Hidden Markov Models

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Outline

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Definitions and Usage

2 Learning the Model Parameters

- Expectation Maximization for HMM
- The Forward-Backward Procedure

Inferring the State Sequences

- Making Predictions
- 5 Practical Considerations

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Hidden Markov Models

 A Hidden Markov Model (HMM) is a Markov chain where we don't know which state the process X^(t) locates in at any time t

• Let
$$\mathbf{z}^{(t)} \in \{0, 1\}^K$$
 be a vector where $z_i^{(t)} = 1$ if $X^{(t)} = S_i$; 0 otherwise

- $P[z^{(t)} = e_i] = P[X^{(t)} = S_i]$ (for brevity, we use the shorthand $P[z_i^{(t)}]$)
- In HMM, $z^{(t)}$ is hidden (not observable) and is a latent variable
- ullet When a state is visited, however, we can record an observation $x^{(t)}$
 - $P[\mathbf{x}^{(t)}|z_i^{(t)}]$ is called the *emission probability* of state *i* at time *t*
 - Like transition probabilities, the emission probabilities are usually assumed to be *time homogeneous*
 - If we assume that the emission probability of state *i* follows some distribution parametrized by θ_i , we can rewrite it as $P[\mathbf{x}^{(t)}|z_i^{(t)}, \theta_i]$
- Markov chain is a special case of HMM where

•
$$m{x}^{(t)}$$
 must be one of the S_1, \cdots, S_K

• $P[\mathbf{x}^{(t)} = S_j | z_i^{(t)}] = 1$ if i = j; 0 otherwise

Graph Representation



• HMM is a candidate for modeling a problem when we are given a sequence $\mathcal{X} = \{\mathbf{x}^{(t)}\}_{t=1}^{T}$ of observations of length T, where $\mathbf{x}^{(t)}$ are **not** i.i.d.

Goals

- HMM is a candidate for modeling a problem when we are given a sequence $\mathcal{X} = \{\mathbf{x}^{(t)}\}_{t=1}^{T}$ of observations of length T, where $\mathbf{x}^{(t)}$ are **not** i.i.d.
- Generally, we want to perform the following tasks:
- Given \mathcal{X} , learn the parameters $\Theta = (\pi^{(1)}, \mathbf{A}, \{\theta_i\}_{i=1}^{K})$ maximizing the likelihood $P[\mathcal{X}|\Theta]$
 - $\pi^{(1)}$ is the initial state probability
 - **A** is the transition matrix
 - θ_i is the parameter of the emission probability of state i
- **3** Given the learned Θ , infer the hidden state sequence $\mathcal{Z} = \{z^{(t)}\}_t^T$ that generated \mathcal{X} with the highest probability $P[\mathcal{X}|\mathcal{Z}, \Theta]$
- **③** Given the learned Θ , evaluate $P[\mathcal{X}^{new}|\Theta]$ for a new sequence \mathcal{X}^{new}

Applications

- For classification, we can model each class as an HMM
 - Learn the parameter Θ_i of each class C_i using a training sequence $\mathcal{X} = \{\mathbf{x}^{(t)}\}_{t=1}^{T}$ (or a set $\mathcal{X} = \{\mathbf{x}^{(n,t)}\}_{n=1,t=1}^{N,T}$ of *n* training sequences)
 - Predict a new sequence \mathcal{X}^{new} to be in class C_i if the posterior $P[C_i|\mathcal{X}^{new}] \propto P[\mathcal{X}^{new}|\Theta_i]P[C_i]$ is the highest

• Applications:

- Pattern recognition (speech recognition, gesture recognition, handwritten character recognition, etc.)
- Sequential data analysis
- Molecular biology, biochemistry, and genetics, etc.
- One most powerful property of an HMM is that *it can accommodate the local warping (compression/stretching) in the time axis*
 - E.g., the likelihood $P[\mathcal{X}^{new}|\Theta] = \sum_{\mathcal{Z}} P[\mathcal{X}^{new}, \mathcal{Z}|\Theta]$ of a speech \mathcal{X}^{new} will not change dramatically when it is spoken slowly, as \mathcal{Z} having more transitions to the same state will contribute to the likelihood more

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Problem Formulation

- Problem: given a sequence $\mathcal{X} = \{\mathbf{x}^{(t)}\}_{t=1}^{T}$ of observations up to time T, we want to find $\Theta = (\pi^{(1)}, \mathbf{A}, \{\theta_i\}_{i=1}^{K})$ that maximizes $P[\mathcal{X}|\Theta]$
- If we know $\mathcal{Z} = \{z^{(t)}\}_{t=1}^{T}$, we have
 - $P[\mathcal{X}|\Theta] = \sum_{\mathcal{Z}} P[\mathcal{X}, \mathcal{Z}|\Theta]$ • $P[\mathcal{X}, \mathcal{Z}|\Theta] = P[\mathcal{X}|\mathcal{Z}, \Theta]P[\mathcal{Z}|\Theta]$ • $P[\mathcal{Z}|\Theta] = P[z^{(1)}, \cdots, z^{(T)}|\Theta] = P[z^{(2)}, \cdots, z^{(T)}|z^{(1)}, \Theta]P[z^{(1)}|\Theta] = P[z^{(3)}, \cdots, z^{(T)}|z^{(2)}, z^{(1)}, \Theta]P[z^{(2)}|z^{(1)}, \Theta]P[z^{(1)}|\pi^{(1)}] = \cdots = P[z^{(1)}|\pi^{(1)}] \left(\prod_{t=1}^{T-1} P[z^{(t+1)}|z^{(t)}, A]\right)$ • $P[\mathcal{X}|\mathcal{Z}, \Theta] = \prod_{t=1}^{T} P[x^{(t)}|z^{(t)}, \theta_{d(z^{(t)})}]$, where $d(z^{(t)})$ is the index of
 - attribute of $oldsymbol{z}^{(t)}$ equal to 1
- Unfortunately, we don't know Z so Θ cannot be solved analytically
 Solution?

