第3章：参数估计(续)

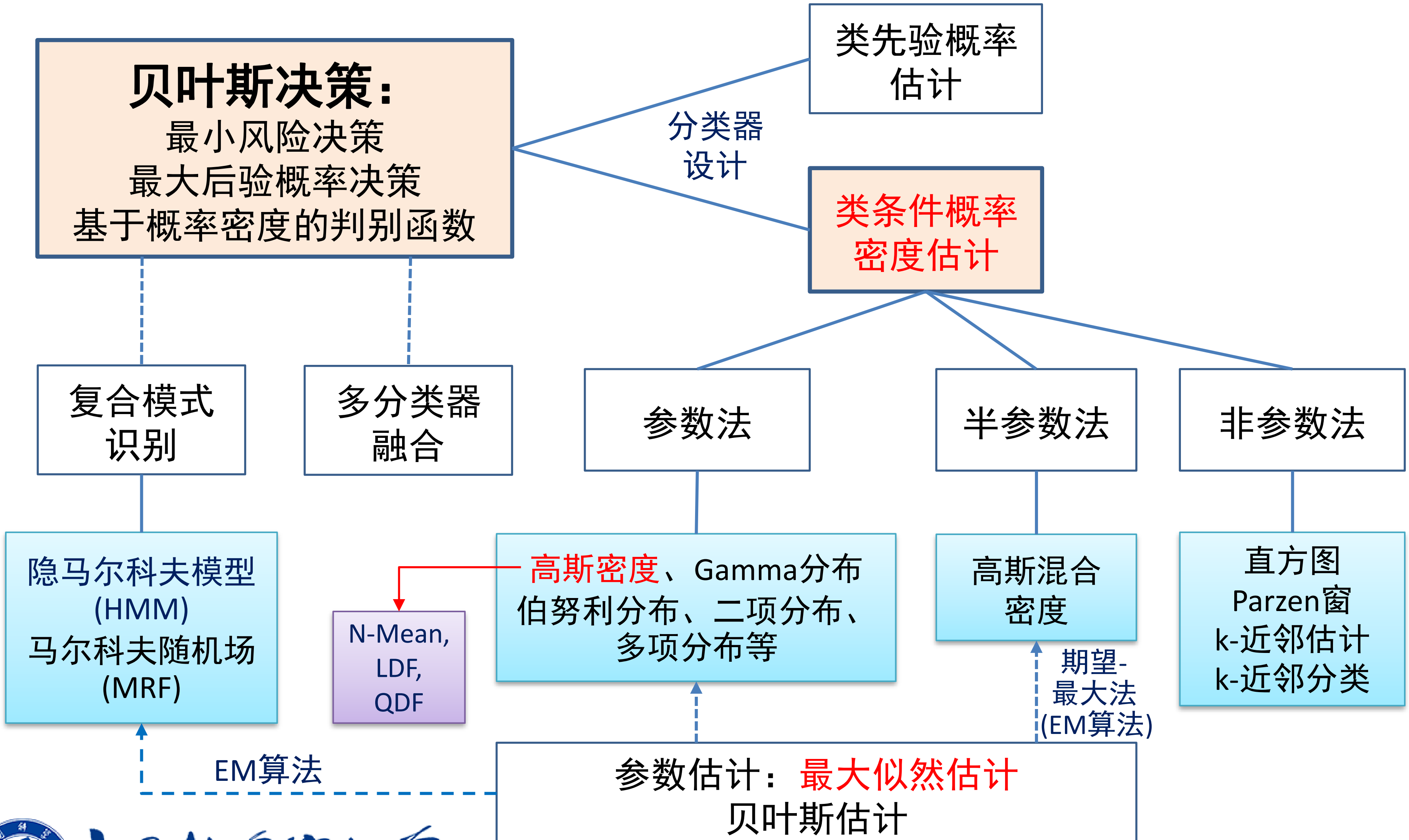
刘成林(liucl@nlpr.ia.ac.cn)

2020年10月7日

助教：敖翔(aoxiang2017@ia.ac.cn)
王瑞琪(ruiqi.wang@nlpr.ia.ac.cn)
赵元兴(zhaoyuanxing2018@ia.ac.cn)

中国科学院大学
University of Chinese Academy of Sciences

基于贝叶斯决策的模式分类框架



公式太多，怎么办？

- 注重宏观思维
  - 先整体，后局部，再回到整体
  - 理解概念最重要！
    - 特征空间、符号、公式的物理意义，形成直觉
    - 高维空间物理意义如何理解：简化到低维，再推广到高维
  - 注重不同方法之间的区别和联系(共性)
  - 理解概念的基础上再去了解细节和数学证明
    - 对主要的方法理解其原理、过程和结论
    - 复杂的数学证明过程可忽略，记住结论即可
      - 简单的情况要清楚细节，如高斯密度函数的最大似然估计求解过程
      - 高斯混合密度的最大似然估计(EM算法)了解主要步骤(E-step, M-step)
      - 低维空间和简单模型能写出详细过程，高维或复杂模型则不要求
  - 数学分析（形式化）和证明的能力对创新研究很重要，但不可能（没有精力）把所有细节都搞懂
    - 善于利用已有概念、原理和结论，理解和会用是基础

上次课主要内容回顾

- 离散变量贝叶斯决策
- 复合模式分类

- 最大似然参数估计
- 贝叶斯估计

高斯分布的情况

Parameter space vs
feature space

二者的区别和联系

提 纲

- 第3章：参数估计
  (贝叶斯分类的参数法、半参数法)
  – 特征维数问题
  – 期望最大法
  – 隐马尔可夫模型

特征维数问题

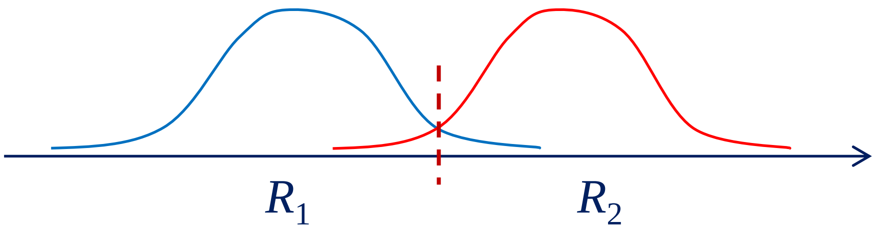
- 统计模式分类
  - 特征空间划分
  - 贝叶斯决策：最小风险规则，MAP
- 增加特征有什么好处
  - 判别性：类别间有差异的特征有助于分类
- 带来什么问题
  - 计算
  - 存储
  - 泛化性能，Overfitting

分类错误率与特征的关系

- 二类高斯分布
  - $p(\mathbf{x}|\omega_j) \sim N(\mu_j, \Sigma)$, j=1,2, 等协方差矩阵
  - Bayes error rate

$$P(e) = \frac{1}{\sqrt{2\pi}} \int_{r/2}^{\infty} e^{-u^2/2} \, du \qquad r^2 = (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)^t \boldsymbol{\Sigma}^{-1} (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)$$

