \ln p(\omega_i)$$

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

$$g_i(\boldsymbol{x}) = -\frac{1}{2}(\boldsymbol{x}-\mu_i)^T \Sigma_i^{-1}(\boldsymbol{x}-\mu_i) - \frac{d}{2}\ln 2\pi - \frac{1}{2}\ln\left|\Sigma_i\right| + \ln p(\omega_i) \qquad (1)$$

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

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

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

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

$$g_i(x) = -\frac{1}{2\sigma^2}\left[x^T x - 2\mu_i^T x + \mu_i^T \mu_i\right] + \ln p(\omega_i)$$

与类别无关，可忽略

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

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

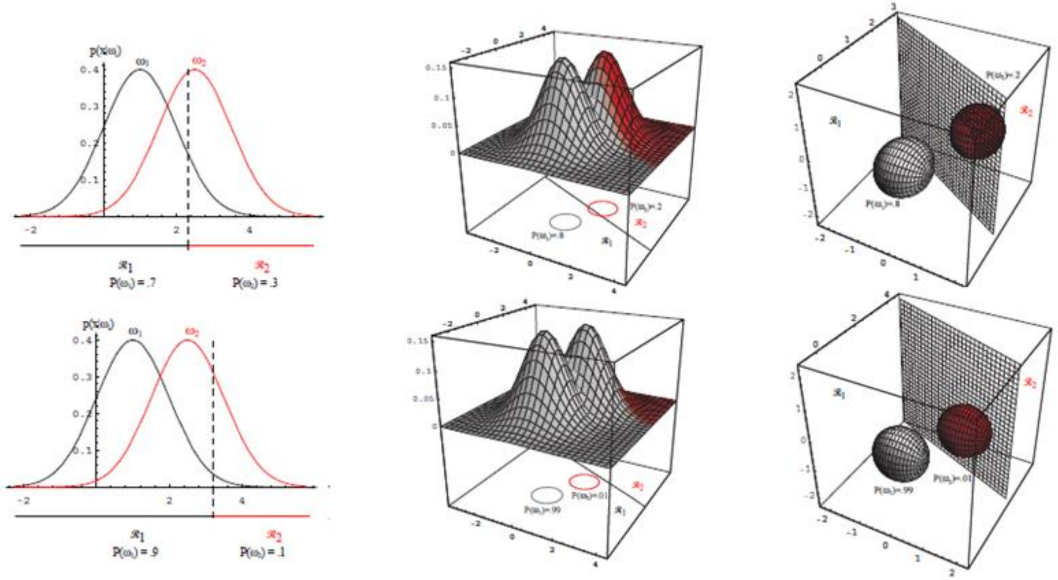
$Case\,1: \Sigma_i = \sigma^2 I$

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

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

$$w = \mu_i - \mu_j$$

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



