

Time Series Analysis

Recap

In the last section, we expanded our framework to include state space models

- There is a hidden or latent process, x_t , called the state process. Assumed to be a Markov process
- There are observations, y_t , that are generated by the state but are otherwise independent
- Linear state space models are a superset of our SARIMAX family of models
 We can rewrite them in state space form
- Dynamic Linear regression
 The weighting coefficients are allowed to change over time
- Kalman Filters
 Enables optimal estimation of state in the presence of noisy measurements

In this section, we'll explore Hidden Markov Models

- Markov Chains
- Viterbi, etc.

State Space Models

When we introduced state space models, we said that they followed two main principles:

- 1. There is a *hidden* or *latent* process, x_t , called the state process.
- The state process is assumed to be a Markov process
- 2. The observations, y_t , are independent given the states x_t
- Any relationship between observations is dictated by the originating states

We've been focused on linear Gaussian state space models, but this is just one (albeit popular) case.

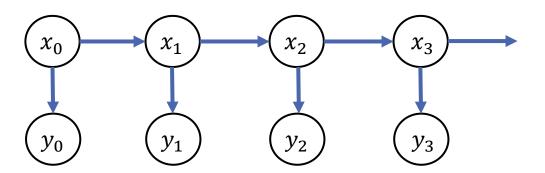
Another well-known case is when the hidden state, x_t , follows a discrete-valued Markov chain.

- The distribution of the possible observations at some time, t, is dictated by the current state at that time.
- The current state is one of m possible states, and the states evolve according to a Markov Chain over time.
- When the underlying state is unknown (we only have the observations), it is termed a hidden Markov model (HMM)

A Markov process is a stochastic process whose future value is only dependent on its current state - not its past.

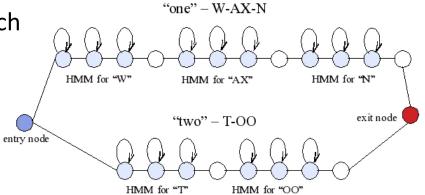
$$p(x_t|x_{t-1}, x_{t-2}, ... x_{t-\infty}) = p(x_t|x_{t-1})$$

- A discrete Markov chain is a specific type of Markoff process, which has a countable number of states.
- Time can also be continuous or discrete (but we'll focus on discrete time)
- In a hidden Markov model, the state is hidden, and we only see a corresponding observation

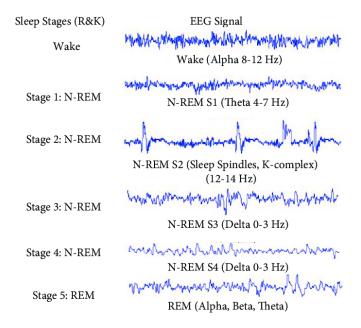


Hidden States: Phonemes of speech

Observations: Acoustic Spectra

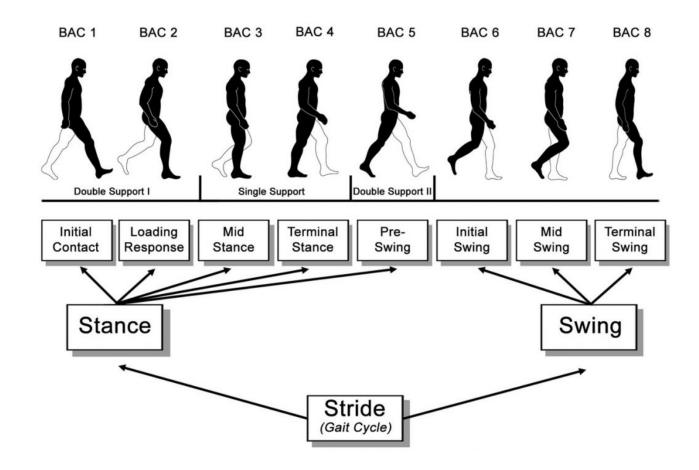


- Hidden States: Stages of sleep
- Observations: EEG signals

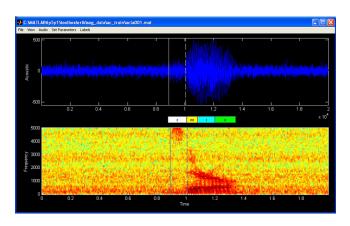


Examples:

- Hidden States: Gait Phase
- Observations: IMU or Video data

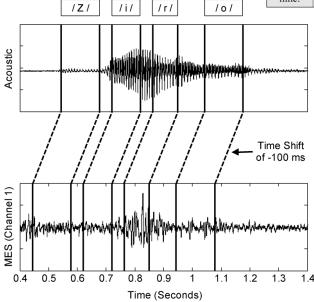


E. J. Scheme, B. Hudgins and P. A. Parker, "Myoelectric Signal Classification for Phoneme-Based Speech Recognition," in *IEEE Transactions on Biomedical Engineering*, vol. 54, no. 4, pp. 694-699, April 2007, doi: 10.1109/TBME.2006.889175.



Word	Phonemes						
zero:	/Z/	/ i /	/ r /	/ o /			
one:	/w/	/ A /	/ n /				
two:	/ t /	/ u /					
three:	/ T /	/ r /	/ i /				
four:	/f/	/ o /	/ r /				
five:	/f/	/ aI /	/ v /				
six:	/s/	/ I /	/ x /				
seven:	/s/	/E/	/ v /	/ n /			
eight:	/ e /	/t/					
nine:	/ n /	/ aI /	/ n /				





HMMs vs Kalman

In Kalman state space models, we assumed that:

- The unobserved state and the observations were Gaussian
- The model evolves continuously according to linear dynamics

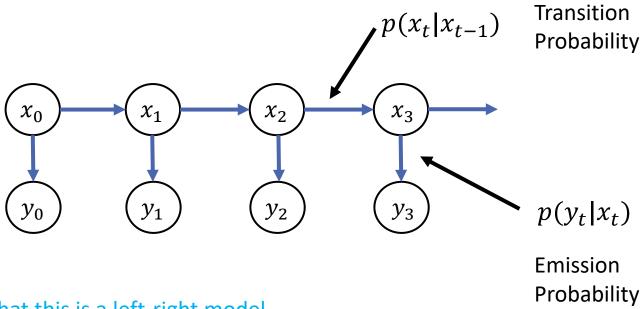
In HMMs, we generally assume that:

- The hidden state is one of a set number of classes (discrete)
- The state/class changes according to a discrete Markov chain
- The observations may be discrete or continuous

In a discrete Markov chain, the observations are deterministic for each given state

The state IS the observable event, so it is not hidden

A discrete hidden Markov model is an extension, where the observation is a probabilistic function of the state

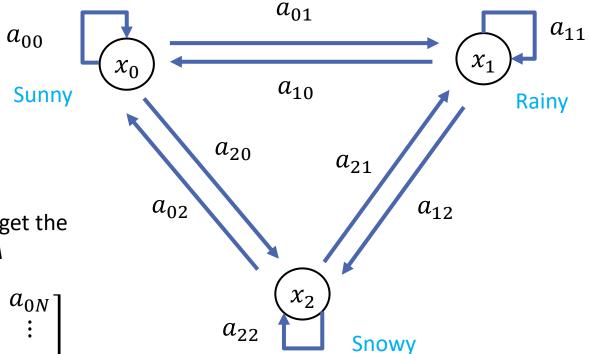


Below, is a 3-state Markov Chain, with transition probabilities:

$$a_{ij} = p(x_j|x_i)$$
 $a_{ij} \ge 0$ $\sum_{j=0}^{N-1} a_{ij} = 1$

$$a_{ij} \ge 0$$

$$\sum_{j=0}^{N-1} a_{ij} = 1$$



For an N-state chain, we get the State Transition Matrix, A

$$A = \begin{bmatrix} a_{00} & \cdots & a_{0N} \\ \vdots & \ddots & \vdots \\ a_{N0} & \cdots & a_{NN} \end{bmatrix}$$

