CSCI567 Machine Learning (Fall 2020)

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U of Southern California

Nov 05, 2020

Administration

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Today's plan:

- one new topic (HMMs)
- HW4 review
- more exercises

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Next week's plan:

- final topics: multi-armed bandits and reinforcement learning
- only multiple-choice questions in Quiz 2

Outline

Markov Models

Markov models are powerful probabilistic tools to analyze **sequential data**:

- text or speech data
- stock market data
- gene data
- $\cdots$

Definition

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

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- $P(Z_{t+1} = s' \mid Z_t = s) = a_{s,s'}$, known as transition probability
- $P(Z_1 = s) = \pi_s$
- $(\{\pi_s\}, \{a_{s,s'}\}) = (\boldsymbol{\pi}, \boldsymbol{A})$ are parameters of the model

Examples

- Example 1 (**Language model**)

  States $[S]$ represent a dictionary of words,

  $$a_{\text{ice,cream}} = P(Z_{t+1} = \text{cream} \mid Z_t = \text{ice})$$

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  is an example of the transition probability.

- Example 2 (**Weather**)

  States $[S]$ represent weather at each day

  $$a_{\text{sunny,rainy}} = P(Z_{t+1} = \text{rainy} \mid Z_t = \text{sunny})$$

High-order Markov chain

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Higher order Markov chains make it more reasonable, e.g.

$$P(Z_{t+1} \mid Z_{1:t}) = P(Z_{t+1} \mid Z_t, Z_{t-1}) \qquad \text{(second-order Markov)}$$

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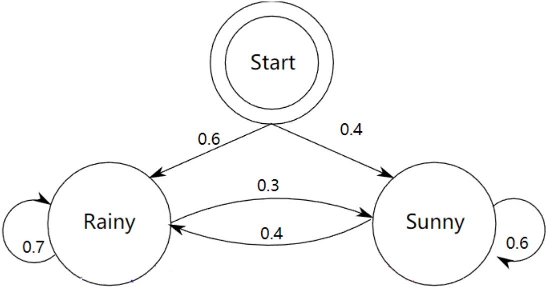
Learning higher order Markov chains is similar, but more expensive.

We only consider standard Markov chains.

Graph Representation

picture from Wikipedia

It is intuitive to represent a Markov model as a **graph**



Learning from examples

Now suppose we have observed N **sequences of examples**:

- $z_{1,1}, \ldots, z_{1,T}$
- $\cdots$
- $z_{n,1}, \ldots, z_{n,T}$
- $\cdots$
- $z_{N,1}, \ldots, z_{N,T}$

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- for simplicity we assume each sequence has the same length T
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From these observations how do we *learn the model parameters* $(\boldsymbol{\pi}, \boldsymbol{A})$?

Finding the MLE

Same story, find the **MLE**.

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&= \sum_{s} \mathbb{I}[z_1 = s] \ln \pi_s + \sum_{s,s'} \left(\sum_{t=2}^{T} \mathbb{I}[z_{t-1} = s, z_t = s'] \right) \ln a_{s,s'}
\end{aligned}$$

Finding the MLE

So MLE is

$$\operatorname*{argmax}_{\boldsymbol{\pi}, \boldsymbol{A}} \sum_{s} (\textbf{\#initial states with value } s) \ln \pi_s + \sum_{s,s'} (\textbf{\#transitions from } s \textbf{ to } s') \ln a_{s,s'}$$

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We have seen this many times. The solution is:

$$\pi_s \propto \#\text{initial states with value } s$$
$$a_{s,s'} \propto \#\text{transitions from } s \text{ to } s'$$

Example

Suppose we observed the following 2 sequences of length 5

- sunny, sunny, rainy, rainy, rainy
- rainy, sunny, sunny, sunny, rainy

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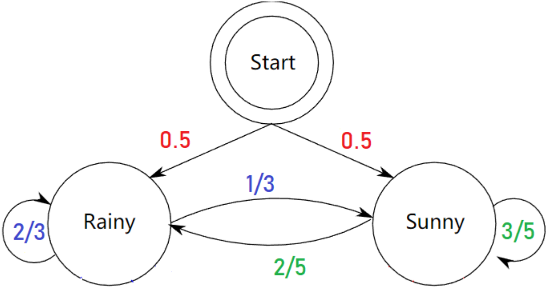
MLE is the following model



Markov Model with outcomes

Now suppose each state Z_t also "emits" some **outcome** $X_t \in [O]$ based on the following model

$$P(X_t = o \mid Z_t = s) = b_{s,o} \qquad \text{(emission probability)}$$

independent of anything else.

