

贝叶斯决策、参数估计

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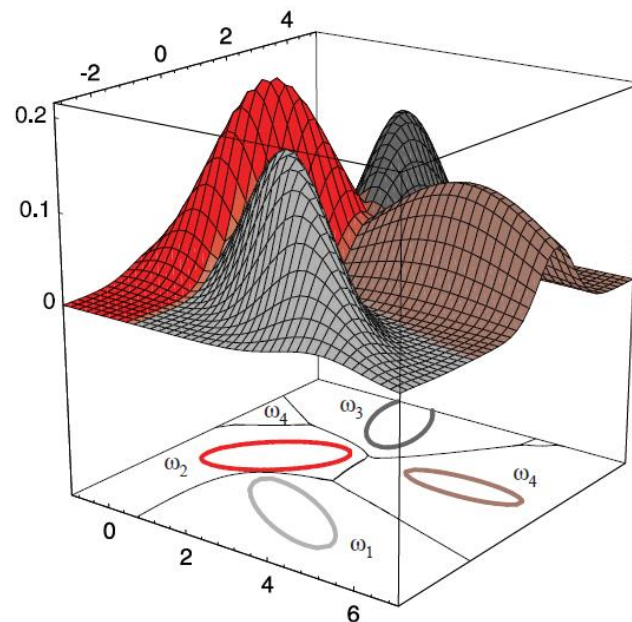
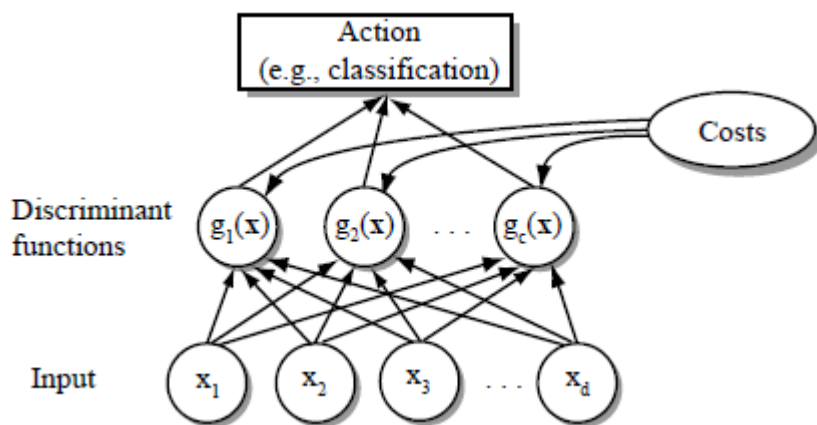
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统计模式分类的基本框架

- 特征空间划分
 - 判别函数(Discriminant function)、决策面(Decision surface)
 - 生成模型(Generative model): $\mathbf{x} \rightarrow p(\mathbf{x} | \omega_i) \rightarrow g_i(\mathbf{x})$
 - 判别模型(Discriminative model): $\mathbf{x} \rightarrow g_i(\mathbf{x})$



上次课主要内容回顾

- 贝叶斯决策
 - 最小风险决策
 - (0-1 loss)最小错误率决策（最大后验概率决策）
- 高斯概率密度（正态分布）
 - 1D, 多维（记住了？）
 - 协方差矩阵特性
 - 等密度点轨迹、马氏距离、特征值分解、正交化
 - 线性变换的高斯密度？
- 高斯密度下的判别函数
 - Quadratic discriminant function (QDF)
 - Three cases, linear discriminant function (LDF)
- 贝叶斯决策的错误率

提 纲

- 第2章
 - 离散变量的贝叶斯决策
 - 复合模式分类
- 第3章
 - 导论：关于参数估计
 - 最大似然参数估计
 - 贝叶斯估计
 - 贝叶斯估计：高斯密度的情况
 - 贝叶斯估计：一般情况

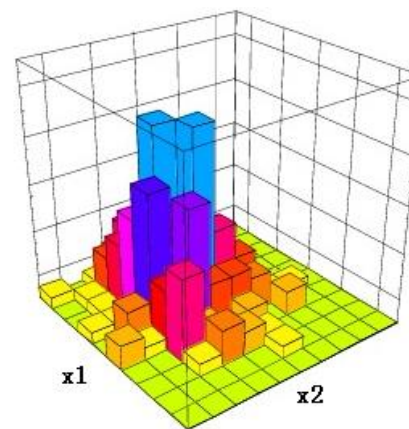
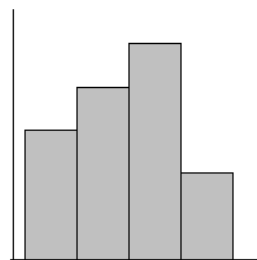
离散变量贝叶斯决策

- 贝叶斯决策

- 最小风险: $\min R(\alpha_i|\mathbf{x}) = \sum_{j=1}^c \lambda(\alpha_i|\omega_j)P(\omega_j|\mathbf{x})$
- 最小错误率(MAP): $\max P(\omega_j|\mathbf{x})$

