## Markov Models

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## Outline

- Introduction
- Markov chains
- Dynamic belief networks
- Hiddem Markov models (HMMs)


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- Time series
- Probabilsitic graphical models
- Markov chains
- Dynamic belief networks
- Hiddem Markov models (HMM)


## What is time series?

- A time series is a sequence of data instance listed in time order.
- In other words, data instances are totally ordered.
- Example: weather forecasting

- Notice: we care about the orderings rather than the exact time.


## Different kinds of time series

- Two properties:


Temperature Prob of rain


## Probabilistic graphical models (PGMs)

- A PGM uses a graph-based representation to represent the conditional distributions over variables.
- Directed acyclic graphs (DAGs)
 Markov model is a subfamily of PGMs on DAGs
- Undirected graph



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- Intuition
- Inference
- Learning
- Dynamic belief networks
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## Modeling time series

Assume a sequence of four weather observations: $y_{1}, y_{2}, y_{3}, y_{4}$


- Possible dependences: $y_{4}$ depends on the previous weather(s)



## Modeling time series

In general observations: $y_{1}, y_{2}, y_{3}, y_{4}$ can be


Fully dependent: E.g. $y_{4}$ depends on all previous observations


Independent:
E.g. $y_{4}$ does not depend on any previous observation

## Modeling time series

- Are there intuitive and convenient dependency models?


Think of the last observation $P\left(y_{4} \mid y_{1} y_{2} y_{3}\right)$
What if we have T observations?
Parameter \#: exponential to \# of observations

## Markov chains

- Markov assumption: Future predictions are independent of all but the most recent observations


Fully dependent


First order Markov chain


Independent

## Markov chains

- Markov assumption: Future predictions are independent of all but the most recent observations



## A formal representation

- Using conditional probabilities to model $y_{1}, y_{2}, y_{3}, y_{4}$
- Fully dependent:
- $P\left(y_{1} y_{2} y_{3} y_{4}\right)=P\left(y_{1}\right) P\left(y_{2} \mid y_{1}\right) P\left(y_{3} \mid y_{1} y_{2}\right) P\left(y_{4} \mid y_{1} y_{2} y_{3}\right)$
- Fully independent:
- $P\left(y_{1} y_{2} y_{3} y_{4}\right)=P\left(y_{1}\right) P\left(y_{2}\right) P\left(y_{3}\right) P\left(y_{4}\right)$
- First-order Markov chain (recent 1 observation):
- $P\left(y_{1} y_{2} y_{3} y_{4}\right)=P\left(y_{1}\right) P\left(y_{2} \mid y_{1}\right) P\left(y_{3} \mid y_{2}\right) P\left(y_{4} \mid y_{3}\right)$
- Second-order Markov chain (recent 2 observations):
- $P\left(y_{1} y_{2} y_{3} y_{4}\right)=P\left(y_{1}\right) P\left(y_{2} \mid y_{1}\right) P\left(y_{3} \mid y_{1} y_{2}\right) P\left(y_{4} \mid y_{2} y_{3}\right)$


## A more formal representation

- Generalizes to T observations
- First-order Markov chain (recent 1 observation):
- $P\left(y_{1} y_{2} \ldots y_{T}\right)=P\left(y_{1}\right) \prod_{t=2}^{T} P\left(y_{t} \mid y_{t-1}\right)$
- Second-order Markov chain (recent 2 observations):
- $P\left(y_{1} y_{2} \ldots y_{T}\right)=P\left(y_{1}\right) P\left(y_{2} \mid y_{1}\right) \prod_{t=3}^{T} P\left(y_{t} \mid y_{t-1} y_{t-2}\right)$
- k-th order Markov chain (recent k observations):
- $P\left(y_{1} y_{2} \ldots y_{T}\right)=P\left(y_{1}\right) P\left(y_{2} \mid y_{1}\right) \ldots P\left(y_{k} \mid y_{1} \ldots y_{k-1}\right) \prod_{t=k+1}^{T} P\left(y_{t} \mid y_{t-k} \ldots y_{t-1}\right)$


