## Hidden Markov Models

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## Outline

(1) Hidden Markov Models

- Definitions and Usage
(2) Learning the Model Parameters
- Expectation Maximization for HMM
- The Forward-Backward Procedure
(3) Inferring the State Sequences
(4) 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 $\boldsymbol{z}^{(t)} \in\{0,1\}^{K}$ be a vector where $z_{i}^{(t)}=1$ if $X^{(t)}=S_{i} ; 0$ otherwise
- $P\left[\boldsymbol{z}^{(t)}=\boldsymbol{e}_{i}\right]=P\left[X^{(t)}=S_{i}\right]$ (for brevity, we use the shorthand $P\left[z_{i}^{(t)}\right]$ )
- In HMM, $\boldsymbol{z}^{(t)}$ is hidden (not observable) and is a latent variable
- When a state is visited, however, we can record an observation $\boldsymbol{x}^{(t)}$
- $P\left[\boldsymbol{x}^{(t)} \mid z_{i}^{(t)}\right]$ 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 $\theta_{i}$, we can rewrite it as $P\left[\boldsymbol{x}^{(t)} \mid z_{i}^{(t)}, \theta_{i}\right]$
- Markov chain is a special case of HMM where
- $\boldsymbol{x}^{(t)}$ must be one of the $S_{1}, \cdots, S_{K}$
- $P\left[\boldsymbol{x}^{(t)}=S_{j} \mid z_{i}^{(t)}\right]=1$ if $i=j ; 0$ otherwise


## Graph Representation



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


## Goals

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


## Applications

- For classification, we can model each class as an HMM
- Learn the parameter $\Theta_{i}$ of each class $C_{i}$ using a training sequence $X=\left\{\boldsymbol{x}^{(t)}\right\}_{t=1}^{T}$ (or a set $X=\left\{\boldsymbol{x}^{(n, t)}\right\}_{n=1, t=1}^{N, T}$ of $n$ training sequences)
- Predict a new sequence $X^{\text {new }}$ to be in class $C_{i}$ if the posterior $P\left[C_{i} \mid X^{\text {new }}\right] \propto P\left[X^{\text {new }} \mid \Theta_{i}\right] P\left[C_{i}\right]$ 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 $P\left[X^{n e w} \mid \Theta\right]=\sum_{z} P\left[X^{\text {new }}, z \mid \Theta\right]$ of a speech $X^{\text {new }}$ will not change dramatically when it is spoken slowly, as $z$ having more transitions to the same state will contribute to the likelihood more


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## Problem Formulation

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


## Problem Formulation

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


## Formulating $Q\left(\Theta ; \Theta^{\text {old }}\right)(1 / 4)$

- Recall that $P[\mathcal{X}, \mathcal{Z} \mid \Theta]=P[\mathcal{X} \mid \mathcal{Z}, \Theta] P[\mathcal{Z} \mid \Theta]=$

$$
\left(\prod_{s=1}^{T} P\left[\boldsymbol{x}^{(s)} \mid z^{(s)}, \theta_{d\left(\mathbf{z}^{(s)}\right)}\right]\right) P\left[\boldsymbol{z}^{(1)} \mid \boldsymbol{\pi}^{(1)}\right]\left(\prod_{t=1}^{T-1} P\left[\boldsymbol{z}^{(t+1)} \mid \boldsymbol{z}^{(t)}, \boldsymbol{A}\right]\right)
$$

- $\mathcal{Q}\left(\Theta ; \Theta^{\text {old }}\right)=E_{Z}\left[\ln (P[X, Z \mid \Theta]) \mid X, \Theta^{\text {old }}\right]$
$=\sum_{z} \ln (P[\mathcal{X}, \mathcal{Z} \mid \Theta]) P\left[\mathcal{Z} \mid X, \Theta^{\text {old }}\right]$
$=\sum_{z} \ln \left(P\left[z^{(1)} \mid \pi^{(1)}\right]\right) P\left[z \mid X, \Theta^{\text {old }}\right]$
$+\sum_{z} \ln \left(\prod_{t=1}^{T-1} P\left[Z^{(t+1)} \mid z^{(t)}, \boldsymbol{A}\right]\right) P\left[z \mid X, \Theta^{\text {old }}\right]$
$+\sum_{z} \ln \left(\prod_{t=1}^{T} P\left[x^{(t)} \mid z^{(t)}, \theta_{d\left(z^{(t)}\right)}\right]\right) P\left[z \mid X, \Theta^{o l d}\right]$


## Formulating $Q\left(\Theta ; \Theta^{\text {old }}\right)(2 / 4)$

The first term $\sum_{z} \ln \left(P\left[z^{(1)} \mid \pi^{(1)}\right]\right) P\left[z \mid X, \Theta^{\text {old }}\right]$
$=\sum_{z} \ln \left(\pi_{d\left(z^{(1)}\right)}^{(1)}\right) P\left[Z \mid X, \Theta^{o l d}\right]$
$=\sum_{\boldsymbol{z}^{(1)}=\boldsymbol{e}_{1}}^{\boldsymbol{e}_{K}} \cdots \sum_{\boldsymbol{z}^{(T)}=\boldsymbol{e}_{1}}^{\boldsymbol{e}_{K}} \ln \left(\pi_{d\left(\boldsymbol{z}^{(1)}\right)}^{(1)}\right) P\left[z^{(1)}, \cdots, z^{(T)} \mid X, \Theta^{\text {old }}\right]$
$=\sum_{z^{(1)}=e_{1}}^{\boldsymbol{e}_{K}} \ln \left(\pi_{d\left(z^{(1)}\right)}^{(1)}\right) \sum_{z^{(2)}=e_{1}}^{\boldsymbol{e}_{K}} \cdots \sum_{z^{(T)}=e_{1}}^{\boldsymbol{e}_{K}} P\left[z^{(1)}, \cdots, z^{(T)} \mid X, \Theta^{\text {old }}\right]$
$=\sum_{\boldsymbol{z}^{(1)}=\boldsymbol{e}_{1}}^{\boldsymbol{e}_{\boldsymbol{1}}} \ln \left(\pi_{d\left(\mathbf{z}^{(1)}\right)}^{(1)}\right) P\left[z^{(1)} \mid X, \Theta^{\text {old }}\right]$
$=\sum_{i=1}^{K} \ln \left(\pi_{i}^{(1)}\right) P\left[z_{i}^{(1)} \mid X, \Theta^{\text {old }}\right]$

