CSCI567 Machine Learning (Spring 2021)

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April 9, 2021

Outline

1. Review of last lecture
2. (Hidden) Markov models II

Logistics for Quiz 2

- There will be 5 questions.
- Only Question 1 will cover cumulative course material, i.e. all topics covered in the class.
- Question 1 will have 5 Multiple Choice Questions (MCQs) and 5 Single CQs.
- Questions 2-5 will be based on material covered after Quiz 1.

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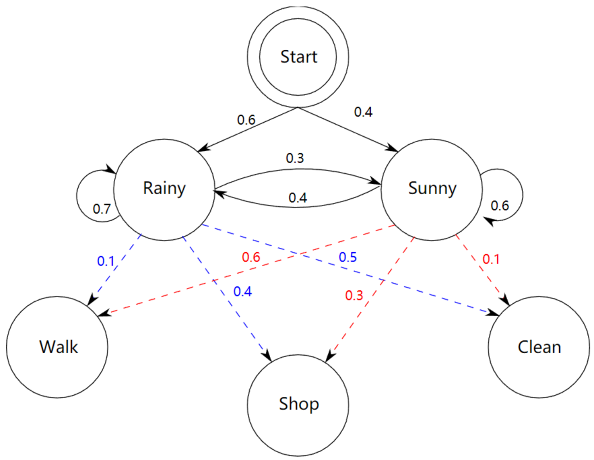
2. (Hidden) Markov models II

An example

picture from Wikipedia

On each day, we also observe **Bob's activity: walk, shop, or clean**, which only depends on the weather of that day.



Definition

A **Markov chain** is a stochastic process with **Markov property**: a sequence of random variables $Z_1, Z_2, \cdots$ s.t.

$$P(Z_{t+1} \mid Z_{1:t}) = P(Z_{t+1} \mid Z_t) \qquad \text{(Markov property)}$$

i.e. *the current state only depends on the most recent state* (notation $Z_{1:t}$ denotes the sequence $Z_1, \ldots, Z_t$).

We consider the following setting:

- All Z_t's take value from the same discrete set $\{1, \ldots, S\}$
- $P(Z_1 = s) = \pi_s$ **initial distribution**
- $P(Z_{t+1} = s' \mid Z_t = s) = a_{s,s'}$, known as **transition probability**
- $P(X_t = o \mid Z_t = s) = b_{s,o}$ **emission probability**
- $(\{\pi_s\}, \{a_{s,s'}\}\{b_{s,o}\}) = (\boldsymbol{\pi}, \boldsymbol{A}, \boldsymbol{B})$ **parameters of the model**

Outline

1 Review of last lecture

2 (Hidden) Markov models II
- Inferring HMMs
- Learning HMMs

What can we infer about an HMM?

Knowing the parameter of an HMM, we can infer

- **the probability of observing some sequence**

$$P(X_{1:T} = x_{1:T})$$

e.g. prob. of observing Bob's activities "walk, walk, shop, clean, walk, shop, shop" for one week

- **the state at some point, given an observation sequence**

$$P(Z_t = s \mid X_{1:T} = x_{1:T})$$

e.g. given Bob's activities for one week, how was the weather like on Wed?

What can we infer for a known HMM?

Knowing the parameter of an HMM, we can infer

- **the transition at some point, given an observation sequence**

$$P(Z_t = s, Z_{t+1} = s' \mid X_{1:T} = x_{1:T})$$

  e.g. given Bob's activities for one week, how was the weather like on Wed and Thu?

- **most likely hidden states path, given an observation sequence**

$$\operatorname*{argmax}_{z_{1:T}} P(Z_{1:T} = z_{1:T} \mid X_{1:T} = x_{1:T})$$

  e.g. given Bob's activities for one week, what's the most likely weather for this week?

