Chapter 3

Maximum-Likelihood and Bayesian Parameter Estimation

Bayes Theorem for Classification

$$P(\omega_j|\mathbf{x}) = \frac{p(\mathbf{x}|\omega_j) \cdot P(\omega_j)}{p(\mathbf{x})} \quad (1 \leq j \leq c) \quad \text{(Bayes Formula)}$$

To compute posterior probability $P(\omega_j|\mathbf{x})$, we need to know:

Prior probability: $P(\omega_j)$ Likelihood: $p(\mathbf{x}|\omega_j)$

The collection of training examples is composed of *c* data sets

$\mathcal{D}_j \ (1 \leq j \leq c)$

- Each example in $\mathcal{D}_j$ is drawn according to the class-conditional pdf, i.e. $p(\mathbf{x}|\omega_j)$
- Examples in $\mathcal{D}_j$ are *i.i.d.* random variables, i.e. **independent and identically distributed (独立同分布)**

Bayes Theorem for Classification (Cont.)

For prior probability: → **no difficulty**

$$P(\omega_j) = \frac{|\mathcal{D}_j|}{\sum_{i=1}^{c} |\mathcal{D}_i|}$$

(Here, $|\cdot|$ returns the **cardinality**, i.e. number of elements, of a set)

For class-conditional pdf:

Ch. 3 ← ☐ **Case I:** $p(\mathbf{x}|\omega_j)$ has certain **parametric form**

$p(\mathbf{x}|\omega_j)$

e.g.: $p(\mathbf{x}|\omega_j) \sim N(\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)$ **(parameters:** $\boldsymbol{\theta}_j = \{\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j\}$**)**

$\mathbf{x} \in \mathbf{R}^d$ → $\boldsymbol{\theta}_j$ contains "$d + d(d+1)/2$" *free* parameters

To show the dependence of $p(\mathbf{x}|\omega_j)$ on $\boldsymbol{\theta}_j$ **explicitly:**

$p(\mathbf{x}|\omega_j) \rightarrow p(\mathbf{x}|\omega_j, \boldsymbol{\theta}_j)$

Ch. 4 ← ☐ **Case II:** $p(\mathbf{x}|\omega_j)$ doesn't have **parametric form**

Estimation Under Parametric Form

Parametric class-conditional pdf: $p(\mathbf{x}|\omega_j, \boldsymbol{\theta}_j)\ (1 \leq j \leq c)$

- **Assumption I: Maximum-Likelihood (ML) estimation (极大似然估计)**

View parameters as quantities whose values are **fixed but unknown** → Estimate parameter values by **maximizing the likelihood** (probability) of observing the actual training examples

- **Assumption II: Bayesian estimation (贝叶斯估计)**

View parameters as **random variables** having some known prior distribution → Observation of the actual training examples transforms parameters' **prior distribution into posterior distribution** (via Bayes theorem)

Maximum-Likelihood Estimation

Settings

Likelihood function for each category is governed by some **fixed but unknown** parameters, i.e. $p(\mathbf{x}|\omega_j, \boldsymbol{\theta}_j)\ (1 \leq j \leq c)$

Task: Estimate $\{\boldsymbol{\theta}_j\}_{j=1}^c$ from $\{\mathcal{D}_j\}_{j=1}^c$

A simplified treatment

Examples in $\mathcal{D}_j$ gives no information about $\boldsymbol{\theta}_i$ if $i \neq j$

$\Downarrow$

Work with each category **separately** and therefore simplify the notations by dropping subscripts w.r.t. categories

without loss of generality: $\mathcal{D}_j \Rightarrow \mathcal{D}$; $\boldsymbol{\theta}_j \Rightarrow \boldsymbol{\theta}$

Maximum-Likelihood Estimation (Cont.)

$\mathbf{x}_k \sim p(\mathbf{x}|\boldsymbol{\theta})$

$(k = 1, \ldots, n)$

$\boldsymbol{\theta}$: Parameters to be estimated

$\mathcal{D}$: A set of *i.i.d.* examples $\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\}$

The objective function

$$p(\mathcal{D}|\boldsymbol{\theta}) = \prod_{k=1}^{n} p(\boldsymbol{x}_k|\boldsymbol{\theta})$$

→ **The likelihood of θ w.r.t. the set of observed examples**

The maximum-likelihood estimation

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

→ **Intuitively, $\hat{\theta}$ best agrees with the actually observed examples**

Maximum-Likelihood Estimation (Cont.)