## Formulating $Q\left(\Theta ; \Theta^{\text {old }}\right)(3 / 4)$

The second term $\sum_{z} \ln \left(\prod_{t=1}^{T-1} P\left[z^{(t+1)} \mid \boldsymbol{z}^{(t)}, \boldsymbol{A}\right]\right) P\left[\mathcal{Z} \mid X, \Theta^{\text {old }}\right]$
$=\sum_{z} \sum_{t=1}^{T-1} \ln \left(P\left[\mathbf{z}^{(t+1)} \mid \boldsymbol{z}^{(t)}, \boldsymbol{A}\right]\right) P\left[\mathcal{Z} \mid \mathcal{X}, \Theta^{\text {old }}\right]$
$\sum_{t=1}^{T-1} \sum_{\boldsymbol{z}^{(1)}=\boldsymbol{e}_{1}}^{\boldsymbol{e}_{K}} \cdots \sum_{\boldsymbol{z}^{(T)}=\boldsymbol{e}_{1}}^{\boldsymbol{e}_{K}} \ln \left(P\left[\boldsymbol{z}^{(t+1)} \mid \boldsymbol{z}^{(t)}, \boldsymbol{A}\right]\right) P\left[\boldsymbol{z}^{(1)}, \cdots, z^{(T)} \mid X, \Theta^{\text {old }}\right]$
$=\sum_{t=1}^{T-1} \sum_{\boldsymbol{z}^{(t)}=\boldsymbol{e}_{\mathbf{1}}}^{\boldsymbol{e}_{K}} \sum_{\boldsymbol{z}^{(t+1)}=\boldsymbol{e}_{\mathbf{1}}}^{\boldsymbol{e}_{K}} \ln \left(P\left[\boldsymbol{z}^{(t+1)} \mid \boldsymbol{z}^{(t)}, \boldsymbol{A}\right]\right) \sum_{\boldsymbol{z}^{(1)}=\boldsymbol{e}_{\mathbf{1}}}^{\boldsymbol{e}_{K}} \cdots \sum_{\boldsymbol{z}^{(t-1)}=\boldsymbol{e}_{1}}^{\boldsymbol{e}_{K}}$ $\sum_{z^{(t+2)}=e_{1}}^{\boldsymbol{e}_{K}} \cdots \sum_{z^{(T)}=e_{1}}^{\boldsymbol{e}_{K}} P\left[z^{(1)}, \cdots, z^{(T)} \mid X, \Theta^{\text {old }}\right]$
$=\sum_{t=1}^{T-1} \sum_{\boldsymbol{z}^{(t)}=\boldsymbol{e}_{1}}^{\boldsymbol{e}_{K}} \sum_{\boldsymbol{z}^{(t+1)}=\boldsymbol{e}_{1}}^{\boldsymbol{e}_{\mathrm{i}}} \ln \left(P\left[\mathbf{z}^{(t+1)} \mid \boldsymbol{z}^{(t)}, \boldsymbol{A}\right]\right) P\left[\mathbf{z}^{(t)}, \boldsymbol{z}^{(t+1)} \mid X, \Theta^{\text {old }}\right]$
$=\sum_{t=1}^{T-1} \sum_{i=1}^{K} \sum_{j=1}^{K} \ln \left(P\left[z_{j}^{(t+1)} \mid z_{i}^{(t)}, \boldsymbol{A}\right]\right) P\left[z_{i}^{(t)}, z_{j}^{(t+1)} \mid \mathcal{X}, \Theta^{o l d}\right]$
$=\sum_{t=1}^{T-1} \sum_{i=1}^{K} \sum_{j=1}^{K} \ln \left(a_{i, j}\right) P\left[z_{i}^{(t)}, z_{j}^{(t+1)} \mid X, \Theta^{o l d}\right]$

## Formulating $Q\left(\Theta ; \Theta^{\text {old }}\right)(4 / 4)$

- Similarly, the third term
$\sum_{z} \ln \left(\prod_{t=1}^{T} P\left[x^{(t)} \mid z^{(t)}, \theta_{d\left(z^{(t)}\right)}\right]\right) P\left[z \mid X, \Theta^{o l d}\right]=$
$\sum_{t=1}^{T} \sum_{i=1}^{K} \ln \left(P\left[x^{(t)} \mid z_{i}^{(t)}, \theta_{i}\right]\right) P\left[z_{i}^{(t)} \mid X, \Theta^{\text {old }}\right]$ [Proof]
- $\mathcal{Q}\left(\Theta ; \Theta^{\text {old }}\right)=\sum_{i=1}^{k} \ln \left(\pi_{i}^{(1)}\right) P\left[z_{i}^{(1)} \mid X, \Theta^{\text {old }}\right]$
$+\sum_{t=1}^{T-1} \sum_{i=1}^{K} \sum_{j=1}^{K} \ln \left(a_{i, j}\right) P\left[z_{i}^{(t)}, z_{j}^{(t+1)} \mid X, \Theta^{o l d}\right]$
$+\sum_{t=1}^{T} \sum_{i=1}^{K} \ln \left(P\left[\boldsymbol{x}^{(t)} \mid z_{i}^{(t)}, \theta_{i}\right]\right) P\left[z_{i}^{(t)} \mid X, \Theta^{\text {old }}\right]$
- In the E-step, we need to evaluate $P\left[z_{i}^{(t)} \mid X, \Theta^{\text {old }}\right]$ and $P\left[z_{i}^{(t)}, z_{j}^{(t+1)} \mid X, \Theta^{o l d}\right]$ for all $t$ (to be discussed later)
- After the evaluation, we denote $\gamma_{i}^{(t)}=P\left[z_{i}^{(t)} \mid X, \Theta^{\text {old }}\right]$ and $\xi_{i, j}^{(t)}=P\left[z_{i}^{(t)}, z_{j}^{(t+1)} \mid \mathcal{X}, \Theta^{\text {old }}\right]$ 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