Problem Formulation

- Problem: given a sequence $\mathcal{X} = \{\mathbf{x}^{(t)}\}_{t=1}^{T}$ of observations up to time T, we want to find $\Theta = (\pi^{(1)}, \mathbf{A}, \{\theta_i\}_{i=1}^{K})$ that maximizes $P[\mathcal{X}|\Theta]$
- If we know $\mathcal{Z} = \{z^{(t)}\}_{t=1}^{T}$, we have
 - $P[\mathfrak{X}|\Theta] = \sum_{\mathfrak{Z}} P[\mathfrak{X}, \mathfrak{Z}|\Theta]$ • $P[\mathfrak{X}, \mathfrak{Z}|\Theta] = P[\mathfrak{X}|\mathfrak{Z}, \Theta]P[\mathfrak{Z}|\Theta]$ • $P[\mathfrak{Z}|\Theta] = P[z^{(1)}, \cdots, z^{(T)}|\Theta] = P[z^{(2)}, \cdots, z^{(T)}|z^{(1)}, \Theta]P[z^{(1)}|\Theta] =$ $P[z^{(3)}, \cdots, z^{(T)}|z^{(2)}, z^{(1)}, \Theta]P[z^{(2)}|z^{(1)}, \Theta]P[z^{(1)}|\pi^{(1)}] = \cdots =$ $P[z^{(1)}|\pi^{(1)}] \left(\prod_{t=1}^{T-1} P[z^{(t+1)}|z^{(t)}, A]\right)$ • $P[\mathfrak{Y}|\mathfrak{T}, \Theta] = \prod_{t=1}^{T} P[\mathbf{x}^{(t)}|z^{(t)}, \Theta, \cdots, z^{(t)}]$ where $d(z^{(t)})$ is the index of
 - $P[\mathfrak{X}|\mathfrak{Z}, \Theta] = \prod_{t=1}^{T} P[\mathbf{x}^{(t)}|\mathbf{z}^{(t)}, \theta_{d(\mathbf{z}^{(t)})}]$, where $d(\mathbf{z}^{(t)})$ is the index of attribute of $\mathbf{z}^{(t)}$ equal to 1
- ullet Unfortunately, we don't know ${\mathfrak Z}$ so Θ cannot be solved analytically
- Solution? Since each $z^{(t)}$ is discrete and corresponds to an instance $x^{(t)}$, we can resort to the EM algorithm

• Recall that
$$P[\mathfrak{X}, \mathfrak{Z}|\Theta] = P[\mathfrak{X}|\mathfrak{Z}, \Theta] P[\mathfrak{Z}|\Theta] = \left(\prod_{s=1}^{T} P[\mathbf{x}^{(s)}|\mathbf{z}^{(s)}, \theta_{d(\mathbf{z}^{(s)})}]\right) P[\mathbf{z}^{(1)}|\mathbf{\pi}^{(1)}] \left(\prod_{t=1}^{T-1} P[\mathbf{z}^{(t+1)}|\mathbf{z}^{(t)}, \mathbf{A}]\right)$$

• $\mathfrak{Q}(\Theta; \Theta^{old}) = E_{\mathfrak{Z}} \left[\ln \left(P[\mathfrak{X}, \mathfrak{Z}|\Theta] \right) |\mathfrak{X}, \Theta^{old} \right]$
 $= \sum_{\mathfrak{Z}} \ln \left(P[\mathfrak{X}, \mathfrak{Z}|\Theta] \right) P[\mathfrak{Z}|\mathfrak{X}, \Theta^{old}]$
 $= \sum_{\mathfrak{Z}} \ln \left(P[\mathbf{z}^{(1)}|\mathbf{\pi}^{(1)}] \right) P[\mathfrak{Z}|\mathfrak{X}, \Theta^{old}]$
 $+ \sum_{\mathfrak{Z}} \ln \left(\prod_{t=1}^{T-1} P[\mathbf{z}^{(t+1)}|\mathbf{z}^{(t)}, \mathbf{A}] \right) P[\mathfrak{Z}|\mathfrak{X}, \Theta^{old}]$
 $+ \sum_{\mathfrak{Z}} \ln \left(\prod_{t=1}^{T} P[\mathbf{x}^{(t)}|\mathbf{z}^{(t)}, \theta_{d(\mathbf{z}^{(t)})}] \right) P[\mathfrak{Z}|\mathfrak{X}, \Theta^{old}]$

$$\begin{split} & \text{The first term } \sum_{\mathcal{Z}} \ln \left(P[z^{(1)} | \pi^{(1)}] \right) P[\mathcal{Z} | \mathcal{X}, \Theta^{old}] \\ &= \sum_{\mathcal{Z}} \ln \left(\pi^{(1)}_{d(z^{(1)})} \right) P[\mathcal{Z} | \mathcal{X}, \Theta^{old}] \\ &= \sum_{z^{(1)} = e_1}^{e_K} \cdots \sum_{z^{(T)} = e_1}^{e_K} \ln \left(\pi^{(1)}_{d(z^{(1)})} \right) P[z^{(1)}, \cdots, z^{(T)} | \mathcal{X}, \Theta^{old}] \\ &= \sum_{z^{(1)} = e_1}^{e_K} \ln \left(\pi^{(1)}_{d(z^{(1)})} \right) \sum_{z^{(2)} = e_1}^{e_K} \cdots \sum_{z^{(T)} = e_1}^{e_K} P[z^{(1)}, \cdots, z^{(T)} | \mathcal{X}, \Theta^{old}] \\ &= \sum_{z^{(1)} = e_1}^{e_K} \ln \left(\pi^{(1)}_{d(z^{(1)})} \right) P[z^{(1)} | \mathcal{X}, \Theta^{old}] \\ &= \sum_{i=1}^{K} \ln \left(\pi^{(1)}_i \right) P[z^{(1)}_i | \mathcal{X}, \Theta^{old}] \end{split}$$