Gradient Operator (梯度算子)

- ✓ Let $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_p)^t \in \mathbf{R}^p$ be a *p*-dimensional vector
- ✓ Let $f : \mathbf{R}^p \rightarrow \mathbf{R}$ be *p*-variate real-valued function over $\boldsymbol{\theta}$

$$\boldsymbol{\nabla}_{\boldsymbol{\theta}} \equiv \begin{bmatrix} \frac{\partial}{\partial \theta_1} \\ \vdots \\ \frac{\partial}{\partial \theta_p} \end{bmatrix}$$

$$f(\boldsymbol{\theta}) = \theta_1^2 + 3\theta_1\theta_2$$

$$\boldsymbol{\nabla}_{\boldsymbol{\theta}} f = \begin{bmatrix} \frac{\partial f}{\partial \theta_1} \\ \frac{\partial f}{\partial \theta_2} \end{bmatrix} = \begin{bmatrix} 2\theta_1 + 3\theta_2 \\ 3\theta_1 \end{bmatrix}$$

$l(\boldsymbol{\theta}) = \ln p(\mathcal{D}|\boldsymbol{\theta})$ is named as the **log-likelihood function**

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

Maximum-Likelihood Estimation (Cont.)

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

$$\underline{\underline{\boldsymbol{\nabla}_{\boldsymbol{\theta}}\, l}} = \boldsymbol{\nabla}_{\boldsymbol{\theta}} \left(\sum_{k=1}^{n} \ln\, p(\mathbf{x}_k|\boldsymbol{\theta}) \right) = \sum_{k=1}^{n} \boldsymbol{\nabla}_{\boldsymbol{\theta}} \underline{\underline{\ln\, p(\mathbf{x}_k|\boldsymbol{\theta})}}$$

p-dimensional vector with each component being a function over $\boldsymbol{\theta}$

p-variate real-valued function over $\boldsymbol{\theta}$ (not over $\mathbf{x}_k$)

Necessary conditions for ML estimate $\hat{\boldsymbol{\theta}}$

$$\boldsymbol{\nabla}_{\boldsymbol{\theta}}\, l \,|_{\boldsymbol{\theta}=\hat{\boldsymbol{\theta}}} = \mathbf{0}$$ **(a set of *p* equations)**

The Gaussian Case: Unknown $\boldsymbol{\mu}$

$\mathbf{x}_k \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$
$(k = 1, \ldots, n)$

suppose $\boldsymbol{\Sigma}$ is known $\Rightarrow$ $\boldsymbol{\theta} = \{\boldsymbol{\mu}\}$

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

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

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

$$\boldsymbol{\nabla}_{\boldsymbol{\mu}} \ln p(\mathbf{x}_k|\boldsymbol{\mu}) = \boldsymbol{\Sigma}^{-1}(\mathbf{x}_k - \boldsymbol{\mu})$$

The Gaussian Case: Unknown $\boldsymbol{\mu}$ (Cont.)

$$l(\boldsymbol{\mu}) = \sum_{k=1}^{n} \ln p(\mathbf{x}_k|\boldsymbol{\mu})$$

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

$$\nabla_{\boldsymbol{\mu}}\, l = \sum_{k=1}^{n} \boldsymbol{\Sigma}^{-1}(\mathbf{x}_k - \boldsymbol{\mu})$$

$\nabla_{\boldsymbol{\mu}} l = \mathbf{0}$ (necessary condition for ML estimate $\hat{\boldsymbol{\mu}}$)

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

Multiply $\boldsymbol{\Sigma}$ on both sides

$$\sum_{k=1}^{n} (\mathbf{x}_k - \hat{\boldsymbol{\mu}}) = \mathbf{0}$$

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

Intuitive result

ML estimate for the unknown $\boldsymbol{\mu}$ is just the arithmetic average of training samples – ***sample mean***