Forward and backward messages

The key to infer all these is to compute two things:

- **forward messages**: for each s and t

$$\alpha_s(t) = P(Z_t = s, X_{1:t} = x_{1:t})$$

- **backward messages**: for each s and t

$$\beta_s(t) = P(X_{t+1:T} = x_{t+1:T} \mid Z_t = s)$$

Computing forward messages

Key: *establish a recursive formula*

$$\begin{aligned}
&\alpha_s(t) \\
&= P(Z_t = s, X_{1:t} = x_{1:t}) \\
&= P(X_t = x_t \mid Z_t = s, X_{1:t-1} = x_{1:t-1}) P(Z_t = s, X_{1:t-1} = x_{1:t-1}) \\
&= b_{s,x_t} \sum_{s'} P(Z_t = s, Z_{t-1} = s', X_{1:t-1} = x_{1:t-1}) \qquad \text{(marginalizing)} \\
&= b_{s,x_t} \sum_{s'} P(Z_t = s | Z_{t-1} = s', X_{1:t-1} = x_{1:t-1}) P(Z_{t-1} = s', X_{1:t-1} = x_{1:t-1}) \\
&= b_{s,x_t} \sum_{s'} a_{s',s} \alpha_{s'}(t-1) \qquad \text{(\textit{recursive form!})}
\end{aligned}$$

Base case: $\alpha_s(1) = P(Z_1 = s, X_1 = x_1) = \pi_s b_{s,x_1}$

Forward procedure

Forward procedure

For all $s \in [S]$, compute $\alpha_s(1) = \pi_s b_{s,x_1}$.

For $t = 2, \ldots, T$

- for each $s \in [S]$, compute

$$\alpha_s(t) = b_{s,x_t} \sum_{s'} a_{s',s} \alpha_{s'}(t-1)$$

It takes $O(S^2 T)$ time and $O(ST)$ space.

Computing backward messages

Again establish a recursive formula

$$
\begin{aligned}
&\beta_s(t) \\
&= P(X_{t+1:T} = x_{t+1:T} \mid Z_t = s) \\
&= \sum_{s'} P(X_{t+1:T} = x_{t+1:T}, Z_{t+1} = s' \mid Z_t = s) && \text{(marginalizing)} \\
&= \sum_{s'} P(Z_{t+1} = s' \mid Z_t = s) P(X_{t+1:T} = x_{t+1:T} \mid Z_{t+1} = s', Z_t = s) \\
&= \sum_{s'} a_{s,s'} P(X_{t+1} = x_{t+1} \mid Z_{t+1} = s') P(X_{t+2:T} = x_{t+2:T} \mid Z_{t+1} = s') \\
&= \sum_{s'} a_{s,s'} b_{s',x_{t+1}} \beta_{s'}(t+1) && \text{(\textit{recursive form!})}
\end{aligned}
$$

Base case: $\beta_s(T) = 1$

Backward procedure

Backward procedure

For all $s \in [S]$, set $\beta_s(T) = 1$.

For $t = T-1, \ldots, 1$

- for each $s \in [S]$, compute

$$\beta_s(t) = \sum_{s'} a_{s,s'} b_{s',x_{t+1}} \beta_{s'}(t+1)$$

Again it takes $O(S^2T)$ time and $O(ST)$ space.

Using forward and backward messages

With forward and backward messages, we can easily infer many things, e.g.

$$
\begin{aligned}
\gamma_s(t) &= P(Z_t = s \mid X_{1:T} = x_{1:T}) \\
&\propto P(Z_t = s, X_{1:T} = x_{1:T}) \\
&= P(Z_t = s, X_{1:t} = x_{1:t}) P(X_{t+1:T} = x_{t+1:T} \mid Z_t = s, X_{1:t} = x_{1:t}) \\
&= \alpha_s(t)\beta_s(t)
\end{aligned}
$$

What constant are we omitting in "$\propto$"? It is exactly

$$P(X_{1:T} = x_{1:T}) = \sum_s \alpha_s(t)\beta_s(t),$$

the probability of observing the sequence $x_{1:T}$.

This is true for any t; a good way to check correctness of your code.