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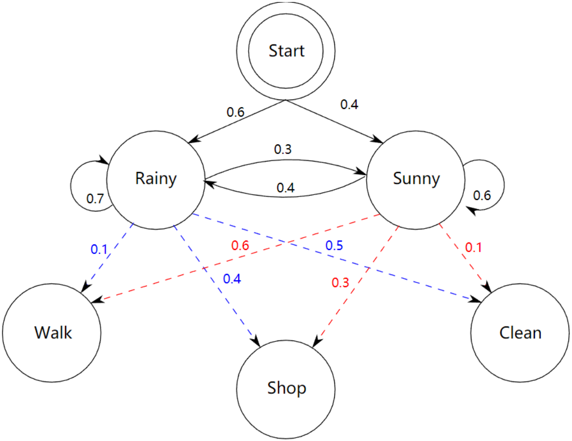
For example, in the language model, X_t is the speech signal for the underlying word Z_t (very useful for speech recognition).

Now the model parameters are $(\{\pi_s\}, \{a_{s,s'}\}, \{b_{s,o}\}) = (\boldsymbol{\pi}, \boldsymbol{A}, \boldsymbol{B})$.

Another 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.



Joint likelihood

The joint log-likelihood of a state-outcome sequence $z_1, x_1, \ldots, z_T, x_T$ is

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(due to all the independence)

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&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{(due to all the independence)} \\
&= \ln \pi_{z_1} + \sum_{t=2}^{T} \ln a_{z_{t-1}, z_t} + \sum_{t=1}^{T} \ln b_{z_t, x_t}
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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 is again very simple (verify yourself):

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

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How to learn HMMs?

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How to learn HMMs? **Roadmap**:

- first discuss how to **infer** when the model is known (key: dynamic programming)

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How to learn HMMs? **Roadmap**:

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- then discuss how to **learn** the model (key: EM)

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- **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**

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

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- **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

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

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

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- **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

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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 $t = 2, \dots, T$

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

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

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

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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)
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&= \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)
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Computing backward messages

Again establish a recursive formula

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Backward procedure

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

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

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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

$$\xi_{s,s'}(t)$$
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\end{aligned}$$

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

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.

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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

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

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

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

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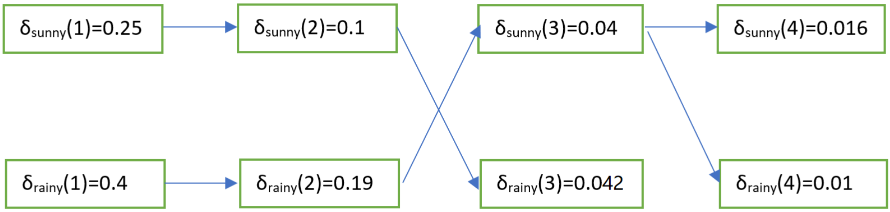
For each $t = T, \ldots, 2$: set $z_{t-1}^* = \Delta_{z_t^*}(t)$.

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

Example

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



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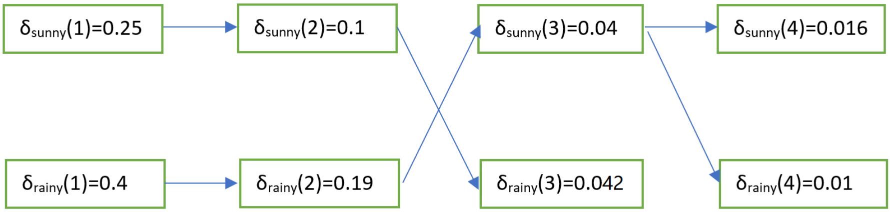

The most likely path is **"rainy, rainy, sunny, sunny"**.