- Problem: $\arg _{\Theta=\left(\boldsymbol{\pi}^{(1)}, \boldsymbol{A},\left\{\theta_{i}\right\}_{i=1}^{K}\right)} \max \mathcal{Q}\left(\Theta ; \Theta^{\text {old }}\right)$, where

$$
\text { - } \begin{aligned}
& Q\left(\Theta ; \Theta^{o l d}\right)=\sum_{i=1}^{K} \ln \left(\pi_{i}^{(1)}\right) \gamma_{i}^{(1)}+\sum_{t=1}^{T-1} \sum_{i=1}^{K} \sum_{j=1}^{K} \ln \left(a_{i, j}\right) \xi_{i, j}^{(t)} \\
& +\sum_{t=1}^{T} \sum_{i=1}^{K} \ln \left(P\left[\boldsymbol{x}^{(t)} \mid z_{i}^{(t)}, \theta_{i}\right]\right) \gamma_{i}^{(t)}
\end{aligned}
$$

- Subject to
- $\sum_{i=1}^{K} \pi_{i}^{(1)}=1$
- $\sum_{j=1}^{K} a_{i, j}=1$ for all $1 \leqslant i \leqslant K$
- We can solve $\boldsymbol{\pi}^{(1)}, \boldsymbol{A}$, and $\left\{\theta_{i}\right\}_{i=1}^{K}$ by considering only the first, second, and third terms respectively


## Solving $\pi^{(1)}$

- Lagrangian: $L\left(\pi^{(1)}, \alpha\right)=\sum_{i=1}^{K} \ln \left(\pi_{i}^{(1)}\right) \gamma_{i}^{(1)}-\alpha\left(\sum_{i=1}^{K} \pi_{i}^{(1)}-1\right)$
- Taking the partial derivatives of $L$ with respect to $\pi_{i}^{(1)}$ and $\alpha$ and then setting them to zero we have $\frac{\gamma_{i}^{(1)}}{\pi_{i}^{(1)}}-\alpha=0 \Rightarrow \pi_{i}^{(1)}=\frac{\gamma_{i}^{(1)}}{\alpha}$ for all $1 \leqslant i \leqslant K$ and $\sum_{i=1}^{K} \pi_{i}^{(1)}=1$
- Summing all equations for $\pi_{i}^{(1)}$ we have $\alpha=\sum_{i=1}^{K} \gamma_{i}^{(1)}$, and therefore $\pi_{i}^{(1)}=\frac{\gamma_{i}^{(1)}}{\sum_{i=1}^{K} \gamma_{i}^{(1)}}=\gamma_{i}^{(1)}$


## Solving A

- Lagrangian: $L\left(\boldsymbol{A},\left\{\alpha_{i}\right\}_{i=1}^{K}\right)=$

$$
\sum_{t=1}^{T-1} \sum_{i=1}^{K} \sum_{j=1}^{K} \ln \left(a_{i, j}\right) \xi_{i, j}^{(t)}-\sum_{i=1}^{K} \alpha_{i}\left(\sum_{j=1}^{K} a_{i, j}-1\right)
$$

- Taking the partial derivatives of $L$ with respect to $a_{i, j}$ and $\alpha_{i}$ 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 $1 \leqslant i \leqslant K$
- Summing the equations for $a_{i, j}$ along $j$ we have
$\alpha_{i}=\sum_{j=1}^{K} \sum_{t=1}^{T-1} \xi_{i, j}^{(t)}$, and therefore $a_{i, j}=\frac{\sum_{t=1}^{T-1} \xi_{i j}^{(t)}}{\sum_{t=1}^{T-1} \sum_{j=1}^{K} \xi_{i, j}^{(t)}}=\frac{\sum_{t=1}^{T-1} \xi_{i,}^{(t)}}{\sum_{t=1}^{T-1} \gamma_{i}^{(t)}}$


## Solving $\left\{\theta_{i}\right\}_{i=1}^{K}(1 / 3)$

- Problem: finding $\left\{\theta_{k}\right\}_{k=1}^{K}$ such that $\sum_{t=1}^{T} \sum_{k=1}^{K} \ln \left(P\left[x^{(t)} \mid z_{k}^{(t)}, \theta_{k}\right]\right) \gamma_{k}^{(t)}$ is maximized
- Suppose $\boldsymbol{x}^{(t)}$ is discrete such that $x_{i}^{(t)}=1$ if the predefined value $O_{i}$ from $\left\{O_{1}, \cdots, O_{d}\right\}$ is observed; 0 otherwise
- We can assume that the emission probability
$P\left[\boldsymbol{x}^{(t)} \mid z_{k}^{(t)}, \theta_{k}\right]=\prod_{i=1}^{d} b_{k, i}^{x_{i}^{(t)}}$ follows the multinomial distribution where $\theta_{k}=\left\{b_{k, i}\right\}_{i=1}^{d}$ and $b_{k, i}$ is the probability that $O_{i}$ is observed in state $k$
- $\sum_{i=1}^{d} b_{k, i}=1$