$$\begin{split} & \text{The second term } \sum_{\mathcal{Z}} \ln \left(\prod_{t=1}^{T-1} P[z^{(t+1)} | z^{(t)}, \mathbf{A}] \right) P[\mathcal{Z} | \mathcal{X}, \Theta^{old}] \\ &= \sum_{\mathcal{Z}} \sum_{t=1}^{T-1} \ln \left(P[z^{(t+1)} | z^{(t)}, \mathbf{A}] \right) P[\mathcal{Z} | \mathcal{X}, \Theta^{old}] \\ &= \sum_{t=1}^{T-1} \sum_{z^{(1)} = \mathbf{e}_{1}}^{\mathbf{e}_{K}} \cdots \sum_{z^{(T)} = \mathbf{e}_{1}}^{\mathbf{e}_{K}} \ln \left(P[z^{(t+1)} | z^{(t)}, \mathbf{A}] \right) P[z^{(1)}, \cdots, z^{(T)} | \mathcal{X}, \Theta^{old}] \\ &= \sum_{t=1}^{T-1} \sum_{z^{(t)} = \mathbf{e}_{1}}^{\mathbf{e}_{K}} \sum_{z^{(t+1)} = \mathbf{e}_{1}}^{\mathbf{e}_{K}} \ln \left(P[z^{(t+1)} | z^{(t)}, \mathbf{A}] \right) \sum_{z^{(1)} = \mathbf{e}_{1}}^{\mathbf{e}_{K}} \cdots \sum_{z^{(t-1)} = \mathbf{e}_{1}}^{\mathbf{e}_{K}} \\ &= \sum_{t=1}^{T-1} \sum_{z^{(t)} = \mathbf{e}_{1}}^{\mathbf{e}_{K}} \sum_{z^{(t+1)} = \mathbf{e}_{1}}^{\mathbf{e}_{K}} \ln \left(P[z^{(t+1)} | z^{(t)}, \mathbf{A}] \right) P[z^{(t)}, z^{(t+1)} | \mathcal{X}, \Theta^{old}] \\ &= \sum_{t=1}^{T-1} \sum_{z^{(t)} = \mathbf{e}_{1}}^{\mathbf{K}} \sum_{z^{(t+1)} = \mathbf{e}_{1}}^{\mathbf{e}_{K}} \ln \left(P[z^{(t+1)} | z^{(t)}, \mathbf{A}] \right) P[z^{(t)}_{i}, z^{(t+1)} | \mathcal{X}, \Theta^{old}] \\ &= \sum_{t=1}^{T-1} \sum_{i=1}^{K} \sum_{j=1}^{K} \ln \left(e_{i,j} \right) P[z^{(t)}_{i}, z^{(t+1)} | \mathcal{X}, \Theta^{old}] \end{split}$$

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Formulating $\Omega(\Theta; \Theta^{old})$ (4/4)

• Similarly, the third term

$$\sum_{\mathcal{Z}} \ln \left(\prod_{t=1}^{T} P[\mathbf{x}^{(t)} | z^{(t)}, \theta_{d(z^{(t)})}] \right) P[\mathcal{Z} | \mathcal{X}, \Theta^{old}] =$$

$$\sum_{t=1}^{T} \sum_{i=1}^{K} \ln \left(P[\mathbf{x}^{(t)} | z_i^{(t)}, \theta_i] \right) P[z_i^{(t)} | \mathcal{X}, \Theta^{old}] \text{ [Proof]}$$
• $\mathcal{Q}(\Theta; \Theta^{old}) = \sum_{i=1}^{K} \ln \left(\pi_i^{(1)} \right) P[z_i^{(1)} | \mathcal{X}, \Theta^{old}]$

$$+ \sum_{t=1}^{T-1} \sum_{i=1}^{K} \sum_{j=1}^{K} \ln (a_{i,j}) P[z_i^{(t)}, z_j^{(t+1)} | \mathcal{X}, \Theta^{old}]$$

$$+ \sum_{t=1}^{T} \sum_{i=1}^{K} \ln \left(P[\mathbf{x}^{(t)} | z_i^{(t)}, \theta_i] \right) P[z_i^{(t)} | \mathcal{X}, \Theta^{old}]$$
• In the E-step, we need to evaluate $P[z_i^{(t)} | \mathcal{X}, \Theta^{old}]$ and $P[z_i^{(t)}, z_j^{(t+1)} | \mathcal{X}, \Theta^{old}]$ for all t (to be discussed later)
• After the evaluation, we denote $\gamma_i^{(t)} = P[z_i^{(t)} | \mathcal{X}, \Theta^{old}]$ and

• After the evaluation, we denote $\gamma_i^{(s)} = P[z_i^{(s)} | \mathcal{X}, \Theta^{old}]$ and $\xi_{i,j}^{(t)} = P[z_i^{(t)}, z_j^{(t+1)} | \mathcal{X}, \Theta^{old}]$ respectively as constants in the M-step • $\gamma_i^{(t)} = \sum_{j=1}^{K} \xi_{i,j}^{(t)}$ and $\sum_{i=1}^{K} \gamma_i^{(t)} = 1$

Solving Θ

• Problem: $\arg_{\Theta = (\pi^{(1)}, \mathbf{A}, \{\theta_i\}_{i=1}^K)} \max \Omega(\Theta; \Theta^{old})$, where

•
$$Q(\Theta; \Theta^{old}) = \sum_{i=1}^{K} \ln\left(\pi_{i}^{(1)}\right) \gamma_{i}^{(1)} + \sum_{t=1}^{T-1} \sum_{i=1}^{K} \sum_{j=1}^{K} \ln\left(a_{i,j}\right) \xi_{i,j}^{(t)}$$

 $+ \sum_{t=1}^{T} \sum_{i=1}^{K} \ln\left(P[\mathbf{x}^{(t)}|z_{i}^{(t)}, \theta_{i}]\right) \gamma_{i}^{(t)}$

Subject to

•
$$\sum_{i=1}^{K} \pi_i^{(1)} = 1$$

• $\sum_{j=1}^{K} a_{i,j} = 1$ for all $1 \leq i \leq K$

• We can solve $\pi^{(1)}$, **A**, and $\{\theta_i\}_{i=1}^K$ by considering only the first, second, and third terms respectively

- Lagrangian: $L(\pi^{(1)}, \alpha) = \sum_{i=1}^{K} \ln\left(\pi_i^{(1)}\right) \gamma_i^{(1)} \alpha\left(\sum_{i=1}^{K} \pi_i^{(1)} 1\right)$

$$\pi_{i}^{(1)} = \frac{\gamma_{i}^{(1)}}{\sum_{i=1}^{K} \gamma_{i}^{(1)}} = \gamma_{i}^{(1)}$$