For a similar 3-state Hidden Markov Model, we have transition probabilities:

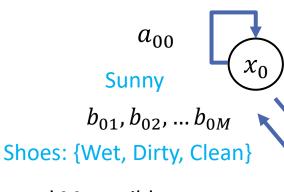
$$a_{ij} = p(x_j | x_i)$$
 $a_{ij} \ge 0$ $\sum_{j=0}^{N-1} a_{ij} = 1$

$$a_{ij} \ge 0$$

$$\sum_{j=0}^{N-1} a_{ij} = 1$$

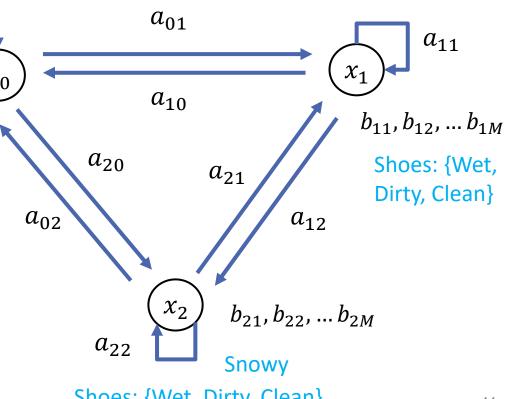
And observation probabilities $b_{ij} = p(y_i|x_i)$

$$b_{ij} = p(y_j|x_i)$$



For N states and M possible observations each, we get the Observation Probability Matrix, B

$$B = \begin{bmatrix} b_{01} & \cdots & b_{0M} \\ \vdots & \ddots & \vdots \\ b_{N1} & \cdots & b_{NM} \end{bmatrix}$$



Shoes: {Wet, Dirty, Clean}

Rainy

HMM Example

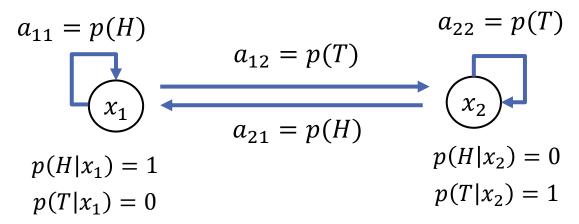
Let's look at a series of coin tosses as a simple example:

- Someone is flipping one or more coins (you can't see them)
- The observation sequence is the corresponding series of heads and tails

Example observations:
$$O = \{o_1, o_2, o_3 \dots o_T\} = \{H \ H \ T \ \dots T\}$$

We could establish several different HMM models for the problem

M1: Assume one coin

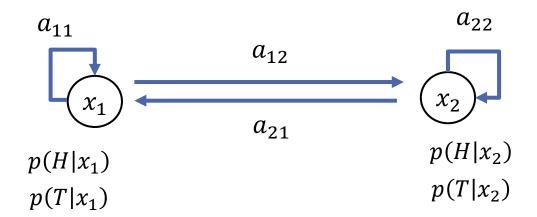


Observation, O={H H T T H T H H T T H}
State Sequence, Q={1 1 2 2 1 2 1 1 2 2 1}

HMM Example

We could establish several different HMM models for the problem

M2: Assume two coins



Observation, O={H H T T H T H H T T H}
State Sequence, Q={2 1 1 2 2 2 1 2 2 1 2}

- In this case, we don't know if the coins are biased (e.g. $p(H) \neq 0.5$) AND we don't know if they are biased equally
- There is a non-zero probability that the same flip result (H or T) can come from either coin

HMM Example

We could establish several different HMM models for the problem

- M3: We could similarly assume that we have three coins, but this would look just like our previous 3-state example
- We might get an example sequence of:

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Observation, O={H H T T H T H H T T H} State Sequence, Q={3 1 2 3 3 1 1 2 3 1 3}
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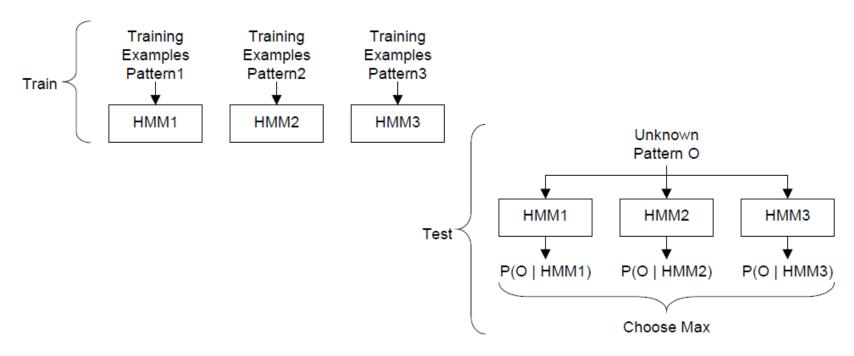
We can explain a sequence of observations with a variety of different models

- In the 2-state example, there were 2^T possible state sequences, whereas
- In the 3-state case, there were 3^T possible state sequences...
- There are an infinite number of HMMs that could explain that particular sequence
- As in all ML, there is a capacity tradeoff, so choice is important

Uses of HMMs

There are two main uses of HMM, in practice

- Modeling: match an HMM to an observation sequence to gain a better understanding of the process
- Pattern Classification: Leverage the temporal information to classify a sequence (e.g. Sign language gesture recognition)



HMMs are defined by a set of 3 main components

For a set of N hidden states, $S = \{S_1, S_2 \dots S_N\}$

and a set of *M possible* observations, $O = \{O_1, O_2, ... O_M\}$

- a. State transition probability matrix, A of size [N, N], composed of $a_{ij} = P(q_{t+1} = S_j | q_t = S_i)$ $(q_t \text{ is the hidden state at time } t)$
- b. State emission probabilities, B of size [N, M], composed of $b_i(k) = P(o_t = O_k | q_t = S_i)$ (o_t is the observation at time t)
- c. Initial distribution vector, π of size [N], where $\pi_i = P(q_1 = S_i)$

From a list of 3000 words from the Oxford Advanced Learner's Dictionary, find the

- Probability of having any word start with a given letter
- Probability of a transition from any one letter to the next

	a	b	C	d	е	f	g	h
<start></start>	7.4	4.8	10.1	5.4	5.5	4.7	2.6	3.1
a	0.0	3.1	6.1	4.9	0.1	1.1	3.3	0.2
b	13.7	0.0	0.0	0.0	17.4	0.0	0.0	0.0
C	11.4	0.0	2.3	0.0	15.8	0.0	0.0	10.7
d	6.7	0.0	0.0	2.4	39.2	0.5	1.7	0.2
е	8.9	0.4	5.5	3.7	3.6	2.1	1.9	0.3
f	12.9	0.0	0.0	0.0	15.9	9.1	0.0	0.0
g	11.2	0.0	0.0	0.0	26.8	0.0	1.6	13.1
h	15.5	0.5	0.0	0.5	26.7	0.0	0.0	0.0

1st row: Initial distribution vector

• 10.1% chance that a word starts with the letter *C*.

All other rows: transition probability matrix, A

 39.2% chance that the letter D is followed by an E.

Question: What use case might lead to non-deterministic state emission probabilities?