## Solving $\left\{\theta_{i}\right\}_{i=1}^{K}(2 / 3)$

- Lagrangian: $L\left(\left\{b_{k, i}\right\}_{k=1, i=1}^{K, d},\left\{\alpha_{k}\right\}_{k=1}^{K}\right)=$

$$
\begin{aligned}
& \sum_{t=1}^{T} \sum_{k=1}^{K} \ln \left(\prod_{i=1}^{d} b_{k, i}^{x_{i}^{(t)}}\right) \gamma_{k}^{(t)}-\sum_{k=1}^{K} \alpha_{k}\left(\sum_{i=1}^{d} b_{k, i}-1\right)= \\
& \sum_{t=1}^{T} \sum_{k=1}^{K} \sum_{i=1}^{d} x_{i}^{(t)} \ln \left(b_{k, i}\right) \gamma_{k}^{(t)}-\sum_{k=1}^{K} \alpha_{k}\left(\sum_{i=1}^{d} b_{k, i}-1\right)
\end{aligned}
$$

- Taking the partial derivatives of $L$ with respect to $b_{k, i}$ and $\alpha_{k}$ and then setting them to zero we have

$$
\begin{aligned}
& \frac{\sum_{t=1}^{T} x_{i}^{(t)} \gamma_{k}^{(t)}}{b_{k, i}^{(0)}}-\alpha_{k}=0 \Rightarrow b_{k, i}=\frac{\sum_{t=1}^{T} x_{i}^{(t)} \gamma_{k}^{(t)}}{\alpha_{k}} \text { and } \sum_{i=1}^{d} b_{k, i}=1 \text { for all } \\
& 1 \leqslant k \leqslant K
\end{aligned}
$$

- 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
$b_{k, i}=\frac{\sum_{t=1}^{T} x_{i}^{(t)} \gamma_{k}^{(t)}}{\sum_{t=1}^{T} \gamma_{k}^{(t)} \sum_{i=1}^{d} x_{i}^{(t)}}=\frac{\sum_{t=1}^{T} x_{i}^{(t)} \gamma_{k}^{(t)}}{\sum_{t=1}^{T} \gamma_{k}^{(t)}}$


## Solving $\left\{\theta_{i}\right\}_{i=1}^{K}(3 / 3)$

- What if $\boldsymbol{x}^{(t)}$ are continuous?


## Solving $\left\{\theta_{i}\right\}_{i=1}^{K}(3 / 3)$

- What if $\boldsymbol{x}^{(t)}$ are continuous?
- We can assume that $P\left[\boldsymbol{x}^{(t)} \mid z_{k}^{(t)}, \theta_{k}\right]$ follows the multivariate normal distribution where $\theta_{k}=\left(\boldsymbol{\mu}_{k}, \boldsymbol{\Sigma}_{k}\right)$
- It can be shown that
- $\mu_{k}=\frac{\sum_{t=1}^{T} \gamma_{k}^{(t)} x^{(t)}}{\sum_{t=1}^{T} \gamma_{k}^{(t)}}$
- $\Sigma_{k}=\frac{\sum_{t=1}^{T} \gamma_{k}^{(t)}\left(x^{(t)}-\mu_{k}\right)\left(x^{(t)}-\mu_{k}\right)^{\top}}{\sum_{t=1}^{T} \gamma_{k}^{(t)}}$ [Homework]


## Learning form Multiple Sequences

- Suppose we are given a set $X=\left\{\boldsymbol{x}^{(n, t)}\right\}_{n=1, t=1}^{N, T}$ of observation sequences, where sequences are independent with each other
- $P[X \mid \Theta]=\prod_{n=1}^{N} P\left[X^{(n)} \mid \Theta\right]$, where $X^{(n)}=\left\{\boldsymbol{x}^{(n, t)}\right\}_{t=1}^{T}$
- Then for discrete $\boldsymbol{x}^{(t)}$ with multinomial emission probability:
- $\pi_{i}^{(1)}=\frac{\sum_{n=1}^{N} \gamma_{i}^{(n, 1)}}{N}$
- $a_{i, j}=\frac{\sum_{n=1}^{N} \sum_{t=1}^{T-1} \xi_{i, j}^{(n, t)}}{\sum_{n=1}^{N} \sum_{t=1}^{T-1} \gamma_{i}^{(n, t)}}$
- $b_{k, i}=\frac{\sum_{n=1}^{N} \sum_{t=1}^{T} x_{i}^{(n, t)} \gamma_{k}^{(n, t)}}{\sum_{n=1}^{N} \sum_{t=1}^{T} \gamma_{k}^{(n, t)}}$
- This is analogous to the estimators of a Markov chain we have seen previously, except that $\gamma_{i}^{(t)}=P\left[z_{i}^{(t)} \mid X, \Theta^{\text {old }}\right]$ and $\xi_{i, j}^{(t)}=P\left[z_{i}^{(t)}, z_{j}^{(t+1)} \mid X, \Theta^{o l d}\right]$ are soft counts of state visits


