

# Chapter 3

## Maximum-Likelihood and Bayesian Parameter Estimation



# Exercise

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

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

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

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

$$\boldsymbol{\mu}_1 = \begin{bmatrix} 3 \\ 6 \end{bmatrix}; \quad \boldsymbol{\Sigma}_1 = \begin{pmatrix} 1/2 & 0 \\ 0 & 2 \end{pmatrix} \text{ and } \boldsymbol{\mu}_2 = \begin{bmatrix} 3 \\ -2 \end{bmatrix}; \quad \boldsymbol{\Sigma}_2 = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$$

Assumes equal prior probabilities,  
What is the decision boundary?



# 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


□ Each example in  $\mathcal{D}_j$  is drawn according to the class-conditional pdf, i.e.  $p(\mathbf{x}|\omega_j)$

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

□ 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**(勢), 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**

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

$p(\mathbf{x}|\omega_j)$   $\mathbf{x} \in \mathbf{R}^d$    $\boldsymbol{\theta}_j$  contains “ $d + d(d + 1)/2$ ” free parameters

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

$$p(\mathbf{x}|\omega_j) \xrightarrow{\text{yellow arrow}} p(\mathbf{x}|\omega_j, \boldsymbol{\theta}_j)$$

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)

# Bayesian vs Frequentist (Revisit)



- The Bayesian billiard game
  - ❑ Alice and Bob **can't** see the billiard table.
  - ❑ The judge rolls a ball down the table, and marks where it lands. Once this **mark** is in place, the judge rolls new balls.
  - ❑ If the ball lands to the left of the mark, Alice gets a point; if it lands to the right of the mark, Bob gets a point.
  - ❑ The first person to reach **6 points** wins the game.
  - ❑ Now say that Alice is leading with **5** points and Bob has **3** points.

**What can be said about the chances of Bob to win the game?**

# Bayesian vs Frequentist (Revisit)

## ■ The Frequentist Approach

- 5 balls out of 8 balls fell on Alice's side
- Maximum likelihood estimate of  $\theta$  that balls land on Alice's side:

- $L(\theta) = p(y|\theta) = \binom{n}{y} \theta^y (1 - \theta)^{n-y}$

- $\log L(\theta) = y \log \theta + (n - y) \log(1 - \theta) + C$

- $\hat{\theta} = \frac{y}{n} = 5/8$

- Assuming this maximum likelihood probability, we can compute the probability that Bob will win, which is given by:

- $P(\text{Bob Wins}) = (1 - 0.675)^3 = 0.052734375$

**Frequentist concludes that Bob got 5.2% chance of winning!**



# 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  $i \neq j$



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

[without loss of generality:  $\mathcal{D}_j \longrightarrow \mathcal{D}$  ;  $\boldsymbol{\theta}_j \longrightarrow \boldsymbol{\theta}$ ]



# Maximum-Likelihood Estimation (Cont.)

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

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

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

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

The objective function

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



The likelihood of  $\boldsymbol{\theta}$  w.r.t. the set of observed examples

The maximum-likelihood estimation

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

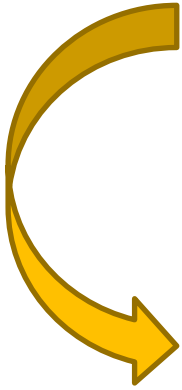


Intuitively,  $\hat{\boldsymbol{\theta}}$  best agrees with the actually observed examples

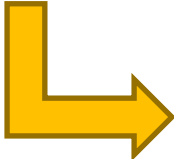
# Maximum-Likelihood Estimation (Cont.)

## Gradient Operator (梯度算子)

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


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

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

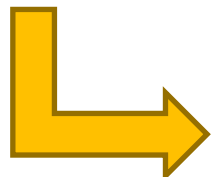

$$\nabla_{\boldsymbol{\theta}} f = \begin{bmatrix} \frac{\partial f}{\partial \theta_1} \\ \frac{\partial f}{\partial \theta_2} \end{bmatrix} = \begin{bmatrix} 2\theta_1 + 3\theta_2 \\ 3\theta_1 \end{bmatrix}$$

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

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

# Maximum-Likelihood Estimation (Cont.)

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


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

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

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

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

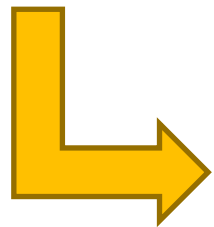
$$\nabla_{\boldsymbol{\theta}} l \big|_{\boldsymbol{\theta}=\hat{\boldsymbol{\theta}}} = \mathbf{0} \text{ (a set of } p \text{ equations)}$$

# The Gaussian Case: Unknown $\mu$

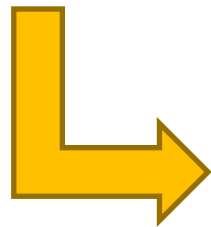
$$\mathbf{x}_k \sim N(\mu, \Sigma) \\ (k = 1, \dots, n)$$

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

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



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



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

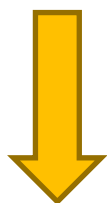
# The Gaussian Case: Unknown $\mu$

## (Cont.)

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

### Intuitive result

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


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

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

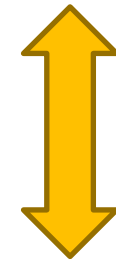

$$\nabla_{\mu} l = \mathbf{0} \text{ (necessary condition}$$

for ML estimate  $\hat{\mu}$ )

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

Multiply  $\Sigma$  on  
both sides

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

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


# The Gaussian Case: Unknown $\mu$ and $\Sigma$

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

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

Consider *univariate* case

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

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

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

# The Gaussian Case: Unknown $\mu$ and $\Sigma$ (Cont.)

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

$$\nabla_{\boldsymbol{\theta}} \ln p(x_k | \boldsymbol{\theta}) =$$

$$\begin{bmatrix} \frac{1}{\theta_2} (x_k - \theta_1) \\ -\frac{1}{2\theta_2} + \frac{(x_k - \theta_1)^2}{2\theta_2^2} \end{bmatrix}$$

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

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

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

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

# The Gaussian Case: Unknown $\mu$ and $\Sigma$ (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**

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



# The Gaussian Case: Unknown $\mu$ and $\Sigma$ (Cont.)

**ML estimate in *multivariate* case**

Intuitive  
result as well!

$$\hat{\mu} = \frac{1}{n} \sum_{k=1}^n \mathbf{x}_k \quad \longrightarrow \quad \text{Arithmetic average of } n \text{ vectors } \mathbf{x}_k$$

$$\hat{\Sigma} = \frac{1}{n} \sum_{k=1}^n (\mathbf{x}_k - \hat{\mu})(\mathbf{x}_k - \hat{\mu})^t \quad \longrightarrow \quad \begin{array}{l} \text{Arithmetic average} \\ \text{of } n \text{ matrices} \\ (\mathbf{x}_k - \hat{\mu})(\mathbf{x}_k - \hat{\mu})^t \end{array}$$

# Bayesian vs Frequentist (Revisit)

## ■ The Bayesian Approach

□ Prior distributions:  $\theta \sim \text{Uniform}(0,1)$

□  $\mathbb{E}(\text{Bob wins}) = \int_0^1 (1 - \theta)^3 P(\theta | A = 5, B = 3) d\theta$

□  $P(\theta | A = 5, B = 3) = \frac{P(\theta)P(A=5, B=3|\theta)}{\int_0^1 P(\theta)P(A=5, B=3|\theta) d\theta}$

□  $P(A = 5, B = 3 | \theta) = \binom{8}{5} \theta^5 (1 - \theta)^3, P(\theta) = 1$

□  $\mathbb{E}(\text{Bob wins}) = \frac{\int_0^1 (1 - \theta)^6 \theta^5 d\theta}{\int_0^1 (1 - \theta)^3 \theta^5 d\theta} = \frac{5!6!/12!}{5!3!/9!} = \frac{1}{11}$

□ Without knowing the Bayesian probability:

■  $\mathbb{E}(\text{Bob Wins}) = 0.091$

$$\int_0^1 p^{m-1} (1-p)^{n-1} dp = \frac{\Gamma(n)\Gamma(m)}{\Gamma(m+n)}$$

$$\Gamma(n+1) = n!$$

**Bayesian concludes that Bob got 9.1% chance of winning!**



# 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!

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

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

# Bayesian Estimation (Cont.)

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

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

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

**Two assumptions**

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

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

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

**Eq.22** [pp.91]

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

**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

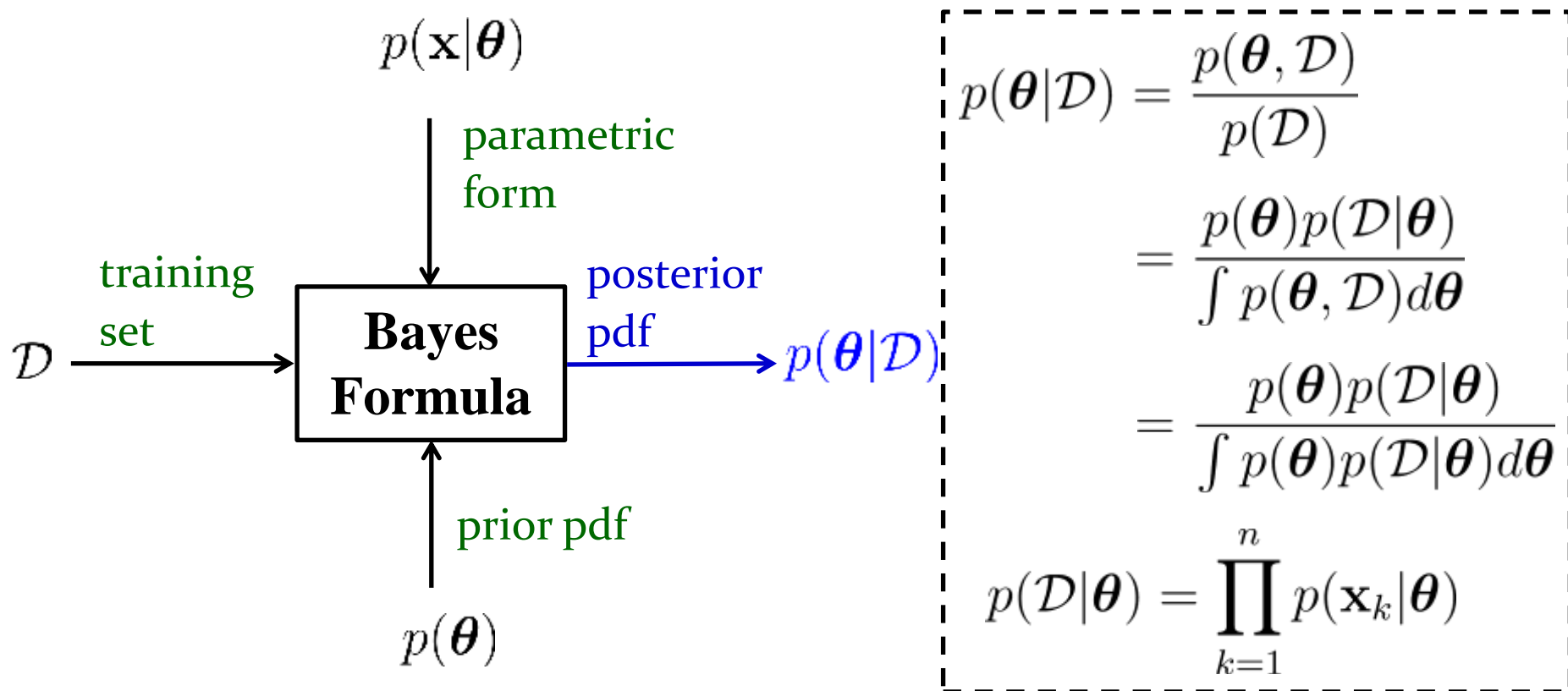


Simplify the *class-conditional pdf*  
notation  $p(\mathbf{x} | \omega_j, \mathcal{D}_j)$  as  $p(\mathbf{x} | \mathcal{D})$

$$\begin{aligned} p(\mathbf{x} | \mathcal{D}) &= \int p(\mathbf{x}, \boldsymbol{\theta} | \mathcal{D}) d\boldsymbol{\theta} \quad (\boldsymbol{\theta} : \text{random variables w.r.t. parametric form}) \\ &= \int p(\mathbf{x} | \boldsymbol{\theta}, \mathcal{D}) p(\boldsymbol{\theta} | \mathcal{D}) d\boldsymbol{\theta} \\ &= \int p(\mathbf{x} | \boldsymbol{\theta}) p(\boldsymbol{\theta} | \mathcal{D}) d\boldsymbol{\theta} \quad (\mathbf{x} \text{ is independent of } \mathcal{D} \text{ given } \boldsymbol{\theta}) \end{aligned}$$

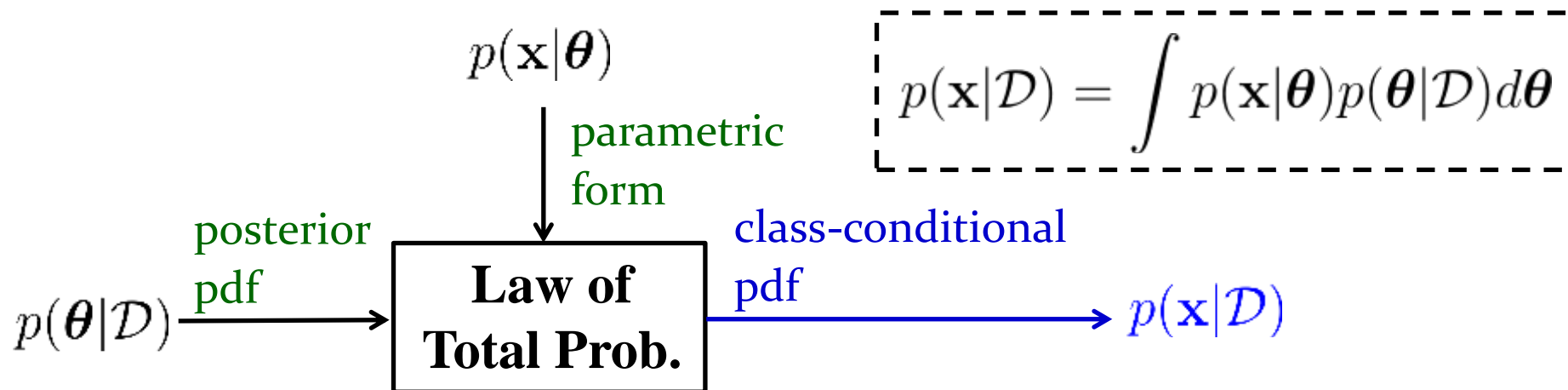
# Bayesian Estimation: The General Procedure

**Phase I:** *prior pdf*  $\Rightarrow$  *posterior pdf* (for  $\theta$ )



# Bayesian Estimation: The General Procedure

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



**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 $\mu$

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

**Phase I:** prior pdf  $\Rightarrow$  posterior pdf (for  $\theta$ )

$$\underline{\underline{p(\mu)}} + \underline{\underline{p(x|\mu)}} + \mathcal{D} \quad \xrightarrow{\text{yellow arrow}} \quad p(\mu|\mathcal{D})$$

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

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 $\mu$

## (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  $\mu$ )

$$= \alpha p(\mu) \prod_{k=1}^n p(x_k|\mu) \quad (\text{examples in } \mathcal{D} \text{ are } \textit{i.i.d.})$$

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

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

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

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



# The Gaussian Case: Unknown $\mu$

## (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  $\mu$



$p(\mu|\mathcal{D})$  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 $\mu$

## (Cont.)

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

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

Equating the  
coefficients in  
both form:

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

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



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

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

# The Gaussian Case: Unknown $\mu$

## (Cont.)

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

$$\underbrace{p(\mu|\mathcal{D})}_{\text{posterior pdf (for } \theta\text{)}} + \underbrace{p(x|\mu)}_{\text{class-conditional pdf (for } \mathbf{x}\text{)}} \xrightarrow{\text{yellow arrow}} p(x|\mathcal{D})$$

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

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

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


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

# The Gaussian Case: Unknown $\mu$

## (Cont.)

Then, phase III  
follows naturally  
for prediction

$$p(x|\mathcal{D}) = \int p(x|\mu)p(\mu|\mathcal{D})d\mu \quad \text{Eq.25 [pp.92]}$$
$$= \int \frac{1}{\sqrt{2\pi}\sigma} \exp \left[ -\frac{1}{2} \left( \frac{x - \mu}{\sigma} \right)^2 \right] \frac{1}{\sqrt{2\pi}\sigma_n} \exp \left[ -\frac{1}{2} \left( \frac{\mu - \mu_n}{\sigma_n} \right)^2 \right] d\mu$$
$$= \beta \cdot \exp \left[ -\frac{1}{2} \frac{(x - \mu_n)^2}{\sigma^2 + \sigma_n^2} \right] \quad \text{Eq.36 [pp.95]}$$

$p(x|\mathcal{D})$  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 $\mu$ (Multivariate)

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



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

$$p(\mu) \sim N(\mu_0, \Sigma_0)$$

$$p(\mu|\mathcal{D}) \sim N(\mu_n, \Sigma_n)$$

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

$$\mu_n = \Sigma_0 \left( \Sigma_0 + \frac{1}{n} \Sigma \right)^{-1} \frac{1}{n} \sum_{k=1}^n \mathbf{x}_k + \frac{1}{n} \Sigma \left( \Sigma_0 + \frac{1}{n} \Sigma \right)^{-1} \mu_0$$

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

# A Few Notes on Parametric Techniques

## ML estimation vs. Bayes estimation

- *Infinite examples*      ML estimation      =      Bayes estimation
- *Complexity*      ML estimation      <      Bayes estimation
- *Interpretability*      ML estimation      >      Bayes estimation
- *Prior knowledge*      ML estimation      <      Bayes estimation

## Source of classification error

Bayes error

+

Model error

+

Estimation error

# Related Topic I

## Hidden Markov Model





# Markov Model

- a **Markov model** is a **stochastic** model used to model **pseudo-randomly** changing systems.
- a **Markov chain** is a stochastic model describing a sequence of events in which the probability of each event depends only on the state of the previous event.



Andrey Andreyevich Markov  
1856-1922  
Russian Mathematics

Markov first worked as a mathematician at the St. Petersburg University. Later during 1908, he quitted being a lecturer became a teacher at a high school.

# Markov Model (Cont.)

## Notations

$\Omega = \{\omega_1, \omega_2, \dots, \omega_c\}$  : A set of  $c$  possible states

$\omega^T = \{\omega(1), \omega(2), \dots, \omega(T)\}$  : A state sequence of length  $T$ , where  $\omega(t) \in \Omega$   
( $1 \leq t \leq T$ )

e.g.:  $\omega^6 = \{\omega_1, \omega_4, \omega_2, \omega_2, \omega_1, \omega_4\}$