The Gaussian Case: Unknown $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$

$$\mathbf{x}_k \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \quad (k = 1, \ldots, n)$$

$\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ unknown $\Rightarrow$ $\boldsymbol{\theta} = \{\boldsymbol{\mu}, \boldsymbol{\Sigma}\}$

Consider *univariate* case

$$p(x_k|\boldsymbol{\theta}) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right] \qquad \left(\boldsymbol{\theta} = \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix} = \begin{bmatrix} \mu \\ \sigma^2 \end{bmatrix}\right)$$

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

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

The Gaussian Case: Unknown $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ (Cont.)

$$l(\boldsymbol{\theta}) = \sum_{k=1}^{n} \ln p(x_k|\boldsymbol{\theta})$$

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

$$\nabla_{\boldsymbol{\theta}} l = \begin{bmatrix} \sum_{k=1}^{n} \frac{1}{\theta_2}(x_k - \theta_1) \\ \sum_{k=1}^{n} \left(-\frac{1}{2\theta_2} + \frac{(x_k-\theta_1)^2}{2\theta_2^2} \right) \end{bmatrix}$$

$\nabla_{\boldsymbol{\theta}} l = 0$ (necessary condition for ML estimate $\hat{\theta}_1$ and $\hat{\theta}_2$)

$$\sum_{k=1}^{n} \frac{1}{\hat{\theta}_2}(x_k - \hat{\theta}_1) = 0$$

$$-\sum_{k=1}^{n} \frac{1}{\hat{\theta}_2} + \sum_{k=1}^{n} \frac{(x_k - \hat{\theta}_1)^2}{\hat{\theta}_2^2} = 0$$

The Gaussian Case: Unknown $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ (Cont.)

$$\sum_{k=1}^{n} \frac{1}{\hat{\theta}_2}(x_k - \hat{\theta}_1) = 0 \quad \Rightarrow \quad \sum_{k=1}^{n}(x_k - \hat{\theta}_1) = 0 \quad \Rightarrow \quad \hat{\theta}_1 = \frac{1}{n}\sum_{k=1}^{n} x_k$$

$$-\sum_{k=1}^{n} \frac{1}{\hat{\theta}_2} + \sum_{k=1}^{n} \frac{(x_k - \hat{\theta}_1)^2}{\hat{\theta}_2^2} = 0 \quad \Rightarrow \quad \hat{\theta}_2 = \frac{1}{n}\sum_{k=1}^{n}(x_k - \hat{\theta}_1)^2$$

ML estimate in *univariate* case

$$\hat{\mu} = \frac{1}{n}\sum_{k=1}^{n} x_k \qquad \hat{\sigma}^2 = \frac{1}{n}\sum_{k=1}^{n}(x_k - \hat{\mu})^2$$

The Gaussian Case: Unknown $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ (Cont.)

Intuitive result as well !

ML estimate in *multivariate* case

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

Arithmetic average of *n* vectors $\mathbf{x}_k$

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

Arithmetic average of *n* matrices $(\mathbf{x}_k - \hat{\boldsymbol{\mu}})(\mathbf{x}_k - \hat{\boldsymbol{\mu}})^t$

Bayesian Estimation

Settings

- The **parametric form** of the likelihood function for each category is known $p(\mathbf{x}|\omega_j, \boldsymbol{\theta}_j)\ (1 \leq j \leq c)$
- However, $\boldsymbol{\theta}_j$ is considered to be **random variables** instead of being fixed (but unknown) values

In this case, we can no longer make a single ML estimate $\hat{\boldsymbol{\theta}}_j$ and then infer $P(\omega_j|\mathbf{x})$ based on $P(\omega_j)$ and $p(\mathbf{x}|\omega_j, \hat{\boldsymbol{\theta}}_j)$

How can we proceed under this situation

Fully exploit training examples!

$$P(\omega_j|\mathbf{x}) \Rightarrow P(\omega_j|\mathbf{x}, \mathcal{D}^*)$$

$$(\mathcal{D}^* = \mathcal{D}_1 \cup \mathcal{D}_2 \cup \cdots \cup \mathcal{D}_c)$$

Bayesian Estimation (Cont.)