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## We Are Not Done Yet

- Given $\Theta^{o l d}$, in the E-step we need to evaluate $\gamma_{i}^{(t)}$ and $\xi_{i, j}^{(t)}$
- $\gamma_{i}^{(t)}=P\left[z_{i}^{(t)} \mid X, \Theta^{\text {old }}\right]=\frac{P\left[X, z_{i}^{(t)} \mid \Theta^{\text {old }}\right]}{P\left[X \mid \Theta^{\text {old }}\right]}$
- $\xi_{i, j}^{(t)}=P\left[z_{i}^{(t)}, z_{j}^{(t+1)} \mid X, \Theta^{\text {old }}\right]=\frac{P\left[X, z_{i}^{(t)}, z_{j}^{(t+1)} \mid \Theta^{\text {old }}\right]}{P\left[X \mid \Theta^{\text {old }}\right]}$
- We can evaluate $\gamma_{i}^{(t)}$ and $\xi_{i, j}^{(t)}$ by considering all possible state sequences:
- $P\left[X \mid \Theta^{\text {old }}\right]=\Sigma_{z} P\left[X, z \mid \Theta^{\text {old }}\right]$
- $P\left[X, z_{i}^{(t)} \mid \Theta^{o l d}\right]=\sum_{z, z^{(t)}=e_{i}} P\left[X, z \mid \Theta^{\text {old }}\right]$
- However, there are exponentially many sequences (specifically, $K^{T}$ and $K^{T-1}$ for $P\left[X \mid \Theta^{o l d}\right]$ and $P\left[X, z_{i}^{(t)} \mid \Theta^{\text {old }}\right]$ respectively)
- The evaluation would be very slow, if not infeasible
- Better idea?


## We Are Not Done Yet

- Given $\Theta^{o l d}$, in the E-step we need to evaluate $\gamma_{i}^{(t)}$ and $\xi_{i, j}^{(t)}$
- $\gamma_{i}^{(t)}=P\left[z_{i}^{(t)} \mid X, \Theta^{\text {old }}\right]=\frac{P\left[X, z_{i}^{(t)} \mid \Theta^{\text {old }}\right]}{P\left[X \mid \Theta^{\text {old }]}\right.}$
- $\xi_{i, j}^{(t)}=P\left[z_{i}^{(t)}, z_{j}^{(t+1)} \mid X, \Theta^{\text {old }}\right]=\frac{P\left[X, z_{i}^{(t)}, z_{j}^{(t+1)} \mid \Theta^{\text {old }}\right]}{P\left[X \mid \Theta^{\text {old }}\right]}$
- We can evaluate $\gamma_{i}^{(t)}$ and $\xi_{i, j}^{(t)}$ by considering all possible state sequences:
- $P\left[X \mid \Theta^{\text {old }}\right]=\Sigma_{z} P\left[X, z \mid \Theta^{\text {old }}\right]$
- $P\left[X, z_{i}^{(t)} \mid \Theta^{o l d}\right]=\sum_{z, z^{(t)}=e_{i}} P\left[X, z \mid \Theta^{\text {old }}\right]$
- However, there are exponentially many sequences (specifically, $K^{T}$ and $K^{T-1}$ for $P\left[X \mid \Theta^{o l d}\right]$ and $P\left[X, z_{i}^{(t)} \mid \Theta^{\text {old }}\right]$ 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 $\gamma_{i}^{(t)}$ and $\xi_{i, j}^{(t)}$
- Given a $\Theta=\left(\boldsymbol{\pi}^{(1)}, \boldsymbol{A},\left\{\theta_{i}\right\}_{i=1}^{K}\right)$, define the forward variable as $\alpha_{i}^{(t)}=P\left[\boldsymbol{x}^{(1)}, \cdots, \boldsymbol{x}^{(t)}, z_{i}^{(t)} \mid \Theta\right]$
- $\alpha_{i}^{(t)}$ denotes the probability that a partial sequence $\left\{\boldsymbol{x}^{(1)}, \cdots, \boldsymbol{x}^{(t)}\right\}$ until time $t$ is observed while the state ends in $S_{i}$ at time $t$
- Similarly, define the backward variable as

$$
\beta_{i}^{(t)}=P\left[x^{(t+1)}, \cdots, x^{(T)} \mid z_{i}^{(t)}, \Theta\right]
$$

- $\beta_{i}^{(t)}$ denotes the probability that a partial sequence $\left\{\boldsymbol{x}^{(t+1)}, \cdots, \boldsymbol{x}^{(\boldsymbol{T})}\right\}$ 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:

$$
\gamma_{i}^{(t)}=\frac{\alpha_{i}^{(t)} \beta_{i}^{(t)}}{\sum_{j=1}^{K} \alpha_{j}^{(t)} \beta_{j}^{(t)}} \text { and } \xi_{i, j}^{(t)}=\frac{\alpha_{i}^{(\boldsymbol{t})} a_{i, j} P\left[\mathbf{x}^{(t+1)} \mid z_{j}^{(t+1)}, \theta_{j}\right] \beta_{j}^{(t+1)}}{\sum_{k=1}^{K} \sum_{l=1}^{K} \alpha_{k}^{(t)} a_{k, l} P\left[x^{(t+1)} \mid z_{l}^{(t+1)}, \theta_{l}\right] \beta_{l}^{(t+1)}}
$$

## Expressing $\gamma_{i}^{(t)}$ Using $\alpha_{i}^{(t)}$ And $\beta_{i}^{(t)}$


$=\frac{P\left[\boldsymbol{x}^{(1)}, \cdots, \mathbf{x}^{(t)} \mid z_{i}^{(t)}, \Theta\right] P\left[x^{(t+1)}, \cdots, \mathbf{x}^{(T)} \mid z_{i}^{(t)}, \Theta\right] P\left[z_{i}^{(t)} \mid \Theta\right]}{P[\mathcal{X} \mid \Theta]}$
$=\frac{P\left[x^{(1)}, \cdots, \boldsymbol{x}^{(t)} z_{i}^{(t)}, \mid \Theta\right] P\left[\boldsymbol{x}^{(t+1)}, \cdots, \boldsymbol{x}^{(T)} \mid z_{i}^{(t)}, \Theta\right]}{P[X \mid \Theta]}$
$=\frac{\alpha_{i}^{(t)} \beta_{i}^{(t)}}{P[X \mid \Theta]}=\frac{\alpha_{i}^{(t)} \beta_{i}^{(t)}}{\sum_{j=1}^{K} P\left[X, z_{j}^{(t)} \mid \Theta\right]}=\frac{\alpha_{i}^{(t)} \beta_{i}^{(t)}}{\sum_{j=1}^{K} \alpha_{j}^{(t)} \beta_{j}^{(t)}}$

