Hidden Markov Models

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Chapter 1

Introduction

The goal of this project is to determine if HMMs are suitable as rain generators.

The first task will be to extend on the work done by Grando. In her testing, she has concluded that HMMs are suitable as rain generators; however, she has used the same data for testing as she used for training. Doing so may, quite likely, have to lead to bias, and thus, we will extend her work by conducting out-of-sample tests.

If possible, we will build the software, so it is user friendly and efficient. With this, we can test data for multiple locations. This will allow us to understand if the result is genuinely significant, at least more than just one location.

Chapter 2

Preliminaries

In this section, we will briefly visit the foundations on which we will build throughout this paper. For most, this will be a simple refresher.

2.1 Mathematical Foundations

We start with a few key mathematical concepts.

2.1.1 Probability Theory

To discuss any probabilistic ideas, we must first understand general probability theory. We will start by defining a probability space.

Definition 2.1. Probability Space
A probability space is defined by $(\Omega, \mathcal{F}, \mathbb{P})$. Ω is the non-empty set of all possible outcomes, such that all events $\omega \in \Omega$. $\mathbb{P}$ is a probability measure, a function $\mathbb{P}$(A) that maps event A to a number within [0,1] based on the likelihood of the event. $\mathcal{F}$ is a σ-algebra on Ω if

1. $\Omega \in \mathcal{F}$
2. A $\in \mathcal{F}$ implies $A^c \in \mathcal{F}$
3. if A_1, A_2, A_3,... are in $\mathcal{F}$ then so is $A_1 \cup A_2 \cup A_3$...

2.1.2 Conditional Probability

Sometimes we require the probability of an event assuming another event has occurred. In such situations, we require a conditional probability. Given two events A and B, the probability of event A occurring conditioned on event B:

$$\mathbb{P}(A|B) = \frac{\mathbb{P}(A \cap B)}{\mathbb{P}(B)},\ \forall A \in \mathcal{F} \tag{2.1}$$

From 2.1 and the fact that for dependednt events $\mathbb{P}$(A $\cap$ B) = $\mathbb{P}$(B $\cap$ A) we can see that:

$$\mathbb{P}(A \cap B) = \mathbb{P}(A|B)\mathbb{P}(B) = \mathbb{P}(B|A)\mathbb{P}(A),\ \forall A, B \in \mathcal{F} \tag{2.2}$$

Subsituting 2.2 into 2.1 we get the famous Bayes Theorem.

Theorem 2.2. *Bayes' Theorem*
For dependent events A and B with probability space $(\Omega, \mathcal{F}, \mathbb{P})$ *, where* $\mathbb{P}$ *(B)* $\neq$ *0,*

$$\mathbb{P}(A|B) = \frac{\mathbb{P}(B|A)\mathbb{P}(A)}{\mathbb{P}(B)},\ \forall A \in \mathcal{F} \tag{2.3}$$

2.1.3 Stochastic Process

To be able to define a Markov model, of any kind, we must first define a stochastic process.

Definition 2.3. Stochastic Process
Given an ordered set T and probability space $(\Omega, \mathcal{F}, \mathbb{P})$ a stochastic process is a collection of random variables X = $\{X_t$; t$\in$T$\}$. Based on t $\in$ T and $\omega \in \Omega$ we get a numerical realization of the process. For simplicity, this may be viewed as a function; $X_t(\omega)$.

2.2 Applied Foundations

Chapter 3

Standard Markov and Markov Property

3.1 History

Andrei Markov discovered the Markov model while analyzing the relationship between consecutive letters from the text in the Russian novel "Eugene Onegin". A translation can be found here Markov, n.d. With a two-state model (states Vowel and Consonant) he proved that the probability of letters being in a particular state is not independent. Given the current state, he could probabilistically predict the next. With various probabilities to and from each state, this chain of states formed the foundation of the Markov Chain.