From a list of 3000 words from the Oxford Advanced Learner's Dictionary, find the

- Probability of having any word start with a given letter
- Probability of a transition from any one letter to the next

Here are some state emission probabilities, B, for a case where you type the right key 70% of the time.

They assume that you hit one of the surrounding keys the rest of the time.

	а	b	С	d	е	f	g	h
a	70.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
b	0.0	70.0	0.0	0.0	0.0	0.0	7.5	0.0
С	0.0	0.0	70.0	7.5	0.0	0.0	0.0	0.0
d	0.0	0.0	5.0	70.0	5.0	5.0	0.0	0.0
е	0.0	0.0	0.0	7.5	70.0	0.0	0.0	0.0
f	0.0	0.0	5.0	5.0	0.0	70.0	5.0	0.0
g	0.0	5.0	0.0	0.0	0.0	5.0	70.0	0.0
h	0.0	5.0	0.0	0.0	0.0	0.0	5.0	70.0

The math associated with HMMs can then be broken into 3 main problems

• Evaluation: Given an HMM, say λ , and a sequence of observations, say O, find the probability of that set of observations being explained (generated) by that model (Forward, Backward algorithms)

$$P(O|\lambda)$$

• Decoding: Given an HMM, λ , and a sequence of observations, O, find the sequence of hidden states, Q that maximizes (Viterbi algorithm)

$$P(O,Q|\lambda)$$

• Learning: Given an unknown HMM, λ , and a sequence of observations, O, find the parameters of $\lambda(A, B, \pi)$ that maximize: (Baum-Welch, Forward-Backward algorithm)

$$P(O|\lambda(A,B,\pi))$$

Evaluation

Evaluation: Given an HMM, say λ , and a sequence of observations, say O, find the probability of that set of observations being explained (generated) by that model:

 $P(0|\lambda)$

Computing this term allows us to determine how well an HMM matches a given observation sequence.

Decoding

Decoding: Given an HMM, λ , and a sequence of observations, O, find the sequence of hidden states, Q that maximizes:

$$P(O,Q|\lambda)$$

Determine the state sequence with the highest probability for a given observation sequence and HMM.

$$argmax\{P(Q \mid 0, \lambda)\}$$

This optimal state sequence, Q_{opt} , is not necessarily the correct state sequence (the true sequence that generated the observation), but it gives some indication about the average statistics of the model and individual states

Learning

Learning: Given an unknown HMM, λ , and a sequence of observations, O, find the parameters of $\lambda(A, B, \pi)$ that maximize:

$$P(O|\lambda(A,B,\pi))$$

The solution of this problem lets us to *train* an HMM based on a set of observed training data.

Evaluation: Direct Computation

There are different ways to execute these three different problems when working with HMMs. Let's first look at the evaluation problem, $P(O|\lambda)$

For a given HMM, we can calculate the probability of a particular observation and state sequence as

$$P(O,Q|\lambda) = \pi_1 \ b_{q_1}(o_1) \ a_{q_1q_2} \ b_{q_2}(o_2) \ a_{q_2q_3} \ b_{q_3}(o_3) \dots a_{q_{T-1}q_T} \ b_{q_T}(o_T)$$

 π_1 is the probability of starting in state q_1 $b_{q_1}(o_1)$ is the probability of observing o_1 , given that we are in state q_1 $a_{q_1q_2}$ is the probability of a state transition from q_1 to q_2 $b_{q_2}(o_2)$ is then the probability of observing o_2 , given that we are in state q_2

Evaluation: Direct Computation

$$P(O,Q|\lambda) = \pi_1 \ b_{q_1}(o_1) \ a_{q_1q_2} \ b_{q_2}(o_2) \ a_{q_2q_3} \ b_{q_3}(o_3) \dots a_{q_{T-1}q_T} \ b_{q_T}(o_T)$$

This is the probability for one specific set of observations AND state sequence, though.

• To determine the probability of a set of observations for a given HMM, we must use the equation determine above for *every possible state sequence* and sum them all.

$$P(O|\lambda) = \sum_{allO} P(O, Q|\lambda)$$

- Each $P(O, Q|\lambda)$ requires the multiplication of 2T terms (where T is the number of observations)
- For an N state HMM, there are N^T of the terms because at every t there are N possible states that can be reached.
- Even for small values of N and T, computing $P(O|\lambda)$ becomes impractical (e.g. N = 5, T = 100, 2T·N^T = 1.57 × 10⁷²)
- Clearly, direct computation of $P(O|\lambda)$ is unfeasible and a more efficient procedure is required.

Instead, we can define the forward variable $\alpha_t(i)$

$$\alpha_t(i) = P(o_1 o_2 \dots o_t, q_t = i | \lambda)$$

as the probability of a partial observation (an observation sequence, O, up to time t), AND being in state i at time t.

This is known as the forward procedure because we start with a partial observation of o_1 and move forward, solving for $\alpha_t(i)$ iteratively until time T so that the entire observation sequence is taken into account.

1. Initialization

$$\alpha_1(i) = \pi_i b_i(o_1) \qquad 1 \le i \le N$$

The forward variable $\alpha_1(i)$ is the probability of observing o_1 in state i.

• the probability of starting in state i multiplied by the probability of observing o_1 while in state i.

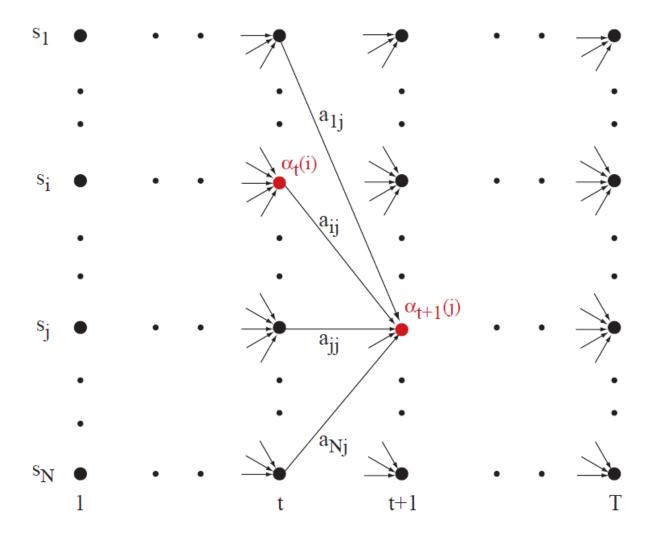
2. Induction

$$\alpha_{t+1}(j) = \left(\sum_{i=1}^{N} \alpha_t(i) \, a_{ij}\right) b_j(o_{t+1}) \qquad 1 \le t \le T-1 \qquad 1 \le j \le N$$

In the induction step, the probability of the partial observation sequence up to time t is assumed to be known.

We can then determine the probability of being in state j at the next time step (t+1) by summing the $\alpha_t(i)a_{ij}$ terms, the probabilities of being in state i and having a state transition into state j

The $b_j(o_{t+1})$ term accounts for the probability of actually observing o_{t+1} given that we are to be in state j



3. Termination

$$P(O|\lambda) = \sum_{i=1}^{N} \alpha_{T}(i)$$

At this point, the forward variable at time *T* is no longer a partial observation because it takes into account the entire observation sequence *O*.

- The term $\alpha_T(i) = P(O, q_T = i | \lambda)$ is the probability of observing O and ending in state i.
- $P(O|\lambda)$ is them just the sum of $\alpha_T(i)$ for all possible ending states.

The calculation of the forward algorithm is on the order of N^2T .