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

$$p(\omega_j,\mathbf{x},\mathcal{D}^*) = p(\mathcal{D}^*)\cdot p(\omega_j,\mathbf{x}|\mathcal{D}^*) = p(\mathcal{D}^*)\cdot P(\omega_j|\mathcal{D}^*)\cdot p(\mathbf{x}|\omega_j,\mathcal{D}^*)$$

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

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

Eq.22 [pp.91]

Two assumptions

$P(\omega_j|\mathcal{D}^*) = P(\omega_j)$

$p(\mathbf{x}|\omega_j,\mathcal{D}^*) = p(\mathbf{x}|\omega_j,\mathcal{D}_j)$

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

Eq.23 [pp.91]

Bayesian Estimation (Cont.)

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

Key problem

Determine $p(\mathbf{x}|\omega_j,\mathcal{D}_j)$

Treat each class independently → Simplify the *class-conditional pdf* notation $p(\mathbf{x}|\omega_j,\mathcal{D}_j)$ as $p(\mathbf{x}|\mathcal{D})$

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

($\boldsymbol{\theta}$: random variables w.r.t. parametric form)

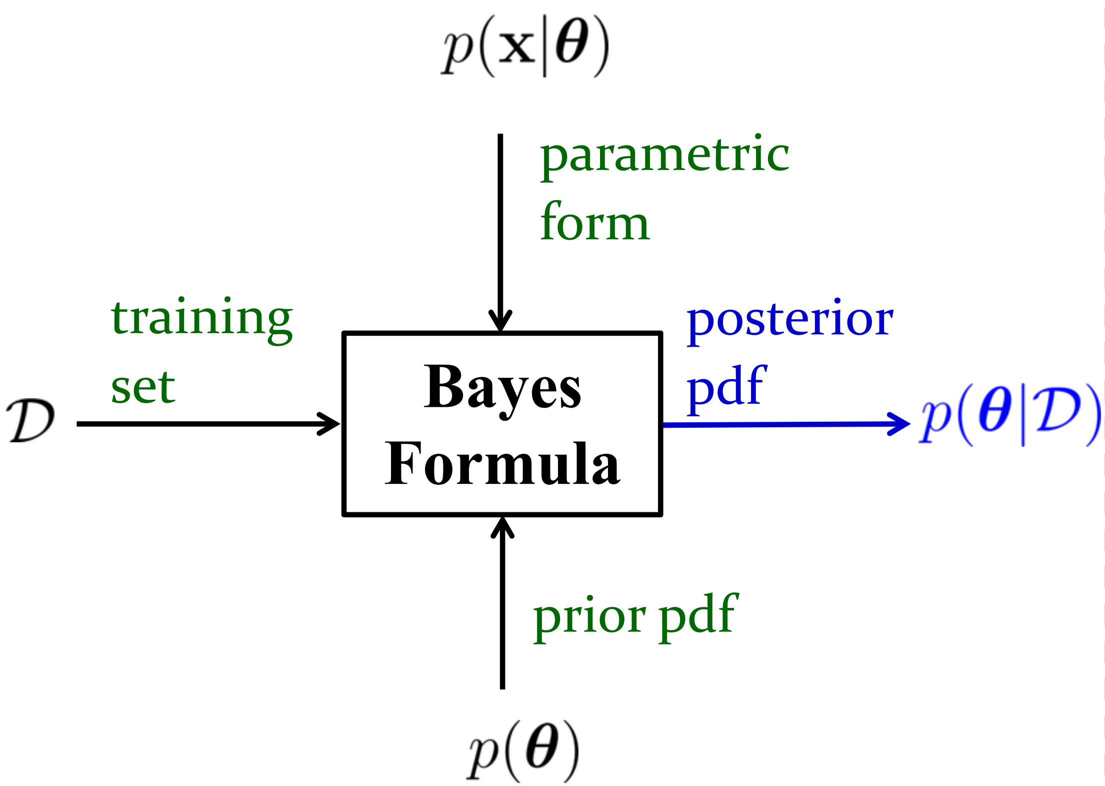
$$= \int p(\mathbf{x}|\boldsymbol{\theta},\mathcal{D})\,p(\boldsymbol{\theta}|\mathcal{D})\,d\boldsymbol{\theta}$$