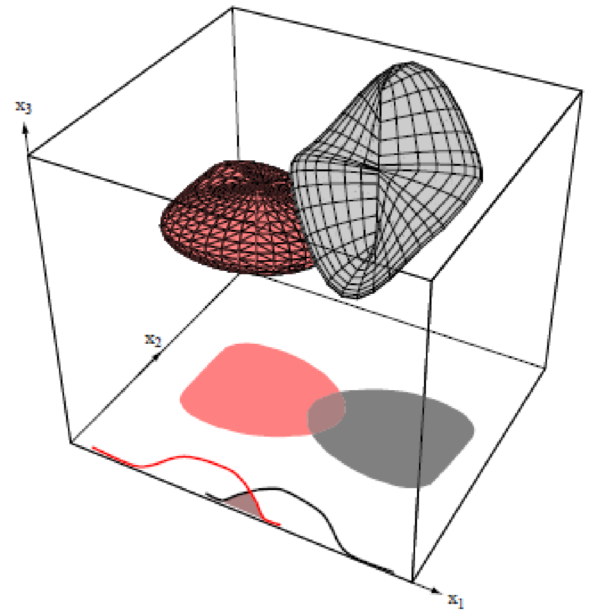
$$\begin{aligned} P(error) &= P(\mathbf{x} \in \mathcal{R}_2, \omega_1) + P(\mathbf{x} \in \mathcal{R}_1, \omega_2) \\ &= P(\mathbf{x} \in \mathcal{R}_2 | \omega_1) P(\omega_1) + P(\mathbf{x} \in \mathcal{R}_1 | \omega_2) P(\omega_2) \\ &= \int_{\mathcal{R}_2} p(\mathbf{x}|\omega_1) P(\omega_1) \, d\mathbf{x} + \int_{\mathcal{R}_1} p(\mathbf{x}|\omega_2) P(\omega_2) \, d\mathbf{x}. \end{aligned}$$



- 二类高斯分布
  - Conditionally independent case $\Sigma = diag(\sigma_1^2, ..., \sigma_d^2)$
    - 每一维二类均值之间距离反映区分度，决定错误率
    - 特征增加有助于减小错误率(r^2增大)

$$r^2 = \sum_{i=1}^{d} \left(\frac{\mu_{i1} - \mu_{i2}}{\sigma_i} \right)^2 \qquad P(e) = \frac{1}{\sqrt{2\pi}} \int_{r/2}^{\infty} e^{-u^2/2}\, du$$

- 特征维数决定可分性的例子
  - 3D空间完全可分
  - 2D和1D投影空间有重叠



然而，增加特征也可能导致分类性能更差，因为有模型估计误差(wrong model)

University of Chinese Academy of Sciences

计算复杂度

- 最大似然估计
  - 高斯分布，*d*维特征，*n*个样本
  - 参数估计的复杂度，主要由Σ决定

$$g(\mathbf{x}) = -\frac{1}{2}(\mathbf{x} - \overset{O(dn)}{\overset{\uparrow}{\hat{\boldsymbol{\mu}}}})^t \overbrace{\widehat{\Sigma}^{-1}}^{O(nd^2)} (\mathbf{x} - \hat{\boldsymbol{\mu}}) - \overbrace{\frac{d}{2}\ln 2\pi}^{O(1)} - \overbrace{\frac{1}{2}\ln|\widehat{\Sigma}|}^{O(d^2n)} + \overbrace{\ln P(\omega)}^{O(n)}$$

$$\widehat{\Sigma} = \frac{1}{n}\sum_{k=1}^{n}(\mathbf{x}_k - \mathbf{m}_n)(\mathbf{x}_k - \mathbf{m}_n)^t$$

- 参数存储复杂度

$$c(d + d(d+1)/2)$$

- 分类复杂度？
  - 计算逆矩阵比较复杂，一般为O(d^3)

University of Chinese Academy of Sciences

过拟合(Overfitting)

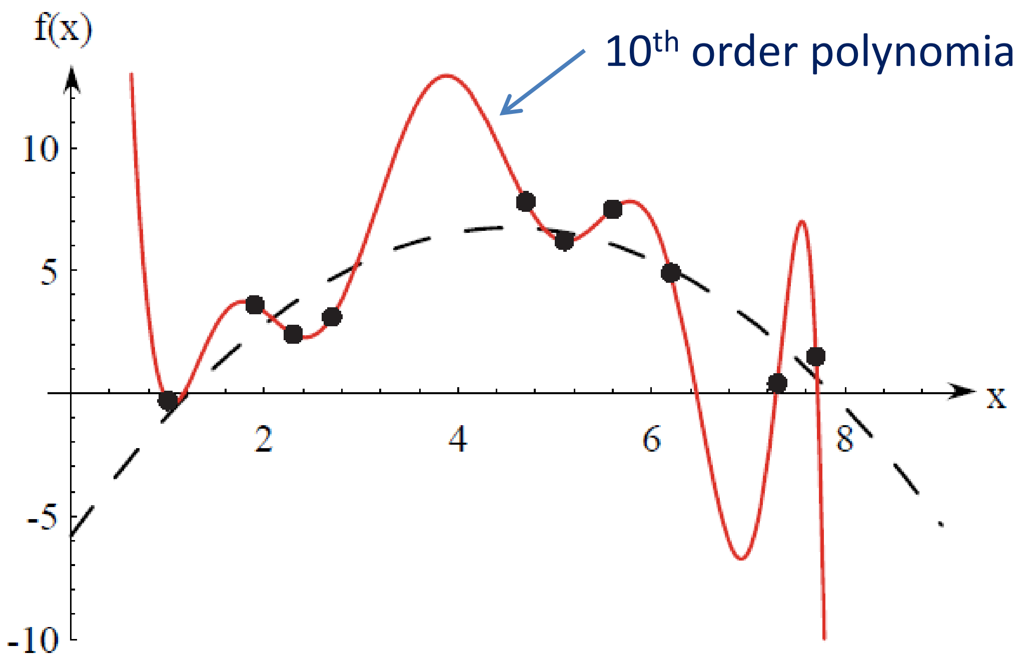
- Overfitting
  - 特征维数高、训练样本少导致模型参数估计不准确
    - 比如协方差矩阵需要样本数在*d*以上
- 克服办法
  - 特征降维：特征提取(变换)、特征选择
  - 参数共享/平滑
    - 共享协方差矩阵Σ_0
    - Shrinkage (a.k.a. Regularized Discriminant Analysis)

$$\mathbf{\Sigma}_i(\alpha) = \frac{(1-\alpha)n_i\mathbf{\Sigma}_i + \alpha n\mathbf{\Sigma}}{(1-\alpha)n_i + \alpha n}$$