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- Lagrangian: $L(\mathbf{A}, \{\alpha_i\}_{i=1}^{K}) = \sum_{t=1}^{T-1} \sum_{i=1}^{K} \sum_{j=1}^{K} \ln(a_{ij}) \xi_{i,j}^{(t)} \sum_{i=1}^{K} \alpha_i \left(\sum_{j=1}^{K} a_{i,j} 1 \right)$
- Taking the partial derivatives of *L* with respect to $a_{i,j}$ and α_i and then setting them to zero we have $\frac{\sum_{t=1}^{T-1} \xi_{i,j}^{(t)}}{a_{i,j}} \alpha_i = 0 \Rightarrow a_{i,j} = \frac{\sum_{t=1}^{T-1} \xi_{i,j}^{(t)}}{\alpha_i}$ and $\sum_{j=1}^{K} a_{i,j} = 1$ for all $1 \leq i \leq K$
- Summing the equations for $a_{i,j}$ along j we have

$$\alpha_i = \sum_{j=1}^{K} \sum_{t=1}^{T-1} \xi_{i,j}^{(t)}, \text{ and therefore } a_{i,j} = \frac{\sum_{t=1}^{T-1} \xi_{i,j}^{(t)}}{\sum_{t=1}^{T-1} \sum_{j=1}^{K} \xi_{i,j}^{(t)}} = \frac{\sum_{t=1}^{T-1} \xi_{i,j}^{(t)}}{\sum_{t=1}^{T-1} \gamma_i^{(t)}}$$

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- Problem: finding $\{\theta_k\}_{k=1}^K$ such that $\sum_{t=1}^T \sum_{k=1}^K \ln\left(P[\mathbf{x}^{(t)}|z_k^{(t)}, \theta_k]\right) \gamma_k^{(t)}$ is maximized
- Suppose x^(t) is discrete such that x_i^(t) = 1 if the predefined value O_i from {O₁, ..., O_d} is observed; 0 otherwise
- We can assume that the emission probability $P[\mathbf{x}^{(t)}|z_k^{(t)}, \theta_k] = \prod_{i=1}^d b_{k,i}^{x_i^{(t)}}$ follows the multinomial distribution where $\theta_k = \{b_{k,i}\}_{i=1}^d$ and $b_{k,i}$ is the probability that O_i is observed in state k• $\sum_{i=1}^d b_{k,i} = 1$

Solving $\{\theta_i\}_{i=1}^{K}$ (2/3)

- Lagrangian: $L(\{b_{k,i}\}_{k=1,i=1}^{K,d}, \{\alpha_k\}_{k=1}^{K}) = \sum_{t=1}^{T} \sum_{k=1}^{K} \ln\left(\prod_{i=1}^{d} b_{k,i}^{x_i^{(t)}}\right) \gamma_k^{(t)} \sum_{k=1}^{K} \alpha_k \left(\sum_{i=1}^{d} b_{k,i} 1\right) = \sum_{t=1}^{T} \sum_{k=1}^{K} \sum_{i=1}^{d} x_i^{(t)} \ln(b_{k,i}) \gamma_k^{(t)} \sum_{k=1}^{K} \alpha_k \left(\sum_{i=1}^{d} b_{k,i} 1\right)$
- Taking the partial derivatives of *L* with respect to $b_{k,i}$ and α_k and then setting them to zero we have $\frac{\sum_{t=1}^{T} x_i^{(t)} \gamma_k^{(t)}}{b_{k,i}} \alpha_k = 0 \Rightarrow b_{k,i} = \frac{\sum_{t=1}^{T} x_i^{(t)} \gamma_k^{(t)}}{\alpha_k} \text{ and } \sum_{i=1}^{d} b_{k,i} = 1 \text{ for all } 1 \leq k \leq K$
- Summing the equations for $b_{k,i}$ along i we have $\alpha_k = \sum_{i=1}^d \sum_{t=1}^T x_i^{(t)} \gamma_k^{(t)}$, and therefore $b_{k,i} = \frac{\sum_{t=1}^T x_i^{(t)} \gamma_k^{(t)}}{\sum_{t=1}^T \gamma_k^{(t)} \sum_{i=1}^d x_i^{(t)}} = \frac{\sum_{t=1}^T x_i^{(t)} \gamma_k^{(t)}}{\sum_{t=1}^T \gamma_k^{(t)}}$

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• What if $x^{(t)}$ are continuous?

- What if $x^{(t)}$ are continuous?
- We can assume that $P[x^{(t)}|z_k^{(t)}, \theta_k]$ follows the multivariate normal distribution where $\theta_k = (\mu_k, \Sigma_k)$
- It can be shown that

•
$$\boldsymbol{\mu}_{k} = \frac{\sum_{t=1}^{T} \boldsymbol{\gamma}_{k}^{(t)} \boldsymbol{x}^{(t)}}{\sum_{t=1}^{T} \boldsymbol{\gamma}_{k}^{(t)}}$$

•
$$\boldsymbol{\Sigma}_{k} = \frac{\sum_{t=1}^{T} \boldsymbol{\gamma}_{k}^{(t)} (\boldsymbol{x}^{(t)} - \boldsymbol{\mu}_{k}) (\boldsymbol{x}^{(t)} - \boldsymbol{\mu}_{k})^{\top}}{\sum_{t=1}^{T} \boldsymbol{\gamma}_{k}^{(t)}}$$
[Homework]

Learning form Multiple Sequences

• Suppose we are given a set $\mathcal{X} = \{x^{(n,t)}\}_{n=1,t=1}^{N,T}$ of observation sequences, where sequences are independent with each other

•
$$P[\mathfrak{X}|\Theta] = \prod_{n=1}^{N} P[\mathfrak{X}^{(n)}|\Theta]$$
, where $\mathfrak{X}^{(n)} = \{\mathbf{x}^{(n,t)}\}_{t=1}^{T}$

• Then for discrete $x^{(t)}$ with multinomial emission probability:

•
$$\pi_i^{(1)} = \frac{\sum_{n=1}^{N} \gamma_i^{(n,1)}}{N}$$

• $a_{i,j} = \frac{\sum_{n=1}^{N} \sum_{t=1}^{T-1} \xi_{i,j}^{(n,t)}}{\sum_{n=1}^{N} \sum_{t=1}^{T-1} \gamma_i^{(n,t)}}$
• $b_{k,i} = \frac{\sum_{n=1}^{N} \sum_{t=1}^{T} \chi_i^{(n,t)} \gamma_k^{(n,t)}}{\sum_{n=1}^{N} \sum_{t=1}^{T} \gamma_k^{(n,t)}}$

• This is analogous to the estimators of a Markov chain we have seen previously, except that $\gamma_i^{(t)} = P[z_i^{(t)}|\mathcal{X}, \Theta^{old}]$ and $\xi_{i,j}^{(t)} = P[z_i^{(t)}, z_j^{(t+1)}|\mathcal{X}, \Theta^{old}]$ are *soft counts* of state visits