$\mathbf{A} = [a_{ij}]_{c \times c}$  : The *transition probability matrix*

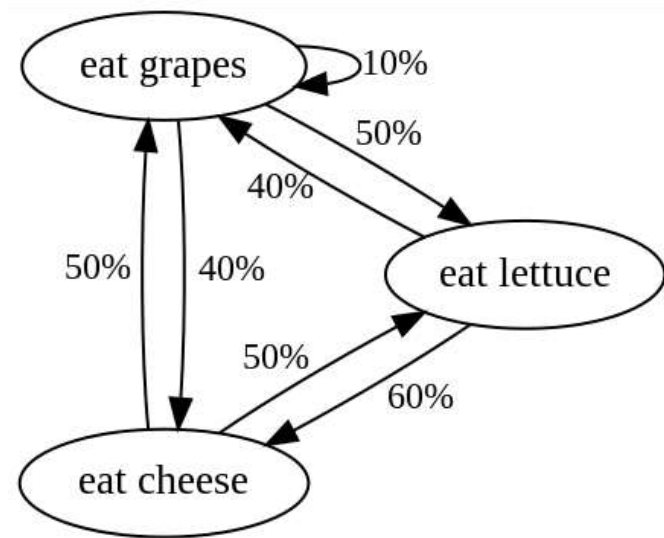
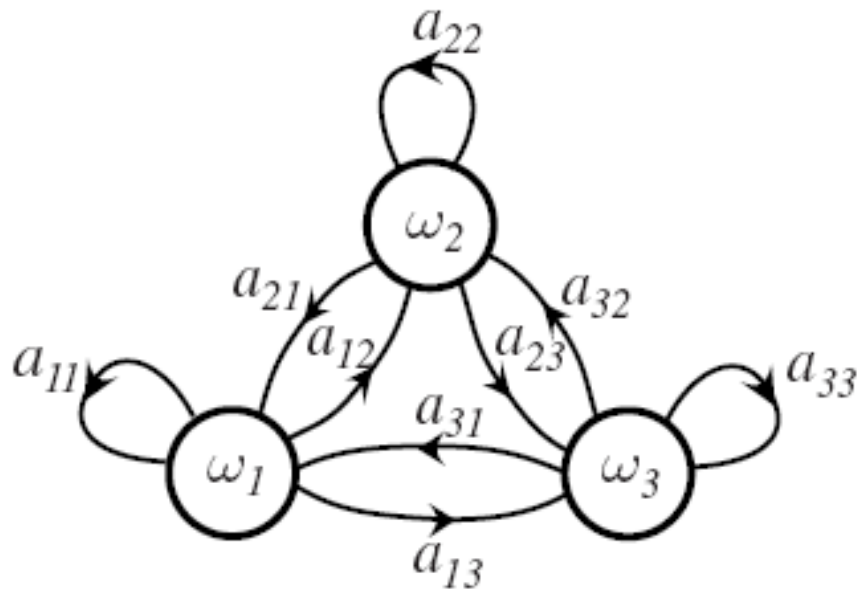
$$\begin{aligned} a_{ij} &= P(\omega(t+1) = \omega_j \mid \omega(t) = \omega_i) \\ &= P(\omega_j \mid \omega_i) \end{aligned}$$

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1c} \\ a_{21} & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ a_{c1} & \cdots & \cdots & a_{cc} \end{bmatrix}$$

(*time-independent*) probability of transferring  
from state  $\omega_i$  to state  $\omega_j$

$$\sum_{j=1}^c a_{ij} = 1, \text{ and in general } a_{ij} \neq a_{ji}$$

# Markov Model (Cont.)

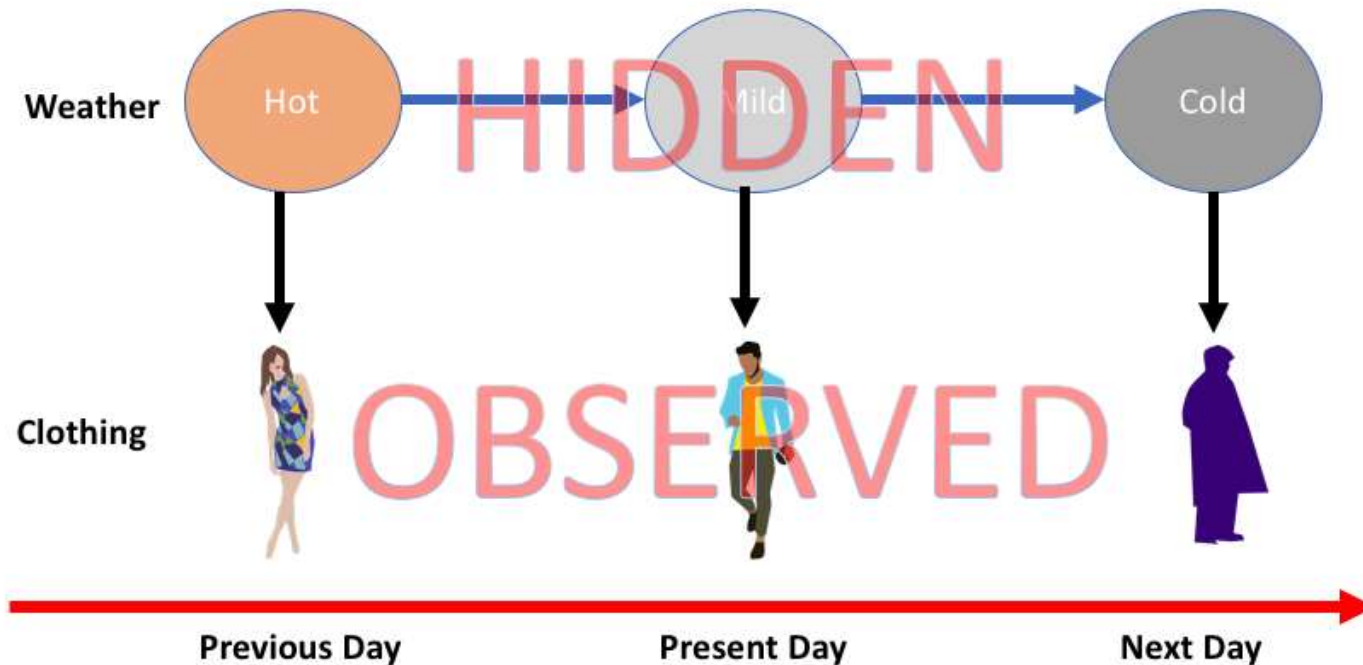


$$\omega^T = \{\omega(1), \omega(2), \dots, \omega(T)\} :$$

$$P(\omega^T) = \prod_{t=1}^T P(\omega(t) \mid \omega(1), \dots, \omega(t-1)) \quad (\text{chain rule})$$

$$= \prod_{t=1}^T P(\omega(t) \mid \omega(t-1)) \quad (\text{first-order assumption})$$

# Hidden Markov Model (HMM)



## Basic assumptions

- ❑ The state at each step is invisible
- ❑ The invisible state emits one visible symbol at each step

# Hidden Markov Model (HMM)

## Basic assumptions

- ❑ The state at each step is invisible
- ❑ The invisible state emits one visible symbol at each step

## A few more notations

$\mathcal{V} = \{v_1, v_2, \dots, v_K\}$  : A set of  $K$  possible symbols

$\mathbf{V}^T = \{v(1), v(2), \dots, v(T)\}$  : An observed symbol sequence of length  $T$ , where  $v(t) \in \mathcal{V}$  ( $1 \leq t \leq T$ )

$\mathbf{B} = [b_{jk}]_{c \times K}$  : The *observation symbol probability* matrix

$\begin{bmatrix} b_{11} & b_{12} & \cdots & b_{1K} \\ \cdots & \cdots & \cdots & \cdots \\ b_{c1} & \cdots & \cdots & b_{cK} \end{bmatrix}$	$b_{jk} = P(v_k \mid \omega_j), \quad \sum_{k=1}^K b_{jk} = 1$ <p><i>probability of emitting symbol <math>v_k</math> at state <math>\omega_j</math></i></p>
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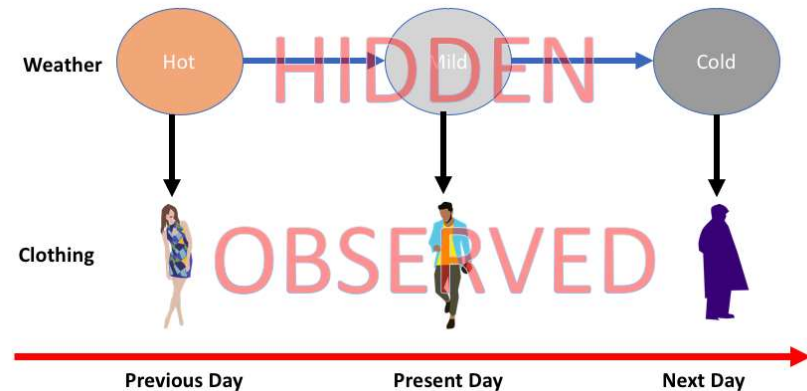
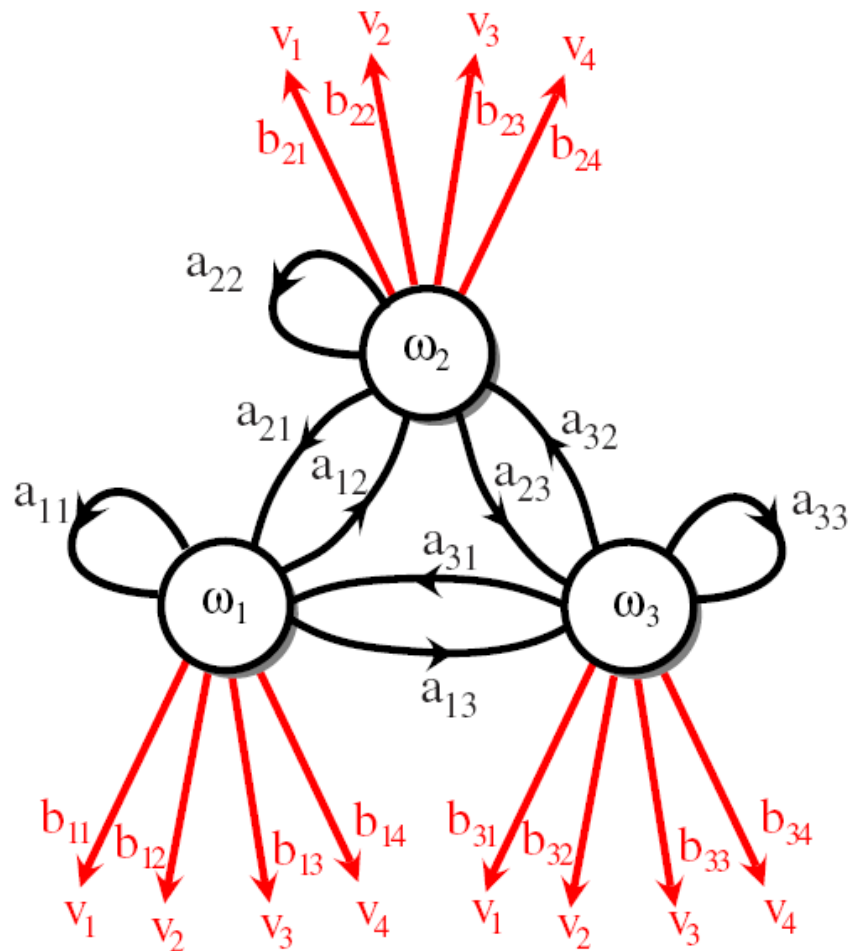
$\boldsymbol{\pi} = (\pi_1, \pi_2, \dots, \pi_c)$  : The *initial state probability*