- 离散特征变量

- 例如：问卷调查，每个问题2个或多个选项；
医疗诊断：是否有某个症状
- 概率密度函数 $p(\mathbf{x}|\omega_i) = p(x_1x_2 \cdots x_d | \omega_i)$
(非参数、直方图表示)



- 独立二值特征(Binary features)

- 独立 $p(\mathbf{x}) = p(x_1 x_2 \cdots x_d) = \prod_{i=1}^d p(x_i)$

- Binary, 概率密度: d个参数 $p_i = \text{Prob}(x_i = 1 | \omega_1)$

- 2-class $q_i = \text{Prob}(x_i = 1 | \omega_2)$

$$P(\mathbf{x} | \omega_1) = \prod_{i=1}^d p_i^{x_i} (1 - p_i)^{1-x_i} \quad P(\mathbf{x} | \omega_2) = \prod_{i=1}^d q_i^{x_i} (1 - q_i)^{1-x_i}$$

- Likelihood ratio $\frac{P(\mathbf{x} | \omega_1)}{P(\mathbf{x} | \omega_2)} = \prod_{i=1}^d \left(\frac{p_i}{q_i} \right)^{x_i} \left(\frac{1 - p_i}{1 - q_i} \right)^{1-x_i}$

- Discriminant function

$$g(\mathbf{x}) = \log \frac{p(\mathbf{x} | \omega_1) P(\omega_1)}{p(\mathbf{x} | \omega_2) P(\omega_2)} = \sum_{i=1}^d \left[x_i \ln \frac{p_i}{q_i} + (1 - x_i) \ln \frac{1 - p_i}{1 - q_i} \right] + \ln \frac{P(\omega_1)}{P(\omega_2)}$$

- Linear $g(\mathbf{x}) = \sum_{i=1}^d w_i x_i + w_0$ w_i 表征每个特征的判别性

$$w_i = \ln \frac{p_i(1 - q_i)}{q_i(1 - p_i)} \quad i = 1, \dots, d \quad w_0 = \sum_{i=1}^d \ln \frac{1 - p_i}{1 - q_i} + \ln \frac{P(\omega_1)}{P(\omega_2)}$$



- An example: 3D binary data

- $P(\omega_1)=0.5, P(\omega_2)=0.5$

- $p_i=0.8, q_i=0.5, i=1,2,3$

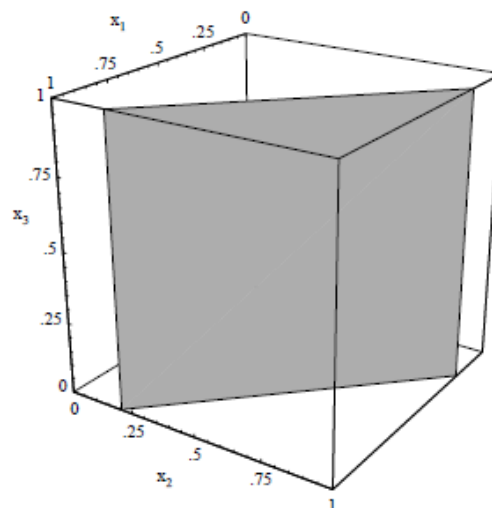
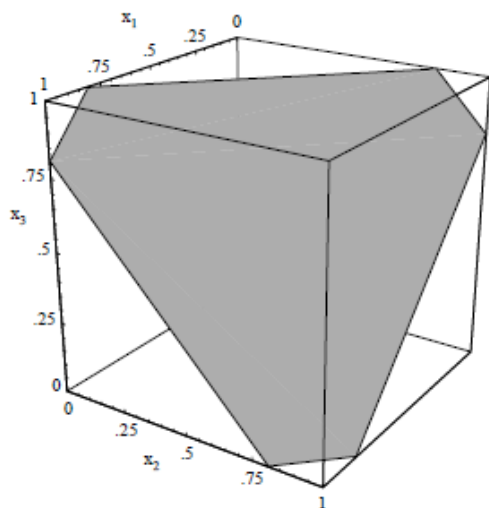
$$P(\mathbf{x}|\omega_1) = \prod_{i=1}^d p_i^{x_i} (1 - p_i)^{1-x_i}$$

$$P(\mathbf{x}|\omega_2) = \prod_{i=1}^d q_i^{x_i} (1 - q_i)^{1-x_i}$$

$$g(\mathbf{x}) = \sum_{i=1}^d w_i x_i + w_0$$

$$w_i = \ln \frac{.8(1 - .5)}{.5(1 - .8)} = 1.3863$$

$$w_0 = \sum_{i=1}^3 \ln \frac{1 - .8}{1 - .5} + \ln \frac{.5}{.5} = 1.2$$



Another case: $p_1=p_2=0.8, q_1=q_2=0.5, p_3=q_3=0.5 \rightarrow w_3=0$

复合模式分类

(*2.12 Compound Bayesian Decision Theory and Context)