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We Are Not Done Yet

• Given Θ^{old} , in the E-step we need to evaluate $\gamma_i^{(t)}$ and $\xi_{i,i}^{(t)}$

•
$$\gamma_i^{(t)} = P[z_i^{(t)} | \mathcal{X}, \Theta^{old}] = \frac{P[\mathcal{X}, z_i^{(t)} | \Theta^{old}]}{P[\mathcal{X} | \Theta^{old}]}$$

• $\xi_{i,j}^{(t)} = P[z_i^{(t)}, z_j^{(t+1)} | \mathcal{X}, \Theta^{old}] = \frac{P[\mathcal{X}, z_i^{(t)}, z_j^{(t+1)} | \Theta^{old}]}{P[\mathcal{X} | \Theta^{old}]}$

• We can evaluate $\gamma_i^{(t)}$ and $\xi_{i,j}^{(t)}$ by considering all possible state sequences:

•
$$P[\mathcal{X}|\Theta^{old}] = \sum_{\mathcal{Z}} P[\mathcal{X}, \mathcal{Z}|\Theta^{old}]$$

• $P[\mathcal{X}, z_i^{(t)}|\Theta^{old}] = \sum_{\mathcal{Z}, z^{(t)} = e_i} P[\mathcal{X}, \mathcal{Z}|\Theta^{old}]$

- However, there are exponentially many sequences (specifically, K^T and K^{T-1} for $P[\mathcal{X}|\Theta^{old}]$ and $P[\mathcal{X}, z_i^{(t)}|\Theta^{old}]$ respectively)
- The evaluation would be very slow, if not infeasible
- Better idea?

We Are Not Done Yet

• Given Θ^{old} , in the E-step we need to evaluate $\gamma_i^{(t)}$ and $\xi_{i,i}^{(t)}$

•
$$\gamma_i^{(t)} = P[z_i^{(t)} | \mathfrak{X}, \Theta^{old}] = \frac{P[\mathfrak{X}, z_i^{(t)} | \Theta^{old}]}{P[\mathfrak{X} | \Theta^{old}]}$$

• $\xi_{i,j}^{(t)} = P[z_i^{(t)}, z_j^{(t+1)} | \mathfrak{X}, \Theta^{old}] = \frac{P[\mathfrak{X}, z_i^{(t)}, z_j^{(t+1)} | \Theta^{old}]}{P[\mathfrak{X} | \Theta^{old}]}$

• We can evaluate $\gamma_i^{(t)}$ and $\xi_{i,j}^{(t)}$ by considering all possible state sequences:

•
$$P[\mathcal{X}|\Theta^{old}] = \sum_{\mathcal{Z}} P[\mathcal{X}, \mathcal{Z}|\Theta^{old}]$$

• $P[\mathcal{X}, z_i^{(t)}|\Theta^{old}] = \sum_{\mathcal{Z}, z^{(t)}=e_i} P[\mathcal{X}, \mathcal{Z}|\Theta^{old}]$

- However, there are exponentially many sequences (specifically, K^T and K^{T-1} for $P[\mathcal{X}|\Theta^{old}]$ and $P[\mathcal{X}, z_i^{(t)}|\Theta^{old}]$ respectively)
- The evaluation would be very slow, if not infeasible
- Better idea? for all $t \Rightarrow$ belief propagation

Forward-Backward Procedure

- There is an algorithm, called the *forward-backward procedure*, that provides an efficient way to evaluate γ^(t)_i and ξ^(t)_{i,i}
- Given a $\Theta = (\pi^{(1)}, \mathbf{A}, \{\theta_i\}_{i=1}^K)$, define the *forward variable* as $\alpha_i^{(t)} = P[\mathbf{x}^{(1)}, \cdots, \mathbf{x}^{(t)}, z_i^{(t)} | \Theta]$
 - $\alpha_i^{(t)}$ denotes the probability that a partial sequence $\{x^{(1)}, \dots, x^{(t)}\}$ until time t is observed while the state ends in S_i at time t
- Similarly, define the **backward variable** as $\beta_i^{(t)} = P[\mathbf{x}^{(t+1)}, \cdots, \mathbf{x}^{(T)} | z_i^{(t)}, \Theta]$
 - $\beta_i^{(t)}$ denotes the probability that a partial sequence $\{x^{(t+1)}, \dots, x^{(T)}\}$ after time t will be observed given a starting state S_i at time t
- We can express $\gamma_i^{(t)}$ and $\xi_{i,j}^{(t)}$ using the forward/backward variables: $\gamma_i^{(t)} = \frac{\alpha_i^{(t)}\beta_i^{(t)}}{\sum_{j=1}^K \alpha_j^{(t)}\beta_j^{(t)}} \text{ and } \xi_{i,j}^{(t)} = \frac{\alpha_i^{(t)}a_{i,j}P[\mathbf{x}^{(t+1)}|z_j^{(t+1)},\theta_j]\beta_j^{(t+1)}}{\sum_{k=1}^K \sum_{l=1}^K \alpha_k^{(t)}a_{k,l}P[\mathbf{x}^{(t+1)}|z_l^{(t+1)}|z_l^{(t+1)},\theta_l]\beta_l^{(t+1)}}$

Expressing $\gamma_i^{(t)}$ Using $\alpha_i^{(t)}$ And $\beta_i^{(t)}$

•
$$\gamma_i^{(t)} = P[z_i^{(t)} | \mathcal{X}, \Theta] = \frac{P[\mathcal{X}, z_i^{(t)} | \Theta]}{P[\mathcal{X} | \Theta]} = \frac{P[\mathcal{X} | z_i^{(t)}, \Theta] P[z_i^{(t)} | \Theta]}{P[\mathcal{X} | \Theta]}$$

$$= \frac{P[\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(t)} | z_i^{(t)}, \Theta] P[\mathbf{x}^{(t+1)}, \dots, \mathbf{x}^{(T)} | z_i^{(t)}, \Theta] P[z_i^{(t)} | \Theta]}{P[\mathcal{X} | \Theta]}$$

$$= \frac{P[\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(t)} z_i^{(t)}, |\Theta] P[\mathbf{x}^{(t+1)}, \dots, \mathbf{x}^{(T)} | z_i^{(t)}, \Theta]}{P[\mathcal{X} | \Theta]}$$

$$= \frac{\alpha_i^{(t)} \beta_i^{(t)}}{P[\mathcal{X} | \Theta]} = \frac{\alpha_i^{(t)} \beta_i^{(t)}}{\sum_{j=1}^{K} P[\mathcal{X}, z_j^{(t)} | \Theta]} = \frac{\alpha_i^{(t)} \beta_i^{(t)}}{\sum_{j=1}^{K} \alpha_j^{(t)} \beta_j^{(t)}}$$