## Stationarity

- Do all states yield to the identical conditional distribution?
- $P\left(y_{t}=j \mid y_{t-1}=i\right)=P\left(y_{t-1}=j \mid y_{t-2}=i\right)$ for all $t, i, j$
- Typically holds
- A transition table A to represent conditional distribution - $A_{i j}=P\left(y_{t}=j \mid y_{t-1}=i\right)$ for all $t=1,2, \ldots, T$ $\left[\begin{array}{ccc}A_{11} & \cdots & A_{1 d} \\ \vdots & \ddots & \vdots \\ A_{d 1} & \cdots & A_{d d}\end{array}\right]$ - $d$ : dimention of $y_{t}$
- A vector $\boldsymbol{\pi}$ to represent the initial distribution - $\pi_{i}=P\left(y_{1}=i\right)$ for all $i=1,2, \ldots, d$


## Inference on a Markov chain

- Probability of a given sequence
- $P\left(y_{1}=i_{1}, \ldots, y_{T}=i_{T}\right)=\pi_{i_{1}} \prod_{t=2}^{T} A_{i_{t} i_{t-1}}$
- Probability of a given state
- Forward iteration: $P\left(y_{t}=i_{t}\right)=\sum_{i_{t-1}} P\left(y_{t-1}=i_{t-1}\right) A_{i_{t} i_{t-1}}$
- Can be calculated iteratively
- Both inferences are efficient
- $P\left(y_{k}=i_{k}, \ldots, y_{T}=i_{T}\right)=P\left(y_{k}=i_{k}\right) \prod_{t=k+1}^{T} A_{i_{t} i_{t-1}}$


## Learning a Markov chain

- MLE of conditional probabilities can be estimated directly.
- $A_{i j}^{M L E}=P\left(y_{t}=j \mid y_{t-1}=i\right)=\frac{P\left(y_{t}=j, y_{t-1}=i\right)}{P\left(y_{t-1}=i\right)}=\frac{N_{i j}}{\sum_{j} N_{i j}}$
- $N_{i j}$ : \# of observations that yields $y_{t}=j, y_{t-1}=i$
- Bayesian parameter estimation
- Prior: $\operatorname{Dir}\left(\theta_{1}, \theta_{2}, \ldots\right)$
- Posterior: $\operatorname{Dir}\left(\theta_{1}+N_{i 1}, \theta_{2}+N_{i 2}, \ldots\right)$
$-A_{i j}^{M A P}=\frac{N_{i j}+\theta_{j}-1}{\sum_{j}\left(N_{i j}+\theta_{j}-1\right)} \quad A_{i j}^{E V}=\frac{N_{i j}+\theta_{j}}{\sum_{j}\left(N_{i j}+\theta_{j}\right)}$


## A toy example - weather forecast

- State 1: rainy state 2 : cloudy state 3: sunny
- Given "sun-sun-sun-rain-rain-sun-cloud-sun", find $A_{33}$
- $A_{33}^{M L E}=\frac{N_{33}}{\sum_{j} N_{3 j}}=\frac{2}{1+1+2}$
- Prior: $\operatorname{Dir}(2,2,2)$
- Posterior: $\operatorname{Dir}(2+1,2+1,2+2)$
- $A_{33}^{M A P}=\frac{N_{33}+\theta_{3}-1}{\sum_{j}\left(N_{3 j}+\theta_{j}-1\right)}=\frac{3}{7} \quad A_{33}^{E V}=\frac{N_{33}+\theta_{3}}{\sum_{j}\left(N_{3 j}+\theta_{j}\right)}=\frac{4}{10}$


## A toy example - weather forecast

- Given $A=\left[\begin{array}{ccc}0.4 & 0.3 & 0.3 \\ 0.2 & 0.6 & 0.2 \\ 0.1 & 0.1 & 0.8\end{array}\right]$, day 1 is sunny
- Find the probability that day $2 \sim 8$ will be "sun-sun-rain-rain-sun-cloud-sun"
- $P\left(y_{1} y_{2} \ldots y_{8}\right)=P\left(y_{1}=s\right) P\left(y_{2}=s \mid y_{1}=s\right)$


$$
\begin{aligned}
& P\left(y_{3}=s \mid y_{2}=s\right) P\left(y_{4}=r \mid y_{3}=s\right) P\left(y_{5}=r \mid y_{4}=r\right) \\
& P\left(y_{6}=s \mid y_{5}=r\right) P\left(y_{7}=c \mid y_{6}=s\right) P\left(y_{8}=s \mid y_{7}=c\right) \\
= & 1 \cdot A_{33} \cdot A_{33} \cdot A_{31} \cdot A_{11} \cdot A_{13} \cdot A_{32} \cdot A_{23} \\
= & 1 \cdot 0.8 \cdot 0.8 \cdot 0.1 \cdot 0.4 \cdot 0.3 \cdot 0.1 \cdot 0.2=1.536 \times 10^{-4}
\end{aligned}
$$