贝叶斯分类器

正态密度的贝叶斯分类器

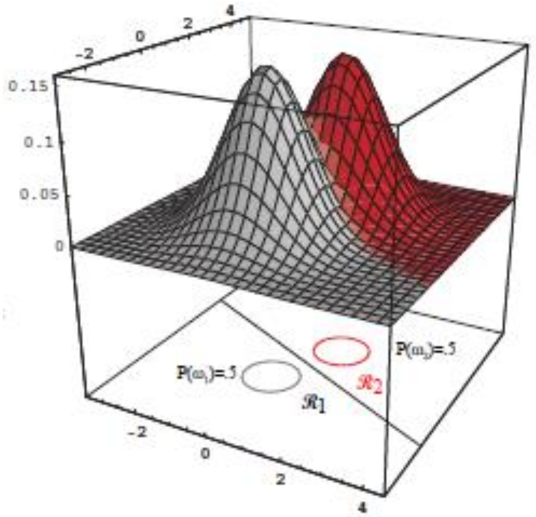
不同高斯参数情况讨论

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

特殊情况，当各个类别先验相等时，退化为最小距离分类器。

$$w = \mu_i - \mu_j$$

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



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

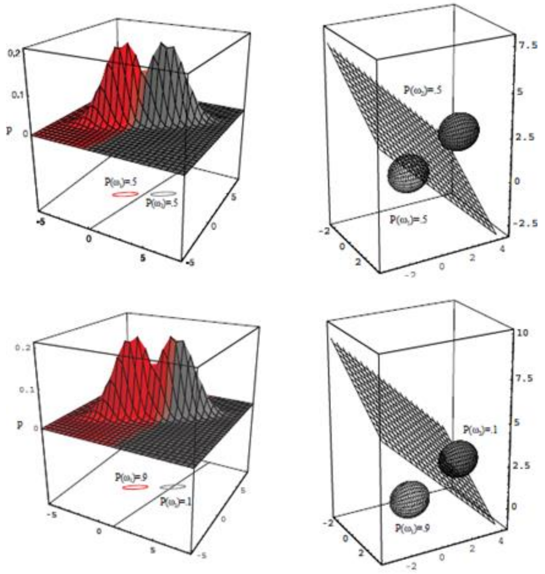
$Case\ 2: \Sigma_i = \Sigma$

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

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

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

$$x_0 = \frac{1}{2}(\mu_i + \mu_j) - \frac{\ln[p(\omega_i)/p(\omega_j)]}{(\mu_i - \mu_j)^T \Sigma^{-1}(\mu_i - \mu_j)}(\mu_i - \mu_j)$$



贝叶斯分类器

正态密度的贝叶斯分类器

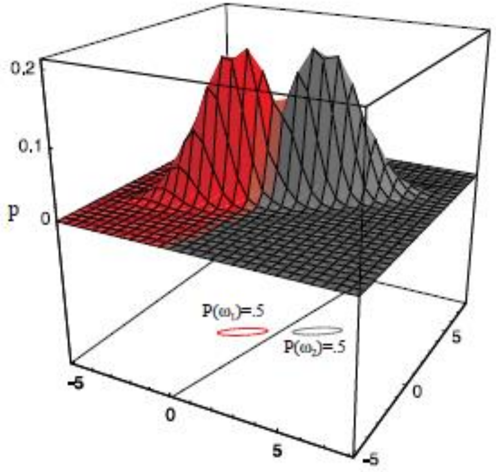
不同高斯参数情况讨论

$Case\ 2: \Sigma_i = \Sigma$

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

$Case\ 3: \Sigma_i = arbitrary$

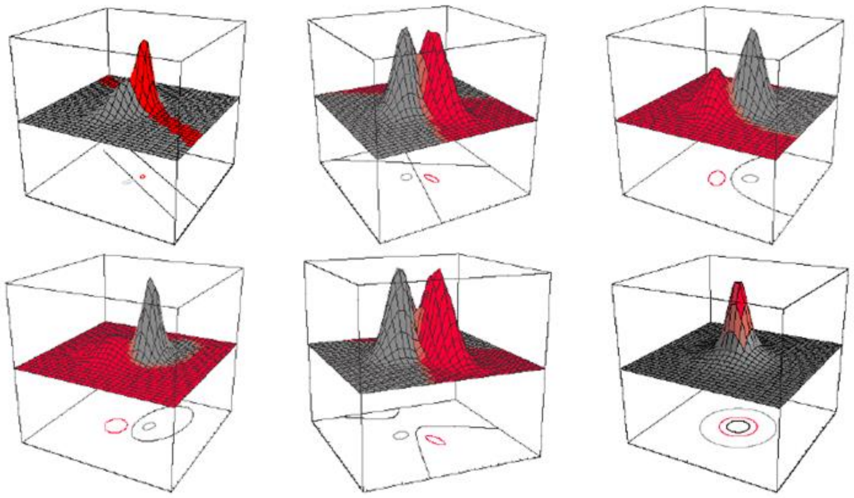
$$g_i(x) = x^T W_i x + w_i^T x + w_{i0}$$