Using forward and backward messages

Another example: the conditional probability of transition s to s' at time t

$$
\begin{aligned}
&\xi_{s,s'}(t) \\
&= P(Z_t = s, Z_{t+1} = s' \mid X_{1:T} = x_{1:T}) \\
&\propto P(Z_t = s, Z_{t+1} = s', X_{1:T} = x_{1:T}) \\
&= P(Z_t = s, X_{1:t} = x_{1:t}) P(Z_{t+1} = s', X_{t+1:T} = x_{t+1:T} \mid Z_t = s, X_{1:t} = x_{1:t}) \\
&= \alpha_s(t) P(Z_{t+1} = s' \mid Z_t = s) P(X_{t+1:T} = x_{t+1:T} \mid Z_{t+1} = s') \\
&= \alpha_s(t) a_{s,s'} P(X_{t+1} = x_{t+1} \mid Z_{t+1} = s') P(X_{t+2:T} = x_{t+2:T} \mid Z_{t+1} = s') \\
&= \alpha_s(t) a_{s,s'} b_{s',x_{t+1}} \beta_{s'}(t+1)
\end{aligned}
$$

The normalization constant is in fact again $P(X_{1:T} = x_{1:T})$

Decoding: Finding the most likely path

Though can't use forward and backward messages directly to find the most likely path, it is very similar to the forward procedure. Key: compute

$$\delta_s(t) = \max_{z_{1:t-1}} P(Z_t = s, Z_{1:t-1} = z_{1:t-1}, X_{1:t} = x_{1:t})$$

the probability of the most likely path for time $1:t$ ending at state s

Computing $\delta_s(t)$

Observe

$$\begin{aligned}
\delta_s(t) &= \max_{z_{1:t-1}} P(Z_t = s, Z_{1:t-1} = z_{1:t-1}, X_{1:t} = x_{1:t}) \\
&= \max_{s'} \max_{z_{1:t-2}} P(Z_t = s, Z_{t-1} = s', Z_{1:t-2} = z_{1:t-2}, X_{1:t} = x_{1:t}) \\
&= \max_{s'} P(Z_t = s \mid Z_{t-1} = s') P(X_t = x_t \mid Z_t = s) \cdot \\
&\qquad \max_{z_{1:t-2}} P(Z_{t-1} = s', Z_{1:t-2} = z_{1:t-2}, X_{1:t-1} = x_{1:t-1}) \\
&= b_{s,x_t} \max_{s'} a_{s',s} \delta_{s'}(t-1) \qquad \text{(}\textit{recursive form!}\text{)}
\end{aligned}$$

Base case: $\delta_s(1) = P(Z_1 = s, X_1 = x_1) = \pi_s b_{s,x_1}$

Exactly the same as forward messages except replacing "sum" by "max"!

Viterbi Algorithm (!)

Viterbi Algorithm

For each $s \in [S]$, compute $\delta_s(1) = \pi_s b_{s,x_1}$.

For each $t = 2, \ldots, T$,

- for each $s \in [S]$, compute

$$\delta_s(t) = b_{s,x_t} \max_{s'} a_{s',s} \delta_{s'}(t-1),$$

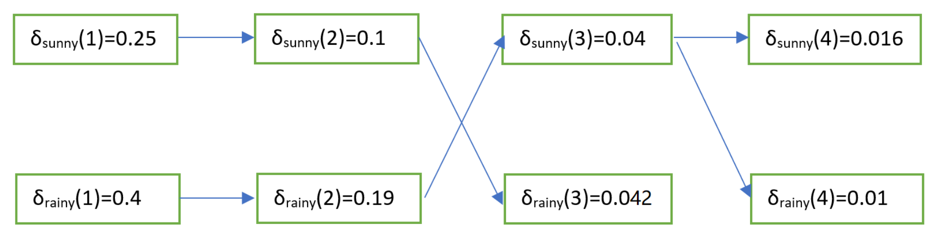
$$\Delta_s(t) = \operatorname*{argmax}_{s'} a_{s',s} \delta_{s'}(t-1).$$

Backtracking: let $z_T^* = \operatorname{argmax}_s \delta_s(T)$.
For each $t = T, \ldots, 2$: set $z_{t-1}^* = \Delta_{z_t^*}(t)$.

Output the most likely path $z_1^*, \ldots, z_T^*$.

Example

Arrows represent the "argmax", i.e. $\Delta_s(t)$.



The most likely path is **"rainy, rainy, sunny, sunny"**.