(e.g. N = 5, T = 100, N² · T =
$$100.5^2$$
 instead of $2T \cdot N^T = 1.57 \times 10^{72}$)

1. Initialization

• Determine the forward variable the probability of observing o_1 in state i.

$$\alpha_1(i) = \pi_i b_i(o_1)$$

2. Induction

We determine the probability of going to state j at the next time step

$$\alpha_{t+1}(j) = \left(\sum_{i=1}^{N} \alpha_t(i) \, a_{ij}\right) b_j(o_{t+1})$$

3. Termination

• We sum the probabilities of observing the sequence O and ending in state i

$$P(O|\lambda) = \sum_{i=1}^{N} \alpha_{T}(i)$$

Note: In the time-series sense, this operation can be viewed as filtering

The backward procedure is like the forward procedure except that we instead start at time T and work our way backwards in time, solving iteratively for the backward variable $\beta_t(i)$.

$$\beta_t(i) = P(o_{t+1}o_{t+2} \dots o_T | q_t = i, \lambda)$$

This backward variable is the probability of the partial observation (observation sequence from time t+1 to time T) given that at time t we are in state i.

In the forward variable, the probability was a joint probability between the partial observation and the state q_t

$$\alpha_t(i) = P(o_1 o_2 \dots o_t, q_t = i | \lambda)$$

• In the backward variable, it is conditional probability between the partial observation and the state q_t

1. Initialization

$$\beta_T(i) = 1$$
 $1 \le i \le N$

We're starting at the end, so we can't define the partial observation sequence from o_{T+1} (beyond our sequence) to o_T . So, for the procedure to work we set $\beta_T(i)$ equal to 1.

2. Induction

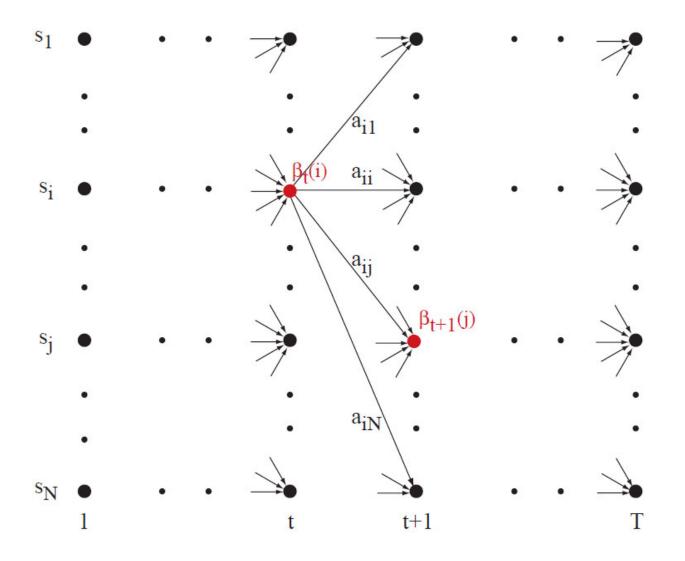
$$\beta_t(i) = \sum_{j=1}^N a_{ij} \, b_j(o_{t+1}) \beta_{t+1}(j) \qquad T - 1 \ge t \ge 1 \qquad 1 \le i \le N$$

In the backward induction step, we know the backward variable from time t+1 to time T

 $\beta_{t+1}(j)$ accounts for everything that happens after t+1, given that we are in state j at time t+1

For a given state i at time t, the induction step must consider transitioning into every state j = 1, 2..., N

Because we know we'll be in $\beta_{t+1}(j)$, we need the single observation probability $b_j(o_{t+1})$, and the transition probabilities a_{ij}



3. Termination

$$P(O|\lambda) = \sum_{i=1}^{N} \pi_i b_i(o_1) \beta_1(i)$$

Finally, $\beta_1(i)$ is the probability of the partial observation $\{o_2o_3 \dots o_T\}$ given that the initial state is state i.

The π_i removes the condition on the probability that the initial state is given to be state i.

The $b_i(o_1)$ is the probability of seeing the observation o_1 at the initial state i.

To compute $P(O|\lambda)$ we need to sum to account for all possible initial states.

Note: In the time-series sense, this operation can be viewed as smoothing

1. Initialization

• We require that $\beta_T(i) = 1$ $1 \le i \le N$

2. Induction

• We determine the probability of going to $\beta_t(i)$ given $\beta_{t+1}(j)$

$$\beta_t(i) = \sum_{j=1}^{N} a_{ij} b_j(o_{t+1}) \beta_{t+1}(j)$$

3. Termination

• We sum the probabilities of the partial observations $\{o_2o_3\dots o_T\}$ given the possible initial states i

$$P(O|\lambda) = \sum_{i=1}^{N} \pi_i b_i(o_1) \beta_1(i)$$

Decoding: Viterbi Algorithm

Remember, in the decoding problem, we need to determine the optimal state sequence for a given set of observations.

• The criteria we used to define 'optimal' was the state sequence that maximized $P(Q|O,\lambda)$.

The formal solution for this is called the Viterbi algorithm.

We define $\delta_t(i)$ to be the highest probability for a partial state sequence $\{q_1, q_2, ..., q_t\}$ ending at state $q_t = i$ for a partial observation sequence $\{o_1, o_2, ..., o_t\}$.

$$\delta_t(i) = \max_{q_1, q_2, \dots q_{t-1}} [P(q_1, q_2, \dots q_{t-1}, q_t = i, o_1, o_2, \dots o_t | \lambda)]$$

The calculation of the Viterbi algorithm is accomplished using dynamic programming.

We can solve for $\delta_t(i)$ inductively using

$$\delta_{t+1}(j) = \max_{i} \left[\delta_t(i) a_{ij} \right] \cdot b_j(o_{t+1})$$

The probability $\delta_t(i)$ is the probability of the optimal path for each state up to time t.

To find the optimal path to state j at time t+1, we calculate, for all i, the probability of moving from state i (given that it was reached optimally at time t) to state j, and take the path with maximum probability.

The term $b_j(o_{t+1})$ is required by the definition of $\delta_t(i)$ because it takes into account the probability of observing o_{t+1} at time t.

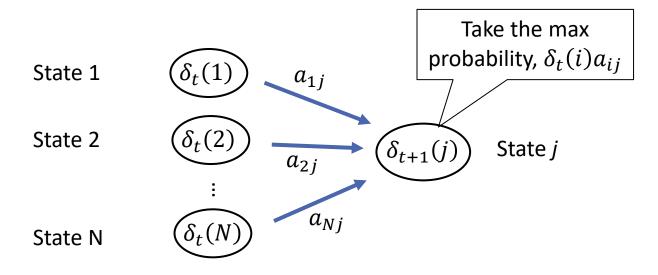
If we track the optimal state transition at each induction step, then we get the optimal state sequence $Q_{opt} = \{q_{opt(1)}, q_{opt(2)}, ..., q_{opt(N)}\}$.

• The array $\psi_1(j)$ is used to keep track of the optimal state transition argument

We can solve for $\delta_t(i)$ inductively using

$$\delta_{t+1}(j) = \max_{i} \left[\delta_t(i) a_{ij} \right] \cdot b_j(o_{t+1})$$

The probability $\delta_t(i)$ is the probability of the optimal path for each state up to time t.



Time t Time t+1

1. Initialization

$$\delta_1(i) = \pi_i b_i(o_1) \quad 1 \le i \le N$$

$$\psi_1(i) = 0 \qquad 1 \le i \le N$$

For time t=1, $\delta_1(i)$ is just the probability of the initial state i multiplied by the probability of observing o_1 when in state i.