- 多个模式同时分类 $\mathbf{X} = \mathbf{x}_1 \mathbf{x}_2 \cdots \mathbf{x}_n$ $\boldsymbol{\omega} = \omega(1)\omega(2)\cdots\omega(n)$

- 比如：字符串识别

tomorrow

- Bayesian decision

$$P(\omega|X) = \frac{p(X|\omega)P(\omega)}{p(X)} = \frac{p(X|\omega)P(\omega)}{\sum_{\omega} p(X|\omega)P(\omega)}$$

- 注意： ω 类别数巨大， $p(X|\omega)$ 存储和估计困难

- Conditionally independent

$$p(X|\omega) = \prod_{i=1}^n p(\mathbf{x}_i|\omega(i))$$

- Prior assumption

- Markov chain

$$P[\omega(1)\omega(2)\cdots\omega(n)] = P[\omega(1)] \prod_{j=2}^n P[\omega(j) | \omega(j-1)]$$

- Hidden Markov model (Chapter 3)

第3章

最大似然和贝叶斯参数估计

关于参数估计

- 分类器设计

- 给定分类器结构/函数形式，从训练样本估计参数
- 统计生成模型：概率密度估计

- 参数法 $p(\mathbf{x}|\omega_i, \theta_i)$, e.g., $N(\mu_i, \Sigma_i)$

- 统计判别模型：判别函数参数估计

- 比如，神经网络

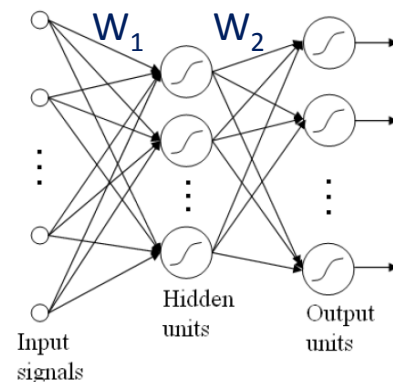
$$g_i(\mathbf{x}) = f(\mathbf{x}, W_1, W_{2,i})$$

- Maximum likelihood (ML)

- 假设参数为固定值，最优估计：似然度最大

- Bayesian estimation (Bayesian learning)

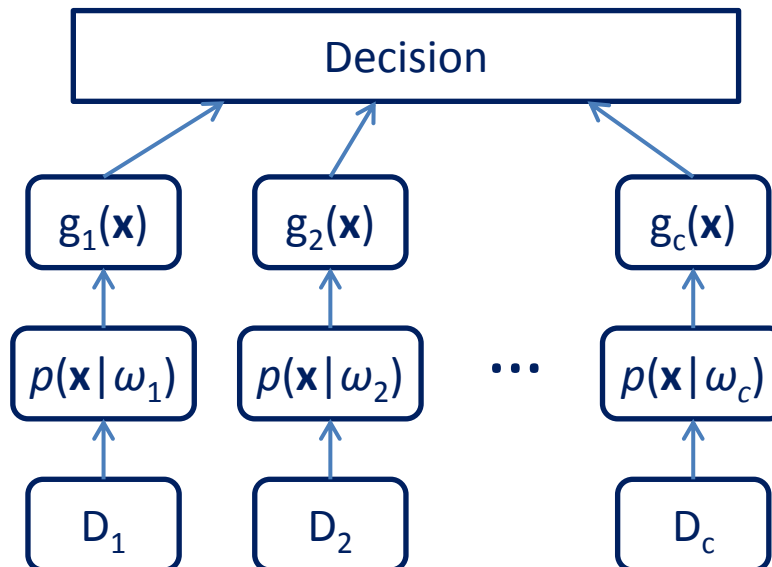
- 假设参数为随机变量，估计其分布



最大似然估计

- 基本原理

- 假设概率密度函数 $p(\mathbf{x}|\omega_i, \theta_i)$, θ_i to be estimated
- 样本数据 D_1, \dots, D_c
 - Samples in D_i assumed to be independent and identically distributed (*i.i.d.*)
 - D_i used to estimate θ_i disregarding the parameters of other classes



– The case for one class

- Likelihood $p(\mathcal{D}|\theta) = \prod_{k=1}^n p(\mathbf{x}_k|\theta)$
- Maximization $\max_{\theta} p(\mathcal{D}|\theta) \leftrightarrow \nabla_{\theta} p(\mathcal{D}|\theta) = 0$
- Gradient: vector in **parameter space**

$$\nabla_{\theta} \equiv \begin{bmatrix} \frac{\partial}{\partial \theta_1} \\ \vdots \\ \frac{\partial}{\partial \theta_p} \end{bmatrix}$$

Parameter space (p-D) versus feature space (d-D)