Exercise 1

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

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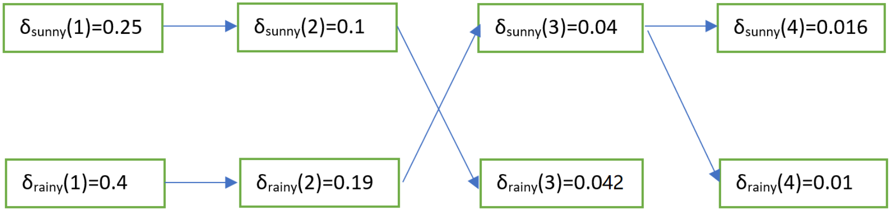

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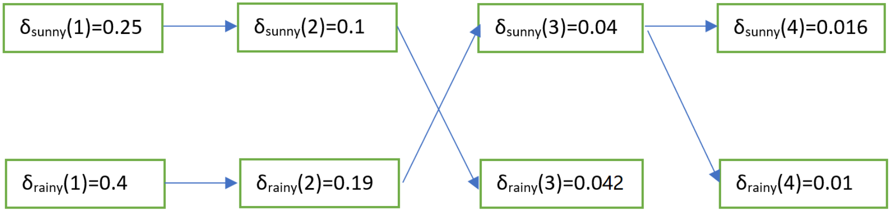
No. It should be

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



Exercise 1

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

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

No. It should be

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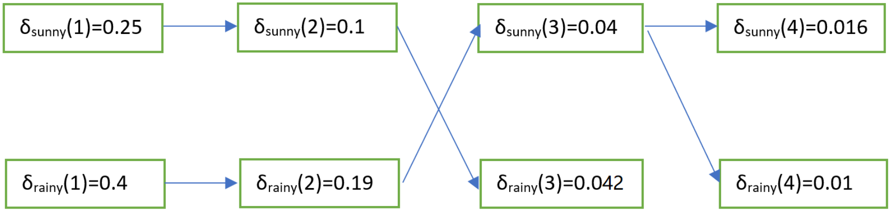

The answer for $T_0 = 3$ is: **"sunny, sunny, rainy"**.

Exercise 2

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Neither. It should be

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

Exercise 2 (cont.)

Reasoning:

$$z^*_{T_0} = \operatorname*{argmax}_s \max_{z_{1:T_0-1}} P(Z_{T_0} = s, Z_{1:T_0-1} = z_{1:T_0-1}, X_{1:T} = x_{1:T})$$

Exercise 2 (cont.)

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z_{T_0}^* &= \operatorname*{argmax}_s \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}) \\
&= \operatorname*{argmax}_s \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})
\end{aligned}
$$

Exercise 2 (cont.)

Reasoning:

$$
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z^*_{T_0} &= \operatorname*{argmax}_s \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}) \\
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&= \operatorname*{argmax}_s \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 \\
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Reasoning:

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&= \operatorname*{argmax}_s \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) \\
&= \operatorname*{argmax}_s \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 $T_0 < T$?

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Again, neither is true.

Exercise 3 (cont.)

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

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

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

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

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Backtracking: let $z_T^* = \operatorname{argmax}_s \delta_s(T)$.

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

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 $z_1^*, \ldots, z_T^*$.

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

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

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&= \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})
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Applying EM: M-Step

The maximizer of complete log-likelihood is simply doing **weighted counting** (compared to the unweighted counting on Slide 16):

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

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

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

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$$\gamma_s^{(n)}(t) = P(Z_{n,t} = s \mid X_{n,1:T} = x_{n,1:T})$$

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Baum–Welch algorithm

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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 25 and 26).

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Step 3 Return to Step 1 if not converged

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

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Several algorithms:

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