## A toy example - weather forecast

- Given $A=\left[\begin{array}{lll}0.4 & 0.3 & 0.3 \\ 0.2 & 0.6 & 0.2 \\ 0.1 & 0.1 & 0.8\end{array}\right]$, day 1 is sunny
- Find the probability that day 3 will be sunny

- $P\left(y_{2}=s\right)=\sum_{i} P\left(y_{1}=i\right) P\left(y_{2}=s \mid y_{1}=i\right)=0 \cdot 0.3+0 \cdot 0.2+1 \cdot 0.8=0.8$
- Similarly, $P\left(y_{2}=r\right)=\sum_{i} P\left(y_{1}=i\right) P\left(y_{2}=r \mid y_{1}=i\right)=0 \cdot 0.4+0 \cdot 0.2+1 \cdot 0.1=0.1$
- $P\left(y_{2}=c\right)=\sum_{i} P\left(y_{1}=i\right) P\left(y_{2}=c \mid y_{1}=i\right)=0 \cdot 0.3+0 \cdot 0.6+1 \cdot 0.1=0.1$
- $P\left(y_{3}=s\right)=\sum_{i} P\left(y_{2}=i\right) P\left(y_{3}=s \mid y_{2}=i\right)=0.1 \cdot 0.3+0.1 \cdot 0.2+0.8 \cdot 0.8=0.69$


## Limitation of Markov chain

- Each state is represented by one variable
- What if each state consists of multiple variables?


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## Modeling multiple variables

- What if each state consists of multiple variables?
- e.g. monitoring a robot
- Location, GPS, Speed

- Modeling all variables in each state jointly
- Is this a good solution?


## Modeling multiple variables



- Each variable only depends on some of the previous or current observations
- Factorization



## Dynamic belief networks

- Also named as dynamic Bayesian networks
$\mathbf{X}_{t}=\left\{S_{t}, L_{t}\right\}$ : transition states
Only dependent on previous
observations
$P\left(\mathbf{X}_{t} \mid \mathbf{X}_{t-1}\right)=$
$\left\{P\left(S_{t} \mid S_{t-1}\right), P\left(L_{t} \mid S_{t-1} L_{t-1}\right)\right\}$ : transition model

$\mathbf{Y}_{t}=\left\{G_{t}\right\}$ : emission states / evidences
Only dependent on current observations $P\left(\mathbf{Y}_{t} \mid \mathbf{X}_{t}\right)=\left\{P\left(G_{t} \mid L_{t}\right)\right\}:$ emission model / sensor model


## Inference on a dynamic BN

- Filtering: given $\mathbf{y}_{1 \ldots . t}$, find $P\left(\mathbf{X}_{t} \mid \mathbf{y}_{1 \ldots t}\right)$
- Exact inference
- using Bayesian rule and the structure of dynamic BN
- $P\left(\mathbf{X}_{t} \mid \mathbf{y}_{1 \ldots t}\right) \quad$ Can be inferred iteratively
$\propto P\left(\mathbf{X}_{t} \mathbf{y}_{t} \mid \mathbf{y}_{1 \ldots t-1}\right)$
$=P\left(\mathbf{y}_{t} \mid \mathbf{X}_{t} \mathbf{y}_{1 \ldots t-1}\right) P\left(\mathbf{X}_{t} \mid \mathbf{y}_{1 \ldots t-1}\right)_{\text {Structure of dynamic BN }}$
$=P\left(\mathbf{y}_{t} \mid \mathbf{X}_{t} \boldsymbol{y}_{\ldots, \ldots-1}\right) \sum_{\mathbf{x}_{t-1}} P\left(\mathbf{X}_{t} \mid \mathbf{x}_{t-1} \boldsymbol{Y}_{\text {Transition model }}\right) P\left(\mathbf{x}_{t-1} \mid \mathbf{y}_{1 \ldots t-1}\right)$