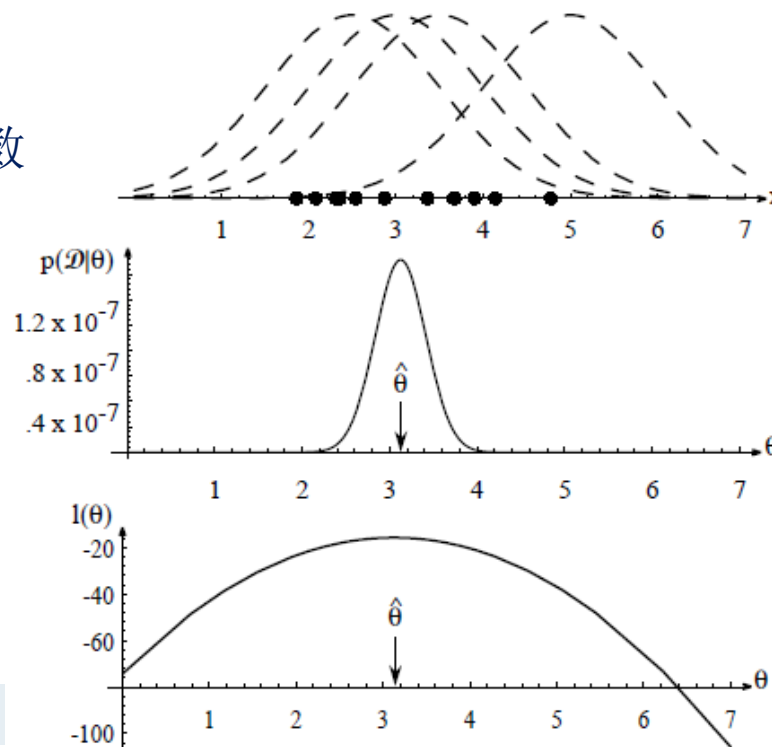
– 最大似然：一个例子

- 假设 σ^2 已知， μ 未知

10个样本点，
4个假设高斯密度函数

Likelihood: μ 的函数

Log-likelihood



- Log-likelihood

$$l(\theta) \equiv \ln p(\mathcal{D}|\theta) \quad l(\theta) = \sum_{k=1}^n \ln p(\mathbf{x}_k|\theta)$$

- ML estimate

$$\hat{\theta} = \arg \max_{\theta} l(\theta)$$

$$\nabla_{\theta} l = \sum_{k=1}^n \nabla_{\theta} \ln p(\mathbf{x}_k|\theta) = 0$$

$$\frac{\partial l}{\partial \theta_j} = 0, \quad j = 1, \dots, p$$

- Maximum a posteriori (MAP) estimator

$$\max_{\theta} l(\theta) p(\theta)$$

- Equivalent to ML when $p(\theta)$ is uniform

- Gaussian case: unknown μ

- Log-likelihood of a single point

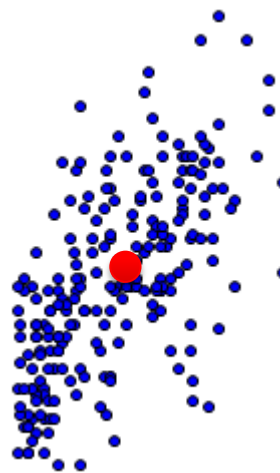
$$\ln p(\mathbf{x}_k | \mu) = -\frac{1}{2} \ln [(2\pi)^d |\Sigma|] - \frac{1}{2} (\mathbf{x}_k - \mu)^t \Sigma^{-1} (\mathbf{x}_k - \mu)$$

$$\nabla_{\theta} \ln p(\mathbf{x}_k | \mu) = \Sigma^{-1} (\mathbf{x}_k - \mu)$$

- ML solution: sample mean

$$\nabla_{\theta} l(\theta) = 0 \Rightarrow \sum_{k=1}^n \Sigma^{-1} (\mathbf{x}_k - \hat{\mu}) = 0$$

$$\Rightarrow \hat{\mu} = \frac{1}{n} \sum_{k=1}^n \mathbf{x}_k$$



- Gaussian case: unknown μ and Σ

- 1D case, $\theta_1 = \mu$ and $\theta_2 = \sigma^2$

$$\ln p(x_k|\theta) = -\frac{1}{2} \ln 2\pi\theta_2 - \frac{1}{2\theta_2}(x_k - \theta_1)^2$$

$$\nabla_{\theta} l = \nabla_{\theta} \ln p(x_k|\theta) = \begin{bmatrix} \frac{1}{\theta_2}(x_k - \theta_1) \\ -\frac{1}{2\theta_2} + \frac{(x_k - \theta_1)^2}{2\theta_2^2} \end{bmatrix}$$