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

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

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

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



贝叶斯分类器

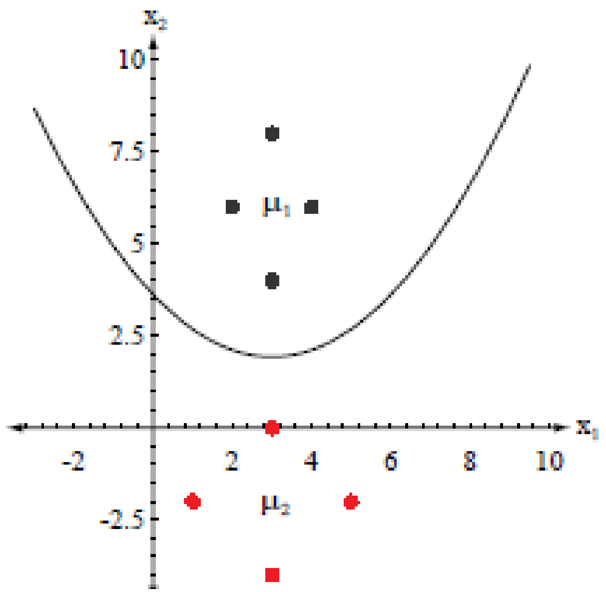
正态密度的贝叶斯分类器

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 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

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**):

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

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

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- 贝努力分布(**Bernoulli**)：

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

- **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 1 0

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

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

（$N_1+N_2=N$）

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 1 0

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

（$N_1+N_2=N$）

(对比)二项式分布：

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

贝叶斯学习

例子 1: Beta 先验分布

- **Prior**

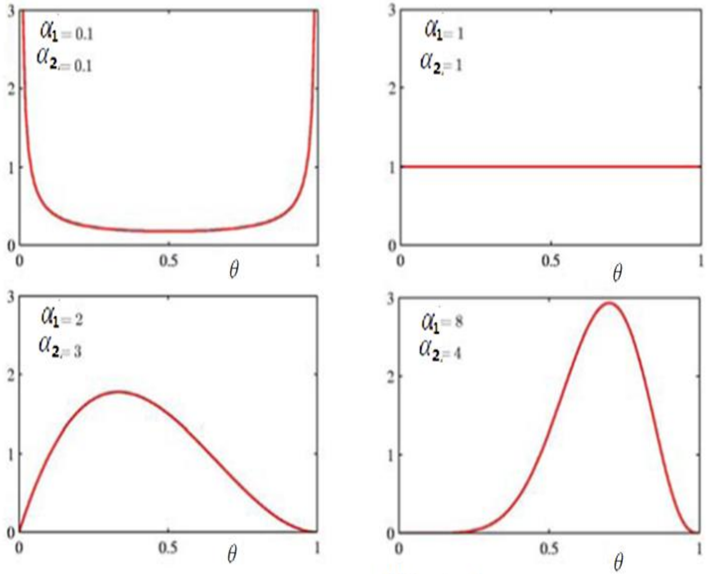
Choice of prior: Beta distribution

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

$\Gamma(x)$ - a Gamma function $\Gamma(x) = (x-1)\Gamma(x-1)$

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

Beta distribution



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贝叶斯学习

例子 1: Beta 先验分布

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$\Gamma(x)$ - a Gamma function $\Gamma(x) = (x-1)\Gamma(x-1)$

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

Why to use Beta distribution?

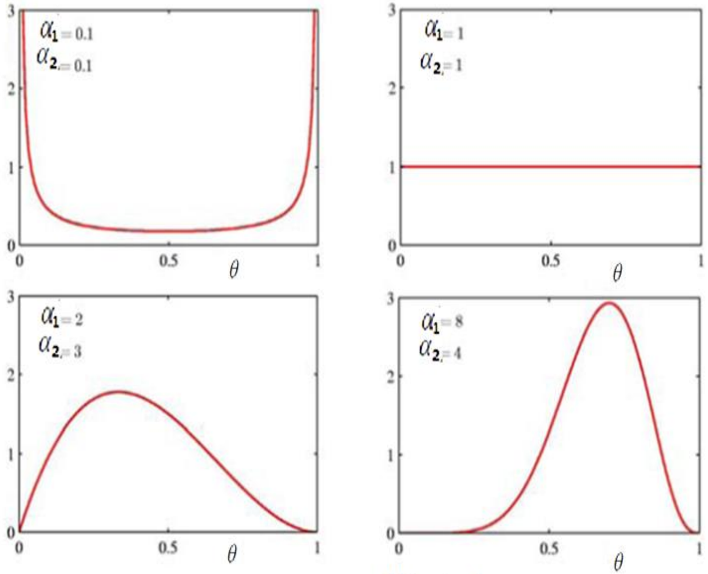
Beta distribution "**fits**" Bernoulli trials - **conjugate choices**