## Approximate inference on a dynamic BN

- Is exact inference useful?
- $P\left(\mathbf{X}_{t} \mid \mathbf{y}_{1 \ldots t}\right)=P\left(\mathbf{y}_{t} \mid \mathbf{X}_{t}\right) \sum_{\mathbf{x}_{t-1}} P\left(\mathbf{X}_{t} \mid \mathbf{x}_{t-1}\right) P\left(\mathbf{x}_{t-1} \mid \mathbf{y}_{1 . . t-1}\right)$
- Needs to enumerate $\mathbf{x}_{t-1}$, exponential to \# of transition variables
- Use approximate inference instead
- Particle filtering


## Particle filtering - a toy example

- $\mathbf{X}_{t}=\left\{S_{t}, L_{t}\right\}, \mathbf{Y}_{t}=\left\{G_{t}\right\}$
- $S_{t}, L_{t}$ only contains 2 outcomes
- $S_{t}=\{$ fast, slow $\} \quad L_{t}=\{$ left, right $\}$

- $P\left(\mathbf{X}_{1}\right)=P\left(S_{1} L_{1}\right)$ a $2 * 2$ table
- $N=10$ : \# of samples in each iteration
- $t$ th iteration $=$ time state $t$


## Particle filtering - a toy example

- Step 1: samples $\mathbf{a}_{1} \ldots \mathbf{a}_{N}$ from prior $P\left(\mathbf{X}_{t-1} \mid \mathbf{y}_{1 \ldots t-1}\right)$
- When $t=1$, samples from $P\left(\mathbf{X}_{1}\right)$
- Step 2: update $\mathbf{a}_{i} \leftarrow$ samples from $P\left(\mathbf{X}_{t} \mid \mathbf{X}_{t-1}=\mathbf{a}_{i}\right)$ for all $i$
- $\mathbf{a}_{i}$ randomly transits based on transition model

| $\stackrel{\infty}{0}$ | 1 | 2 |
| :--- | :--- | :--- |
| $\stackrel{\rightharpoonup}{\circ}$ | 3 | 4 |

Location

| $\stackrel{0}{0}$ | 2 | 3 |
| :---: | :---: | :---: |
| $\stackrel{\infty}{2}$ | 2 | 3 |
|  |  | Location |

## Particle filtering - a toy example

- Step 3: given $\mathbf{y}_{t}$ and $\mathbf{a}_{i}$, define $w_{i}=P\left(\mathbf{y}_{t} \mid \mathbf{X}_{t}=\mathbf{a}_{i}\right)$
- In step 1 of next iteration, we sample from $\mathbf{a}_{1} \ldots \mathbf{a}_{N}$ where the weight of $\mathbf{a}_{i}$ is $w_{i}$
- Should be the same as sampling from $P\left(\mathbf{X}_{t} \mid \mathbf{y}_{1 \ldots t}\right)$
- Is this true?

| $\stackrel{y}{\|c\|}$ | 1 | 2 |
| :---: | :---: | :---: |
|  | 3 | 4 |
|  |  |  | Location |
|  |  |  |





## Correctness of particle filtering

- Can be proved using induction
- Let $N\left(\mathbf{x}_{t-1} \mid \mathbf{y}_{1 \ldots t-1}\right)$ denotes population of $\mathbf{x}_{t-1}$ given $\mathbf{y}_{1 \ldots t-1}$
- After step 1: $\frac{N\left(\mathbf{x}_{t-1} \mid \mathbf{y}_{1 \ldots t-1}\right)}{N}=P\left(\mathbf{x}_{t-1} \mid \mathbf{y}_{1 \ldots t-1}\right)$
- After step 2, we have population of $\mathbf{x}_{t}$ :
- $N\left(\mathbf{x}_{t} \mid \mathbf{y}_{1 \ldots t-1}\right)=\sum_{\mathbf{x}_{t-1}} P\left(\mathbf{x}_{t} \mid \mathbf{x}_{t-1}\right) N\left(\mathbf{x}_{t-1} \mid \mathbf{y}_{1 \ldots t-1}\right)$