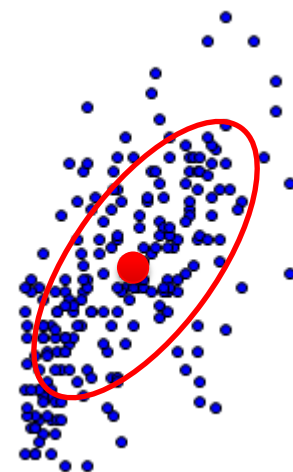
$$\begin{aligned} \nabla_{\theta} l(\theta) = 0 &\Rightarrow \sum_{k=1}^n \frac{1}{\hat{\theta}_2}(x_k - \hat{\theta}_1) = 0 \Rightarrow \hat{\mu} = \frac{1}{n} \sum_{k=1}^n x_k \\ &\quad \searrow \quad \quad \quad \nearrow \\ &\quad -\sum_{k=1}^n \frac{1}{\hat{\theta}_2} + \sum_{k=1}^n \frac{(x_k - \hat{\theta}_1)^2}{\hat{\theta}_2^2} = 0 \Rightarrow \hat{\sigma}^2 = \frac{1}{n} \sum_{k=1}^n (x_k - \hat{\mu})^2 \end{aligned}$$

- Multivariate case (Problem 6, Chapter 3)

记住结论即可

$$\hat{\mu} = \frac{1}{n} \sum_{k=1}^n \mathbf{x}_k$$


$$\hat{\Sigma} = \frac{1}{n} \sum_{k=1}^n (\mathbf{x}_k - \hat{\mu})(\mathbf{x}_k - \hat{\mu})^t$$



- ML estimate of variance/covariance is biased

$$\mathcal{E} \left[\frac{1}{n} \sum_{i=1}^n (x_i - \bar{x})^2 \right] = \frac{n-1}{n} \sigma^2 \neq \sigma^2$$

$\bar{x} = \frac{1}{n} \sum_{i=1}^n x_i$



- Unbiased estimate (sample covariance matrix)

$$\mathcal{E} \left[\frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})^2 \right] = \sigma^2$$
$$\mathbf{C} = \frac{1}{n-1} \sum_{k=1}^n (\mathbf{x}_k - \hat{\boldsymbol{\mu}})(\mathbf{x}_k - \hat{\boldsymbol{\mu}})^t$$

- 不能说哪个对或错，实际使用中几乎没有区别

Break

贝叶斯参数估计

- 贝叶斯估计
 - 参数被视为随机变量，估计其后验分布
 - 模型使用：MAP, sampled models combination
- Class-conditional densities

$$P(\omega_i | \mathbf{x}, \mathcal{D}) = \frac{p(\mathbf{x} | \omega_i, \mathcal{D}) P(\omega_i | \mathcal{D})}{\sum_{j=1}^c p(\mathbf{x} | \omega_j, \mathcal{D}) P(\omega_j | \mathcal{D})}$$

- Prior probabilities assumed known

$$P(\omega_i | \mathbf{x}, \mathcal{D}) = \frac{p(\mathbf{x} | \omega_i, \mathcal{D}_i) P(\omega_i)}{\sum_{j=1}^c p(\mathbf{x} | \omega_j, \mathcal{D}_j) P(\omega_j)}$$

- \mathcal{D}_i used to estimate θ_i disregarding the parameters of other classes

- Parameter distribution

- Assume known density function $p(\mathbf{x}|\boldsymbol{\theta})$, known prior density $p(\boldsymbol{\theta})$
- To estimate posterior density $p(\boldsymbol{\theta}|\mathcal{D})$
- Estimated density

$$\begin{aligned} p(\mathbf{x}|\mathcal{D}) &= \int p(\mathbf{x}, \boldsymbol{\theta}|\mathcal{D}) d\boldsymbol{\theta} \\ &= \int p(\mathbf{x}|\boldsymbol{\theta}) \underline{p(\boldsymbol{\theta}|\mathcal{D})} d\boldsymbol{\theta} \end{aligned}$$

- Model usage

- **Model average** (weighting density functions)
- If $p(\boldsymbol{\theta}|\mathcal{D})$ peaks sharply, MAP $p(\mathbf{x}|\mathcal{D}) \simeq p(\mathbf{x}|\hat{\boldsymbol{\theta}})$

高斯密度贝叶斯估计

- 1D case: $p(\mu | \mathcal{D})$ $p(x|\mu) \sim N(\mu, \sigma^2)$ Assume known σ^2
 - Assume prior density $p(\mu) \sim N(\mu_0, \sigma_0^2)$
 - Posterior density

$$\begin{aligned} p(\mu | \mathcal{D}) &= \frac{p(\mathcal{D} | \mu) p(\mu)}{\int p(\mathcal{D} | \mu) p(\mu) d\mu} \\ &= \alpha \prod_{k=1}^n p(x_k | \mu) p(\mu) \quad \alpha: \text{normalization factor} \end{aligned}$$