- The numerator $\alpha_{i}^{(t)} \beta_{i}^{(t)}$ explains the whole observation sequence $\left\{\boldsymbol{x}^{(1)}, \cdots, \boldsymbol{x}^{(t)}\right\}$ 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 $\xi_{i, j}^{(t)}$ <br> Using $\alpha_{i}^{(t)}$ And $\beta_{i}^{(t)}$ <br> $(1 / 2)$

$$
\begin{aligned}
& \text { - } \xi_{i j}^{(t)}=P\left[z_{i}^{(t)}, z_{j}^{(t+1)} \mid x, \Theta\right]=\frac{P\left(x, z_{i}^{(t)}, z_{i}^{(t+1)} \mid \Theta\right]}{P[|\theta|} \\
& =\frac{P\left(x\left|z_{i}^{(t)} z_{j}^{(t+1)}, \Theta\right| P \mid z_{i}^{(t)}\left(z_{j}^{(t+1)} \mid \theta\right]\right.}{P|x| \theta)} \\
& =\frac{P\left(x \mid z_{i}^{(t)}, z_{j}^{(t+1)}, \Theta\right] P\left[z_{2}^{(t+1)}\left|z_{i}^{(t)}, \Theta\right| P\left[z_{i}^{(t)} \mid \Theta\right]\right.}{P(x \mid \theta \theta} \\
& =\left(\frac{1}{\rho(x \mid \Theta)}\right) P\left[x^{(1)} \cdots, x^{(t)} \mid z_{i}^{(t)}, \Theta\right] P\left[x^{(t+1)} \mid z_{j}^{(t+1)}, \Theta\right] \\
& P\left[x^{(t+2)} \ldots, x^{(T)} \mid z_{j}^{(t+1)}, \Theta\right] a_{i j} P\left[z_{i}^{(t)} \mid \Theta\right] \\
& =\frac{P\left[\boldsymbol{x}^{(1)} \cdots, x^{(t)}, z_{i}^{(t)} \mid \Theta\right] P\left[x^{(t+1)} \mid z_{j}^{(t+1)}, \Theta\right] P\left[x^{(t+2)} \cdots, x^{(T)} \mid z_{j}^{(t+1)}, \Theta\right] a_{i, j}}{P[X \mid \Theta]} \\
& =\frac{\alpha_{i}^{(t)} a_{i, j} P\left[x^{(t+1)} \mid z_{j}^{(t+1)}, \Theta\right] \beta_{j}^{(t+1)}}{P[X \mid \Theta]}=\frac{\alpha_{i}^{(t)} a_{i, j} P\left[x^{(t+1)} \mid z_{j}^{(t+1)}, \Theta\right] \beta_{j}^{(t+1)}}{\sum_{k=1}^{K} \sum_{l=1}^{K} P\left[X, z_{k}^{(t)}, z_{l}^{(t+1)} \mid \Theta\right]} \\
& =\frac{\alpha_{i}^{(t)} a_{i, j} P\left[x^{(t+1)} \mid z_{j}^{(t+1)}, \theta_{j}\right] \beta_{j}^{(t+1)}}{\sum_{k=1}^{K} \sum_{I=1}^{K} \alpha_{k}^{(t)} a_{k, I} P\left[x^{(t+1)} \mid z_{I}^{(t+1)}, \theta_{I}\right] \beta_{I}^{(t+1)}}
\end{aligned}
$$