## Correctness of particle filtering

- After step 3, population of $\mathbf{x}_{t}$ is weighted by $P\left(\mathbf{y}_{t} \mid \mathbf{x}_{t}\right)$
- $P\left(\mathbf{y}_{t} \mid \mathbf{x}_{t}\right) N\left(\mathbf{x}_{t} \mid \mathbf{y}_{1 \ldots t-1}\right)$

$$
\begin{aligned}
& =P\left(\mathbf{y}_{t} \mid \mathbf{x}_{t}\right) \sum_{\mathbf{x}_{t-1}} P\left(\mathbf{x}_{t} \mid \mathbf{x}_{t-1}\right) N\left(\mathbf{x}_{t-1} \mid \mathbf{y}_{1 \ldots t-1}\right) \\
& =N P\left(\mathbf{y}_{t} \mid \mathbf{x}_{t}\right) \sum_{\mathbf{x}_{t-1}} P\left(\mathbf{x}_{t} \mid \mathbf{x}_{t-1}\right) P\left(\mathbf{x}_{t-1} \mid \mathbf{y}_{1 \ldots t-1}\right) \\
& =N P\left(\mathbf{y}_{t} \mid \mathbf{x}_{t}\right) P\left(\mathbf{x}_{t} \mid \mathbf{y}_{1 \ldots t-1}\right) \\
& =N P\left(\mathbf{y}_{t} \mathbf{x}_{t} \mid \mathbf{y}_{1 \ldots t-1}\right) \propto P\left(\mathbf{x}_{t} \mid \mathbf{y}_{1 \ldots t}\right)
\end{aligned}
$$

## Learning a dynamic BN

- Given the structure of the dynamic BN...
- Learning transition models and emission models is same as in Markov chain
- How to learn the structure?
- For $P\left(\mathbf{X}_{t} \mid \mathbf{X}_{t-1}\right)$, take each $\mathbf{X}_{t}^{(i)} \in \mathbf{X}_{t}$ as label and $\mathbf{X}_{t-1}$ as features
- For $P\left(\mathbf{Y}_{t} \mid \mathbf{X}_{t}\right)$, take each $\mathbf{Y}_{t}^{(i)} \in \mathbf{Y}_{t}$ as label and $\mathbf{X}_{t}$ as features
- Converts to feature reduction


## Limitation

- Current assumption: all states are observable, which is unrealistic

- The actual location $L$ of the robot may never be observed
- What if some variables are hidden?


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- Applications \& APIs


## Hidden variables

- Some variables in the dynamic BN can be hidden

- Transistion variables can be hidden
- HMM: think of only one transition \& one emission variable


## Hidden Markov models (HMMs)

- Overview

- A sequence of length T
- Evidence / emission variable: $\left\{y_{t}\right\}$ is categorical or continuous
- Hidden variable: $\left\{x_{t}\right\}$ is categorical
- $P\left(y_{1} \ldots y_{T}, x_{1} \ldots x_{T}\right)=P\left(x_{1}\right) \prod_{t=2}^{T} P\left(x_{t} \mid x_{t-1}\right) \prod_{t=1}^{T} P\left(y_{t} \mid x_{t}\right)$


## Transition table

- Let d as the dimention of $x_{t}$
- Transition table A is a $\mathrm{d}^{*} \mathrm{~d}$ matrix

$$
A=\left[\begin{array}{ccc}
A_{11} & \cdots & A_{1 d} \\
\vdots & \ddots & \vdots \\
A_{d 1} & \cdots & A_{d d}
\end{array}\right]
$$

- $A_{i j}=P\left(x_{t}=j \mid x_{t-1}=i\right)$
- Clearly, $\sum_{j=1}^{d} A_{i j}=1$ for all i


## Emission function

- When $y_{t}$ is categorical, let K as the dimension of $y_{t}$
- Emission function B can be represented as a d*K matrix

$$
B=\left[\begin{array}{ccc}
B_{11} & \cdots & B_{1 K} \\
\vdots & \ddots & \vdots \\
B_{d 1} & \cdots & B_{d K}
\end{array}\right]
$$

- $B_{i j}=P\left(y_{t}=j \mid x_{t}=i\right)$
- Clearly, $\sum_{j=1}^{K} B_{i j}=1$ for all i