$$\pi_j = P(\omega(1) = \omega_j)$$



# Hidden Markov Model (Cont.)

## State transition diagram



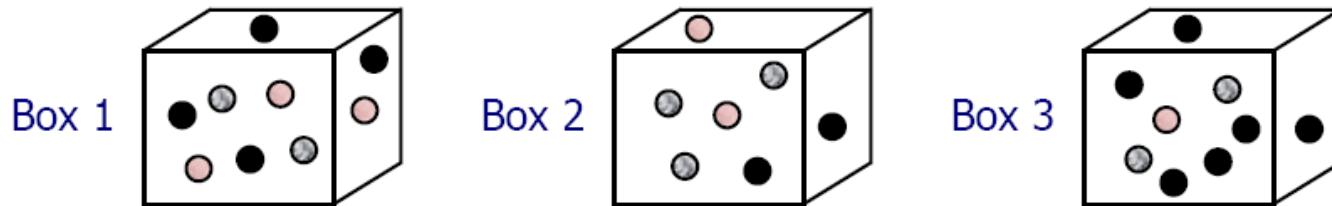
$$P(\mathbf{V}^T | \boldsymbol{\omega}^T) = \prod_{t=1}^T P(v(t) | \omega(t))$$

$$= \prod_{t=1}^T b_{\omega(t)v(t)}$$

*The probability of emitting one symbol at each step only depends on the state at that step*

# Hidden Markov Model (Cont.)

## An illustrative example



Hidden state: box

Visible symbol: ball

Observation symbol probability:  $P(\bullet | \text{box } i)$ ,  $P(\bullet\!\!\circ | \text{box } i)$ ,  $P(\circ | \text{box } i)$

Observed symbol sequence:  $\bullet \bullet \bullet\!\!\circ \circ \bullet \circ \circ \bullet \bullet\!\!\circ$



Given the observed symbol sequence, what are the central problems in HMM?

# Hidden Markov Model (Cont.)

## Three central problems in HMM

$\theta = \{A, B, \pi\}$  : the complete set of HMM parameters

$V^T$  : the observed symbol sequence

### Evaluation

Given  $\theta$ , determine the probability of generating  $V^T$

*to evaluate  $P(V^T | \theta)$*

### Learning

Given  $V^T$ , determine model parameters  $\theta$

*to identify  $\theta$  which maximizes  $P(V^T | \theta)$*

### Decoding

Given  $\theta$  and  $V^T$ , determine the most likely hidden state sequence

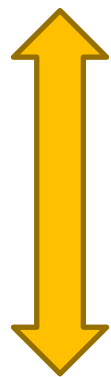
*to identify  $\omega^T$  which maximizes  $P(\omega^T | V^T, \theta)$*



# The Evaluation Problem for HMM

## A straightforward evaluation

$$P(\mathbf{V}^T | \boldsymbol{\theta}) = \sum_{\boldsymbol{\omega}^T} P(\mathbf{V}^T | \boldsymbol{\omega}^T, \boldsymbol{\theta}) P(\boldsymbol{\omega}^T | \boldsymbol{\theta})$$



$$P(\boldsymbol{\omega}^T | \boldsymbol{\theta}) = \prod_{t=1}^T a_{\omega(t-1)\omega(t)} \quad (\text{with abuse of notation: } a_{\omega(0)\omega(1)} = \pi_{\omega(1)})$$

$$P(\mathbf{V}^T | \boldsymbol{\omega}^T, \boldsymbol{\theta}) = \prod_{t=1}^T b_{\omega(t)v(t)}$$

$$P(\mathbf{V}^T | \boldsymbol{\theta}) = \sum_{\boldsymbol{\omega}^T} \prod_{t=1}^T a_{\omega(t-1)\omega(t)} b_{\omega(t)v(t)}$$


Computational complexity:  $\mathcal{O}(c^T \cdot T)!$

e.g.:  $c=10, T=20 \rightarrow \sim 10^{21}$  calculations

Infeasible!

# The Evaluation Problem for HMM (Cont.)

## HMM forward algorithm


$$P(\mathbf{V}^T \mid \boldsymbol{\theta}) = \sum_{j=1}^c \alpha_j(T)$$

Let  $\alpha_j(t) = P(v(1), v(2), \dots, v(t), \omega(t) = \omega_j \mid \boldsymbol{\theta})$

*the probability of being in hidden state  $\omega_j$  at step  $t$  and having generated the first  $t$  symbols of  $\mathbf{V}^T$*

Then,  $\alpha_j(t)$  ( $1 \leq j \leq c, 1 \leq t \leq T$ ) can be calculated recursively as:

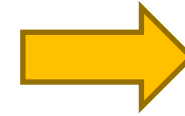
$$\begin{aligned}\alpha_j(1) &= P(v(1), \omega(1) = \omega_j \mid \boldsymbol{\theta}) = P(\omega(1) = \omega_j \mid \boldsymbol{\theta}) \cdot P(v(1) \mid \omega_j, \boldsymbol{\theta}) \\ &= \pi_j b_{jv(1)}\end{aligned}$$

$$\begin{aligned}\alpha_j(t) &= \sum_{i=1}^c P(v(1), \dots, v(t-1), \omega(t-1) = \omega_i, v(t), \omega(t) = \omega_j \mid \boldsymbol{\theta}) \\ &= \sum_{i=1}^c P(v(1), \dots, v(t-1), \omega(t-1) = \omega_i \mid \boldsymbol{\theta}) \cdot P(\omega_j \mid \omega_i, \boldsymbol{\theta}) \cdot P(v(t) \mid \omega_j, \boldsymbol{\theta}) \\ &= \left[ \sum_{i=1}^c \alpha_i(t-1) a_{ij} \right] b_{jv(t)}\end{aligned}$$

# The Evaluation Problem for HMM (Cont.)

$\theta = \{A, B, \pi\}$  : the complete set of HMM parameters

$V^T$  : the observed symbol sequence



*to evaluate*  
 $P(V^T | \theta)$

## Pseudo-code for HMM forward algorithm

1. **Initialize**  $t = 1$  and  $\alpha_j(t) = \pi_j b_{jv(t)}$  ( $1 \leq j \leq c$ )
2. **For**  $t = 2$  to  $T$
3.   **For**  $j = 1$  to  $c$
4.      $\alpha_j(t) = \left[ \sum_{i=1}^c \alpha_i(t-1) a_{ij} \right] b_{jv(t)}$
5.   **End**
6. **End**
7. **Return**  $P(V^T | \theta) = \sum_{j=1}^c \alpha_j(T)$

Computational  
complexity

$$\mathcal{O}(c^T \cdot T)$$



$$\mathcal{O}(c^2 \cdot T)$$

# The Evaluation Problem for HMM (Cont.)

$\theta = \{\mathbf{A}, \mathbf{B}, \pi\}$  : the complete set of HMM parameters

$\mathbf{V}^T$  : the observed symbol sequence



*to evaluate*  
 $P(\mathbf{V}^T | \theta)$

Let  $\alpha_j(t) = P(v(1), v(2), \dots, v(t), \omega(t) = \omega_j | \theta)$

*the probability of being in hidden state  $\omega_j$  at step  $t$  and having generated the first  $t$  symbols of  $\mathbf{V}^T$*

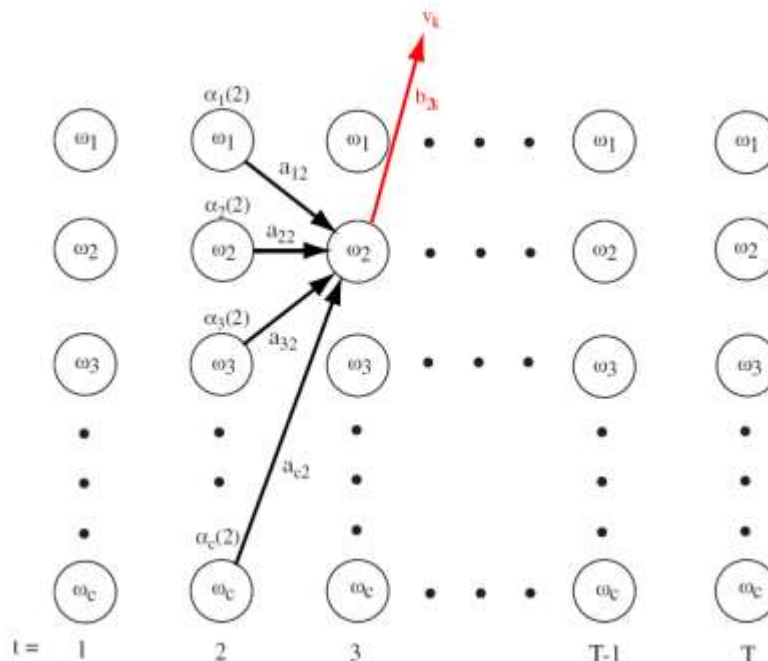
A trellis diagram (网格图)

$$\alpha_2(3) = \left[ \sum_{i=1}^c \alpha_i(2) a_{i2} \right] b_{2k}$$

$$t = 3$$

$$j = 2$$

$$v(t) = v_k$$



# The Evaluation Problem for HMM (Cont)

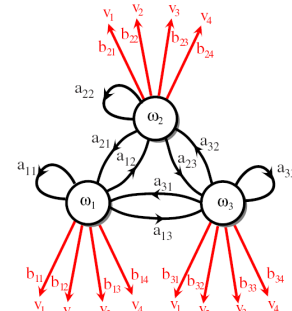
## An illustrative example

$$\Omega = \{\omega_1, \omega_2, \dots, \omega_4\} \quad (c = 4) \quad \mathcal{V} = \{v_1, v_2, \dots, v_5\} \quad (K = 5)$$

$$\mathbf{A} = [a_{ij}]_{c \times c} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0.2 & 0.3 & 0.1 & 0.4 \\ 0.2 & 0.5 & 0.2 & 0.1 \\ 0.8 & 0.1 & 0.0 & 0.1 \end{pmatrix}$$

$$\mathbf{B} = [b_{jk}]_{c \times K} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0.3 & 0.4 & 0.1 & 0.2 \\ 0 & 0.1 & 0.1 & 0.7 & 0.1 \\ 0 & 0.5 & 0.2 & 0.1 & 0.2 \end{pmatrix}$$

$$\boldsymbol{\pi} = (\pi_1, \pi_2, \dots, \pi_c) = (0, 1, 0, 0)$$



### *Specific properties for $\theta = \{\mathbf{A}, \mathbf{B}, \boldsymbol{\pi}\}$*

- ❑  $\omega_1$  can be viewed as an **absorbing** state, which won't transit to other states once entered
- ❑ at state  $\omega_1$ , **only the symbol  $v_1$  is emitted**
- ❑ at states other than  $\omega_1$ , **the symbol  $v_1$  won't be emitted**
- ❑ the **initial state** should be  $\omega_2$