- The numerator $\alpha_i^{(t)}\beta_i^{(t)}$ explains the whole observation sequence $\{x^{(1)}, \cdots, x^{(t)}\}$ and that at time t, the state is S_i
- $\alpha_i^{(t)} \beta_i^{(t)}$ is normalized by dividing over all possible intermediate states at time t to ensure that $\sum_{i=1}^{K} \gamma_i^{(t)} = 1$

Expressing $\xi_{i,i}^{(t)}$ Using $\alpha_i^{(t)}$ And $\beta_i^{(t)}$ (1/2)

$$\begin{split} \bullet \ & \xi_{i,j}^{(t)} = P[z_i^{(t)}, z_j^{(t+1)} | \mathcal{X}, \Theta] = \frac{P[\mathcal{X}, z_i^{(t)}, z_j^{(t+1)} | \Theta]}{P[\mathcal{X}|\Theta]} \\ &= \frac{P[\mathcal{X}|z_i^{(t)}, z_j^{(t+1)}, \Theta] P[z_i^{(t)}, z_j^{(t+1)} | \Theta]}{P[\mathcal{X}|\Theta]} \\ &= \frac{P[\mathcal{X}|z_i^{(t)}, z_j^{(t+1)}, \Theta] P[z_j^{(t+1)} | z_i^{(t)}, \Theta] P[z_i^{(t)} | \Theta]}{P[\mathcal{X}|\Theta]} \\ &= \left(\frac{1}{P[\mathcal{X}|\Theta]}\right) P[\mathbf{x}^{(1)} \cdots, \mathbf{x}^{(t)} | z_i^{(t)}, \Theta] P[\mathbf{x}^{(t+1)} | z_j^{(t+1)}, \Theta] \\ &P[\mathbf{x}^{(t+2)} \cdots, \mathbf{x}^{(T)} | z_j^{(t+1)}, \Theta] a_{i,j} P[z_i^{(t)} | \Theta] \\ &= \frac{P[\mathbf{x}^{(1)} \cdots, \mathbf{x}^{(t)}, z_i^{(t)} | \Theta] P[\mathbf{x}^{(t+1)} | z_j^{(t+1)}, \Theta] P[\mathbf{x}^{(t+2)} \cdots, \mathbf{x}^{(T)} | z_j^{(t+1)}, \Theta] a_{i,j}}{P[\mathcal{X}|\Theta]} \\ &= \frac{\alpha_i^{(t)} a_{i,j} P[\mathbf{x}^{(t+1)} | z_j^{(t+1)}, \Theta] \beta_j^{(t+1)}}{P[\mathcal{X}|\Theta]} = \frac{\alpha_i^{(t)} a_{i,j} P[\mathbf{x}^{(t+1)} | z_j^{(t+1)}, \Theta] \beta_j^{(t+1)}}{\sum_{k=1}^{K} \sum_{l=1}^{K} P[\mathcal{X}, z_k^{(t)}, z_l^{(t+1)} | \Theta]} \\ &= \frac{\alpha_i^{(t)} a_{i,j} P[\mathbf{x}^{(t+1)} | z_j^{(t+1)} | z_j^{(t+1)}, \Theta] \beta_j^{(t+1)}}}{\sum_{k=1}^{K} \sum_{l=1}^{K} P[\mathcal{X}, z_k^{(t)}, z_l^{(t+1)} | \Theta]} \end{aligned}$$

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Expressing $\xi_{i,i}^{(t)}$ Using $\alpha_i^{(t)}$ And $\beta_i^{(t)}$ (2/2)

•
$$\xi_{i,j}^{(t)} = \frac{\alpha_i^{(t)} a_{ij} P[x^{(t+1)} | z_j^{(t+1)}, \theta_j] \beta_j^{(t+1)}}{\sum_{k=1}^{K} \sum_{l=1}^{K} \alpha_k^{(t)} a_{k,l} P[x^{(t+1)} | z_l^{(t+1)}, \theta_l] \beta_l^{(t+1)}}$$

- α_i^(t) in the numerator explains the first t observations and ends in state S_i at time t
- At time t + 1, the process moves on to sate S_j with probability $a_{i,j}$, and generates the (t + 1)st observation
- Continue from S_j at time t+1, $\beta_j^{(t+1)}$ explains the rest observations
- Finally, normalize by dividing all possible pairs of states at time t and t+1

Evaluating $\alpha_i^{(t)}$ And $\beta_i^{(t)}$ (1/2)

• The merit of the forward-backward procedure is that $\alpha_i^{(t)}$ and $\beta_i^{(t)}$ can be evaluated efficiently • $\alpha_i^{(1)} = P[\mathbf{x}^{(1)}, z_i^{(1)}|\Theta] = P[\mathbf{x}^{(1)}|z_i^{(1)}, \Theta]P[z_i^{(1)}|\Theta] = P[\mathbf{x}^{(1)}|z_i^{(1)}, \Theta_i]\pi_i^{(1)}$ • $\alpha_i^{(t+1)} = P[\mathbf{x}^{(1)}, \cdots, \mathbf{x}^{(t+1)}, z_i^{(t+1)}|\Theta] =$ $P[\mathbf{x}^{(1)}, \cdots, \mathbf{x}^{(t+1)} | z_i^{(t+1)}, \Theta] P[z_i^{(t+1)} | \Theta]$ $= P[\mathbf{x}^{(1)}, \cdots, \mathbf{x}^{(t)} | z_i^{(t+1)}, \Theta] P[\mathbf{x}^{(t+1)} | z_i^{(t+1)}, \Theta] P[z_i^{(t+1)} | \Theta]$ $= P[\mathbf{x}^{(1)}, \cdots, \mathbf{x}^{(t)}, z_i^{(t+1)} | \Theta] P[\mathbf{x}^{(t+1)} | z_i^{(t+1)}, \Theta]$ $= P[\mathbf{x}^{(t+1)}|z_i^{(t+1)}, \Theta] \sum_{i=1}^{K} P[\mathbf{x}^{(1)}, \cdots, \mathbf{x}^{(t)}, z_i^{(t)}, z_i^{(t+1)}|\Theta]$ $= P[\mathbf{x}^{(t+1)}|z_i^{(t+1)}, \Theta] \sum_{i=1}^{K} P[\mathbf{x}^{(1)}, \cdots, \mathbf{x}^{(t)}, z_i^{(t+1)}|z_i^{(t)}, \Theta] P[z_i^{(t)}|\Theta]$ $= P[\mathbf{x}^{(t+1)}|z_{i}^{(t+1)},\Theta]$ $\sum_{i=1}^{K} P[\mathbf{x}^{(1)}, \cdots, \mathbf{x}^{(t)} | z_i^{(t)}, \Theta] P[z_i^{(t+1)} | z_i^{(t)}, \Theta] P[z_i^{(t)} | \Theta]$ $= P[\mathbf{x}^{(t+1)}|z_i^{(t+1)}, \Theta] \sum_{i=1}^{K} P[\mathbf{x}^{(1)}, \cdots, \mathbf{x}^{(t)}, z_i^{(t)}|\Theta] P[z_i^{(t+1)}|z_i^{(t)}, \Theta]$ $= \left(\sum_{i=1}^{K} \alpha_{i}^{(t)} a_{i,i}\right) P[\mathbf{x}^{(t+1)} | z_{i}^{(t+1)}, \theta_{i}]$