3.2 Markov Chain

A Markov chain is a network of connected states. At any given time the model is said to be in a particular state. At a regular discrete interval, the model can change states depending on the probabilities. To define a Markov chain, we must first address the Markov property GRIMMETT et al., 2020.

Definition 3.1. Markov Property
Let $\{X_t$; t $\in \mathbb{N}_0\}$ denote a stochastic proccess 2.3, where t represents time. The process has the Markov property if and only if,

$$\mathbb{P}\{X_{n+1} = i_{n+1} | X_n = i_n, X_{n-1} = i_{n-1}, ..., X_0 = i_0\} = \mathbb{P}\{X_{n+1} = i_{n+1} | X_n = i_n\} \tag{3.1}$$

We can now define a Markov chain.

Definition 3.2. Markov Chain
A stochastic process $\{X_t$; t $> 0\}$ is a Markov Chain if and only if it satisfies the Markov property 3.1.

To store the sequence of states a Markov chain has been through, we use the set $Q = \{q_t; t \in \mathbb{N}_0\}$, where q_t represents the state at time t. We will use this notation throughout the paper.

Example 3.3. Given a Markov Model with states S = $\{S_1, S_2, S_3\}$, if the model starts at S_2 and then goes to S_3 and then back to S_2 the state sequence Q will be $Q = \{q_1 = S_2, q_2 = S_3, q_3 = S_2\}$.

From the Markov property, we can see that the only thing that influences q_t is q_{t-1}. We can use this to make predictions for q_{t+1} based on the outward transition probabilities from state q_t. By calculating all outward transition probabilities from the state at q_t, we can construct a probability measure that we may use to predict future states.
i.e.
Given a Markov chain with N states including i and j and discrete time $t \in \mathbb{N}_0$, we can use

$$\mathbb{P}(q_t = S_j | q_{t-1} = S_i)_{1 \leq i,j \leq N} \tag{3.2}$$

as a probility measure to help predict future states.

These probabilities can vary with time, but this can make the model quite complicated. Thus, we usually assume the probabilities are constant. These unique Markov models are called time-homogenous.

Definition 3.4. Time homogenous
Let $\{X_t$; t $\in \mathbb{N}_0\}$ denote a stochastic proccess 2.3, where t represents discrete time, and $p(i, j)$ represent the transition probability from state i to state j. If

$$\mathbb{P}\{X_n = j | X_{n-1} = i\} = p(i, j), \forall n \in \mathbb{N}_0 \tag{3.3}$$

then the process is time-homogenous.

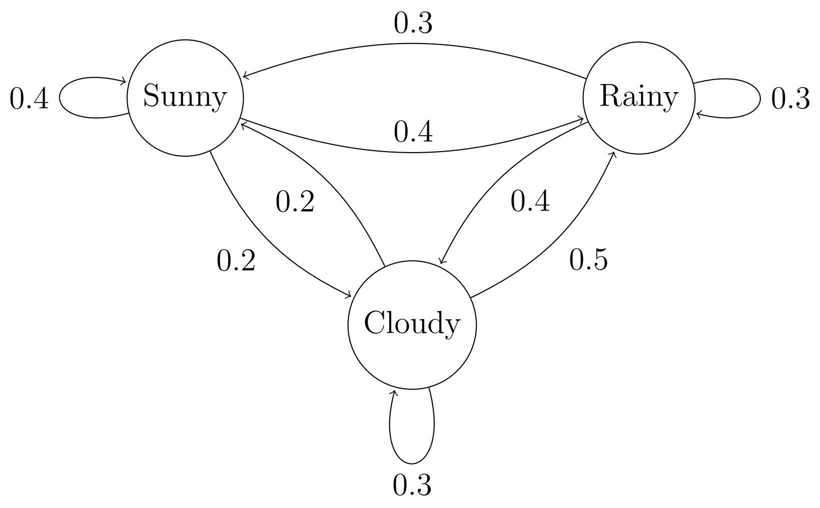
For a discrete Markov model with N states, there are N^2 total transitions, where $p(i, j) = 0$ represents an impossible transition. We must store each of these probabilities. Given a time-homogenous Markov chain, we can create a 2-dimensional N x N matrix of transition probabilities p. Unique Markov chains have unique transition matrices. These matrices can be defined as below:

$$p = \{p(i, j) = \mathbb{P}\{X_n = j | X_{n-1} = i\}\}_{1 \leq i,j \leq N} \tag{3.4}$$