# The Evaluation Problem for HMM (Cont.)

The forward procedure for evaluating  $P(\mathbf{V}^5 \mid \boldsymbol{\theta})$  with  $\mathbf{V}^5 = \{v_4, v_2, v_4, v_3, v_1\}$

	$v_4$	$v_2$	$v_4$	$v_3$	$v_1$	
$\omega_1$	0	0	0	0	.0011	$\mathbf{A} = [a_{ij}]_{c \times c} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0.2 & 0.3 & 0.1 & 0.4 \\ 0.2 & 0.5 & 0.2 & 0.1 \\ 0.8 & 0.1 & 0.0 & 0.1 \end{pmatrix}$
$\omega_2$	1	.09	.0052	.0024	0	$\mathbf{B} = [b_{jk}]_{c \times K} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0.3 & 0.4 & 0.1 & 0.2 \\ 0 & 0.1 & 0.1 & 0.7 & 0.1 \\ 0 & 0.5 & 0.2 & 0.1 & 0.2 \end{pmatrix}$
$\omega_3$	0	.01	.0077	.0002	0	$\boldsymbol{\pi} = (\pi_1, \pi_2, \dots, \pi_c) = (0, 1, 0, 0)$
$\omega_4$	0	.20	.0057	.0007	0	<i>The value of <math>\alpha_j(t)</math> is shown in the circles of the trellis</i>
$t =$	1	2	3	4	5	$\alpha_j(t) = \left[ \sum_{i=1}^c \alpha_i(t-1) a_{ij} \right] b_{jv(t)}$

# The Evaluation Problem for HMM (Cont.)

HMM backward algorithm   $P(\mathbf{V}^T \mid \boldsymbol{\theta}) = \sum_{j=1}^c \pi_j b_{jv(1)} \beta_j(1)$

Let  $\beta_j(t) = P(v(t+1), v(t+2), \dots, v(T) \mid \omega(t) = \omega_j, \boldsymbol{\theta})$

*the probability of observing the rest  $T - t$  symbols in  $\mathbf{V}^T$  given that the hidden state at step  $t$  is  $\omega_j$*

Then,  $\beta_j(t)$  ( $1 \leq j \leq c, 1 \leq t \leq T$ ) can be calculated recursively as:

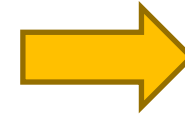
$$\beta_j(T) = 1$$

$$\begin{aligned} \beta_j(t) &= \sum_{i=1}^c P(v(t+1), \omega(t+1) = \omega_i, v(t+2), \dots, v(T) \mid \omega(t) = \omega_j, \boldsymbol{\theta}) \\ &= \sum_{i=1}^c P(v(t+2), \dots, v(T) \mid \omega(t+1) = \omega_i, \boldsymbol{\theta}) \cdot P(\omega_i \mid \omega_j, \boldsymbol{\theta}) \cdot P(v(t+1) \mid \omega_i, \boldsymbol{\theta}) \\ &= \sum_{i=1}^c \beta_i(t+1) a_{ji} b_{iv(t+1)} \end{aligned}$$

# The Evaluation Problem for HMM (Cont.)

$\theta = \{A, B, \pi\}$  : the complete set of HMM parameters

$V^T$  : the observed symbol sequence



*to evaluate*  
 $P(V^T | \theta)$

## Pseudo-code for HMM backward algorithm

1. **Initialize**  $t = T$  **and**  $\beta_j(T) = 1$  ( $1 \leq j \leq c$ )

2. **For**  $t = T - 1$  to 1

3. **For**  $j = 1$  to  $c$

4.  $\beta_j(t) = \sum_{i=1}^c \beta_i(t+1) a_{ji} b_{iv(t+1)}$

5. **End**

6. **End**

7. **Return**  $P(V^T | \theta) = \sum_{j=1}^c \pi_j b_{jv(1)} \beta_j(1)$

Computational  
complexity

$$\mathcal{O}(c^T \cdot T)$$



$$\mathcal{O}(c^2 \cdot T)$$



# The Decoding Problem for HMM

$\theta = \{A, B, \pi\}$  : the HMM parameters

$V^T$  : the observed symbol sequence



*to identify the state sequence*

$$\omega^* = \arg \max_{\omega^T} P(\omega^T | V^T, \theta)$$

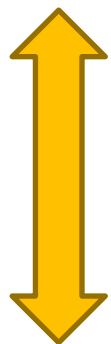
$$\omega^* = \arg \max_{\omega^T} P(\omega^T | V^T, \theta)$$



$$\omega^* = \arg \max_{\omega^T} P(\omega^T, V^T | \theta)$$

A straightforward decoding

$$\omega^* = \arg \max_{\omega^T} P(\omega^T, V^T | \theta)$$



$$P(\omega^T | \theta) = \prod_{t=1}^T P(\omega(t) | \omega(t-1)) \quad (\text{let } P(\omega(1) | \omega(0)) = \pi_{\omega(1)})$$

$$P(V^T | \omega^T, \theta) = \prod_{t=1}^T b_{\omega(t)v(t)}$$

$$\omega^* = \arg \max_{\omega^T} \prod_{t=1}^T P(\omega(t) | \omega(t-1)) \cdot b_{\omega(t)v(t)}$$

Computational  
complexity:  $\mathcal{O}(c^T \cdot T)!$

**Infeasible!**

# The Decoding Problem for HMM (Cont.)

## The Viterbi algorithm

Let  $\delta_j(t) = \max_{\omega(1), \dots, \omega(t-1)} P(\omega(1), \dots, \omega(t-1), \omega(t) = \omega_j, v(1), \dots, v(t) \mid \theta)$

*the **highest probability** (best score) of the state sequence and observed symbols **till step t**, where the state at step t is  $\omega_j$*

*Similar to the forward and backward evaluation algorithm,  $\delta_j(t)$  ( $1 \leq j \leq c, 1 \leq t \leq T$ ) can be calculated recursively based on dynamic programming (动态规划)*



**Andrew J. Viterbi**  
*Founder of Qualcomm*  
**(1935- )**

# The Decoding Problem for HMM (Cont.)

$\delta_j(t)$  ( $1 \leq j \leq c, 1 \leq t \leq T$ ) can be calculated recursively as:

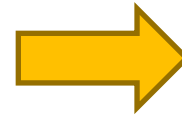
$$\begin{aligned}\delta_j(1) &= P(\omega(1) = \omega_j, v(1) \mid \boldsymbol{\theta}) = P(\omega(1) = \omega_j \mid \boldsymbol{\theta}) \cdot P(v(1) \mid \omega_j, \boldsymbol{\theta}) \\ &= \pi_j b_{jv(1)}\end{aligned}$$

$$\begin{aligned}\delta_j(t) &= \max_{\omega(1), \dots, \omega(t-1)} P(\omega(1), \dots, \omega(t-1), \omega(t) = \omega_j, v(1), \dots, v(t) \mid \boldsymbol{\theta}) \\ &= \max_{\omega(t-1)} \left[ \max_{\omega(1), \dots, \omega(t-2)} P(\omega(1), \dots, \omega(t-1), \omega(t) = \omega_j, v(1), \dots, v(t) \mid \boldsymbol{\theta}) \right] \\ &= \max_{1 \leq i \leq c} \left[ \max_{\omega(1), \dots, \omega(t-2)} P(\omega(1), \dots, \omega(t-2), \omega(t-1) = \omega_i, v(1), \dots, v(t-1) \mid \boldsymbol{\theta}) \right. \\ &\quad \left. \cdot P(\omega_j \mid \omega_i, \boldsymbol{\theta}) \cdot P(v(t) \mid \omega_j, \boldsymbol{\theta}) \right] \\ &= \left[ \max_{1 \leq i \leq c} \delta_i(t-1) a_{ij} \right] b_{jv(t)}\end{aligned}$$

# The Decoding Problem for HMM (Cont.)

$\theta = \{A, B, \pi\}$  : the HMM parameters

$V^T$  : the observed symbol sequence



*to identify the state sequence*

$$\omega^* = \arg \max_{\omega^T} P(\omega^T | V^T, \theta)$$

## Pseudo-code for the Viterbi algorithm

1. **Initialize**  $\delta_j(1) = \pi_j b_{jv(1)}$  **and**  $\psi_j(1) = 0$  ( $1 \leq j \leq c$ )
2. **For**  $t = 2$  to  $T$
3.   **For**  $j = 1$  to  $c$
4.      $\delta_j(t) = \left[ \max_{1 \leq i \leq c} \delta_i(t-1) a_{ij} \right] b_{jv(t)}$ ;  $\psi_j(t) = \arg \max_{1 \leq i \leq c} \delta_i(t-1) a_{ij}$
5.   **End**
6. **End**
7. **Decode**  $\omega^*(T) = \arg \max_{1 \leq j \leq c} \delta_j(T)$
8. **Decode**  $\omega^*(t) = \psi_{\omega^*(t+1)}(t+1)$  ( $1 \leq t \leq T-1$ ) **with path backtracking (路径回溯)**