$$\mathbf{\Sigma}(\beta) = (1-\beta)\mathbf{\Sigma} + \beta\mathbf{I}$$

University of Chinese Academy of Sciences

- 过拟合的例子



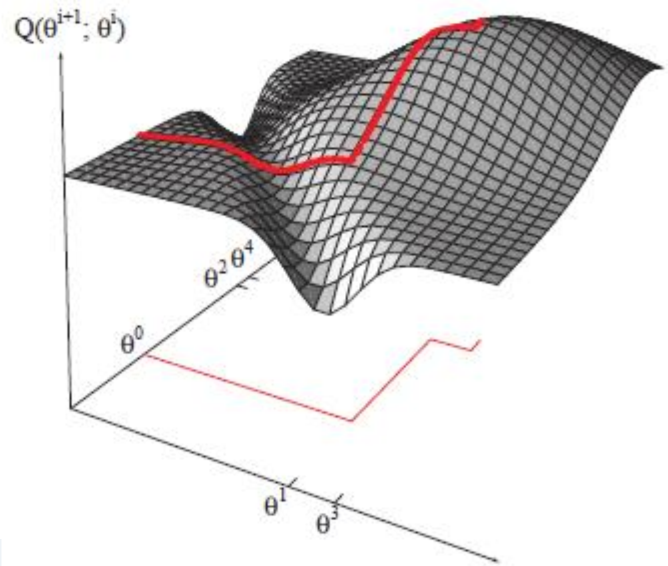
$$f(x) = ax^2 + bx + c + \epsilon \text{ where } p(\epsilon) \sim N(0, \sigma^2)$$

期望-最大法(EM)

- 数据缺失情况下的参数估计
  - Good features, missing/bad features $\mathbf{x}_k = \{\mathbf{x}_{kg}, \mathbf{x}_{kb}\}$

    $$\mathcal{D} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\} = \mathcal{D}_g \cup \mathcal{D}_b$$
  - 已知参数值θ^i情况下估计新参数值θ
    - 对缺失数据求期望(marginalize)

      max $Q(\boldsymbol{\theta}; \boldsymbol{\theta}^i) = \mathcal{E}_{\mathcal{D}_b}[\ln p(\mathcal{D}_g, \mathcal{D}_b; \boldsymbol{\theta}) | \mathcal{D}_g; \boldsymbol{\theta}^i]$



中国科学院大学
University of Chinese Academy of Sciences

- Expectation-Maximization (EM)

Algorithm 1 (Expectation-Maximization)

$$
\begin{array}{l}
\underline{\textbf{begin}}\ \underline{\textbf{initialize}}\ \theta^0, T, i = 0 \\
\qquad\qquad \underline{\textbf{do}}\ i \leftarrow i + 1 \\
\qquad\qquad\qquad \textbf{E step}: \text{compute } Q(\theta;\ \theta^i) \\
\qquad\qquad\qquad \textbf{M step}: \theta^{i+1} \leftarrow \arg\max_{\theta} Q(\theta;\ \theta^i) \\
\qquad\qquad \underline{\textbf{until}}\ Q(\theta^{i+1};\ \theta^i) - Q(\theta^i;\ \theta^{i-1}) \leq T \\
\qquad \underline{\textbf{return}}\ \hat{\theta} \leftarrow \theta^{i+1} \\
\underline{\textbf{end}}
\end{array}
$$

The EM algorithm guarantees that the log-likelihood of good data increases monotonically.

- Example: EM for a 2D Gaussian

$$\mathcal{D} = \{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4\} = \left\{ \binom{0}{2}, \binom{1}{0}, \binom{2}{2}, \binom{*}{4} \right\}$$

parameters $\boldsymbol{\theta} = \begin{pmatrix} \mu_1 \\ \mu_2 \\ \sigma_1^2 \\ \sigma_2^2 \end{pmatrix}$ initially $\boldsymbol{\theta}^0 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \end{pmatrix}$

$$\begin{aligned}
Q(\boldsymbol{\theta};\, \boldsymbol{\theta}^0) &= \mathcal{E}_{x_{41}}[\ln p(\mathbf{x}_g, \mathbf{x}_b;\, \boldsymbol{\theta}|\boldsymbol{\theta}^0;\, \mathcal{D}_g)] \\
&= \int_{-\infty}^{\infty} \left[\sum_{k=1}^{3} \ln p(\mathbf{x}_k|\boldsymbol{\theta}) + \ln p(\mathbf{x}_4|\boldsymbol{\theta}) \right] p(x_{41}|\boldsymbol{\theta}^0;\, x_{42}=4)\, dx_{41} \\
&= \sum_{k=1}^{3} [\ln p(\mathbf{x}_k|\boldsymbol{\theta})] + \int_{-\infty}^{\infty} \ln p\left(\left. \binom{x_{41}}{4} \right| \boldsymbol{\theta} \right) \frac{p\left(\binom{x_{41}}{4} | \boldsymbol{\theta}^0 \right)}{\underbrace{\left(\int_{-\infty}^{\infty} p\left(\left. \binom{x'_{41}}{4} \right| \boldsymbol{\theta}^0 \right) dx'_{41} \right)}_{\equiv K}} dx_{41}
\end{aligned}$$

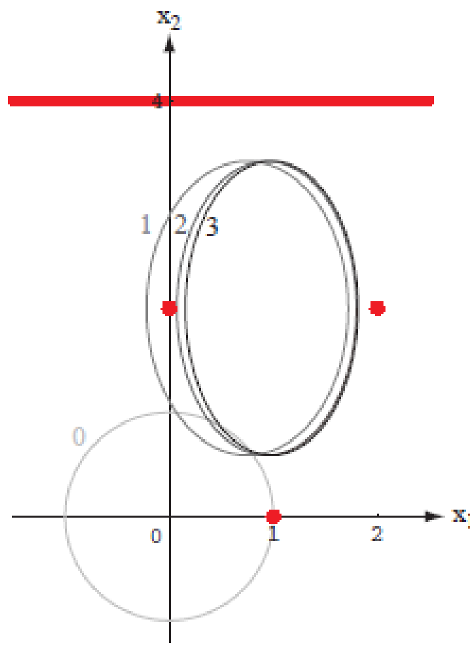
$$\begin{aligned}
Q(\boldsymbol{\theta};\, \boldsymbol{\theta}^0) &= \sum_{k=1}^{3} [\ln p(\mathbf{x}_k|\boldsymbol{\theta})] + \frac{1}{K} \int_{-\infty}^{\infty} \ln p\left(\left. \binom{x_{41}}{4} \right| \boldsymbol{\theta} \right) \frac{1}{2\pi \left| \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right|} \exp\left[-\frac{1}{2}(x_{41}^2 + 4^2) \right] dx_{41} \\
&= \sum_{k=1}^{3} [\ln p(\mathbf{x}_k|\boldsymbol{\theta})] - \frac{1+\mu_1^2}{2\sigma_1^2} - \frac{(4-\mu_2)^2}{2\sigma_2^2} - \ln\, (2\pi\sigma_1\sigma_2).
\end{aligned}$$