The array $\psi_1(i)$ is set arbitrarily to zero at time t=1, but is never be actually used in the algorithm

there was no state to transition from prior to this

2. Recursion

$$\delta_{t+1}(j) = \max_{i} \left[\delta_{t}(i) a_{ij} \right] \cdot b_{j}(o_{t+1})$$

$$\psi_{t}(i) = \arg \left[\max_{i} \left[\delta_{t}(i) a_{ij} \right] \right]$$

$$1 \le j \le N \qquad 2 \le t \le T$$

The probability $\delta_t(i)$ is determined recursively as we just walked through.

The argument that indicates the optimal state transition is stored for each state at each time t.

3. Termination

$$P_{opt} = \max_{i} [\delta_T(i)]$$

$$q_{opt}(T) = arg\left[\max_{i}[\delta_{T}(i)]\right]$$

 P_{opt} is the probability of the optimal state sequence (the sequence with the maximum probability) for the observation sequence

• has an end state of $q_{opt}(T)$

4. Path Backtracking

$$q_{opt}(t) = \psi_{t+1} \left(q_{opt}(t+1) \right) \qquad T-1 \ge t \ge 1$$

Now that we know that the optimal path ends at $q_{opt}(T)$, and we know the optimal state transitions, we can trace backwards to find the optimal path.

We start with $q_{opt}(T)$ and work backwards in time to find the optimal sequence of states, Q_{opt} .

Start

State 1 State 2

State 3

$$\pi = \begin{bmatrix} 1/6 \\ 3/6 \\ 2/6 \end{bmatrix} \quad A = \begin{bmatrix} 4/6 & 1/6 & 1/6 \\ 2/6 & 2/6 & 2/6 \\ 1/6 & 1/6 & 4/6 \end{bmatrix}$$

$$B = \begin{bmatrix} 3/6 & 3/6 \\ 5/6 & 1/6 \\ 2/6 & 4/6 \end{bmatrix}$$

$$0 = [1 \ 2 \ 1 \ 1 \ 2]$$

$$Q_{opt} = ?$$

1. Initialization

$$\delta_1(i) = \pi_i b_i(o_1)$$
$$\psi_1(i) = 0$$

Start
$$\psi_{1}(1)=0$$

$$\psi_{1}(2)=0$$

$$\psi_{1}(2)=0$$

$$\delta_{1}(2)=15/6^{2}$$

$$V_{1}(3)=0$$

$$\delta_{1}(3)=4/6^{2}$$

$$\pi = \begin{bmatrix} 1/6\\3/6\\2/6 \end{bmatrix}$$

$$A = \begin{bmatrix} 4/6 & 1/6 & 1/6\\2/6 & 2/6 & 2/6\\1/6 & 1/6 & 4/6 \end{bmatrix}$$

$$B = \begin{bmatrix} 3/6 & 3/6\\5/6 & 1/6\\2/6 & 4/6 \end{bmatrix}$$

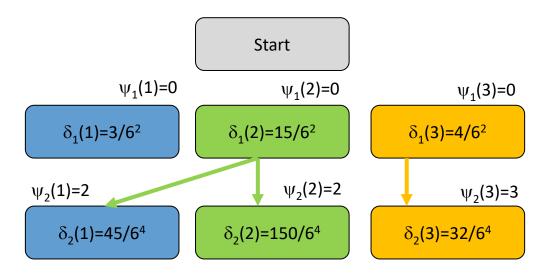
$$O = \begin{bmatrix} 1 & 2 & 1 & 1 & 2 \end{bmatrix}$$

$$Q_{opt} = ?$$

1. Initialization

$$\delta_1(i) = \pi_i b_i(o_1)$$

$$\psi_1(i) = 0$$



$$\pi = \begin{bmatrix} 1/6 \\ 3/6 \\ 2/6 \end{bmatrix} \quad A = \begin{bmatrix} 4/6 & 1/6 & 1/6 \\ 2/6 & 2/6 & 2/6 \\ 1/6 & 1/6 & 4/6 \end{bmatrix}$$

$$B = \begin{bmatrix} 3/6 & 3/6 \\ 5/6 & 1/6 \\ 2/6 & 4/6 \end{bmatrix}$$

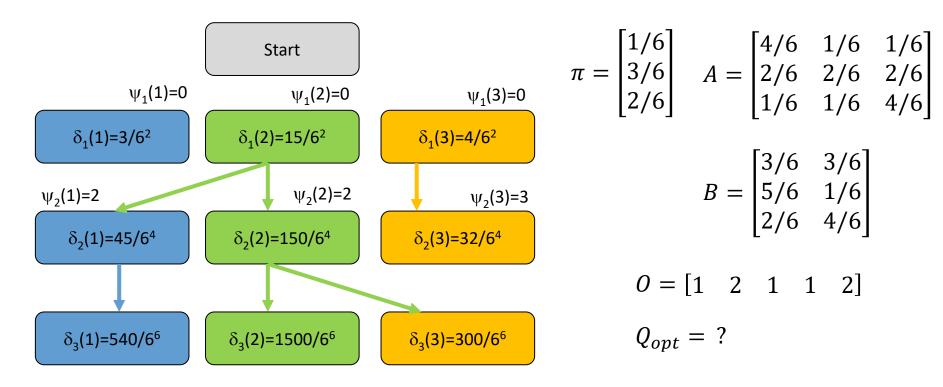
$$O = \begin{bmatrix} 1 & 2 & 1 & 1 & 2 \end{bmatrix}$$

$$Q_{opt} = ?$$

2. Recursion

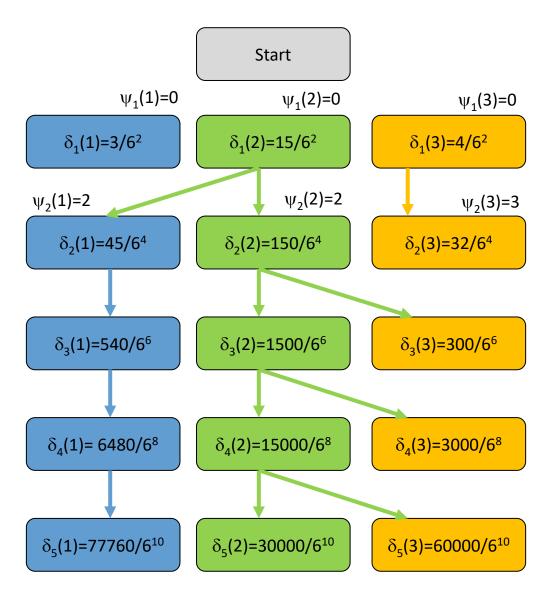
$$\delta_{t+1}(j) = \max_{i} \left[\delta_{t}(i) a_{ij} \right] \cdot b_{j}(o_{t+1})$$

$$\psi_{t}(i) = \arg \left[\max_{i} \left[\delta_{t}(i) a_{ij} \right] \right]$$



2. Recursion

$$\delta_{t+1}(j) = \max_{i} \left[\delta_{t}(i) a_{ij} \right] \cdot b_{j}(o_{t+1})$$
$$\psi_{t}(i) = \arg \left[\max_{i} \left[\delta_{t}(i) a_{ij} \right] \right]$$



$$\pi = \begin{bmatrix} 1/6 \\ 3/6 \\ 2/6 \end{bmatrix} \quad A = \begin{bmatrix} 4/6 & 1/6 & 1/6 \\ 2/6 & 2/6 & 2/6 \\ 1/6 & 1/6 & 4/6 \end{bmatrix}$$