Computational complexity

$$\mathcal{O}(c^T \cdot T)$$



$$\mathcal{O}(c^2 \cdot T)$$

# The Learning Problem for HMM

$V^T$  : the observed symbol sequence  to identify  $\theta = \{A, B, \pi\}$  which  
which maximizes  $P(V^T | \theta)$

Generally, there is **no known algorithm** which can obtain the  
**optimal solution** to the above problem



Try to find a **local optimum** based on iterative updating:  
in each iteration, update  $\theta$  to  $\hat{\theta}$  such that  $P(V^T | \hat{\theta}) \geq P(V^T | \theta)$

## The Baum-Welch algorithm

a.k.a. **forward-backward algorithm**,  
which is an instantiation of the  
famous **Expectation-Maximization**  
**(EM)** procedure



Leonard E. Baum  
(1931-2017)



Lloyd R. Welch  
(1927-2024)

# The Learning Problem for HMM (Cont.)

## The Baum-Welch algorithm

Let  $\gamma_{ij}(t) = P(\omega(t) = \omega_i, \omega(t+1) = \omega_j \mid \mathbf{V}^T, \boldsymbol{\theta})$

*the probability of being in state  $\omega_i$  at step  $t$ , and state  $\omega_j$  at step  $t+1$ , given the observed symbol sequence*

$$\begin{aligned}\gamma_{ij}(t) &= P(\omega(t) = \omega_i, \omega(t+1) = \omega_j \mid \mathbf{V}^T, \boldsymbol{\theta}) \\ &= \frac{P(v(1), \dots, v(t), \omega(t) = \omega_i, \omega(t+1) = \omega_j, v(t+1), \dots, v(T) \mid \boldsymbol{\theta})}{P(\mathbf{V}^T \mid \boldsymbol{\theta})} \\ &= \frac{\alpha_i(t) a_{ij} b_{jv(t+1)} \beta_j(t+1)}{P(\mathbf{V}^T \mid \boldsymbol{\theta})} \\ &= \frac{\alpha_i(t) a_{ij} b_{jv(t+1)} \beta_j(t+1)}{\sum_{i=1}^c \sum_{j=1}^c \alpha_i(t) a_{ij} b_{jv(t+1)} \beta_j(t+1)}\end{aligned}$$



# The Learning Problem for HMM (Cont.)

## Pseudo-code for the Baum-Welch algorithm

1. **Randomly initialize**  $\theta = \{A, B, \pi\}$
2. **Repeat**
3.   **Estimate**  $\alpha_j(t)$  ( $1 \leq j \leq c, 1 \leq t \leq T$ ) **by invoking the forward algorithm**
4.   **Estimate**  $\beta_j(t)$  ( $1 \leq j \leq c, 1 \leq t \leq T$ ) **by invoking the backward algorithm**
5.   **Set**  $\gamma_{ij}(t) = \frac{\alpha_i(t) a_{ij} b_{jv(t+1)} \beta_j(t+1)}{\sum_{i=1}^c \sum_{j=1}^c \alpha_i(t) a_{ij} b_{jv(t+1)} \beta_j(t+1)}$  ( $1 \leq i, j \leq c, 1 \leq t \leq T-1$ )
6.   **Set**  $\hat{\theta} = \{\hat{A}, \hat{B}, \hat{\pi}\}$  **such that**  $\forall 1 \leq i, j \leq c, 1 \leq k \leq K :$   
$$\hat{\pi}_i = \sum_{j=1}^c \gamma_{ij}(1) \quad \hat{a}_{ij} = \frac{\sum_{t=1}^{T-1} \gamma_{ij}(t)}{\sum_{t=1}^{T-1} \sum_{j=1}^c \gamma_{ij}(t)} \quad \hat{b}_{ik} = \frac{\sum_{t=1, v(t)=v_k}^{T-1} \sum_{j=1}^c \gamma_{ij}(t)}{\sum_{t=1}^{T-1} \sum_{j=1}^c \gamma_{ij}(t)}$$
7.   **Update**  $\theta \leftarrow \hat{\theta}$
8. **Until convergence**  $\leftarrow$  *practical convergence condition:  $\|\theta - \hat{\theta}\| \leq \epsilon$*





# To have the full story on HMM.....

L. R. Rabiner. A tutorial on hidden Markov models and selected applications in speech recognition. *Proceedings of the IEEE*, 1989, 77(2): 257-286

A tutorial on hidden Markov models and selected applications in speech recognition

LR Rabiner - Proceedings of the IEEE, 1989 - [ieeexplore.ieee.org](http://ieeexplore.ieee.org)

This tutorial provides an overview of the basic theory of hidden Markov models (HMMs) as originated by LE Baum and T. Petrie (1966) and gives practical details on methods of implementation of the theory along with a description of selected applications of the theory to distinct problems in speech recognition. Results from a number of original sources are combined to provide a single source of acquiring the background required to pursue further this area of research. The author first reviews the theory of discrete Markov chains and ...

☆ 保存 引用 被引用次数: 31166 相关文章 所有 61 个版本



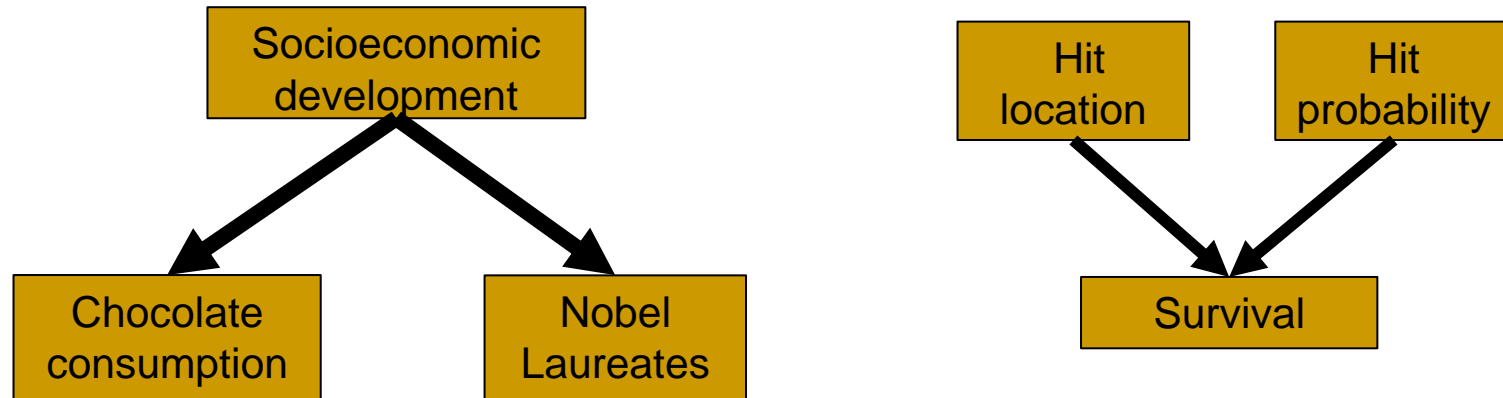


# Related Topic II

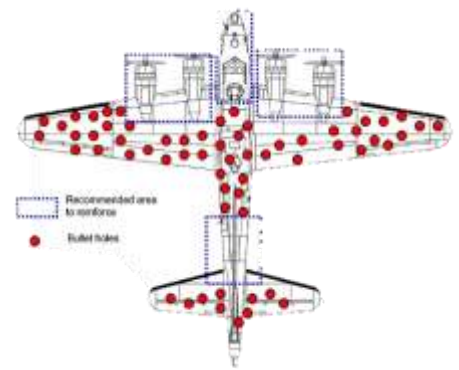
## Bayesian Belief Network



# Decision: a tale of two sides (Cont.)



- The first example is called “confounding bias”
- The second example is called “selection bias”



# Directed Acyclic Graph (DAG; 有向无环图)

$$G = (V, E)$$

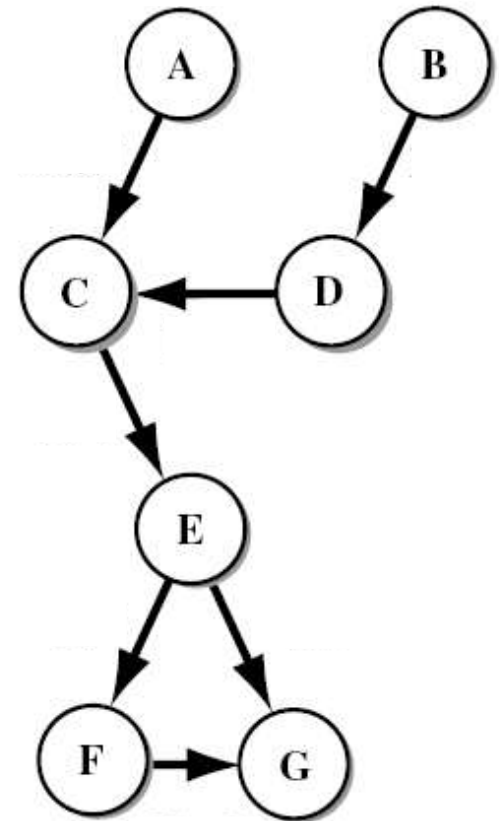
- $V$ : a set of **nodes** in graph  $G$
- $E$ : a set of **directed edges** in  $G$

**Basic assumption: no directed loop in  $G$**

## An illustrative example

$$V = \{A, B, C, D, E, F, G\} \quad (|V| = 7)$$

$$E = \{(A, C), (B, D), (D, C), (C, E), \\ (E, F), (E, G), (F, G)\} \quad (|E| = 7)$$