## Expressing $\xi_{i, j}^{(t)}$ Using $\alpha_{i}^{(t)}$ And $\beta_{i}^{(t)}(2 / 2)$

- $\xi_{i, j}^{(t)}=\frac{\alpha_{i}^{(t)} a_{i, j} P\left[x^{(t+1)} \mid z_{j}^{(t+1)}, \theta_{j}\right] \beta_{j}^{(t+1)}}{\sum_{k=1}^{K} \sum_{l=1}^{K} \alpha_{k}^{(t)} a_{k, I} P\left[x^{(t+1)} \mid z_{l}^{(t+1)}, \theta_{l}\right] \beta_{l}^{(t+1)}}$
- $\alpha_{i}^{(t)}$ 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
- $\alpha_{i}^{(1)}=P\left[x^{(1)}, z_{i}^{(1)} \mid \Theta\right]=P\left[x^{(1)} \mid z_{i}^{(1)}, \Theta\right] P\left[z_{i}^{(1)} \mid \Theta\right]=P\left[x^{(1)} \mid z_{i}^{(1)}, \theta_{i}\right] \pi_{i}^{(1)}$
- $\alpha_{j}^{(t+1)}=P\left[x^{(1)}, \cdots, x^{(t+1)}, z_{j}^{(t+1)} \mid \Theta\right]=$
$P\left[x^{(1)}, \cdots, x^{(t+1)} \mid z_{j}^{(t+1)}, \Theta\right] P\left[z_{j}^{(t+1)} \mid \Theta\right]$
$=P\left[\boldsymbol{x}^{(1)}, \cdots, \boldsymbol{x}^{(t)} \mid z_{j}^{(t+1)}, \Theta\right] P\left[\boldsymbol{x}^{(t+1)} \mid z_{j}^{(t+1)}, \Theta\right] P\left[z_{j}^{(t+1)} \mid \Theta\right]$
$=P\left[x^{(1)}, \cdots, x^{(t)}, z_{j}^{(t+1)} \mid \Theta\right] P\left[x^{(t+1)} \mid z_{j}^{(t+1)}, \Theta\right]$
$=P\left[x^{(t+1)} \mid z_{j}^{(t+1)}, \Theta\right] \sum_{i=1}^{K} P\left[x^{(1)}, \cdots, x^{(t)}, z_{i}^{(t)}, z_{j}^{(t+1)} \mid \Theta\right]$
$=P\left[x^{(t+1)} \mid z_{j}^{(t+1)}, \Theta\right] \sum_{i=1}^{K} P\left[x^{(1)}, \cdots, x^{(t)}, z_{j}^{(t+1)} \mid z_{i}^{(t)}, \Theta\right] P\left[z_{i}^{(t)} \mid \Theta\right]$
$=P\left[x^{(t+1)} \mid z_{j}^{(t+1)}, \Theta\right]$
$\sum_{i=1}^{K} P\left[x^{(1)}, \cdots, x^{(t)} \mid z_{i}^{(t)}, \Theta\right] P\left[z_{j}^{(t+1)} \mid z_{i}^{(t)}, \Theta\right] P\left[z_{i}^{(t)} \mid \Theta\right]$
$=P\left[\boldsymbol{x}^{(t+1)} \mid z_{j}^{(t+1)}, \Theta\right] \sum_{i=1}^{K} P\left[\boldsymbol{x}^{(1)}, \cdots, \boldsymbol{x}^{(t)}, z_{i}^{(t)} \mid \Theta\right] P\left[z_{j}^{(t+1)} \mid z_{i}^{(t)}, \Theta\right]$
$=\left(\sum_{i=1}^{K} \alpha_{i}^{(t)} a_{i, j}\right) P\left[x^{(t+1)} \mid z_{j}^{(t+1)}, \theta_{j}\right]$


## Evaluating $\alpha_{i}^{(t)}$ And $\beta_{i}^{(t)}(2 / 2)$

- Based on the recurrence relation

$$
\left\{\begin{array}{l}
\alpha_{i}^{(1)}=P\left[\boldsymbol{x}^{(1)} \mid z_{i}^{(1)}, \theta_{i}\right] \pi_{i}^{(1)} \\
\alpha_{j}^{(t+1)}=\left(\sum_{i=1}^{K} \alpha_{i}^{(t)} a_{i, j}\right) P\left[\boldsymbol{x}^{(t+1)} \mid z_{j}^{(t+1)}, \theta_{j}\right], \alpha_{j}^{(t+1)} \text { has the }
\end{array}\right.
$$

optimal substructure that it can be evaluated efficiently within $O(K)$ time if all $\alpha_{i}^{(t)}, 1 \leqslant i \leqslant K$, are known

- We can evaluate all $\alpha_{i}^{(t)}, 1 \leqslant i \leqslant K$ and $1 \leqslant t \leqslant T$, within $O\left(K^{2} T\right)$ time using the dynamic programming from $t=1$ to $T$
- Similarly, we can derive the recurrence relation for $\beta_{i}^{(t)}$ as

$$
\left\{\begin{array}{l}
\beta_{i}^{(T)}=1 \\
\left.\beta_{i}^{(t)}=\sum_{j=1}^{K} a_{i, j} P\left[\boldsymbol{x}^{(t+1)} \mid z_{j}^{(t+1)}, \theta_{j}\right] \beta_{j}^{(t+1)} \quad \text { [Proof] }\right]
\end{array}\right.
$$

- All $\beta_{i}^{(t)}$ can also be evaluated within $O\left(K^{2} T\right)$ 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 $O\left(K^{2}\right)$ time respectively
- The total time complexity for an E-step is $O\left(K^{2} T\right)$


## The recurrence relations



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## Problem Formulation

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


## The Optimal Substructure

- $P[X, z \mid \Theta]=P[X \mid z, \Theta] P[Z \mid \Theta]$

$$
\begin{aligned}
& =\left(\prod_{s=1}^{T} P\left[\boldsymbol{x}^{(s)} \mid \boldsymbol{z}^{(s)}, \theta_{d\left(\mathbf{z}^{(s)}\right)}\right]\right) P\left[\boldsymbol{z}^{(1)} \mid \boldsymbol{\pi}^{(1)}\right]\left(\prod_{t=1}^{T-1} P\left[\boldsymbol{z}^{(t+1)} \mid \boldsymbol{z}^{(t)}, \boldsymbol{A}\right]\right) \\
& =\left(P\left[\boldsymbol{z}^{(1)} \mid \boldsymbol{\pi}^{(1)}\right] P\left[\boldsymbol{x}^{(1)} \mid \boldsymbol{z}^{(1)}, \theta_{d\left(\mathbf{z}^{(1)}\right)}\right]\right) \\
& \quad \quad\left(\prod_{t=1}^{T-1} a_{d\left(\boldsymbol{z}^{(t)}\right), d\left(\mathbf{z}^{(t+1)}\right)} P\left[\boldsymbol{x}^{(t+1)} \mid \boldsymbol{z}^{(t+1)}, \theta_{d\left(\boldsymbol{z}^{(t+1)}\right)}\right]\right)
\end{aligned}
$$

- Define

$$
\delta_{i}^{(t)}=\max _{z^{(1)}, \cdots, z^{(t-1)}} P\left[x^{(1)}, \cdots, x^{(t)}, z^{(1)}, \cdots, z^{(t-1)}, z^{(t)}=e_{i} \mid \Theta\right]
$$