中国科学院大学
University of Chinese Academy of Sciences

$$\max \sum_{k=1}^{3}[\ln p(\mathrm{x}_k|\boldsymbol{\theta})] - \frac{1+\mu_1^2}{2\sigma_1^2} - \frac{(4-\mu_2)^2}{2\sigma_2^2} - \ln\,(2\pi\sigma_1\sigma_2)$$

$$\theta^1 = \begin{pmatrix} 0.75 \\ 2.0 \\ 0.938 \\ 2.0 \end{pmatrix}$$

After 3 iterations $\boldsymbol{\mu} = \binom{1.0}{2.0}$, and $\boldsymbol{\Sigma} = \begin{pmatrix} 0.667 & 0 \\ 0 & 2.0 \end{pmatrix}$



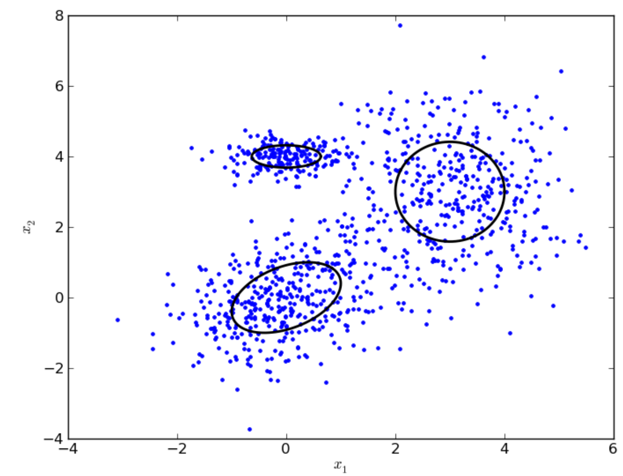
x_{41} unknown

What if $x_4=(1,4)^T$

- EM for Gaussian mixture
  - 参数型概率密度函数，可以表示复杂的分布

$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k p(\mathbf{x} | \theta_k)$$

$$\text{subject to } \sum_{k=1}^{K} \pi_k = 1$$



- Gaussian component

$$p(\mathbf{x} | \theta_k) = \mathcal{N}(\mathbf{x} | \mu_k, \Sigma_k)$$

  - 参数估计：Maximum Likelihood (ML)

$$\max LL = \log \prod_{n=1}^{N} p(\mathbf{x}_n) = \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k p(\mathbf{x}_n | \theta_k)$$

$$\nabla_{\pi_k} LL = 0, \quad \nabla_{\mu_k} LL = 0, \quad \nabla_{\Sigma_k} LL = 0$$

不能解析求解

- EM Algorithm for Gaussian mixture
  - Incomplete data X, complete data {X,Z}

missing $z_{nk} \in \{0,1\}, \quad k = 1,\ldots,K$

  - Expectation of complete data log-likelihood

$$Q(\Theta,\Theta^{old}) = \sum_{\mathbf{Z}} [\log p(\mathbf{X},\mathbf{Z}\,|\,\Theta)]\, p(\mathbf{Z}\,|\,\mathbf{X},\Theta^{old})$$

1. Choose an initial set of parameters for Θ^{old}
2. Do

   E-step: Evaluate p(Z|X, Θ^{old})

   M-step: Update parameters

$$\Theta^{new} = \arg\max_{\Theta} Q(\Theta,\Theta^{old})$$

   If convergence condition is not satisfied

$$\Theta^{old} \leftarrow \Theta^{new}$$

3. End

(C.M. Bishop, *Pattern Recognition and Machine Learning*, 2006)

- EM Algorithm for Gaussian mixture

E-step $p(\mathbf{X},\mathbf{Z}\,|\,\Theta)=\prod_{n=1}^{N}\prod_{k=1}^{K}\pi_k^{z_{nk}}\mathcal{N}(\mathbf{x}_n\,|\,\mu_k,\Sigma_k)^{z_{nk}}$

$$Q(\Theta,\Theta^{old})=\mathrm{E}_{\mathbf{Z}}[\log p(\mathbf{X},\mathbf{Z}\,|\,\Theta)]=\sum_{n=1}^{N}\sum_{k=1}^{K}\gamma(z_{nk})\{\log\pi_k+\log\mathcal{N}(\mathbf{x}\,|\,\mu_k,\Sigma_k)\}$$

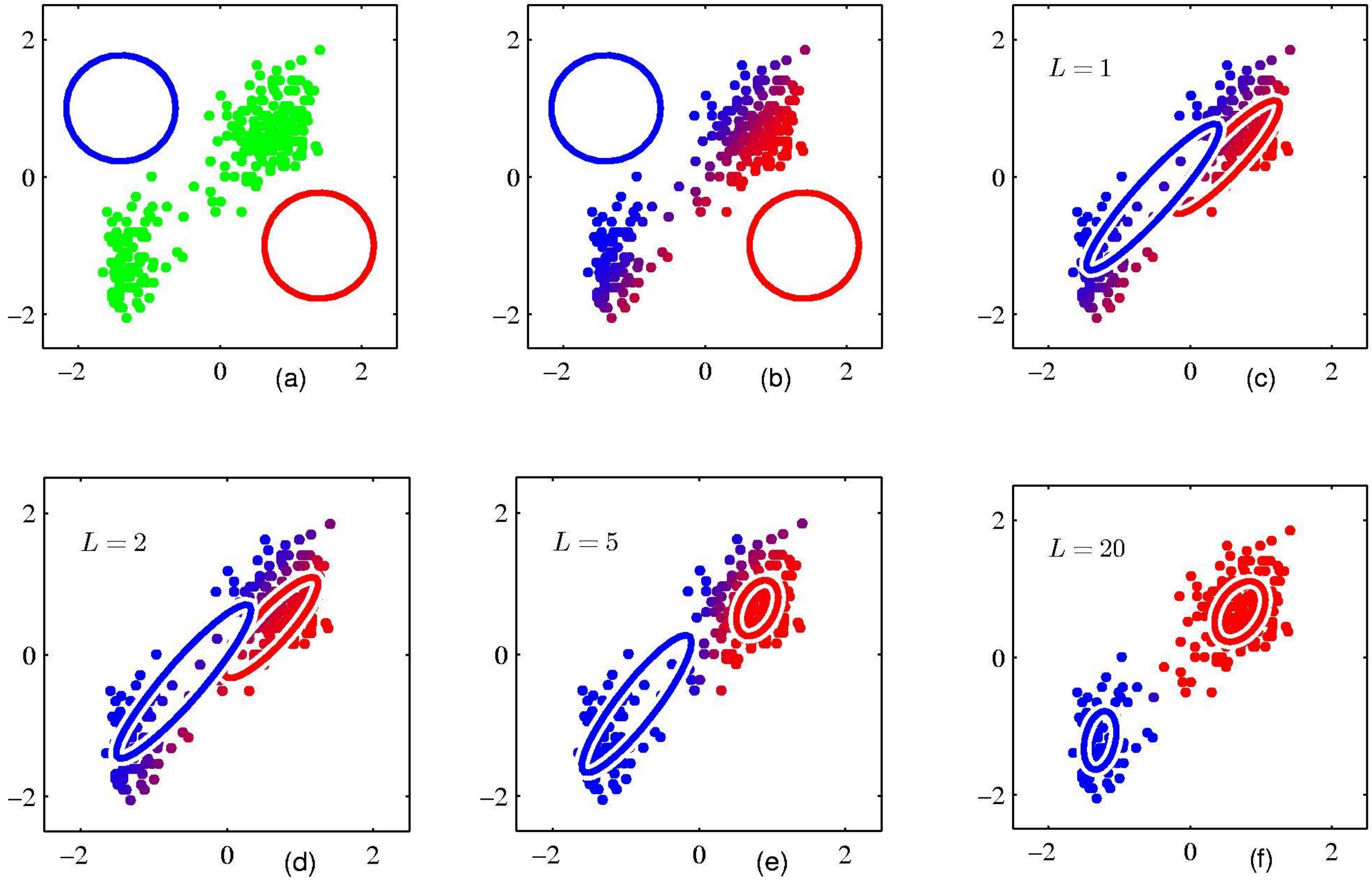
$$\boxed{\gamma(z_{nk})=P(z_{nk}=1\,|\,\mathbf{x}_n)=\frac{\pi_k N(\mathbf{x}_n\,|\,\mu_k,\Sigma_k)}{\sum_{j=1}^{K}\pi_j N(\mathbf{x}_n\,|\,\mu_j,\Sigma_j)}}$$