## Emission function

- When $y_{t}$ is continuous, $p\left(y_{t} \mid x_{t}\right)$ is a PDF
- Emission function B is the set of parameters of different PDFs
- When $p\left(y_{t} \mid x_{t}\right)$ is Gaussian
- $B=\left\{\mu_{1} \ldots \mu_{d}, \Sigma_{1} \ldots \Sigma_{d}\right\}$


## Inference on an HMM

- Given the HMM, what can we do?
- Given an observation sequence, find its probability
- Filtering: find the distribution of the last hidden variable
- Smoothing: find the distribution of the a hidden variable in the middle
- Given an observation sequence, find the most likely (ML) hidden variable sequence


## Probability of an observed sequence

- $P\left(y_{1} \ldots y_{T}\right)=\sum_{i=1}^{d} P\left(y_{1} \ldots y_{T}, x_{T}=i\right)$
- Let's expand one step more:
- $P\left(y_{\frac{1}{d}} \ldots y_{T}, x_{T}=i\right)=\sum_{j=1}^{d} P\left(y_{1} \ldots y_{T}, x_{T}=i, x_{T-1}=j\right)$
$=\sum_{j=1} P\left(y_{1} \ldots y_{T-1}, x_{T-1}=j\right) P\left(x_{T}=i \mid x_{T-1}=j\right) P\left(y_{T} \mid x_{T}=i\right)$
- Can be calculated iteratively


## Forward algorithm

- Let $\alpha_{t}(i)=P\left(y_{1} \ldots y_{t}, x_{t}=i\right)$
- Iteration:

$$
\alpha_{t}(i)=\sum_{j=1}^{d} \alpha_{t-1}(j) A_{j i} P\left(y_{t} \mid x_{t}=i\right)
$$

- Base: $\quad \alpha_{1}(i)=P\left(y_{1}, x_{1}=i\right)=\pi_{i} P\left(y_{1} \mid x_{1}=i\right)$
- Output: $\quad \sum_{i=1}^{d} \alpha_{T}(i)$


## Forward algorithm

- $P\left(y_{1} \ldots y_{t}, x_{t}=i\right)=\sum_{j=1}^{d} P\left(y_{1} \ldots y_{t-1}, x_{t-1}=j\right) P\left(y_{t}, x_{t}=i \mid x_{t-1}=j\right)$
- $\alpha_{t}(i)=P\left(y_{1} \ldots y_{t}, x_{t}=i\right)$
- $\alpha_{t-1}(j)=P\left(y_{1} \ldots y_{t-1}, x_{t-1}=j\right)$
- $P\left(y_{t}, x_{t}=i \mid x_{t-1}=j\right)=A_{j i} P\left(y_{t} \mid x_{t}=i\right)$



## Backward algorithm

- Iterates reversely
- Let $\beta_{t}(i)=P\left(y_{t+1} \ldots y_{T} \mid x_{t}=i\right)$
- Iteration:

$$
\beta_{t}(i)=\sum_{j=1}^{d} \beta_{t+1}(j) A_{i j} P\left(y_{t+1} \mid x_{t+1}=i\right)
$$

- Base: $\quad \beta_{T}(i)=1$
- Output: $\quad \sum_{i=1}^{d} \pi_{i} P\left(y_{1} \mid x_{1}=i\right) \beta_{1}(i)$


## Filtering and smoothing

- Filtering: find $P\left(x_{T}=i \mid y_{1} \ldots y_{T}\right)$
- $P\left(x_{T}=i \mid y_{1} \ldots y_{T}\right) \propto P\left(y_{1} \ldots y_{T}, x_{T}=i\right)=\alpha_{t}(i)$
- Directly applies forward algorithm
- Smoothing: find $P\left(x_{t}=i \mid y_{1} \ldots y_{T}\right)$ where $t<T$
- $P\left(x_{t}=i \mid y_{1} \ldots y_{T}\right) \propto P\left(y_{1} \ldots y_{T}, x_{t}=i\right)$

$$
=P\left(y_{1} \ldots y_{t}, x_{t}=i\right) P\left(y_{t+1} \ldots y_{T} \mid x_{t}=i\right)=\alpha_{t}(i) \beta_{t}(i)
$$