- $z^{*}$ is the sequence having $\delta^{(T) *}=\max _{1 \leqslant i \leqslant K} \delta_{i}^{(T)}$
- Notice that we can calculate $\delta_{j}^{(T)}$ efficiently if we already know $\delta_{i}^{(T-1)}$ for all $1 \leqslant i \leqslant K$

$$
\text { - } \delta_{j}^{(t)}=\left(\max _{1 \leqslant i \leqslant K} \delta_{i}^{(t-1)} a_{i, j}\right) P\left[\boldsymbol{x}^{(t)} \mid z_{j}^{(t)}, \theta_{j}\right]
$$

- $\delta_{j}^{(t)}$ has the optimal substructure and can be evaluated efficiently using dynamic programming
- We can obtain $z^{*}$ by backtracking


## The Viterbi Algorithm

Input: $\mathcal{X} \leftarrow\left\{\boldsymbol{x}^{(t)}\right\}_{t=1}^{T}$ and $\Theta \leftarrow\left(\boldsymbol{\pi}^{(1)}, \boldsymbol{A},\left\{\theta_{i}\right\}_{i=1}^{K}\right)$
Output: $\mathcal{Z} \leftarrow\left\{\boldsymbol{z}^{(t)}\right\}_{t=1}^{T}$ resulting the highest $P[\mathcal{X}, \mathcal{Z} \mid \Theta]$
for $i \leftarrow 1$ to $K$ do

```
    \(\delta_{i}^{(1)} \leftarrow \pi_{i}^{(1)} P\left[x^{(1)} \mid z_{i}^{(1)}, \theta_{i}\right] ;\)
    \(\psi_{i}^{(1)} \leftarrow\) null;
end
for \(t \leftarrow 2\) to \(T\) do
    for \(j \leftarrow 1\) to \(K\) do
        \(\delta_{j}^{(t)} \leftarrow\left(\max _{1 \leqslant i \leqslant K} \delta_{i}^{(t-1)} a_{i, j}\right) P\left[x^{(t)} \mid z_{j}^{(t)}, \theta_{j}\right] ;\)
        \(\psi_{j}^{(t)} \leftarrow \arg _{1 \leqslant i \leqslant K} \max \delta_{i}^{(t-1)} a_{i, j} ; / /\) previous state
    end
end
\(d\left(z^{(T)}\right) \leftarrow \arg _{1 \leqslant i \leqslant K} \max \delta_{i}^{(T)} ;\)
for \(t \leftarrow T-1\) to 1 do
    \(d\left(z^{(t)}\right) \leftarrow \psi_{d\left(z^{(t+1)}\right)}^{(t+1)} ; / /\) backtracking
end
```

Algorithm 1: The Viterbi algorithm of time complexity $O\left(K^{2} T\right)$.

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## Making Predictions

- When HMM is used to model a class, we predict a new sequence $X^{n e w}$ to be in class $C_{i}$ if the posterior $P\left[C_{i} \mid X^{\text {new }}\right] \propto P\left[X^{\text {new }} \mid \Theta_{i}\right] P\left[C_{i}\right]$ is the highest
- Problem: given parameters $\Theta$ and a sequence $X$, we want to know $P[\mathcal{X} \mid \Theta]$
- Again, we can try out all possible z using $P[X \mid \Theta]=\sum_{z} P[X, Z \mid \Theta]$, but this is cost prohibitive
- Better way?


## Making Predictions

- When HMM is used to model a class, we predict a new sequence $X^{\text {new }}$ to be in class $C_{i}$ if the posterior $P\left[C_{i} \mid X^{\text {new }}\right] \propto P\left[X^{\text {new }} \mid \Theta_{i}\right] P\left[C_{i}\right]$ is the highest
- Problem: given parameters $\Theta$ and a sequence $X$, we want to know $P[\mathcal{X} \mid \Theta]$
- Again, we can try out all possible z using $P[X \mid \Theta]=\sum_{z} P[X, Z \mid \Theta]$, but this is cost prohibitive
- Better way?
- Notice that $P[X \mid \Theta]=\sum_{i=1}^{K} P\left[X, z_{i}^{(t)} \mid \Theta\right]=\sum_{i=1}^{K} \alpha_{i}^{(T)}$
- Calculate the forward variables $\alpha_{i}^{(T)}$ for all $1 \leqslant i \leqslant K$ first, which takes $O\left(K^{2} T\right)$ time
- Obtain $P[X \mid \Theta]$ 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

$$
\begin{aligned}
& \alpha_{j}^{(t)}=\left(\sum_{i=1}^{K} \alpha_{i}^{(t-1)} a_{i, j}\right) P\left[x^{(t)} \mid z_{j}^{(t)}, \theta_{j}\right] \\
& \beta_{i}^{(t)}=\sum_{j=1}^{K} a_{i, j} P\left[x^{(t+1)} \mid z_{j}^{(t+1)}, \theta_{j}\right] \beta_{j}^{(t+1)}, \text { and } \\
& \delta_{j}^{(t)}=\left(\max _{1 \leqslant i \leqslant K} \delta_{i}^{(t-1)} a_{i, j}\right) P\left[x^{(t)} \mid z_{j}^{(t)}, \theta_{j}\right] \text { are all multiplication of small } \\
& \quad \text { numbers }
\end{aligned}
$$

- 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 $P[\mathcal{X} \mid \Theta]$ by $P[\mathcal{X} \mid \Theta]=\sum_{i=1}^{K} \alpha_{i}^{(T)}=\frac{1}{\prod_{t=1}^{T} c_{t}} \sum_{i=1}^{K} \widetilde{\alpha}_{i}^{(T)}=\frac{1}{\prod_{t=1}^{T} c_{t}}$
- 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 $K, K^{\prime}<K$, that can be transited to
- This reduces the complexity of forward-backward procedure and Viterbi algorithm to $O\left(K K^{\prime} T\right)$
- 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).