All p matrices have some essential properties. The first is that all values within p must be within $[0, 1]$ which comes naturally as all values are probabilities and thus by definition, it must lie within $[0, 1]$. The second is that all rows, columns or both form stochastic vectors. If it is the rows, then the matrix is defined as a right-stochastic matrix; if it is the columns, it is called a left-stochastic matrix.

To demonstrate, we will present an example where the states represent the weather.

Example 3.5. Let $\{X_t; t \in \mathbb{N}_0\}$ denote a Markov Chain, with state-space S = {rainy, sunny, cloudy}, where t represents the number of days from the start. Since all states can eventually reach all other states, we say this model is ergodic. When all states within a model connect to all others, the model is always ergodic.



Arrows indicated the transition between states and adjacent values correspond to the probability of this transition.

Using 3.5 we can create a matrix p. To make this clear, we first create a table with our states labelled for rows and columns, where the $p(i, j)$ is the cell corresponding to row i and column j.

x	Sunny	Rainy	Cloudy
Sunny	0.4	0.4	0.2
Rainy	0.3	0.3	0.4
Cloudy	0.2	0.5	0.3

This content of this table forms the matrix p.

$$p = \begin{bmatrix} 0.4 & 0.4 & 0.2 \\ 0.3 & 0.3 & 0.4 \\ 0.2 & 0.5 & 0.3 \end{bmatrix} \tag{3.5}$$

Now that we have a Markov Model with its p, we must reflect on its potential uses. Some natural questions one may ask are:

1. Given at time t the state was S_i, what is the most likely state time $t + 1$?

2. What is the probability of getting a particular state sequence O?

3. What is the probability of staying within a state for d time steps?

This first problem we will address using the matrix p. The motivation for creating the matrix p was to build a matrix where p_{ij} contains the probability of moving from state i to state j. Thus, we look at the current row and find the maximum probability and its corresponding j.

Example 3.6. Let us refer back to 3.5 and assume the current state is Cloudy. We can see that $0.2 < 0.3 < 0.5$ and that 0.5 corresponds to Rainy. Thus our the most likely next state would be Rainy.

Note: If the current state were sunny, we would have two maximums of 0.4. In such a case, the process is equally likely to go to either.

The second problem provides a state sequence $Q = \{q_t, q_{t+1}, q_{t+2}...\}$ and asks what the probability of this occuring is, i.e. $\mathbb{P}(Q|model)$. This can be simplified quite easily as shown below.

$$\begin{aligned}
\mathbb{P}(Q|model) &= \mathbb{P}(\{q_t, q_{t+1}, q_{t+2}...\}|model) &(3.6)\\
&= \mathbb{P}(q_t)\mathbb{P}(q_{t+1}|q_t)\mathbb{P}(q_{t+2}|q_{t+1})... &(3.7)\\
&= \mathbb{P}(q_t)p(q_t, q_{t+1})p(q_{t+1}q_{t+2})... &(3.8)
\end{aligned}$$

Example 3.7. We can now use 3.6 to demonstrate the probability of a state squence from 3.5. Let $Q = \{\text{Sunny, Sunny, Cloudy, Rainy}\}$. Given that we start from Sunny:

$$\begin{aligned}
\mathbb{P}(Q|model) &= \mathbb{P}(\{Sunny, Sunny, Cloudy, Rainy\}|model) &(3.9)\\
&= \mathbb{P}(Sunny)\mathbb{P}(Sunny|Sunny)\mathbb{P}(Cloudy|Sunny)\mathbb{P}(Rainy|Cloudy) &(3.10)\\
&= 1 * 0.4 * 0.2 * 0.5 &(3.11)\\
&= 0.04 &(3.12)
\end{aligned}$$