M-step $\nabla_{\pi_k}Q=0,\quad \nabla_{\mu_k}Q=0,\quad \nabla_{\Sigma_k}Q=0$

$$\left\{\begin{aligned}
\mu_k^{new}&=\frac{1}{N_k}\sum_{n=1}^{N}\gamma(z_{nk})\mathbf{x}_n\\
\Sigma_k^{new}&=\frac{1}{N_k}\sum_{n=1}^{N}\gamma(z_{nk})(\mathbf{x}_n-\mu_k^{new})(\mathbf{x}_n-\mu_k^{new})^T\\
\pi_k^{new}&=\frac{N_k}{N}
\end{aligned}\right.$$

$$N_k=\sum_{n=1}^{N}\gamma(z_{nk})$$

An example, from (C.M. Bishop, *Pattern Recognition and Machine Learning*, 2006. Figure 9.8)



Break

隐马尔可夫模型

- Sequential (Temporal) Pattern
  - Variable length
  - Distortion
  - Ambiguous boundary between primitives (symbols)
- Bayesian Classification
  - Sequence of patterns (observations) $\mathbf{O} = O_1 O_2 \cdots O_T$
  - Sequence class (states) $\mathbf{q} = q_1 q_2 \cdots q_T$
  - Posterior probability $$P(\mathbf{q} \mid \mathbf{O}) = \frac{p(\mathbf{O} \mid \mathbf{q}) P(\mathbf{q})}{p(\mathbf{O})}$$
- Hidden Markov Model (HMM)
  - Model $p(\mathbf{O}|\mathbf{q})$, $p(\mathbf{O},\mathbf{q})$

Markov Chain

- Sequence of States (classes)

$$P(q_1 q_2 \cdots q_T) = P(q_1)P(q_2 \mid q_1)P(q_3 \mid q_1 q_2)\cdots P(q_T \mid q_1 \cdots q_{T-1})$$

$$q_t \in \{S_1, \ldots, S_N\}$$

  – First-Order Markov chain

$$P(q_t = S_j \mid q_{t-1} = S_i, q_{t-2} = S_k, \cdots) = P(q_t = S_j \mid q_{t-1} = S_i)$$

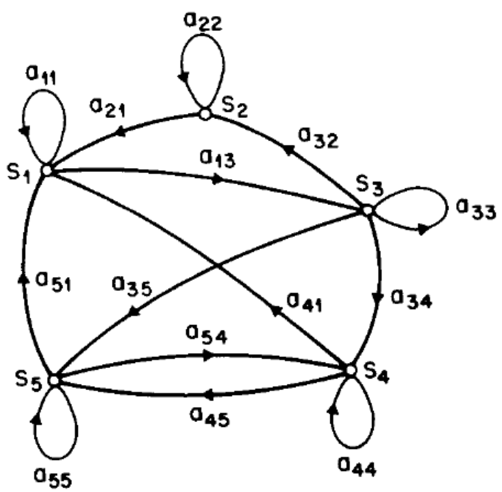
$$P(q_1 q_2 \cdots q_T) =$$

$$P(q_1)P(q_2 \mid q_1)P(q_3 \mid q_2)\cdots P(q_T \mid q_{T-1})$$

State transition probabilities

$$a_{ij} = P(q_t = S_j \mid q_{t-1} = S_i), \quad 1 \le i, j \le N$$

$$\sum_{j=1}^{N} a_{ij} = 1$$



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

– State duration (self-transition)

$$O = \{S_i, S_i, S_i, \ldots, S_i, S_j \neq S_i\}$$

1 2 3 d d+1

$$P(O \mid \text{Model}, q_1 = S_i) = (a_{ii})^{d-1}(1 - a_{ii}) = p_i(d)$$

– Expected duration of specific state

$$\bar{d}_i = \sum_{d=1}^{\infty} d \; p_i(d)$$

$$= \sum_{d=1}^{\infty} d(a_{ii})^{d-1}(1 - a_{ii}) = \frac{1}{1 - a_{ii}}$$

- Example: Transition of Weather

State 1: rain or (snow)
State 2: cloudy
State 3: sunny

$$\mathbf{A} = \{a_{ij}\} = \begin{bmatrix} 0.4 & 0.3 & 0.3 \\ 0.2 & 0.6 & 0.2 \\ 0.1 & 0.1 & 0.8 \end{bmatrix}$$

Expected number of days for sunny and cloudy?

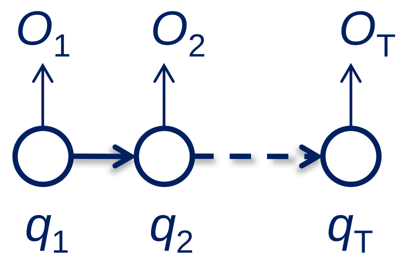
Hidden Markov Model (HMM)

- Markov Chain: States are Observable
- Hidden States: An Example
  - Imagine you are in a un-windowed room, cannot see the weather outside. Instead, you can guess the weather from the temperature and humidity in room
    - Observations: temperature, humidity
    - Hidden states: weather
  - Hidden Markov Model (HMM): Doubly embedded stochastic process

    $P(O_1,O_2,\ldots,O_T)$

    $P(q_1,q_2,\ldots,q_T)$

    - Infer states from observations



$q_i \in \{S_1,S_2,\ldots,S_N\}$

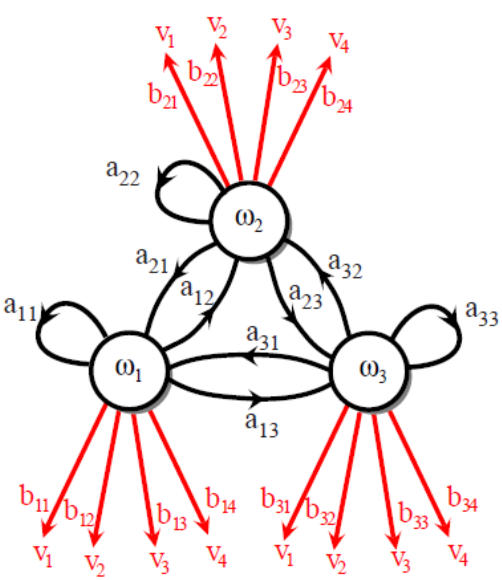
University of Chinese Academy of Sciences