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Evaluating $\alpha_i^{(t)}$ And $\beta_i^{(t)}$ (2/2)

• Based on the recurrence relation $\begin{cases} \alpha_i^{(1)} = P[\mathbf{x}^{(1)}|z_i^{(1)}, \theta_i]\pi_i^{(1)} \\ \alpha_j^{(t+1)} = \left(\sum_{i=1}^{K} \alpha_i^{(t)} a_{i,j}\right) P[\mathbf{x}^{(t+1)}|z_j^{(t+1)}, \theta_j] \\ optimal substructure that it can be evaluated efficiently within$

O(K) time if all $lpha_i^{(t)}$, $1\leqslant i\leqslant K$, are known

- We can evaluate all $\alpha_i^{(t)}$, $1 \leq i \leq K$ and $1 \leq t \leq T$, within $O(K^2T)$ time using the dynamic programming from t = 1 to T
- Similarly, we can derive the recurrence relation for $\beta_i^{(t)}$ as $\begin{cases} \beta_i^{(T)} = 1 \\ \beta_i^{(t)} = \sum_{j=1}^{K} a_{i,j} P[\mathbf{x}^{(t+1)} | z_j^{(t+1)}, \theta_j] \beta_j^{(t+1)} \end{cases} \text{ [Proof]}$

• All $\beta_i^{(t)}$ can also be evaluated within $O(K^2T)$ time from t = T to 1

- Once obtaining $\alpha_i^{(t)}$ and $\beta_i^{(t)}$, we can derive all $\gamma_i^{(t)}$ and $\xi_{i,j}^{(t)}$ within O(K) and $O(K^2)$ time respectively
- The total time complexity for an E-step is $O(K^2 T)$

The recurrence relations







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NetDB-ML, Spring 2015

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- Problem: given a sequence \mathcal{X} and parameters Θ , we want to infer the hidden state sequence $\mathcal{Z}^* = \{z^{(t)}\}_t^T$ such that it has the highest posterior $P[\mathcal{Z}|\mathcal{X}, \Theta]$
 - ullet This helps us understand the "reason" behind ${\mathfrak X}$
 - A common task in time series analysis
- Since $P[\mathcal{Z}|\mathcal{X}, \Theta] = \frac{P[\mathcal{X}, \mathcal{Z}|\Theta]}{P[\mathcal{X}|\Theta]}$ and $P[\mathcal{X}|\Theta]$ is independent with \mathcal{Z} , we only need to find \mathcal{Z}^* maximizing $P[\mathcal{X}, \mathcal{Z}|\Theta]$
- Objective: $\arg_{\mathcal{Z}} \max P[\mathcal{X}, \mathcal{Z}|\Theta]$
- \bullet We can try out all possible $\mathcal{Z},$ at the cost of exponential time complexity
- Efficient solution?

The Optimal Substructure

•
$$P[\mathfrak{X}, \mathfrak{Z}|\Theta] = P[\mathfrak{X}|\mathfrak{Z}, \Theta] P[\mathfrak{Z}|\Theta]$$

= $\left(\prod_{s=1}^{T} P[\mathbf{x}^{(s)}|\mathbf{z}^{(s)}, \theta_{d(\mathbf{z}^{(s)})}]\right) P[\mathbf{z}^{(1)}|\pi^{(1)}] \left(\prod_{t=1}^{T-1} P[\mathbf{z}^{(t+1)}|\mathbf{z}^{(t)}, \mathbf{A}]\right)$
= $\left(P[\mathbf{z}^{(1)}|\pi^{(1)}] P[\mathbf{x}^{(1)}|\mathbf{z}^{(1)}, \theta_{d(\mathbf{z}^{(1)})}]\right)$
 $\left(\prod_{t=1}^{T-1} a_{d(\mathbf{z}^{(t)}), d(\mathbf{z}^{(t+1)})} P[\mathbf{x}^{(t+1)}|\mathbf{z}^{(t+1)}, \theta_{d(\mathbf{z}^{(t+1)})}]\right)$
• Define
 $\delta_{i}^{(t)} = \max_{\mathbf{z}^{(1)}, \dots, \mathbf{z}^{(t-1)}} P[\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(t)}, \mathbf{z}^{(1)}, \dots, \mathbf{z}^{(t-1)}, \mathbf{z}^{(t)} = \mathbf{e}_{i}|\Theta]$
• \mathcal{X}^{*} is the sequence having $\delta^{(T)*} = \max_{1 \leq i \leq K} \delta_{i}^{(T)}$
• Notice that we can calculate $\delta_{j}^{(T)}$ efficiently if we already know
 $\delta_{i}^{(T-1)}$ for all $1 \leq i \leq K$
• $\delta_{j}^{(t)} = \left(\max_{1 \leq i \leq K} \delta_{i}^{(t-1)} a_{i,j}\right) P[\mathbf{x}^{(t)}|\mathbf{z}_{j}^{(t)}, \theta_{j}]$
• $\delta_{j}^{(t)}$ has the optimal substructure and can be evaluated efficiently
using dynamic programming
• We can obtain \mathcal{X}^{*} by backtracking