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

($\mathbf{x}$ is independent of $\mathcal{D}$ given $\boldsymbol{\theta}$)

Bayesian Estimation: The General Procedure

Phase I: *prior pdf* ➔ *posterior pdf* (for $\boldsymbol{\theta}$)



$$p(\boldsymbol{\theta}|\mathcal{D}) = \frac{p(\boldsymbol{\theta}, \mathcal{D})}{p(\mathcal{D})}$$

$$= \frac{p(\boldsymbol{\theta})p(\mathcal{D}|\boldsymbol{\theta})}{\int p(\boldsymbol{\theta}, \mathcal{D})d\boldsymbol{\theta}}$$

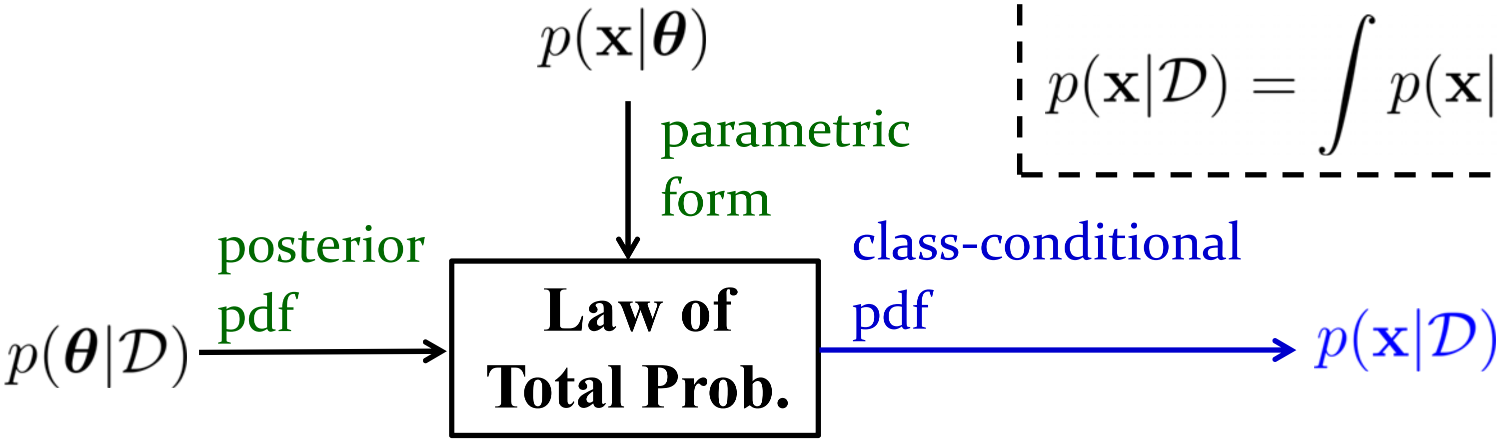
$$= \frac{p(\boldsymbol{\theta})p(\mathcal{D}|\boldsymbol{\theta})}{\int p(\boldsymbol{\theta})p(\mathcal{D}|\boldsymbol{\theta})d\boldsymbol{\theta}}$$

$$p(\mathcal{D}|\boldsymbol{\theta}) = \prod_{i=1}^{n} p(\mathbf{x}_k|\boldsymbol{\theta})$$

Bayesian Estimation: The General Procedure

Phase II: *posterior pdf* (for $\boldsymbol{\theta}$) ➔ *class-conditional pdf* (for $\mathbf{x}$)

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



Phase III: $$P(\omega_j|\mathbf{x},\mathcal{D}^*) = \frac{P(\omega_j)\cdot p(\mathbf{x}|\omega_j,\mathcal{D}_j)}{\sum_{i=1}^{c} P(\omega_i)\cdot p(\mathbf{x}|\omega_i,\mathcal{D}_i)}$$

The Gaussian Case: Unknown $\boldsymbol{\mu}$

Consider *univariate* case: $\boldsymbol{\theta} = \{\mu\}$ (σ^2 is known)

Phase I: *prior pdf* ➔ *posterior pdf* (for $\boldsymbol{\theta}$)

$$\underline{\underline{p(\mu)}} + \underline{\underline{p(x|\mu)}} + \mathcal{D} \Longrightarrow p(\mu|\mathcal{D})$$

$$p(x|\mu) \sim N(\mu, \sigma^2)$$

Gaussian parametric form

$$p(\mu) \sim N(\mu_0, \sigma_0^2)$$

- Prior pdf still takes Gaussian form
- Other form of prior pdf could be assumed as well

How would $p(\mu|\mathcal{D})$ look like in this case?