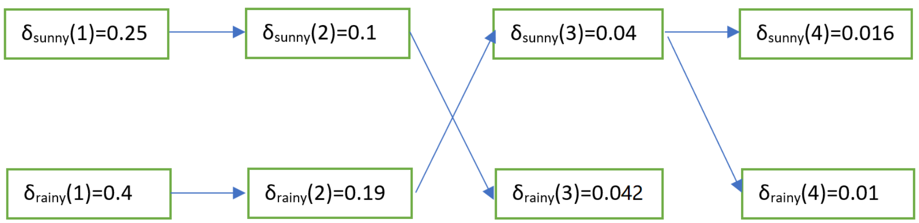
Exercise 1

What is the most likely sequence $z^*_{1:T_0}$ given $x_{1:T_0}$ for some $T_0 < T$?

- Is it the first T_0 outputs of the Viterbi algorithm (with all data)?

No. It should be

- $z^*_{T_0} = \text{argmax}_s \, \delta_s(T_0)$
- for each $t = T_0, \ldots, 2$: $z^*_{t-1} = \Delta_{z^*_t}(t)$



The answer for $T_0 = 3$ is: **"sunny, sunny, rainy"**.

Exercise 2

What is the most likely sequence $z^*_{1:T_0}$ given $x_{1:T}$ for some $T_0 < T$?

- Is it the same as Exercise 1?
- Is it the first T_0 outputs of the Viterbi algorithm (with all data)?

Neither. It should be

- $z^*_{T_0} = \text{argmax}_s \, \delta_s(T_0)\beta_s(T_0)$
- for each $t = T_0, \ldots, 2$: $z^*_{t-1} = \Delta_{z^*_t}(t)$

Exercise 2 (cont.)

Reasoning:

$$
\begin{aligned}
z^*_{T_0} &= \underset{s}{\text{argmax}} \max_{z_{1:T_0-1}} P(Z_{T_0} = s, Z_{1:T_0-1} = z_{1:T_0-1}, X_{1:T} = x_{1:T}) \\
&= \underset{s}{\text{argmax}} \max_{z_{1:T_0-1}} P(Z_{T_0} = s, Z_{1:T_0-1} = z_{1:T_0-1}, X_{1:T_0} = x_{1:T_0}) \cdot \\
&\qquad P(X_{T_0+1,T} = x_{T_0+1:T} \mid Z_{T_0} = s, Z_{1:T_0-1} = z_{1:T_0-1}, X_{1:T_0} = x_{1:T_0}) \\
&= \underset{s}{\text{argmax}} \left(\max_{z_{1:T_0-1}} P(Z_{T_0} = s, Z_{1:T_0-1} = z_{1:T_0-1}, X_{1:T_0} = x_{1:T_0}) \right) \cdot \\
&\qquad P(X_{T_0+1,T} = x_{T_0+1:T} \mid Z_{T_0} = s) \\
&= \underset{s}{\text{argmax}} \; \delta_s(T_0)\beta_s(T_0)
\end{aligned}
$$

Exercise 3

What is the most likely sequence $z^*_{1:T}$ given $x_{1:T_0}$ for some $T_0 < T$?

- Is it the same as the Viterbi algorithm (with all data)?
- Are the first T_0 states the same as Exercise 1?

Again, neither is true.

Exercise 3 (cont.)

Viterbi Algorithm with partial data $x_{1:T_0}$

For each $s \in [S]$, compute $\delta_s(1) = \pi_s b_{s,x_1}$.

For each $t = 2, \ldots, T$,

- for each $s \in [S]$, compute

$$\delta_s(t) = \begin{cases} b_{s,x_t} \max_{s'} a_{s',s}\delta_{s'}(t-1) & \text{if } t \le T_0 \\ \max_{s'} a_{s',s}\delta_{s'}(t-1) & \text{else} \end{cases}$$

$$\Delta_s(t) = \operatorname*{argmax}_{s'} a_{s',s}\delta_{s'}(t-1).$$

Backtracking: let $z_T^* = \operatorname{argmax}_s \delta_s(T)$.
For each $t = T, \ldots, 2$: set $z_{t-1}^* = \Delta_{z_t^*}(t)$.

Output the most likely path $z_1^*, \ldots, z_T^*$.

Learning the parameters of an HMM

All previous inferences depend on knowing the parameters $(\boldsymbol{\pi}, \boldsymbol{A}, \boldsymbol{B})$.

How do we learn the parameters based on N observation sequences $x_{n,1}, \ldots, x_{n,T}$ for $n = 1, \ldots, N$?