- Elements of an HMM $\boldsymbol{\lambda} = (\mathbf{A}, \mathbf{B}, \boldsymbol{\pi})$
  - N: number of states in the model, $S=\{S_1,S_2,\ldots,S_N\}$
  - M: number of observation symbols, $V=\{v_1,v_2,\ldots,v_M\}$
  - State transition probability distribution $A=\{a_{ij}\}$

$$a_{ij} = P(q_{t+1} = S_j \mid q_t = S_i), \quad 1 \le i, j \le N$$

  - Observation symbol (emission) probability distribution $B=\{b_j(k)\}$ $b_j(k) = P(v_k \text{ at } t \mid q_t = S_j), \ 1 \le j \le N, \ 1 \le k \le M$
  - Initial state distribution $\boldsymbol{\pi} = \{\pi_i\}$

$$\pi_i = P(q_1 = S_i), \ 1 \le i \le N$$



- Three Basic Problems of HMM
  - Problem 1 (Evaluation):

    How to efficiently compute the probability of observation sequence $P(O|\lambda)$

  - Problem 2 (Decoding):

    How to choose the best state sequence responding to an observation sequence

  - Problem 3 (Training):

    How to estimate the model parameters

Evaluation Problem

- Given model $\boldsymbol{\lambda} = (\mathbf{A}, \mathbf{B}, \boldsymbol{\pi})$ and observation sequence $O=O_1O_2...O_T$, compute $P(O \mid \boldsymbol{\lambda})$
  - Direct computation

$$\boxed{\begin{aligned} P(O \mid \boldsymbol{\lambda}) &= \sum_{all\ Q} P(O \mid Q, \boldsymbol{\lambda}) P(Q \mid \boldsymbol{\lambda}) \\ &= \sum_{q_1, q_2, \ldots, q_T} \pi_{q_1} b_{q_1}(O_1) a_{q_1 q_2} b_{q_2}(O_\mathbf{2}) \cdots a_{q_{T-1} q_T} b_{q_T}(O_\mathbf{T}) \end{aligned}}$$

Conditional independence

$$\begin{aligned} P(O \mid Q, \boldsymbol{\lambda}) &= \prod_{t=1}^{T} P(O_t \mid q_t, \boldsymbol{\lambda}) \\ &= b_{q_1}(O_1) b_{q_2}(O_\mathbf{2}) \cdots b_{q_T}(O_\mathbf{T}) \end{aligned}$$

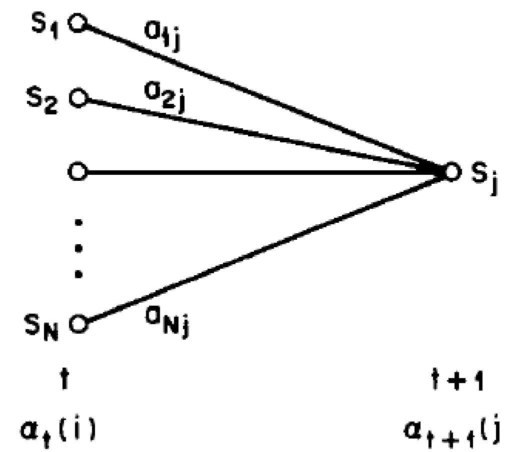
$$P(Q \mid \boldsymbol{\lambda}) = \pi_{q_1} a_{q_1 q_2} a_{q_2 q_3} \cdots a_{q_{T-1} q_T}$$

Markov chain of states

  - Complexity: O(2TN^T)!

- Evaluation: Forward Procedure
  - Define forward variable $\boxed{\alpha_t(i) = P(O_1 O_2 \cdots O_t, q_t = S_i \mid \lambda)}$
  - Initialization $\alpha_1(i) = \pi_i b_i(O_1),\ 1 \le i \le N$
  - Induction

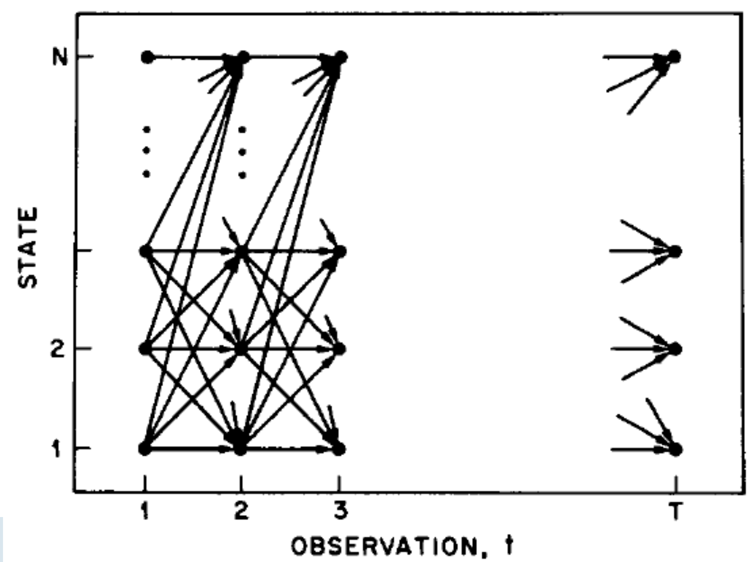
$$\boxed{\begin{gathered}\alpha_{t+1}(j) = \left[\sum_{i=1}^{N} \alpha_t(i) a_{ij}\right] b_j(O_{t+1}), \\ 1 \le t \le T-1, \qquad 1 \le j \le N.\end{gathered}}$$



  - Termination

$$P(O \mid \lambda) = \sum_{i=1}^{N} \alpha_T(i)$$

  - Complexity: O(TN^2)



- Evaluation: Backward Procedure
  - Define backward variable

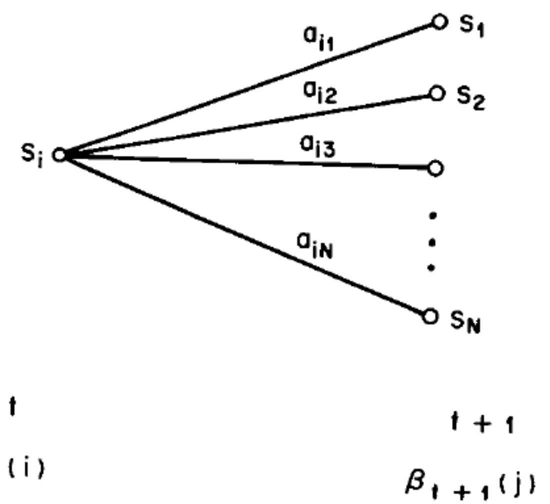
$$\beta_t(i) = P(O_{t+1}, \ldots, O_T \mid q_t = S_i, \lambda)$$

  - Initialization

$$\beta_T(i) = 1, \quad 1 \le i \le N$$

  - Induction

$$\boxed{\begin{gathered}\beta_t(i) = \sum_{j=1}^{N} a_{ij} b_j(O_{t+1}) \beta_{t+1}(j), \\ 1 \le t \le T-1, \quad 1 \le i \le N\end{gathered}}$$



  - Termination

$$P(O \mid \lambda) = \sum_{i=1}^{N} \pi_i b_i(O_1) \beta_1(i) = \sum_{i=1}^{N} \alpha_1(i) \beta_1(i)$$

  - Complexity?