The third problem asks how long is the model likely to stay in any given state. Assume that the model stays in state S_i for d days. We can create a state sequence for this, $Q = \{q_t = S_i, q_{t+1} = S_i, ..., q_{t+d-1} = S_i, q_{t+d} \neq S_i\}$. Using the state sequence probabililty calculation from before we can compute the following equation:

$$\mathbb{P}(Q|model) = p(i,i)^{d-1}(1 - p(i,i)) = p_i(d) \tag{3.13}$$

We label this $p_i(d)$ to represent the discrete probability density function of the duration d in state i. From this we can calculate the expected stay in any particular state. This is done using the following formula:

$$\begin{aligned}
\bar{d_i} &= \sum_{d=1}^{\infty} dp_i(d) &(3.14)\\
&= \frac{1}{1 - p(i,i)} &(3.15)
\end{aligned}$$

Example 3.8. Reffering back to 3.5, suppose we would like to see how many days in a row we expect it to be sunny. We see that $p(Sunny, Sunny) = 0.4$. Now we can use 3.14 to find,

$$\begin{aligned}
\bar{d}_{Sunny} &= \sum_{d=1}^{\infty} dp_{Sunny}(d) &(3.16)\\
&= \frac{1}{1 - p(Sunny, Sunny)} &(3.17)\\
&= \frac{1}{1 - 0.4} &(3.18)\\
&= 1.67 &(3.19)
\end{aligned}$$

Thus we expect it to remain sunny for 1.67 days. Since we are dealing with discrete data, it is more appropriate to round up to 2 days.

The Markov model we have been discussing so far is observable as we can observe its events. Not all Markov models, however, are observable.

3.3 Motivating the Hidden Markov Model

Sometimes we do not observe our states but only see the effect of a state change. To help develop this idea, we borrow an example from Rabiner and Juang, 1986.

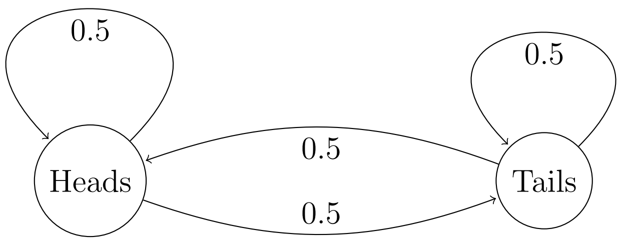
Example 3.9. Suppose someone is hiding behind a barrier or curtain, where we cannot see what they are doing. This person is doing some experiment with flipping coins and shouting heads or tails at regular intervals. We do not know:

i How many coins there are.

ii If the coin/s is/are fair.

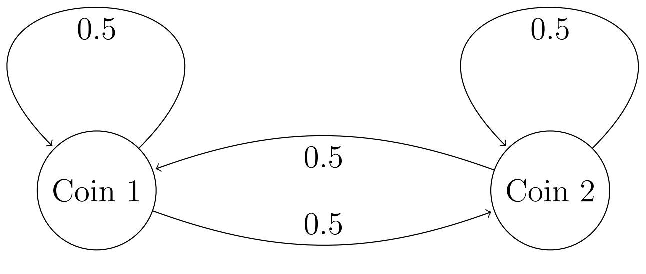
Since the problem is quite vague, we must experiment with various models and see which fits best the data. Since the only thing we can observe is the outcome, heads or tails, we will refer to this as our observation. Let us start with the simplest.

1. 1-Fair Coin
   In this model we have two states, heads and tails. There is a 0.5 probability for the model to change state and equally for staying in the same. The simplicity of this model comes at the cost of many assumptions that may not necessarily hold.