$$\begin{aligned} p(\mu | \mathcal{D}) &= \alpha \prod_{k=1}^n \overbrace{\frac{1}{\sqrt{2\pi}\sigma} \exp \left[-\frac{1}{2} \left(\frac{x_k - \mu}{\sigma} \right)^2 \right]}^{p(x_k | \mu)} \overbrace{\frac{1}{\sqrt{2\pi}\sigma_0} \exp \left[-\frac{1}{2} \left(\frac{\mu - \mu_0}{\sigma_0} \right)^2 \right]}^{p(\mu)} \\ &= \alpha' \exp \left[-\frac{1}{2} \left(\sum_{k=1}^n \left(\frac{\mu - x_k}{\sigma} \right)^2 + \left(\frac{\mu - \mu_0}{\sigma_0} \right)^2 \right) \right] \\ &= \alpha'' \exp \left[-\frac{1}{2} \left[\left(\frac{n}{\sigma^2} + \frac{1}{\sigma_0^2} \right) \mu^2 - 2 \left(\frac{1}{\sigma^2} \sum_{k=1}^n x_k + \frac{\mu_0}{\sigma_0^2} \right) \mu \right] \right] \end{aligned}$$

$p(\mu | \mathcal{D})$ 仍为正态分布! $p(\mu)$: conjugate prior

– Estimate from n samples

$$p(\mu|\mathcal{D}) \sim N(\mu_n, \sigma_n^2)$$

$$p(\mu|\mathcal{D}) = \frac{1}{\sqrt{2\pi}\sigma_n} \exp \left[-\frac{1}{2} \left(\frac{\mu - \mu_n}{\sigma_n} \right)^2 \right]$$

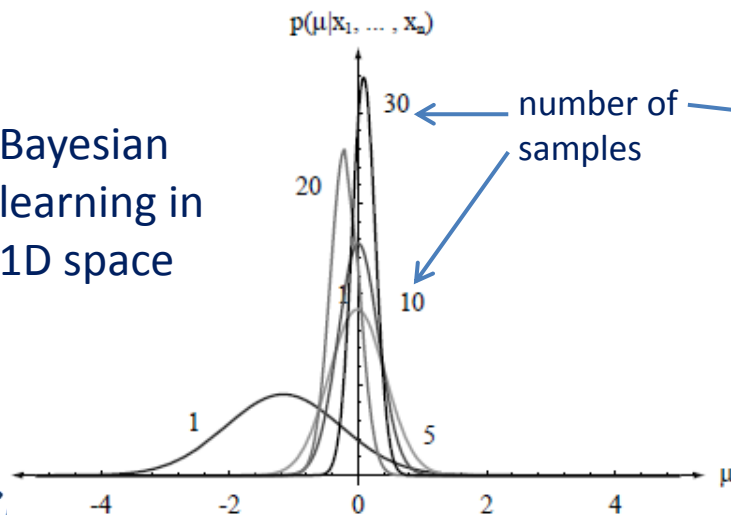
$$\frac{1}{\sigma_n^2} = \frac{n}{\sigma^2} + \frac{1}{\sigma_0^2} \quad \frac{\mu_n}{\sigma_n^2} = \frac{n}{\sigma^2} \hat{\mu}_n + \frac{\mu_0}{\sigma_0^2} \quad \leftarrow \hat{\mu}_n = \frac{1}{n} \sum_{k=1}^n x_k$$

$$\mu_n = \left(\frac{n\sigma_0^2}{n\sigma_0^2 + \sigma^2} \right) \hat{\mu}_n + \frac{\sigma^2}{n\sigma_0^2 + \sigma^2} \mu_0$$

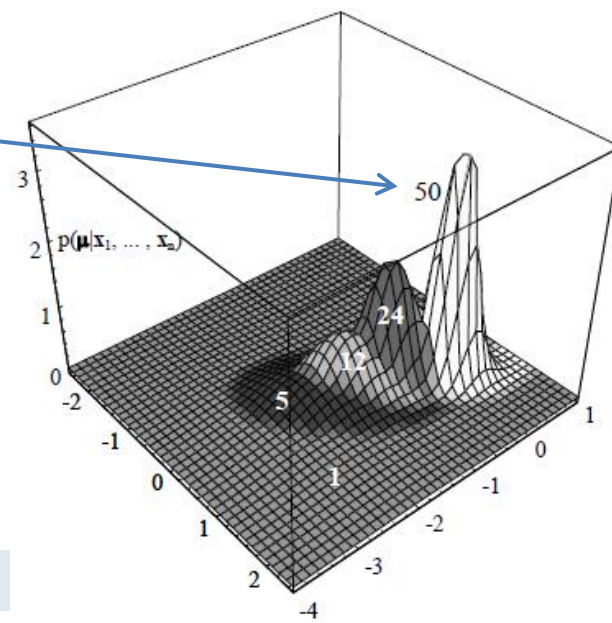
$$\sigma_n^2 = \frac{\sigma_0^2 \sigma^2}{n\sigma_0^2 + \sigma^2}$$