Decoding Problem

- This is Pattern Recognition
- Optimal Sequence of States

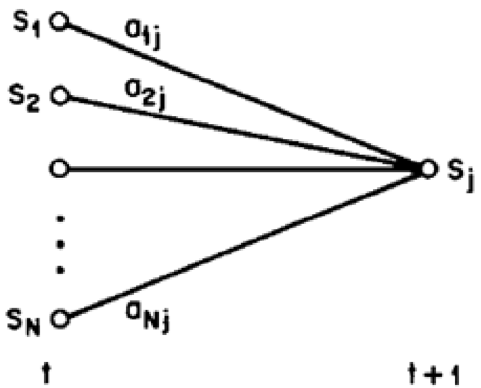
$$\max_{q_1 q_2 \cdots q_T} P(q_1 q_2 \cdots q_T \mid O, \boldsymbol{\lambda}) = \max_{q_1 q_2 \cdots q_T} P(q_1 q_2 \cdots q_T, O \mid \boldsymbol{\lambda})$$

- Viterbi Algorithm (DP: dynamic programming)
  - Define variable

$$\delta_t(i) = \max_{q_1, q_2, \cdots, q_{t-1}} P(q_1 q_2 \cdots q_t = i, O_1 O_2 \cdots O_t / \boldsymbol{\lambda})$$

  - DP

$$\delta_{t+1}(j) = \left[\max_i \delta_t(i) a_{ij} \right] \cdot b_j(O_{t+1})$$



  - Initialization

$$\delta_1(i) = \pi_i b_i(O_1), \quad 1 \le i \le N$$
$$\psi_1(i) = 0.$$

$$\delta_t(i) = \max_{q_1, q_2, \ldots, q_{t-1}} P(q_1 q_2 \cdots q_t = i, O_1 O_2 \cdots O_t \mid \lambda)$$

- Viterbi Algorithm (Cont.)
  - Recursion

$$\boxed{\begin{aligned} &\delta_t(j) = \left[\max_{1\le i\le N} \delta_{t\text{-}1}(i) a_{ij}\right] b_j(O_t), \\ &\psi_{\text{t}}(j) = \arg\max_{1\le i\le N} \delta_{t\text{-}1}(i) a_{ij}, \\ &\quad 2 \le t \le T, \quad 1 \le j \le N \end{aligned}}$$

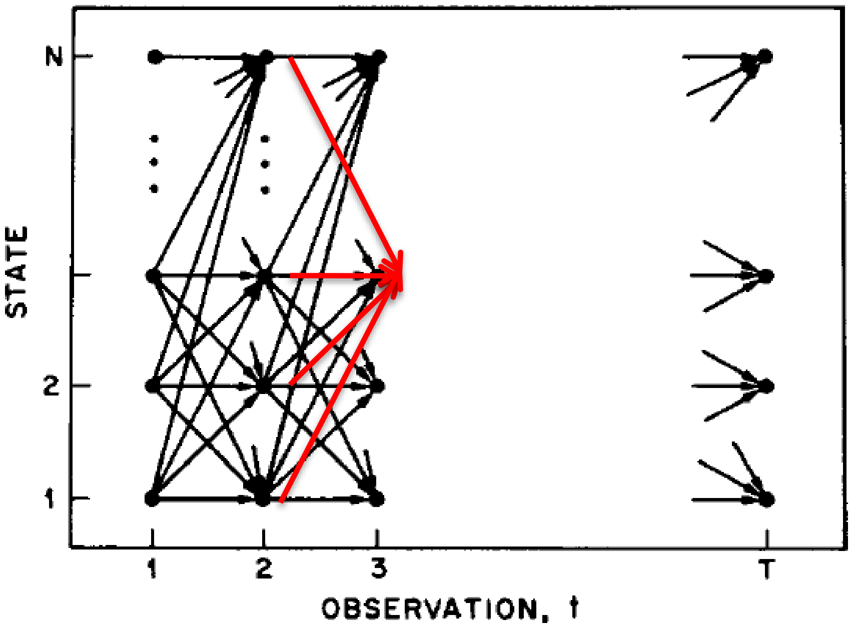
  - Termination

$$P^* = \max_{1\le i\le N} \delta_T(i)$$

$$q_T^{\ *} = \arg\max_{1\le i\le N} \delta_T(i)$$

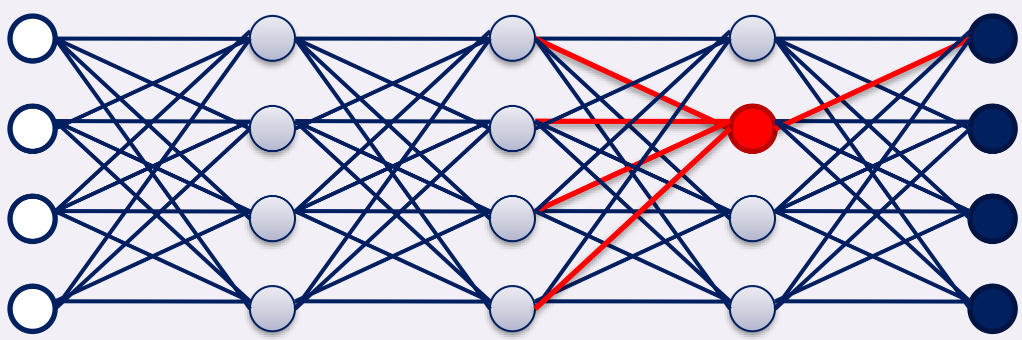
  - Backtracking

$$q_t^* = \psi_{t+1}(q_{t+1}^*),$$
$$1 \le t \le T-1$$



Complexity: O(TN^2)

- Appendix: Dynamic Programming (DP) Principle (Bellman Principle of Optimality)
  - The best path through a particular, intermediate place is the best way from start to it, followed by the best way from it to the goal.
  - Implication: from multiple ways reaching an intermediate place, only retain the best one
  - Often used in sequence matching and HMMs



Training Problem

- Maximum Likelihood (ML) $\max_{A,B,\pi} P(O \mid \lambda)$
- Baum-Welch Algorithm (EM)