The Gaussian Case: Unknown $\boldsymbol{\mu}$ (Cont.)

$$p(\mu|\mathcal{D}) = \frac{p(\mu,\mathcal{D})}{p(\mathcal{D})} = \frac{p(\mu)p(\mathcal{D}|\mu)}{\int p(\mu)p(\mathcal{D}|\mu)\,d\mu}$$

$$= \alpha\, p(\mu)\, p(\mathcal{D}|\mu)$$

($\int p(\mu)p(\mathcal{D}|\mu)\,d\mu$ is a constant not related to μ)

$$= \alpha\, p(\mu) \prod_{k=1}^{n} p(x_k|\mu)$$

(examples in $\mathcal{D}$ are *i.i.d.*)

$$p(\mu) \sim N(\mu_0, \sigma_0^2)$$

$$p(\mu) = \frac{1}{\sqrt{2\pi}\sigma_0} \exp\left[-\frac{1}{2}\left(\frac{\mu-\mu_0}{\sigma_0}\right)^2\right]$$

$$p(x|\mu) \sim N(\mu, \sigma^2)$$

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

The Gaussian Case: Unknown $\boldsymbol{\mu}$ (Cont.)

$$p(\mu|\mathcal{D}) = \alpha\, p(\mu) \prod_{k=1}^{n} p(x_k|\mu)$$

$p(\mu|\mathcal{D})$ is an exponential function of a quadratic function of μ ⇒ $p(\mu|\mathcal{D})$ is a normal pdf as well

$$= \alpha \cdot \frac{1}{\sqrt{2\pi}\sigma_0} \exp\left[-\frac{1}{2}\left(\frac{\mu-\mu_0}{\sigma_0}\right)^2\right] \cdot \prod_{k=1}^{n} \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{1}{2}\left(\frac{x_k-\mu}{\sigma}\right)^2\right]$$

$$= \alpha' \cdot \exp\left[-\frac{1}{2}\left(\left(\frac{\mu-\mu_0}{\sigma_0}\right)^2 + \sum_{k=1}^{n}\left(\frac{\mu-x_k}{\sigma}\right)^2\right)\right]$$

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

$$= \alpha'' \cdot \exp\left[-\frac{1}{2}\left[\left(\frac{n}{\sigma^2}+\frac{1}{\sigma_0^2}\right)\mu^2 - 2\left(\frac{1}{\sigma^2}\sum_{k=1}^{n} x_k + \frac{\mu_0}{\sigma_0^2}\right)\mu\right]\right]$$

The Gaussian Case: Unknown $\boldsymbol{\mu}$ (Cont.)

$$p(\mu|\mathcal{D}) = \alpha'' \cdot \exp\left[-\frac{1}{2}\left[\boxed{\left(\frac{n}{\sigma^2}+\frac{1}{\sigma_0^2}\right)}\mu^2 - 2\boxed{\left(\frac{1}{\sigma^2}\sum_{k=1}^{n} x_k + \frac{\mu_0}{\sigma_0^2}\right)}\mu\right]\right]$$

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

Equating the coefficients in both form:

$$\frac{1}{\sigma_n^2} = \frac{n}{\sigma^2} + \frac{1}{\sigma_0^2}$$

$$\frac{\mu_n}{\sigma_n^2} = \frac{1}{\sigma^2}\sum_{k=1}^{n} x_k + \frac{\mu_0}{\sigma_0^2}$$

$\Rightarrow$

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

$$\mu_n = \frac{\sigma_n^2}{\sigma^2}\sum_{k=1}^{n} x_k + \frac{\sigma_n^2}{\sigma_0^2}\mu_0$$

The Gaussian Case: Unknown $\boldsymbol{\mu}$ (Cont.)