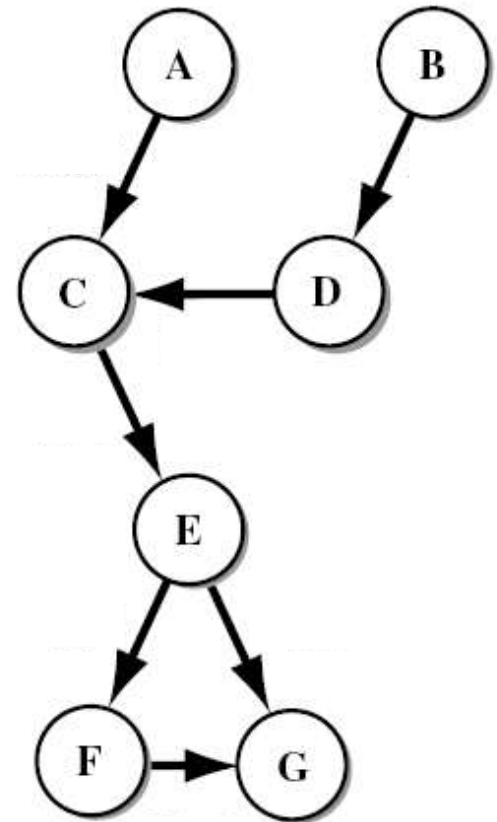
# Bayesian Belief Network (贝叶斯置信网)

## The goal of Bayesian belief network

Model the **joint distribution of a set of random variables** w.r.t. the network's DAG structure

## Notations

- Node:  $A, B, \dots$
- Random Variable:  $a, b, \dots$
- Values of Random Variable:  $\{a_1, a_2, \dots\}, \dots$
- Parent variables:  $\mathcal{G}(a), \mathcal{G}(b), \dots$   
e.g.  $\mathcal{G}(c) = \{a, d\}, \mathcal{G}(f) = \{e\}$

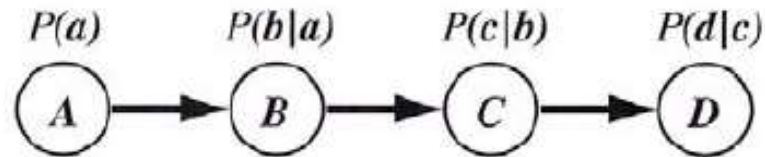


**joint distribution**  
w.r.t. the DAG

The joint distribution can **be factorized into the product of the conditional probability** of each random variable given its parent variables

# Bayesian Belief Network (Cont.)

## DAG Example I



$$\begin{aligned} P(\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d}) &= P(\mathbf{a} \mid \mathcal{G}(\mathbf{a})) \cdot P(\mathbf{b} \mid \mathcal{G}(\mathbf{b})) \cdot P(\mathbf{c} \mid \mathcal{G}(\mathbf{c})) \cdot P(\mathbf{d} \mid \mathcal{G}(\mathbf{d})) \\ &= P(\mathbf{a}) \cdot P(\mathbf{b} \mid \mathbf{a}) \cdot P(\mathbf{c} \mid \mathbf{b}) \cdot P(\mathbf{d} \mid \mathbf{c}) \end{aligned}$$

$$\begin{aligned} P(\mathbf{d}) &= \sum_{\mathbf{a}, \mathbf{b}, \mathbf{c}} P(\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d}) = \sum_{\mathbf{a}, \mathbf{b}, \mathbf{c}} P(\mathbf{a}) \cdot P(\mathbf{b} \mid \mathbf{a}) \cdot P(\mathbf{c} \mid \mathbf{b}) \cdot P(\mathbf{d} \mid \mathbf{c}) \\ &= \sum_{\mathbf{c}} P(\mathbf{d} \mid \mathbf{c}) \underbrace{\sum_{\mathbf{b}} P(\mathbf{c} \mid \mathbf{b}) \sum_{\mathbf{a}} P(\mathbf{b} \mid \mathbf{a}) P(\mathbf{a})}_{P(\mathbf{b})} \\ &\quad \underbrace{\hspace{10em}}_{P(\mathbf{c})} \\ &\quad \underbrace{\hspace{15em}}_{P(\mathbf{d})} \end{aligned}$$

# Bayesian Belief Network (Cont.)

## DAG Example II

$$P(\mathbf{e}, \mathbf{f}, \mathbf{g}, \mathbf{h})$$

$$= P(\mathbf{e} \mid \mathcal{G}(\mathbf{e})) \cdot P(\mathbf{f} \mid \mathcal{G}(\mathbf{f})) \cdot P(\mathbf{g} \mid \mathcal{G}(\mathbf{g})) \cdot P(\mathbf{h} \mid \mathcal{G}(\mathbf{h}))$$

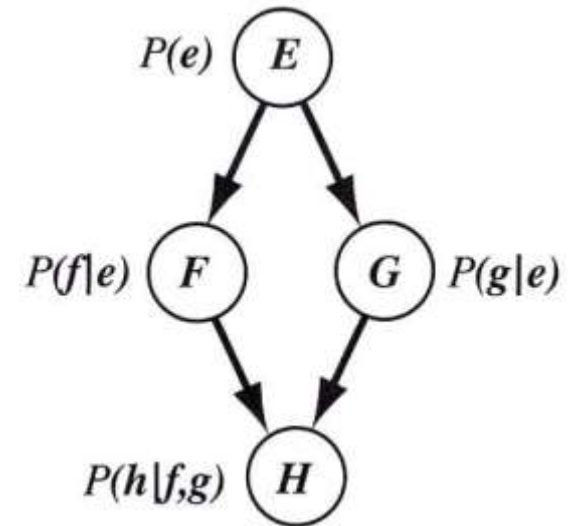
$$= P(\mathbf{e}) \cdot P(\mathbf{f} \mid \mathbf{e}) \cdot P(\mathbf{g} \mid \mathbf{e}) \cdot P(\mathbf{h} \mid \mathbf{f}, \mathbf{g})$$

$$P(\mathbf{f}, \mathbf{g}, \mathbf{h}) = \sum_{\mathbf{e}} P(\mathbf{e}, \mathbf{f}, \mathbf{g}, \mathbf{h})$$

$$= P(\mathbf{h} \mid \mathbf{f}, \mathbf{g}) \sum_{\mathbf{e}} P(\mathbf{e}) \cdot P(\mathbf{f} \mid \mathbf{e}) \cdot P(\mathbf{g} \mid \mathbf{e})$$

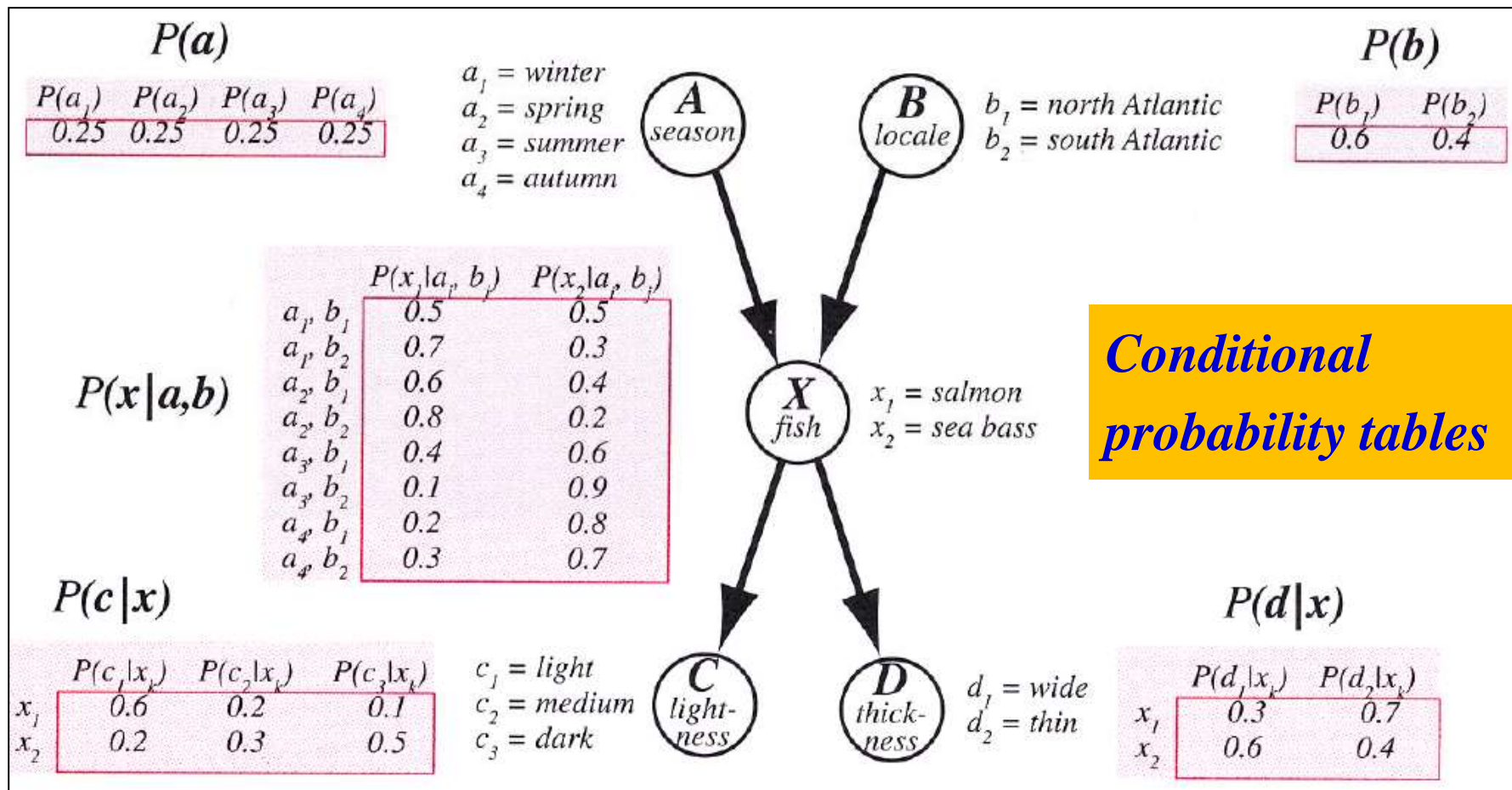
$$P(\mathbf{h}) = \sum_{\mathbf{e}, \mathbf{f}, \mathbf{g}} P(\mathbf{e}, \mathbf{f}, \mathbf{g}, \mathbf{h})$$

$$= \sum_{\mathbf{e}} P(\mathbf{e}) \sum_{\mathbf{f}, \mathbf{g}} P(\mathbf{f} \mid \mathbf{e}) \cdot P(\mathbf{g} \mid \mathbf{e}) \cdot P(\mathbf{h} \mid \mathbf{f}, \mathbf{g})$$