当 n 增大, μ_n 趋近 $\hat{\mu}_n$, σ_n^2 趋近 σ^2/n

Bayesian
learning in
1D space



Bayesian
learning in
2D space



- 1D case: class-conditional density

$$\begin{aligned}
 p(x|\mathcal{D}) &= \int p(x|\mu)p(\mu|\mathcal{D}) d\mu \\
 &= \int \frac{1}{\sqrt{2\pi}\sigma} \exp \left[-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2 \right] \frac{1}{\sqrt{2\pi}\sigma_n} \exp \left[-\frac{1}{2} \left(\frac{\mu-\mu_n}{\sigma_n} \right)^2 \right] d\mu \\
 &= \frac{1}{2\pi\sigma\sigma_n} \exp \left[-\frac{1}{2} \frac{(x-\mu_n)^2}{\sigma^2 + \sigma_n^2} \right] f(\sigma, \sigma_n),
 \end{aligned}$$

where
$$f(\sigma, \sigma_n) = \int \exp \left[-\frac{1}{2} \frac{\sigma^2 + \sigma_n^2}{\sigma^2 \sigma_n^2} \left(\mu - \frac{\sigma_n^2 x + \sigma^2 \mu_n}{\sigma^2 + \sigma_n^2} \right)^2 \right] d\mu$$

- Bayesian estimation

$$p(x|\mathcal{D}) \sim N(\mu_n, \sigma^2 + \sigma_n^2)$$

- C.f. ML estimation

$$p(x|D) = N(\hat{\mu}_n, \sigma^2)$$

$$\begin{aligned}
 \mu_n &= \left(\frac{n\sigma_0^2}{n\sigma_0^2 + \sigma^2} \right) \hat{\mu}_n + \frac{\sigma^2}{n\sigma_0^2 + \sigma^2} \mu_0 \\
 \sigma_n^2 &= \frac{\sigma_0^2 \sigma^2}{n\sigma_0^2 + \sigma^2}
 \end{aligned}$$

- Multivariate case, with Σ known

$$p(\mathbf{x}|\mu) \sim N(\mu, \Sigma) \quad \text{and} \quad p(\mu) \sim N(\mu_0, \Sigma_0) \quad \text{注意：不同空间！}$$

- Parameter posterior distribution

$$\begin{aligned} p(\mu|\mathcal{D}) &= \alpha \prod_{k=1}^n p(\mathbf{x}_k|\mu)p(\mu) \\ &= \alpha' \exp \left[-\frac{1}{2} \left(\mu^t (n\Sigma^{-1} + \Sigma_0^{-1})\mu - 2\mu^t \left(\Sigma^{-1} \sum_{k=1}^n \mathbf{x}_k + \Sigma_0^{-1} \mu_0 \right) \right) \right] \\ &= \alpha'' \exp \left[-\frac{1}{2} (\mu - \mu_n)^t \Sigma_n^{-1} (\mu - \mu_n) \right] \sim N(\mu_n, \Sigma_n) \end{aligned}$$

$$\Sigma_n^{-1} = n\Sigma^{-1} + \Sigma_0^{-1} \quad \Sigma_n^{-1} \mu_n = n\Sigma^{-1} \hat{\mu}_n + \Sigma_0^{-1} \mu_0 \quad \hat{\mu}_n = \frac{1}{n} \sum_{k=1}^n \mathbf{x}_k$$

$$\mu_n = \Sigma_0 \left(\Sigma_0 + \frac{1}{n} \Sigma \right)^{-1} \hat{\mu}_n + \frac{1}{n} \Sigma \left(\Sigma_0 + \frac{1}{n} \Sigma \right)^{-1} \mu_0$$

$$\Sigma_n = \Sigma_0 \left(\Sigma_0 + \frac{1}{n} \Sigma \right)^{-1} \frac{1}{n} \Sigma$$

- Data (feature) posterior distribution

$$p(\mathbf{x}|\mathcal{D}) = \int p(\mathbf{x}|\mu)p(\mu|\mathcal{D}) d\mu \sim N(\mu_n, \Sigma + \Sigma_n)$$

贝叶斯估计：一般情况

- 基本条件

- Known density function $p(\mathbf{x}|\boldsymbol{\theta})$ with unknown parameters
- Prior parameter distribution $p(\boldsymbol{\theta})$
- Dataset D of n samples independently drawn according to $p(\mathbf{x})$

- Steps

- Posterior parameter distribution

$$p(\boldsymbol{\theta}|D) = \frac{p(D|\boldsymbol{\theta})p(\boldsymbol{\theta})}{\int p(D|\boldsymbol{\theta})p(\boldsymbol{\theta}) d\boldsymbol{\theta}} \quad p(D|\boldsymbol{\theta}) = \prod_{k=1}^n p(\mathbf{x}_k|\boldsymbol{\theta})$$

- Posterior data distribution

$$p(\mathbf{x}|D) = \int p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta}|D) d\boldsymbol{\theta}$$