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Hidden Markov Models

The Viterbi Algorithm

Input:
$$\mathcal{X} \leftarrow \{\mathbf{x}^{(t)}\}_{t=1}^{T}$$
 and $\Theta \leftarrow (\pi^{(1)}, \mathbf{A}, \{\theta_i\}_{i=1}^{K})$
Output: $\mathcal{Z} \leftarrow \{\mathbf{z}^{(t)}\}_{t=1}^{T}$ resulting the highest $P[\mathcal{X}, \mathcal{Z}|\Theta]$
for $i \leftarrow 1$ to K do
 $\begin{vmatrix} \delta_i^{(1)} \leftarrow \pi_i^{(1)} P[\mathbf{x}^{(1)}|\mathbf{z}_i^{(1)}, \theta_i]; \\ \psi_i^{(1)} \leftarrow \text{null}; \end{vmatrix}$
end
for $t \leftarrow 2$ to T do
 $\begin{cases} \text{for } j \leftarrow 1$ to K do
 $\begin{vmatrix} \delta_j^{(t)} \leftarrow (\max_{1 \le i \le K} \delta_i^{(t-1)} \mathbf{a}_{i,j}) P[\mathbf{x}^{(t)}|\mathbf{z}_j^{(t)}, \theta_j]; \\ \psi_j^{(t)} \leftarrow \arg_{1 \le i \le K} \max_i^{(t-1)} \mathbf{a}_{i,j}; // \text{ previous state} \end{vmatrix}$
end
end

end

$$\begin{aligned} & d(z^{(T)}) \leftarrow \arg_{1 \leqslant i \leqslant K} \max \delta_i^{(T)}; \\ & \text{for } t \leftarrow T - 1 \text{ to } 1 \text{ do} \\ & | \quad d(z^{(t)}) \leftarrow \psi_{d(z^{(t+1)})}^{(t+1)}; // \text{ backtracking} \\ & \text{end} \end{aligned}$$

Algorithm 1: The Viterbi algorithm of time complexity $O(K^2T)$.

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- When HMM is used to model a class, we predict a new sequence X^{new} to be in class C_i if the posterior P[C_i|X^{new}] ∝ P[X^{new}|Θ_i]P[C_i] is the highest
- Problem: given parameters Θ and a sequence $\mathcal{X},$ we want to know $P[\mathcal{X}|\Theta]$
- Again, we can try out all possible \mathcal{Z} using $P[\mathcal{X}|\Theta] = \sum_{\mathcal{Z}} P[\mathcal{X}, \mathcal{Z}|\Theta]$, but this is cost prohibitive
- Better way?

- When HMM is used to model a class, we predict a new sequence X^{new} to be in class C_i if the posterior P[C_i|X^{new}] ∝ P[X^{new}|Θ_i]P[C_i] is the highest
- Problem: given parameters Θ and a sequence $\mathcal{X},$ we want to know $P[\mathcal{X}|\Theta]$
- Again, we can try out all possible \mathcal{Z} using $P[\mathcal{X}|\Theta] = \sum_{\mathcal{Z}} P[\mathcal{X}, \mathcal{Z}|\Theta]$, but this is cost prohibitive
- Better way?
- Notice that $P[\mathcal{X}|\Theta] = \sum_{i=1}^{K} P[\mathcal{X}, z_i^{(t)}|\Theta] = \sum_{i=1}^{K} \alpha_i^{(T)}$
 - Calculate the forward variables $\alpha_i^{(T)}$ for all $1 \le i \le K$ first, which takes $O(K^2T)$ time
 - Obtain $P[\mathcal{X}|\Theta]$ by summing $\alpha_i^{(T)}$

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Implementation Issues

• When calculating $\alpha_j^{(t)}$, $\beta_i^{(t)}$, and $\delta_j^{(t)}$ in a program, we risk getting the underflow

•
$$\alpha_j^{(t)} = \left(\sum_{i=1}^K \alpha_i^{(t-1)} a_{i,j}\right) P[\mathbf{x}^{(t)}|z_j^{(t)}, \theta_j],$$

 $\beta_i^{(t)} = \sum_{j=1}^K a_{i,j} P[\mathbf{x}^{(t+1)}|z_j^{(t+1)}, \theta_j] \beta_j^{(t+1)},$ and
 $\delta_j^{(t)} = \left(\max_{1 \leq i \leq K} \delta_i^{(t-1)} a_{i,j}\right) P[\mathbf{x}^{(t)}|z_j^{(t)}, \theta_j]$ are all multiplication of small numbers

- We can calculate the normalized $\widetilde{\alpha}_i^{(t)}$ and $\widetilde{\beta}_i^{(t)}$ by multiplying $\alpha_i^{(t)}$ and $\beta_i^{(t)}$ by $c_t = \sum_{j=1}^{K} \frac{1}{\alpha_j^{(t)}}$ (note $\sum_{j=1}^{K} \beta_j^{(t)} \neq 1$) at each step of the dynamic programming, and then denormalize the related targets
 - E.g., since $\widetilde{\alpha}_i^{(T)} = \alpha_i^{(T)} \prod_{t=1}^T c_t$ and $\sum_{i=1}^K \widetilde{\alpha}_i^{(T)} = 1$, we denormalize $P[\mathfrak{X}|\Theta]$ by $P[\mathfrak{X}|\Theta] = \sum_{i=1}^K \alpha_i^{(T)} = \frac{1}{\prod_{t=1}^T c_t} \sum_{i=1}^K \widetilde{\alpha}_i^{(T)} = \frac{1}{\prod_{t=1}^T c_t}$
- For $\delta_j^{(t)}$, we can simply calculate $\widetilde{\delta}_j^{(t)} = \log \delta_j^{(t)}$ at each step, and then exponent the related targets

Model Selection

- Reduce the number of states, K
 - The optimal K can be determined using the cross validation
- Or, constrain the model structure
 - Limit the number of states K, K' < K, that can be transited to
 - This reduces the complexity of forward-backward procedure and Viterbi algorithm to O(KK'T)
 - In particular, the *left-to-right HMM* is commonly used (e.g., in speech recognition)



Figure : An example left-to-right HMM. The process never moves to a state with a smaller index (i.e., $a_{i,j} = 0$ if j < i), and a big jump in state index is not allowed (i.e., $a_{i,j} = 0$ for j > i + c, where c = 2 in this case).