$$B = \begin{bmatrix} 3/6 & 3/6 \\ 5/6 & 1/6 \\ 2/6 & 4/6 \end{bmatrix}$$

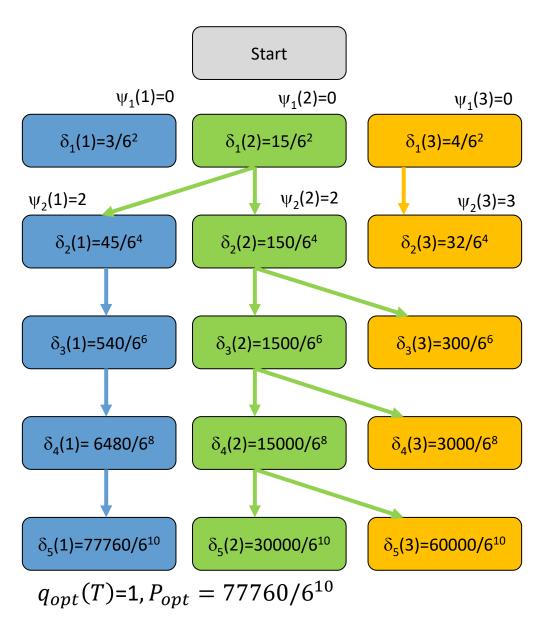
$$0 = [1 \ 2 \ 1 \ 1 \ 2]$$

$$Q_{opt} = ?$$

2. Recursion

$$\delta_{t+1}(j) = \max_{i} \left[\delta_{t}(i) a_{ij} \right] \cdot b_{j}(o_{t+1})$$

$$\psi_{t}(i) = \arg \left[\max_{i} \left[\delta_{t}(i) a_{ij} \right] \right]$$



$$\pi = \begin{bmatrix} 1/6 \\ 3/6 \\ 2/6 \end{bmatrix} \quad A = \begin{bmatrix} 4/6 & 1/6 & 1/6 \\ 2/6 & 2/6 & 2/6 \\ 1/6 & 1/6 & 4/6 \end{bmatrix}$$

$$B = \begin{bmatrix} 3/6 & 3/6 \\ 5/6 & 1/6 \\ 2/6 & 4/6 \end{bmatrix}$$

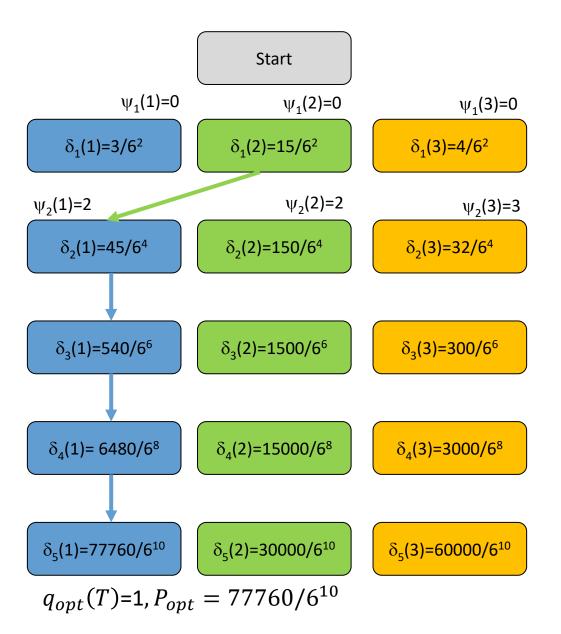
$$0 = [1 \ 2 \ 1 \ 1 \ 2]$$

$$Q_{opt} = ?$$

3. Termination

$$P_{opt} = \max_{i} [\delta_{T}(i)]$$

$$q_{opt}(T) = arg \left[\max_{i} [\delta_{T}(i)] \right]$$



$$\pi = \begin{bmatrix} 1/6 \\ 3/6 \\ 2/6 \end{bmatrix} \quad A = \begin{bmatrix} 4/6 & 1/6 & 1/6 \\ 2/6 & 2/6 & 2/6 \\ 1/6 & 1/6 & 4/6 \end{bmatrix}$$

$$B = \begin{bmatrix} 3/6 & 3/6 \\ 5/6 & 1/6 \\ 2/6 & 4/6 \end{bmatrix}$$

$$0 = [1 \ 2 \ 1 \ 1 \ 2]$$

$$Q_{opt} = ?$$

4. Path Backtracking

$$Q_{opt} = [2 \ 1 \ 1 \ 1 \ 1]$$

Learning (HMM Training)

If you remember in the 3rd problem, learning, we needed to find the parameters of an HMM, $\lambda(A, B, \pi)$, that maximize the probability of having observed a given sequence, O:

$$P(O|\lambda(A,B,\pi))$$

The goal here, is therefore to learn, or train, the HMM hyperparameters based on a set of training data.

- That is, we need to learn the A (all the a_{ij} 's),B (all the $b_j(k)$), and π
- Here, we'll discuss the popular Baum-Welch method (also known as the forward-backward method)

The Baum-Welch method is a dynamic programming approach and a special case of *expectation maximization* (EM)

• The goal is to iteratively tune the parameters such that we maximize the likelihood that the model "generated" the observations.

1. Initialization

• Initialize the A, B, π using prior knowledge if possible (otherwise random)

2. Forward Phase

• Compute the forward algorithm

$$\alpha_{t+1}(j) = \left(\sum_{i=1}^{N} \alpha_t(i) \, a_{ij}\right) b_j(o_{t+1})$$

3. Backward Phase

Compute the backward algorithm

$$\beta_t(i) = \sum_{j=1}^{N} a_{ij} b_j(o_{t+1}) \beta_{t+1}(j)$$

4. Re-Estimation

Compute the new parameters

First, let's define $\gamma_t(i)$ as the probability of being in state i at time t, given an observation sequence.

$$\gamma_t(i) = P(q_t = i | O, \lambda) = \frac{P(q_t = i | \lambda)}{P(O | \lambda)}$$
using Bayes' theorem

This numerator is equal to the product of the forward and backward variables for state i at time t, which we previously described.

$$\gamma_t(i) = P(q_t = i|0, \lambda) = \frac{\alpha_t(i)\beta_t(i)}{P(0|\lambda)}$$

- The forward variable $\alpha_t(i)$ takes into account the partial observation sequence $\{o_1\ o_2\ ...\ o_t\}$ ending at state i at time t
- The backward variable $\beta_t(i)$ takes into account the remainder of the observation $\{o_{t+1} \ o_{t+2} \ ... \ o_T\}$ given state i at time t.

Now, let's define $\xi_t(i,j)$ as the probability of having a state transition from i to j at time t, given an observation sequence.

$$\xi_t(i,j) = P(q_t = i, q_{t+1} = j | O, \lambda) = \frac{P(O, q_t = i, q_{t+1} = j | \lambda)}{P(O | \lambda)}$$
Again, using Bayes' theorem

The numerator is similar to what we found for $\gamma_t(i)$ and can again be simplified:

$$\xi_t(i,j) = \frac{\alpha_t(i)a_{ij}b_j(o_{t+1})\beta_{t+1}(j)}{P(O|\lambda)}$$

- The forward variable $\alpha_t(i)$ takes into account the partial observation sequence $\{o_1\ o_2\ ...\ o_t\}$ ending at state i at time t
- The backward variable $\beta_{t+1}(j)$ takes into account the remainder of the observation $\{o_{t+1}\ o_{t+2}\ ...\ o_T\}$ given state j at time t+1

Now we can explore the re-estimation of the HMM model.