MLE is intractable due to the hidden variables $Z_{n,t}$'s (similar to GMMs)

Need to apply **EM** again! Known as the **Baum–Welch algorithm**.

Applying EM: E-Step

Recall in the E-Step we fix the parameters and find the **posterior distributions q of the hidden states** (for each sample n), which leads to the complete log-likelihood:

$$\begin{aligned} &\mathbb{E}_{z_{1:T}\sim q}\left[\ln P(Z_{1:T} = z_{1:T}, X_{1:T} = x_{1:T})\right] \\ &= \mathbb{E}_{z_{1:T}\sim q}\left[\ln \pi_{z_1} + \sum_{t=1}^{T-1} \ln a_{z_t,z_{t+1}} + \sum_{t=1}^{T} \ln b_{z_t,x_t}\right] \\ &= \sum_s \gamma_s(1)\ln \pi_s + \sum_{t=1}^{T-1}\sum_{s,s'} \xi_{s,s'}(t)\ln a_{s,s'} + \sum_{t=1}^{T}\sum_s \gamma_s(t)\ln b_{s,x_t} \end{aligned}$$

We have discussed how to compute

$$\gamma_s(t) = P(Z_t = s \mid X_{1:T} = x_{1:T})$$
$$\xi_{s,s'}(t) = P(Z_t = s, Z_{t+1} = s' \mid X_{1:T} = x_{1:T})$$

Applying EM: M-Step

The maximizer of complete log-likelihood is simply doing **weighted counting** (compared to the unweighted counting on Slide 18 Lecture 21):

$$\pi_s \propto \sum_n \gamma_s^{(n)}(1) = \mathbb{E}_q\left[\ \textbf{\#initial states with value } s\right]$$

$$a_{s,s'} \propto \sum_n \sum_{t=1}^{T-1} \xi_{s,s'}^{(n)}(t) = \mathbb{E}_q\left[\ \textbf{\#transitions from } s \textbf{ to } s'\right]$$

$$b_{s,o} \propto \sum_n \sum_{t:x_t=o} \gamma_s^{(n)}(t) = \mathbb{E}_q\left[\ \textbf{\#state-outcome pairs } (s,o)\right]$$

where

$$\gamma_s^{(n)}(t) = P(Z_{n,t} = s \mid X_{n,1:T} = x_{n,1:T})$$
$$\xi_{s,s'}^{(n)}(t) = P(Z_{n,t} = s, Z_{n,t+1} = s' \mid X_{n,1:T} = x_{n,1:T})$$

Slide 18 Lecture 21: Learning the model

If we observe N state-outcome sequences: $z_{n,1}, x_{n,1}, \ldots, z_{n,T}, x_{n,T}$ for $n = 1, \ldots, N$, the MLE can again be obtained in a similar way (verify yourself):

$$\pi_s \propto \textbf{\#initial states with value } s$$
$$a_{s,s'} \propto \textbf{\#transitions from } s \textbf{ to } s'$$
$$b_{s,o} \propto \textbf{\#state-outcome pairs } (s,o)$$

Baum–Welch algorithm

Step 0 Initialize the parameters $(\boldsymbol{\pi}, \boldsymbol{A}, \boldsymbol{B})$

Step 1 (E-Step) Fixing the parameters, compute forward and backward messages for all sample sequences, then use these to compute $\gamma_s^{(n)}(t)$ and $\xi_{s,s'}^{(n)}(t)$ for each n, t, s, s' (see Slides 15 and 16).

Step 2 (M-Step) Update parameters:

$$\pi_s \propto \sum_n \gamma_s^{(n)}(1), \quad a_{s,s'} \propto \sum_n \sum_{t=1}^{T-1} \xi_{s,s'}^{(n)}(t), \quad b_{s,o} \propto \sum_n \sum_{t:x_t=o} \gamma_s^{(n)}(t)$$

Step 3 Return to Step 1 if not converged

Summary

Very important models: **Markov chains**, **hidden Markov models**

Several algorithms:

- forward and backward procedures
- inferring HMMs based on forward and backward messages
- Viterbi algorithm
- Baum–Welch algorithm

Additional Resources:

- `https://web.stanford.edu/~jurafsky/slp3/A.pdf`
- MLaPP 17.3