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

Posterior distribution is again a Beta distribution

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

Beta distribution



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

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

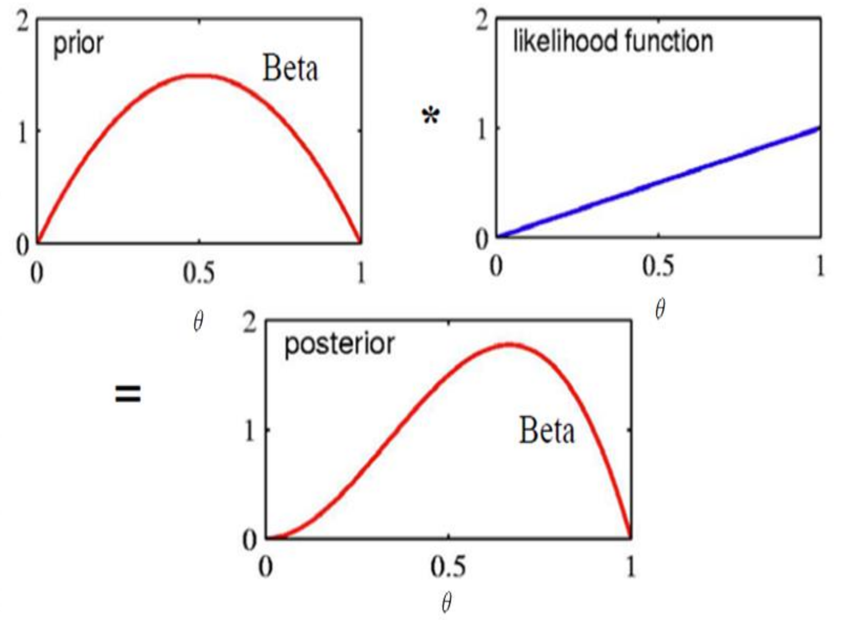
- **Posterior:**

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

$$= \frac{\Gamma(\alpha_1 + \alpha_2 + N_1 + N_2)}{\Gamma(\alpha_1 + N_1)\Gamma(\alpha_2 + N_2)} \theta^{N_1+\alpha_1-1}(1-\theta)^{N_2+\alpha_2-1}$$

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

Posterior distribution



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

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

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

最大化

似然函数 likelihood：

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

Maximum Likelihood

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

转化为求 log-likelihood 极大的问题

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

求解过程

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

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

$$\theta_{\mathrm{ML}} = \frac{1}{N}\sum_{n=1}^{N} x_n \qquad \theta_{\mathrm{ML}} = \frac{m}{N}$$

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

最优的参数：

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

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

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 u

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

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

- Log-likelihood:

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

极大似然估计

例子 2：高斯分布的 ML-估计 u

Taking the gradient with respect to $\boldsymbol{\mu}$, we obtain

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

or

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

极大似然估计

例子 3：高斯分布的 ML-估计方差

Assume that N data points, $x_1, x_2, \ldots, x_N$, 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

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

$$= -\frac{N}{2}\ln(2\pi\sigma^2) - \frac{1}{2\sigma^2}\sum_{k=1}^{N}(x_k-\mu)^2$$

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

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

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)。

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

最大化

贝叶斯公式中

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

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

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**

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

$$= \frac{\Gamma(\alpha_1 + \alpha_2 + N_1 + N_2)}{\Gamma(\alpha_1 + N_1)\Gamma(\alpha_2 + N_2)} \theta^{N_1+\alpha_1-1} (1-\theta)^{N_2+\alpha_2-1}$$

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

MAP Solution: $\theta_{MAP} = \dfrac{\alpha_1 + N_1 - 1}{\alpha_1 + \alpha_2 + N_1 + N_2 - 2}$

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 H T T T H T H H H H T H H H H T
    - **Heads:** 15
    - **Tails:** 10
  - Assume $p(\theta \mid \alpha) = Beta(\theta \mid 5,5)$

  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：θ_{ML} =15/25=0.6， θ_{MAP} =19/33=0.5758

最大后验估计

例子 2：高斯分布的 MAP-估计 u

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

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

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

The MAP estimate is given by the solution of

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

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

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

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

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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