- A re-estimated model, $\lambda^*(A, B, \pi)$ can be derived to maximize $P(O|\lambda)$ such that $P(O|\lambda^*) > P(O|\lambda)$
- This process is repeated iteratively, each time updating the model based on the previous estimates
- Unfortunately, the likelihood function for an HMM is quite complex and has many local maxima to which the re-estimation may converge.

We'll explain concepts without getting too deep into these, but be aware

The re-estimated initial state probabilities, π_i^* , are just:

 $\pi_i^* = \text{Expected number of times in state } i \text{ at time } (t=1)$

$$\pi_i^* = \gamma_1(i)$$

The re-estimated transition probabilities, a_{ij}^* , are given by:

$$a_{ij}^* = \frac{\text{expected number of transitions from state } i \text{ to } j}{\text{expected number of transitions from state } i} = \frac{\sum_{t=1}^{T-1} \xi_t(i,j)}{\sum_{t=1}^{T-1} \gamma_t(i)}$$

- Recall that $\xi_t(i,j)$ is the probability of going from state i to state j at time t.
- So, the numerator (the sum of $\xi_t(i,j)$ over all time) is the expected number of transitions from state i to state j.
- Recall that $\gamma_t(i)$ is the probability of being in state i at time t.
- Then, the denominator (the sum of $\gamma_t(i)$ over all time) is the expected number of transitions from state i.

The re-estimated transition probabilities, a_{ij}^* , are given by:

$$a_{ij}^* = \frac{\text{expected number of transitions from state } i \text{ to } j}{\text{expected number of transitions from state } i} = \frac{\sum_{t=1}^{T-1} \xi_t(i,j)}{\sum_{t=1}^{T-1} \gamma_t(i)}$$

Substituting in the formulas for $\xi_t(i,j)$ and $\xi_t(i)$, we get:

$$a_{ij}^* = \frac{\sum_{t=1}^{T-1} \frac{\alpha_t(i) a_{ij} b_j(o_{t+1}) \beta_{t+1}(j)}{P(O|\lambda)}}{\sum_{t=1}^{T-1} \frac{\alpha_t(i) \beta_t(i)}{P(O|\lambda)}} = \frac{\sum_{t=1}^{T-1} \alpha_t(i) a_{ij} b_j(o_{t+1}) \beta_{t+1}(j)}{\sum_{t=1}^{T-1} \alpha_t(i) \beta_t(i)}$$

So, the result is simply composed of:

- The forward result
- The backward result
- The previous transition probabilities
- The previous observation probabilities

The re-estimated observation probabilities, $b_i^*(k)$, are given by:

$$b_j^*(k) = \frac{\text{expected number of times observing } o_k \text{ when in state } j}{\text{expected number of times in state } j} \quad = \frac{\sum_{t=1,o_k}^T \gamma_t(j)}{\sum_{t=1}^T \gamma_t(j)}$$

- The denominator (the sum of $\gamma_t(j)$ over all time) is the same as before (the expected number of transitions from state j), except that it now includes the full 1:T
- The numerator is similar to the denominator, except that we only include terms for which we are in state j AND observing symbol o_k
- If we define $\delta(o_t,o_k) = \begin{cases} 1 & \text{if } o_t = o_k \\ 0 & \text{otherwise} \end{cases}$, and substitute the formula derived for $\gamma_t(i)$,

$$b_j^*(k) = \frac{\sum_{t=1}^T \frac{\alpha_t(i)\beta_t(i)}{P(O|\lambda)} \delta(o_t, o_k)}{\sum_{t=1}^T \frac{\alpha_t(i)\beta_t(i)}{P(O|\lambda)}} = \frac{\sum_{t=1}^T \alpha_t(i)\beta_t(i) \delta(o_t, o_k)}{\sum_{t=1}^T \alpha_t(i)\beta_t(i)}$$

Using these formulas, we can iterative over the re-estimation until the results converge, such that $P(O|\lambda^*) \approx P(O|\lambda)$

$$\pi_i^* = \gamma_1(i)$$

$$a_{ij}^* = \frac{\sum_{t=1}^{T-1} \alpha_t(i) a_{ij} b_j(o_{t+1}) \beta_{t+1}(j)}{\sum_{t=1}^{T-1} \alpha_t(i) \beta_t(i)} \qquad b_j^*(k) = \frac{\sum_{t=1}^{T} \alpha_t(i) \beta_t(i) \delta(o_t, o_k)}{\sum_{t=1}^{T} \alpha_t(i) \beta_t(i)}$$

Note that these derivations have assumed that the observations were discrete

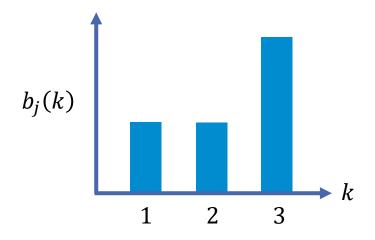
We could count the number of times each observation occurred for each state

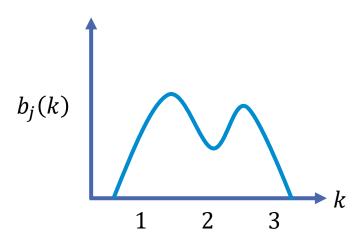
Note that these derivations have assumed that the observations were discrete

We could count the number of times each observation occurred for each state

In practice, this is often not true, requiring the consideration of continuous observation densities

• π and A stay the same, but now we estimate the probability density function (pdf) for each state, instead of the (discrete) probability mass function, $b_i(k)$.





Whereas re-estimating the pmf, $b_i^*(k)$ was achieved using

$$b_j^*(k) = \frac{\sum_{t=1}^T \alpha_t(i)\beta_t(i)\delta(o_t, o_k)}{\sum_{t=1}^T \alpha_t(i)\beta_t(i)}$$

Estimation of the pdf is most often achieved using Gaussian Mixture Models

• We describe the pdf as a weighted sum of M Gaussian distributions, η

$$b_j(\bar{o}) = \sum_{k=1}^M c_{jk} \eta(\bar{o}, \bar{\mu}_{jk}, \bar{U}_{jk}) \quad 1 \le j \le N$$

- Here, $\bar{\mu}_{jk}$ is the mean vector, and \bar{U}_{jk} is the covariance matrix for the k^{th} mixture component in state j.
- The coefficients c_{jk} are the mixture coefficients, which weight the contribution of the Gaussians, subject to:

$$\sum_{k=1}^{M} c_{jk} = 1 \qquad c_{jk} \ge 0 \qquad 1 \le j \le N, 1 \le k \le M$$

The training of a continuous observation HMM is similar to before, but requires the additional re-estimation of these c_{jk} , $\bar{\mu}_{jk}$, and \bar{U}_{jk} parameters.

As before, we need to defined a helpful variable.

• $\gamma_t(j,k)$ is the probability of being in state j at time t with the k^{th} mixture component accounting for the observation vector \bar{o}_t

$$\gamma_t(j,k) = \left[\frac{\alpha_t(j)\beta_t(j)}{\sum_{j=1}^N \alpha_t(j)\beta_t(j)} \right] \left[\frac{c_{jk}\eta(\bar{o}_t,\bar{\mu}_{jk},\bar{U}_{jk})}{\sum_{m=1}^M c_{jm}\eta(\bar{o}_t,\bar{\mu}_{jm},\bar{U}_{jm})} \right]$$

- The first term is exactly the same as the discrete HMM equivalent, $\gamma_t(j)$.
- The second term is the ratio between the probability that the k^{th} mixture of state j can account for the observation vector \bar{o}_t and the probability that the observation vector \bar{o}_t can be accounted for in state j, in general.