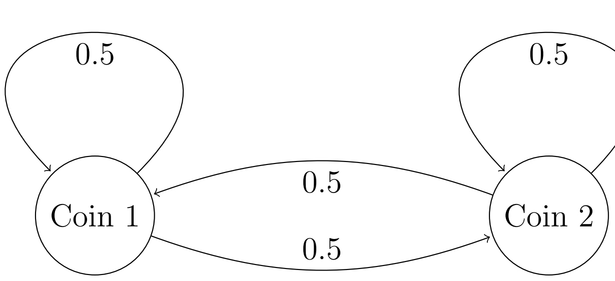
$\mathbb{P}(Heads)$	0.5
$\mathbb{P}(Tails)$	0.5

2. 2-Fair Coins
   This model also has two states, but this time they represent two different coins. Both can produce heads and tails. Thus we do not know which produced the observation. The fact that they are both fair coins means that as an external observer, we will not see a difference between this model and the 1-Fair Coin. However, it is clear that the observations are now independent of the hidden states transitions, as they are equally likely regardless of the state. In the 1-Fair Coin model, we can determine perfectly which state the model is in from the observation, but here this is no longer possible.



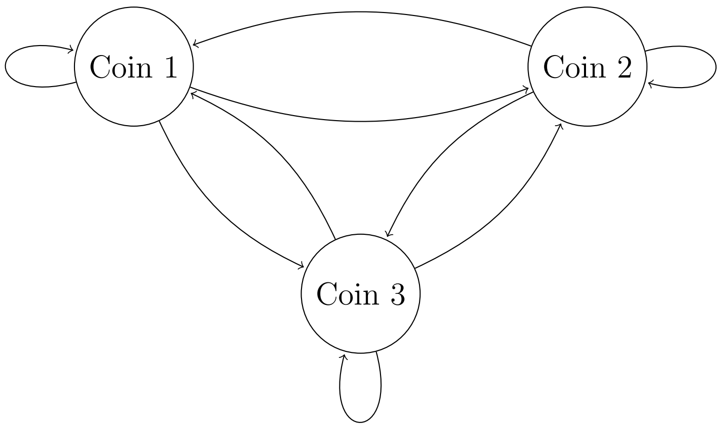
	$\mathbb{P}(Coin1)$	$\mathbb{P}(Coin2)$
$\mathbb{P}(Heads)$	0.5	0.5
$\mathbb{P}(Tails)$	0.5	0.5

3. 2-Biased Coins
   Although this model is similar to 2-Fair Coins, the change in $\mathbb{P}(Heads)$ and $\mathbb{P}(Tails)$ for each state has a large impact on the observation probabilities. If the model is in state one heads is more likely and if the state is in state two tails is more likely. As an observer we can now say if we see tails, it was most likely from state two and if we see heads, it was most likely from state one. The change between these two states must be an unrelated probability, such as a third coin or another source of randomness.



	$\mathbb{P}(Coin1)$	$\mathbb{P}(Coin2)$
$\mathbb{P}(Heads)$	0.75	0.25
$\mathbb{P}(Tails)$	0.25	0.75

4. 3-Biased Coins
   Similar to the 2-Biased Coins model, the probabilities for heads and tails vary with the three states.



	$\mathbb{P}(Coin1)$	$\mathbb{P}(Coin2)$	$\mathbb{P}(Coin3)$
$\mathbb{P}(Heads)$	0.6	0.25	0.45
$\mathbb{P}(Tails)$	0.4	0.75	0.55

After contemplating which model is best, an important conclusion one may make, is that it is quite challenging to decide on the number of states without a priori information. We must ensure that there are enough states, such that the model does not overgeneralize but also not so many that it requires too much data to train. Naturally, one would assume choosing the larger number of states is more suitable as they can take the shape of a model with fewer states, while it is not for the opposite. However, larger models require much more data to be statistically reliable, as there are too many unknown variables. Below we show this for our models and where the unknowns come from (-s being from the state transition probabilities and -O being from the observation probabilities).