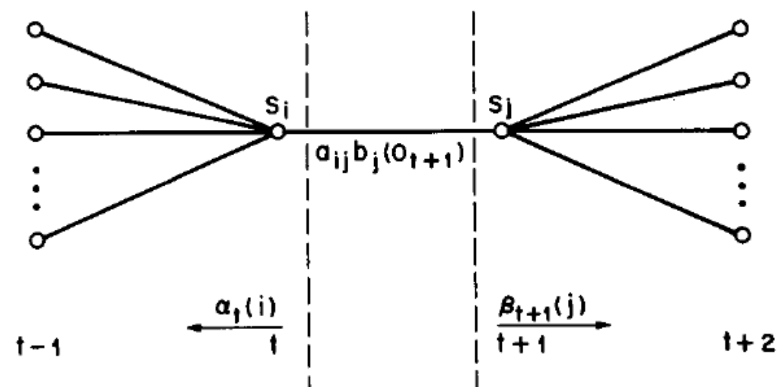
$$\max_{\bar{\lambda}} Q(\lambda, \bar{\lambda}) = \sum_{Q} [\log P(Q, O \mid \bar{\lambda})] P(Q, O \mid \lambda)$$

– Define variable $\boxed{\xi_t(i, j) = P(q_t = S_i, q_{t+1} = S_j \mid O, \boldsymbol{\lambda})}$

$$\xi_t(i, j) = \frac{\alpha_t(i) a_{ij} b_j(O_{t+1}) \beta_{t+1}(j)}{P(O \mid \boldsymbol{\lambda})}$$

$$\alpha_t(i) a_{ij} b_j(O_{t+1}) \beta_{t+1}(j) \leftarrow P(O, q_t = S_i, q_{t+1} = S_j \mid \lambda)$$

$$= \frac{\alpha_t(i) a_{ij} b_j(O_{t+1}) \beta_{t+1}(j)}{\sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_t(i) a_{ij} b_j(O_{t+1}) \beta_{t+1}(j)}$$



– Define probability

$$\gamma_t(i) = P(q_t = S_i \mid O, \boldsymbol{\lambda}) = \frac{\alpha_t(i) \beta_t(i)}{P(O \mid \boldsymbol{\lambda})} = \frac{\alpha_t(i) \beta_t(i)}{\sum_{i=1}^{N} \alpha_t(i) \beta_t(i)} = \sum_{j=1}^{N} \xi_t(i, j)$$

- Baum-Welch Algorithm (Cont.)
  - Reestimation formulas

$$\bar{\pi}_i = \text{expected frequency (number of times) in state } S_i \text{ at time (t=1)} = \gamma_1(i)$$

$$\bar{a}_{ij} = \frac{\text{expected number of transitions from state } S_i \text{ to state } S_j}{\text{expected number of transitions from state } S_i}$$

$$= \frac{\sum_{t=1}^{T-1} \xi_t(i,j)}{\sum_{t=1}^{T-1} \gamma_t(i)} = \frac{\sum_{t=1}^{T-1} \alpha_t(i) a_{ij} b_j(O_{t+1}) \beta_{t+1}(j)}{\sum_{t=1}^{T-1} \alpha_t(i)\beta_t(i)}$$

$$\bar{b}_j(k) = \frac{\text{expected number of times in state } j \text{ and observing symbol } v_k}{\text{expected number of times in state } j}$$

$$= \frac{\sum_{t=1,\ \text{s.t.}\ O_t = v_k}^{T-1} \gamma_t(j)}{\sum_{t=1}^{T-1} \gamma_t(j)} = \frac{\sum_{t=1,\ \text{s.t.}\ O_t = v_k}^{T} \alpha_t(j)\beta_t(j)}{\sum_{t=1}^{T} \alpha_t(j)\beta_t(j)}$$

Continuous Density HMM

- Handling Continuous Observations
  - Continuous features: vector $\boldsymbol{O}_T$
  - Discretization: vector quantization (VQ)
    - Each vector replaced with its closest codevector, which is viewed as a symbol
    - Small codebook: distortion
    - Large codebook: large data required in emission probability estimation
  - Continuous emission density: Gaussian mixture (GM)

$$b_j(O) = \sum_{m=1}^{M} c_{jm} \mathcal{N}(O; \mu_{jm}, U_{jm}), \quad 1 \le j \le N$$

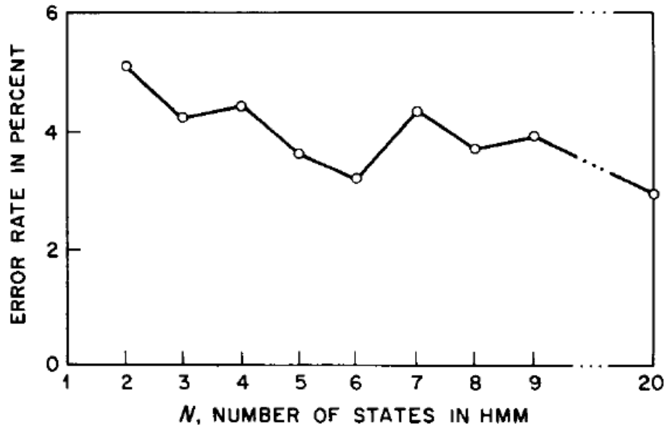
- Parameter Estimation of Continuous HMM (omitted)

Application to Speech Recognition

- Isolated Word Recognition
  - Given HMM λ^v for each word in the vocabulary
  - Input observation sequence ***O***, Bayes decision (assuming equal prior probabilities)

$$v^* = \arg\max_{1\le v\le V} P(\boldsymbol{\lambda}^v \mid O) = \arg\max_{1\le v\le V} P(O \mid \boldsymbol{\lambda}^v)$$

  - Acoustic features ($\boldsymbol{O}_t$) (details omitted)
  - Vector quantization (discrete observation symbols)
  - Choice of model parameters
    - Number of states: empirical (cross-validation), can be equal for all word models
    - Number of components in GM



University of Chinese Academy of Sciences

Extensions of HMM

- Hybrid HMM/Neural
  - HMM: parametric $b_j(O_t)=p(O_t|q_t=S_j)$, conditional independence
  - Neural: discriminative emission probability $p(q_t=S_j|O_t)$
    - Neural network outputs approximate posterior probabilities
  - Replace $p(O_t|q_t)$ with $p(q_t|O_t)/p(q_t)$

$$\frac{p(O_t \mid q_t)}{p(O_t)} = \frac{p(q_t \mid O_t)}{P(q_t)}$$

  - ANN may input multiple frames to learn the correlation

$$p(q_t = S_j \mid \ldots O_{t-1} O_t O_{t+1} \ldots)$$

- Latest: deep neural networks

讨论

- 特征维数与过拟合
  - 克服过拟合的方法？
- 期望最大法(EM)
  - 对数似然度对缺失数据的期望
  - EM for Gaussian mixture
- 隐马尔可夫模型(HMM)
  - Three basic problems
  - Viterbi Algorithm
  - Extensions

下次课内容

- 第4章 非参数法
  - 密度估计
  - Parzen窗方法
  - K近邻估计
  - 最近邻规则
  - 距离度量
  - Reduced Coulomb Energy Network
  - Approximation by Series Expansion