- Using both forward and backward algorithm


## Viterbi algorithm

- Find $\underset{\operatorname{argmax}^{2}}{ } P\left(x_{1} \ldots x_{T} \mid y_{1} \ldots y_{T}\right)$

$$
x_{1} \ldots x_{T}
$$

- $\underset{x_{1} \ldots x_{T}}{\operatorname{argmax}} P\left(x_{1} \ldots x_{T} \mid y_{1} \ldots y_{T}\right)=\underset{x_{1} \ldots x_{T}}{\operatorname{argmax}} P\left(y_{1} \ldots y_{T}, x_{1} \ldots x_{T}\right)$
- Let $\delta_{t}(i)=\max _{x_{1} \ldots x_{t-1}} P\left(y_{1} \ldots y_{t}, x_{1} \ldots x_{t-1}, x_{t}=i\right)$
- Represents the highest probability of a hidden variable sequence $x_{1} \ldots x_{t}$ ending with $x_{t}=i$
- Iteration: $\quad \delta_{t}(i)=P\left(y_{t} \mid x_{t}=i\right) \max _{j}\left[\delta_{t-1}(j) A_{j i}\right]$
- $A_{j i}$ and $P\left(y_{t} \mid x_{t}=i\right)$ are independent of $y_{1} \ldots y_{t-1}, x_{1} \ldots x_{t-2}$
- Base: $\quad \delta_{1}(i)=P\left(y_{1}, x_{1}=i\right)=\pi_{i} P\left(y_{1} \mid x_{1}=i\right)$


## Learning an HMM

- Given $y_{1} \ldots y_{T}$, find the MLE of $\pi, A, B$
- Some notations (for simplicity):
$\mathbf{~} \mathbf{x}=\left\{x_{1} \ldots x_{t}\right\} \quad \mathbf{y}=\left\{y_{1} \ldots y_{T}\right\}$
- $x_{t i}$ : binary variable, 1 if $x_{t}=i$ and 0 otherwise
- $\gamma\left(x_{t i}\right)=P\left(x_{t}=i \mid \mathbf{y}\right)$
- $\eta\left(x_{t-1, j} x_{t i}\right)=P\left(x_{t-1}=j, x_{t}=i \mid \mathbf{y}\right)$
- Using Baum-Welch algorithm (EM)


## Q function

- 

$$
\max _{\mathbf{\pi}, A, B} \mathbb{E}_{\mathbf{x} \mid \mathbf{y}} \log P(\mathbf{y}, \mathbf{x})
$$

- $\sum_{\mathbf{x}} P(\mathbf{x} \mid \mathbf{y}) \log P(\mathbf{y}, \mathbf{x})=\sum_{\mathbf{x}} P(\mathbf{x} \mid \mathbf{y})\left[\log P\left(x_{1}\right)+\sum_{t=2}^{T} P\left(x_{t} \mid x_{t-1}\right)+\sum_{t=1}^{T} P\left(y_{t} \mid x_{t}\right)\right]$
$=\sum_{x_{1}} P\left(x_{1} \mid \mathbf{y}\right) \log P\left(x_{1}\right)+\sum_{t=2}^{T} \sum_{x_{t-1} x_{t}} P\left(x_{t-1} x_{t} \mid \mathbf{y}\right) \log P\left(x_{t} \mid x_{t-1}\right)+\sum_{t=1}^{T} \sum_{x_{t}} P\left(x_{t} \mid \mathbf{y}\right) \log P\left(y_{t} \mid x_{t}\right)$
$=\sum_{k=1}^{d} \gamma\left(x_{1 k}\right) \log \pi_{k}+\sum_{t=2}^{T} \sum_{j=1}^{d} \sum_{k=1}^{d} \eta\left(x_{t-1, j} x_{t k}\right) \log A_{j k}+\sum_{t=1}^{T} \sum_{k=1}^{d} \gamma\left(x_{t k}\right) \log P\left(y_{t} \mid x_{t}=k\right)$


## M-step

$\sum_{k=1}^{d} \gamma\left(x_{1 k}\right) \log \pi_{k}+\sum_{t=2}^{T} \sum_{j=1}^{d} \sum_{k=1}^{d} \eta\left(x_{t-1, j} x_{t k}\right) \log A_{j k}+\sum_{t=1}^{T} \sum_{k=1}^{d} \gamma\left(x_{t k}\right) \log P\left(y_{t} \mid x_{t}=k\right)$