The mixture gains, c_{ik} , can then be re-estimated as

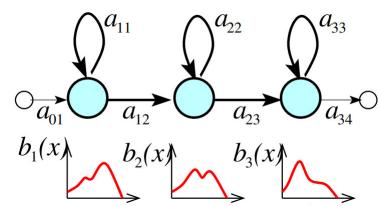
$$c_{jk} = \frac{\sum_{t=1}^{T} \gamma_t(j, k)}{\sum_{t=1}^{T} \sum_{k=1}^{M} \gamma_t(j, k)}$$

• which is the ratio between the expected number of times the system is in state j, using the kth mixture component, and the total number of times the system is in state j.

The means and covariances of the Gaussian mixtures can be re-estimated using

$$\bar{\mu}_{jk} = \frac{\sum_{t=1}^{T} \gamma_t(j,k) \cdot \bar{o}_t}{\sum_{t=1}^{T} \gamma_t(j,k)} \qquad \bar{U}_{jk} = \frac{\sum_{t=1}^{T} \gamma_t(j,k) \cdot (\bar{o}_t - \bar{\mu}_{ij}) (\bar{o}_t - \bar{\mu}_{ij})'}{\sum_{t=1}^{T} \gamma_t(j,k)}$$

• where the numerators are the sum of the probabilities of being in state j, using the $k^{\rm th}$ mixture, weighted by the observation vector \bar{o}_t (for the mean) or the covariance.



Hidden Markov Models

Using priori knowledge about the problem, we can constrain HMMs for better performance or efficiency. We can:

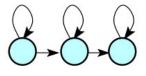
constrain models to be left-right model (state index is non-decreasing)

$$a_{ij} = 0$$
 $j < i$

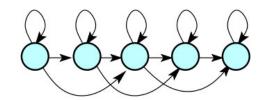
limit how far 'ahead' a model can jump

$$a_{ij} = 0$$
 $j > i + \Delta i$

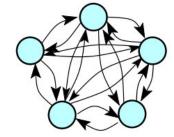
Force the model to start in state 1, or end in state N



left-to-right model



parallel path left-to-right model



ergodic model

$$\left(\begin{array}{ccc}
a_{11} & a_{12} & 0 \\
0 & a_{22} & a_{23} \\
0 & 0 & a_{33}
\end{array}\right)$$

$$\begin{pmatrix} a_{11} & a_{12} & 0 \\ 0 & a_{22} & a_{23} \\ 0 & 0 & a_{33} \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} & a_{13} & 0 & 0 \\ 0 & a_{22} & a_{23} & a_{24} & 0 \\ 0 & 0 & a_{33} & a_{34} & a_{35} \\ 0 & 0 & 0 & a_{44} & a_{45} \\ 0 & 0 & 0 & 0 & a_{55} \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} & a_{15} \\ a_{21} & a_{22} & a_{23} & a_{24} & a_{25} \\ a_{31} & a_{32} & a_{33} & a_{34} & a_{35} \\ a_{41} & a_{42} & a_{43} & a_{44} & a_{45} \\ a_{51} & a_{52} & a_{53} & a_{54} & a_{55} \end{pmatrix}$$

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} & a_{15} \\ a_{21} & a_{22} & a_{23} & a_{24} & a_{25} \\ a_{31} & a_{32} & a_{33} & a_{34} & a_{35} \\ a_{41} & a_{42} & a_{43} & a_{44} & a_{45} \\ a_{51} & a_{52} & a_{53} & a_{54} & a_{55} \end{pmatrix}$$

Hierarchical Hidden Markov Models

Complex HMMs can be designed to be more efficient by carefully constraining the transitions matrix, A

However, they can sometimes be hard to interpret directly

Several extensions have therefore been proposed, particularly to embed or emphasis known structure.

A particularly interesting (and more common) variant is the hierarchical HMM

- As the name implies, hHMMs combines multiple HMMs in a hierarchical (or tree-like) arrangement
- Each state of the original (top) model is comprised of its own HMM
- In this way, the observations associated with a given state in the upper level(s) are informed by the state sequence through the associated 'leaf' HMM.

As an example, consider the English language

- Sentences are formed from sequences of words
- Words are formed from sequences of syllables
- Syllables are formed from sequences of phonemes

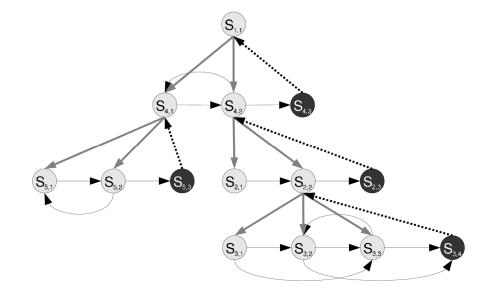
Hierarchical Hidden Markov Models

A hierarchical HMM could then be designed where the top level models the flow of words through a sentence

- For each word, and new hierarchical HMM could model the flow of syllables within that word
- And a final HMM could model the flow of phonemes through those syllables

Within each level of a hierarchical HMM, there is a sequence of states

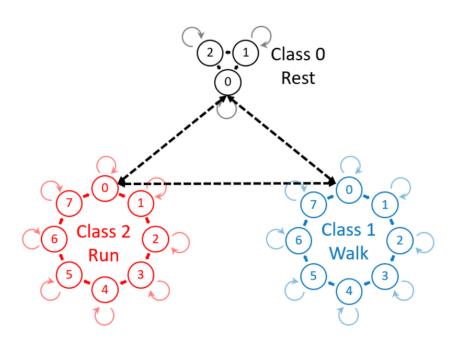
- An output is only returned to the next level up once the sequence has been completed
- That is, the first and middle states of each HMM are 'non-producing', and only inform the observation that is generated by the last state.

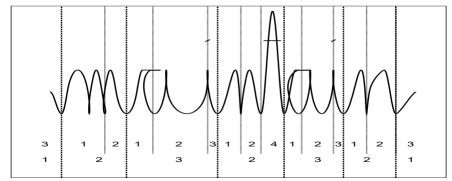


Hierarchical Hidden Markov Models

Recent applications of hHMMs include

- Speech
- Gesture and human activity recognition
- Gait
- Genetic sequencing





Fine, Shai, Singer, Yoram, Tishby, Naftali, The Hierarchical Hidden Markov Model: Analysis and Applications, Machine Learning, 32, 41–62 (1998)

Martindale, Christine & Hoenig, Florian & Strohrmann, Christina & Eskofier, Bjoern. (2017). Smart Annotation of Cyclic Data Using Hierarchical Hidden Markov Models. Sensors. 17. 2328. 10.3390/s17102328.

Summary

In this section, we continued with another common state-space model; the Hidden Markov Model

- A sequence of latent states, which each generate some observable output
 The observations can be deterministic, discrete, or continuous (based on a pdf)
- State progression is governed by the probabilities in a state transition matrix
 Observations depend only on the current state
- HMMs can be used for time series modeling, or for classification of temporal sequences
 - We focused on the classification task
- Three main "problems" Evaluation (forward, backward), Decoding (Viterbi), Learning (Baum-Welch)
- The models can be constrained for more efficient learning or to better represent known structure/semantics
 - Left-right vs ergodic models, hierarchical HMMs

In the next section, we'll jump again and look at deep learning models

- Regression & Gradient Descent
- RNN, LSTM, maybe CNN (as time allows)