- Model usage: parameter sampling or MAP

If $p(\boldsymbol{\theta}|D)$ peaks at $\boldsymbol{\theta} = \hat{\boldsymbol{\theta}}$, $p(\mathbf{x}|D)$ will be approximately $p(\mathbf{x}|\hat{\boldsymbol{\theta}})$



- Recursive Bayes Learning

- Incremental data $\mathcal{D}^n = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$

$$p(\mathcal{D}^n|\theta) = p(\mathbf{x}_n|\theta)p(\mathcal{D}^{n-1}|\theta)$$

- Recursive update of posterior parameter density

$$p(\theta|\mathcal{D}) = \frac{p(\mathcal{D}|\theta)p(\theta)}{\int p(\mathcal{D}|\theta)p(\theta) d\theta} \longrightarrow p(\theta|\mathcal{D}^n) = \frac{p(\mathbf{x}_n|\theta)p(\theta|\mathcal{D}^{n-1})}{\int p(\mathbf{x}_n|\theta)p(\theta|\mathcal{D}^{n-1}) d\theta}$$

- Need to retain all samples $1 \dots n-1$?

- Sufficient statistics: contain all needed information for parameter.

e.g., in Gaussian case

$$\frac{1}{n} \sum_{k=1}^n \mathbf{x}_k$$
$$\frac{1}{n} \sum_{k=1}^n \mathbf{x}_k \mathbf{x}_k^t$$

- Recursive Bayes: An example

- Parametric density: uniform distribution

$$p(x|\theta) \sim U(0, \theta) = \begin{cases} 1/\theta & 0 \leq x \leq \theta \\ 0 & \text{otherwise} \end{cases}$$

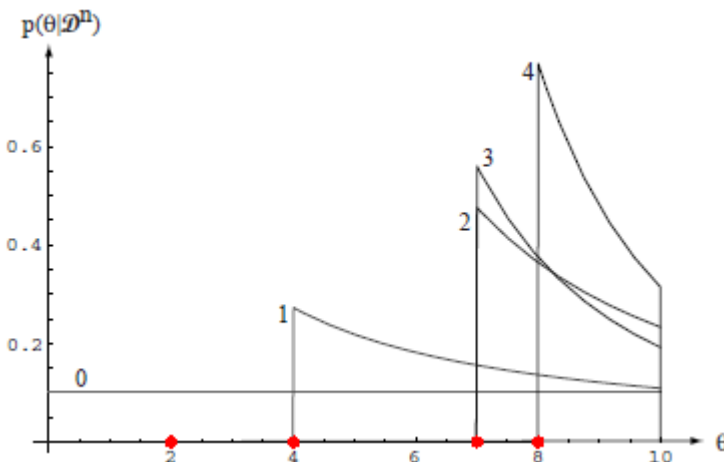
- Parameter prior $p(\theta|D^0) = p(\theta) = U(0, 10)$

- Data samples $D = \{4, 7, 2, 8\}$

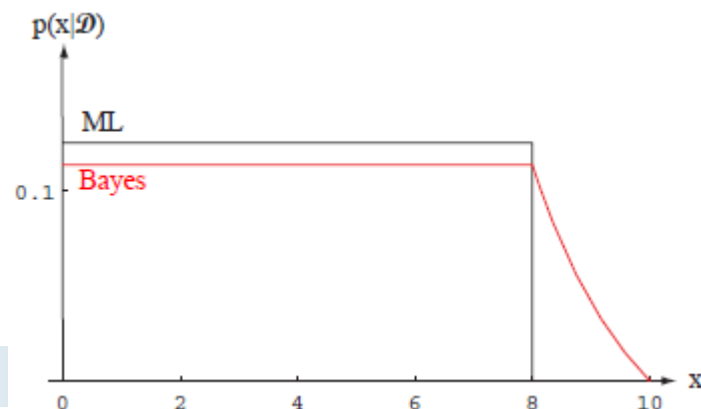
- Recursive

$$p(\theta|D^1) \propto p(x|\theta)p(\theta|D^0) = \begin{cases} 1/\theta & \text{for } 4 \leq \theta \leq 10 \\ 0 & \text{otherwise,} \end{cases} \quad \theta \geq x!$$

$$p(\theta|D^2) \propto p(x|\theta)p(\theta|D^1) = \begin{cases} 1/\theta^2 & \text{for } 7 \leq \theta \leq 10 \\ 0 & \text{otherwise,} \end{cases} \quad \begin{matrix} n=3? \\ n=4? \end{matrix}$$



ML estimation: $p(x|D) \sim U(0, 8)$ Why?



讨论

- Maximum-likelihood versus Bayesian estimation (BL)
 - When n approaches infinite, ML and BL are equivalent
 - ML: computationally simple
 - BL: incorporating prior (sometime very informative), theoretically incremental, gives uncertainty of parameters

下次课内容

- 第3章
 - 特征维数问题
 - 期望最大法
 - 隐马尔可夫模型