- We can maximize Q regarding $\pi, A, B$ separately
- Can be achieved using Lagrange multipliers


## Maximize $Q$ regarding $\pi$

- For $\boldsymbol{\pi}=\left\{\pi_{1} \ldots \pi_{d}\right\}$, we always have $\sum_{k=1}^{d} \pi_{k}=1$
- We incorporate such constraint, and set the derivative as 0 :

$$
\frac{\partial}{\partial \pi_{k}}\left[\sum_{k=1}^{d} \gamma\left(x_{1 k}\right) \log \pi_{k}+\varphi\left(\sum_{k=1}^{d} \pi_{k}-1\right)\right]=\frac{\gamma\left(x_{1 k}\right)}{\pi_{k}}+\varphi=0
$$

- In other words, $\gamma\left(x_{1 k}\right)+\varphi \pi_{k}=0$ holds for all k . Their sum is also 0

$$
\sum_{k=1}^{d} \gamma\left(x_{1 k}\right)+\varphi \sum_{k=1}^{d} \pi_{k}=\sum_{k=1}^{d} \gamma\left(x_{1 k}\right)+\varphi=0
$$

- Take $\varphi$ back to the derivative for each $\pi_{k}$, we obtain $\pi_{k}=\frac{\gamma\left(x_{1 k}\right)}{\sum_{j=1}^{d} \gamma\left(x_{1 j}\right)}$


## Maximize Q regarding $A, B$

- Using similar technique, A and B can also be optimized
- $A_{j k}=\frac{\sum_{t=2}^{T} \eta\left(x_{t-1, j} x_{t k}\right)}{\sum_{l=1}^{d} \sum_{t=2}^{T} \eta\left(x_{t-1, j} x_{t l}\right)}$
- When $y_{t}$ is categorical:
- $P\left(y_{t} \mid x_{t}=k\right)=\prod_{i=1}^{K} \mu_{i k} y_{t i x_{t k}}$ where $\mu_{i k}=\frac{\sum_{t=1}^{T} \gamma\left(x_{t k}\right) y_{t i}}{\sum_{t=1}^{T} \gamma\left(x_{t k}\right)}$
- When $y_{t}$ is continuous: $P\left(y_{t} \mid x_{t}=k\right) \sim \mathcal{N}\left(\mu_{k}, \Sigma_{k}\right)$
- $\mu_{k}=\frac{\sum_{t=1}^{T} \gamma\left(x_{t k}\right) y_{t}}{\sum_{t=1}^{T} \gamma\left(x_{t k}\right)}$

$$
\Sigma_{k}=\frac{\sum_{t=1}^{T} \gamma\left(x_{t k}\right)\left(y_{t}-\mu_{k}\right)\left(y_{t}-\mu_{k}\right)^{T}}{\Sigma_{t=1}^{T} \gamma\left(x_{t k}\right)}
$$

## E-step

- Compute $\gamma\left(x_{t k}\right)$ and $\eta\left(x_{t-1, j} x_{t k}\right)$ for all t,j,k
- Remember:
- $\gamma\left(x_{t k}\right)=P\left(x_{t}=k \mid \mathbf{y}\right)$
- $\eta\left(x_{t-1, j} x_{t k}\right)=P\left(x_{t-1}=j, x_{t}=k \mid \mathbf{y}\right) \quad$ Similar to smoothing!
- $\gamma\left(x_{t k}\right) \propto P\left(x_{t}=k, \mathbf{y}\right)=\alpha_{t}(k) \beta_{t}(k)$
- $\eta\left(x_{t-1, j} x_{t k}\right) \propto P\left(x_{t-1}=j, x_{t}=k, \mathbf{y}\right)=\alpha_{t-1}(j) \beta_{t}(k) A_{j k} P\left(y_{t} \mid x_{t}=k\right)$


## Applications

- Speech recognition
- Natural language processing


Part Of Speech Tagging

- Bio-sequence analysis


## APIs

- Python: hmmlearn (compatible with scikit-learn)
- https://github.com/hmmlearn/hmmlearn (or pip install hmmlearn)
- Matlab (integrated)
- https://www.mathworks.com/help/stats/hidden-markov-modelshmm.html
- C++: HTK3
- http://htk.eng.cam.ac.uk/


## Thank You!

Markov models