# Bayesian Belief Network (Cont.)

## DAG Example III Bayesian network for fish



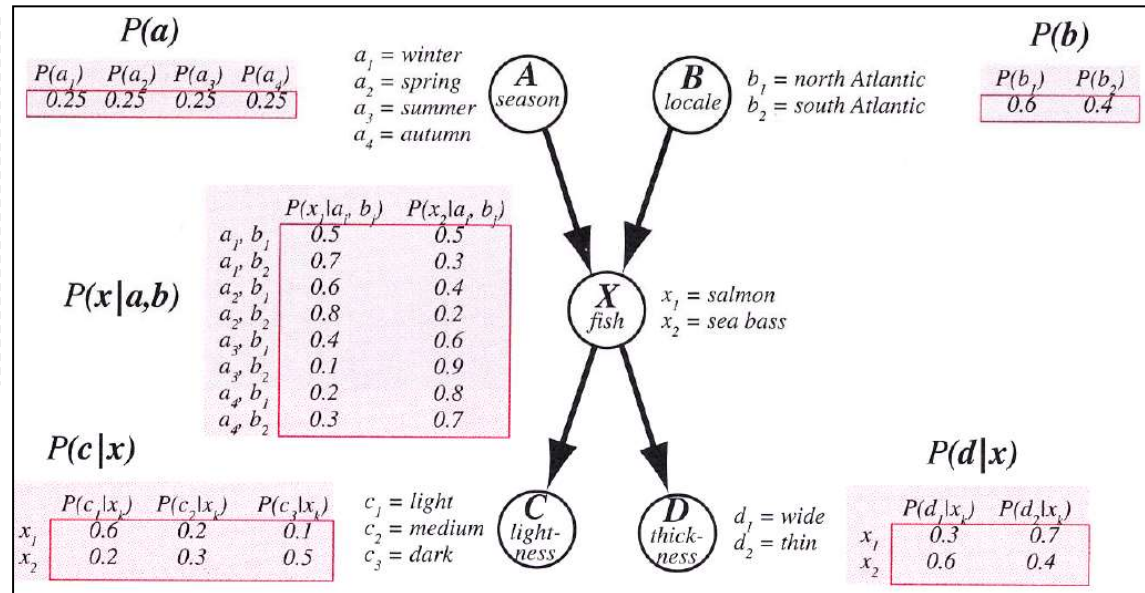


# Bayesian Belief Network (Cont.)

*What is the probability that the fish was caught in the **summer** in the **north Atlantic** and is **sea bass** that is **dark** and **thin**?*

$\mathbf{a} = a_3$      $\mathbf{b} = b_1$

$\mathbf{x} = x_2$      $\mathbf{c} = c_3$      $\mathbf{d} = d_2$



$$\begin{aligned}
 P(a_3, b_1, x_2, c_3, d_2) &= P(a_3) \cdot P(b_1) \cdot P(x_2 | a_3, b_1) \cdot P(c_3 | x_2) \cdot P(d_2 | x_2) \\
 &= 0.25 \times 0.6 \times 0.6 \times 0.5 \times 0.4 \\
 &= 0.018
 \end{aligned}$$



# Bayesian Belief Network (Cont.)

Suppose we know a fish is **light** and caught in the **south Atlantic**, **how shall we classify the fish?**

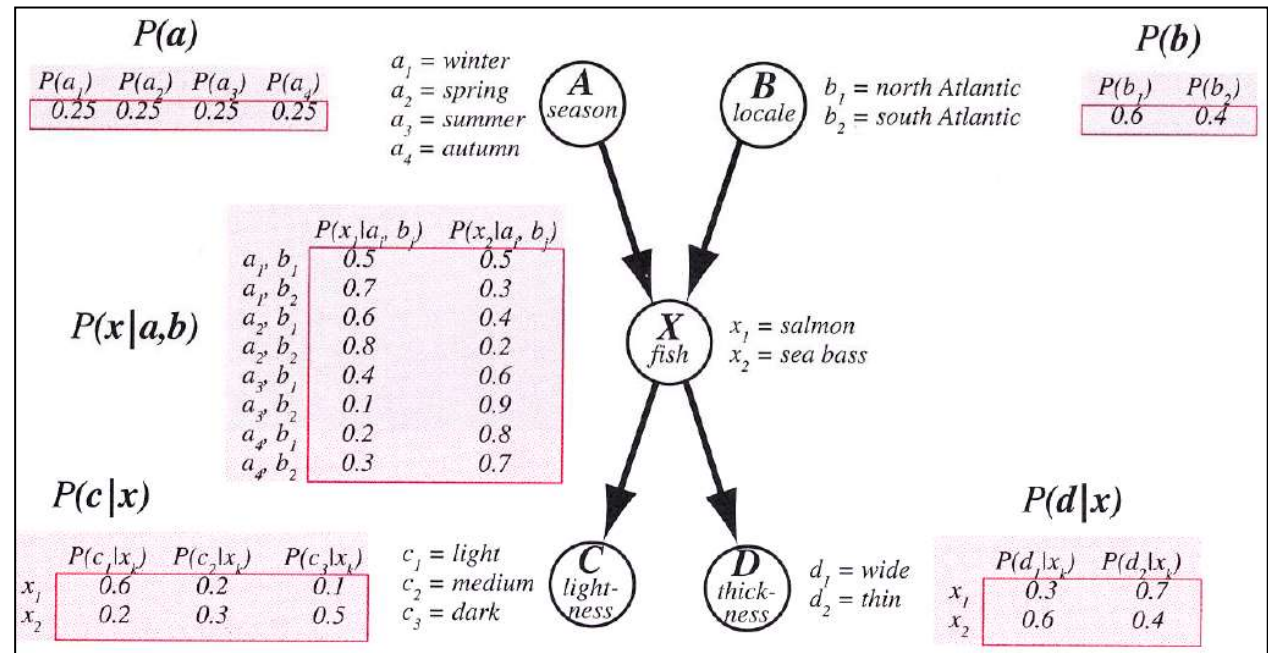
$\mathbf{b} = b_2 \quad \mathbf{c} = c_1$

**evidence**

$$P(\mathbf{x} = x_1 \mid b_2, c_1)$$

**VS**

$$P(\mathbf{x} = x_2 \mid b_2, c_1)$$



# Bayesian Belief Network (Cont.)

$$P(x_1 | b_2, c_1)$$

$$= P(x_1, b_2, c_1) / P(b_2, c_1)$$

$$= \alpha \sum_{\mathbf{a}, \mathbf{d}} P(\mathbf{a}, x_1, b_2, c_1, \mathbf{d})$$

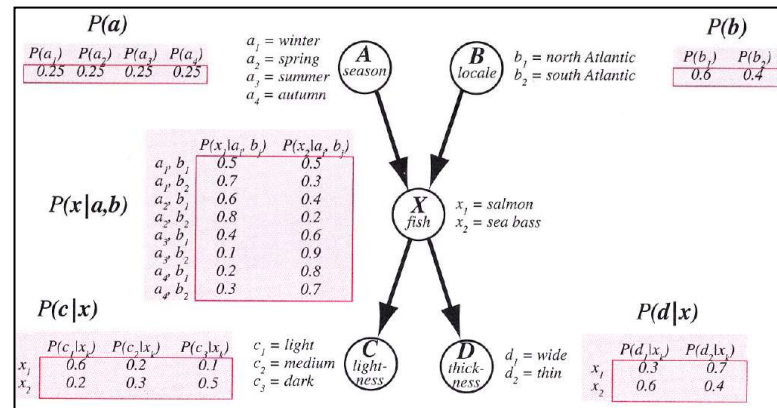
$$= \alpha \sum_{\mathbf{a}, \mathbf{d}} P(\mathbf{a}) P(b_2) P(x_1 | \mathbf{a}, b_2) P(c_1 | x_1) P(\mathbf{d} | x_1)$$

$$= \alpha P(b_2) P(c_1 | x_1) \left[ \sum_{\mathbf{a}} P(\mathbf{a}) P(x_1 | \mathbf{a}, b_2) \right] \left[ \sum_{\mathbf{d}} P(\mathbf{d} | x_1) \right]$$

$$= \alpha (0.4) (0.6) [(0.25)(0.7) + (0.25)(0.8) + (0.25)(0.1) + (0.25)(0.3)] (1.0)$$

$$= \alpha 0.114 \quad \text{Similarly, we can have } P(x_2 | b_2, c_1) = \alpha 0.042$$

$$P(x_1 | b_2, c_1) = 0.73 \quad P(x_2 | b_2, c_1) = 0.27$$



# Bayesian Belief Network (Cont.)

Further Example

**Bayesian network for xxx**



# 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  $\mu$
    - Unknown  $\mu$  and  $\Sigma$



# Summary (Cont.)

- Bayesian estimation

- Settings: **parameters as random variables**

- The general procedure

- Phase I: *prior pdf*  $\rightarrow$  *posterior pdf* (for  $\theta$ )

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

- Phase III: *prediction* (Eq.22 [pp.91])

- The Gaussian case

- Unknown  $\Sigma$  : univariate and multivariate

# Summary (Cont.)

## ■ Hidden Markov Model (HMM)

- Parameters in HMM:  $\theta = \{A, B, \pi\}$
- Observed symbol sequence:  $V^T$
- Three central problems in HMM
  - **Evaluation:**  $P(V^T | \theta)$ , the forward/backward algorithm
  - **Decoding:**  $\arg \max_{\omega^T} P(\omega^T | V^T, \theta)$ , the Viterbi algorithm
  - **Learning:**  $\arg \max_{\theta} P(V^T | \theta)$ , the Baum-Welch algorithm

## ■ Bayesian Belief Network

- The **DAG structure** for modeling joint distribution
- Conditional probability tables