Phase II: *posterior pdf* (for $\boldsymbol{\theta}$) ➔ *class-conditional pdf* (for **x**)

$$\underline{\underline{p(\mu|\mathcal{D})}} + \underline{\underline{p(x|\mu)}} \Longrightarrow p(x|\mathcal{D})$$

$$p(x|\mu) \sim N(\mu, \sigma^2)$$

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

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

$$\mu_n = \frac{\sigma_n^2}{\sigma^2}\sum_{k=1}^{n} x_k + \frac{\sigma_n^2}{\sigma_0^2}\mu_0$$

How would $p(x|\mathcal{D})$ look like in this case?

The Gaussian Case: Unknown $\boldsymbol{\mu}$ (Cont.)

Then, phase III follows naturally for prediction

$$p(x|\mathcal{D}) = \int p(x|\mu)p(\mu|\mathcal{D})d\mu$$ **Eq.25** [pp.92]

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

$$= \beta\cdot\exp\left[-\frac{1}{2}\frac{(x-\mu_n)^2}{\sigma^2+\sigma_n^2}\right]$$ **Eq.36** [pp.95]

$p(x|\mathcal{D})$ is an exponential function of a quadratic function of x ⇒ $p(x|\mathcal{D})$ is a normal pdf as well

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

The Gaussian Case: Unknown $\boldsymbol{\mu}$ (Multivariate)

$\boldsymbol{\theta} = \{\boldsymbol{\mu}\}$ ($\boldsymbol{\Sigma}$ is known)

$$p(\mathbf{x}|\boldsymbol{\mu}) \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

$$p(\boldsymbol{\mu}) \sim N(\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0)$$

$$p(\boldsymbol{\mu}|\mathcal{D}) \sim N(\boldsymbol{\mu}_n, \boldsymbol{\Sigma}_n) \qquad p(\mathbf{x}|\mathcal{D}) \sim N(\boldsymbol{\mu}_n, \boldsymbol{\Sigma} + \boldsymbol{\Sigma}_n)$$

$$\boldsymbol{\mu}_n = \boldsymbol{\Sigma}_0 \left(\boldsymbol{\Sigma}_0 + \frac{1}{n}\boldsymbol{\Sigma}\right)^{-1} \frac{1}{n}\sum_{k=1}^{n}\mathbf{x}_k + \frac{1}{n}\boldsymbol{\Sigma}\left(\boldsymbol{\Sigma}_0 + \frac{1}{n}\boldsymbol{\Sigma}\right)^{-1}\boldsymbol{\mu}_0$$

$$\boldsymbol{\Sigma}_n = \boldsymbol{\Sigma}_0 \left(\boldsymbol{\Sigma}_0 + \frac{1}{n}\boldsymbol{\Sigma}\right)^{-1} \frac{1}{n}\boldsymbol{\Sigma}$$

Summary

- Key issue for PR
  - Estimate prior and class-conditional pdf from training set
  - Basic assumption on training examples: *i.i.d.*
- Two strategies to the key issue
  - Parametric form for class-conditional pdf
    - Maximum likelihood (ML) estimation
    - Bayesian estimation
  - No parametric form for class-conditional pdf

Summary (Cont.)

- Maximum likelihood estimation
  - Settings: parameters as fixed but unknown values
  - The objective function: Log-likelihood function
  - Necessary conditions for ML estimation: gradient for the objective function should be zero vector
  - The Gaussian case
    - Unknown $\boldsymbol{\mu}$
    - Unknown $\boldsymbol{\mu}$ and Σ

Summary (Cont.)

- Bayesian estimation
  - Settings: parameters as random variables
  - The general procedure
    - Phase I: *prior pdf* ➔ *posterior pdf* (for $\boldsymbol{\theta}$)
    - Phase II: *posterior pdf* (for $\boldsymbol{\theta}$) ➔ *class-conditional pdf* (for $\mathbf{x}$)
    - Phase III: *prediction* (Eq.22 [pp.91])
  - The Gaussian case
    - Unknown $\boldsymbol{\mu}$: univariate and multivariate