Model	Number of Unknowns	From
1-Fair Coin	0	-
2-Fair Coins	1	1-S
2-Biased Coins	4	2-S 2-O
3-Biased Coins	9	6-S 3-O

Hence, the best approach is to base the model state size on the amount of available data, which is not always guaranteed to give reliable results but can sometimes be the only option. For example, when limited by data.

One may notice that the first model has 0 unknowns. It has this because each state links with only one observation. Thus, as an observer, we can assert what state the model is in from an observation. Thus, the states are no longer hidden, and the model is simply a standard Markov model.

Another essential detail the avid reader may have noticed is in the case of 2-Biased Coins and 3-Biased Coins it is possible to make a reasonable guess of what state the model is in, i.e. which coin is flipped, based on the observation. Furthermore, the statistical properties of predictions generated using 1-Fair Coin and 2-Fair Coins should be identical but for 2-Biased Coins and 3-Biased Coins be somewhat unique. Due to this, unless the underlying system is entirely fair, like in one and two, it should be possible to determine which model best fits the data and determine the model.

We now arrive at the core idea behind hidden Markov models. Although we cannot directly observe the model or its properties, we can create a model that fits the data the best through sufficient observation data.

Chapter 4

Hidden Markov Model

4.1 Definition

A hidden Markov model is a doubly stochastic process, where the underlying process is markovian and hidden Rabiner and Juang, 1986, which comes from the fact that there are two stochastic processes, one determining the transition between states and one determining the output observation. Braum and his colleagues developed this in Leonard E Baum, Eagon, et al., 1967 and Leonard E. Baum and Petrie, 1966.

To define a hidden Markov model, we need five things.

1. N

   i N is the number of hidden states. Usually based on something in the real world but sometimes can be unknown, as in 3.9.

   ii The states are usually ergodic, i.e. from any given state, we can eventually reach another, but this is unnecessary.

   iii The states are from the state space $S = \{S_1, S_2, ..., S_N\}$.

2. M

   i M is the number of observable outputs.

   ii These make a discrete alphabet of observations called $V = \{v_1, v_2, ..., v_M\}$.

3. A

   i A is the state transition matrix.

   ii This is the same as the p matrix 3.4.

   iii A $= \{a_{ij}\}$

   iv $a_{ij} = \{p(i,j) = \mathbb{P}\{X_n = j | X_{n-1}\}$

4. B

   i B is the observation probability matrix.

   ii B $= \{b_j(k)\}$

   iii $b_j(k) = \mathbb{P}(V_k \ at \ t | q_t = S_j)_{1 \leq j \leq N, 1 \leq k \leq M}$

5. π

   i π is a vector containing all inital state probabilities.

   ii $\pi = \{\pi_i\}$

   iii $\pi_i = \mathbb{P}(q_1 = S_i) for 1 \leq i \leq N$

We can now combine the above to provide a formal definition of hidden markov models.

Definition 4.1. Hidden Markov Model
A Hidden Markov Model is a 5-tuple $\{N, M, A, B, \pi\}$ that is used to represent a doubly stochastic process where the hidden process is markovian.

Before we continue, we will also provide some notation used for the rest of the paper.

i We will continue to use Q 3.3 to represent the Markov model's state sequence, i.e. the hidden process.

ii We will use $O = \{O_1, O_2, ..., O_T\},\ O_i \in V$ to represent the observation sequence.

iii we will occasionally represent the hidden markov model as $\{N, M, \lambda\}$ where $\lambda = \{A, B, \pi\}$

4.2 Using HMM

As with any mathematical model, we can use HMMs to predict future observations. As with simple Markov models 3.2, we can create probability measures, but this time we must use conditioning.

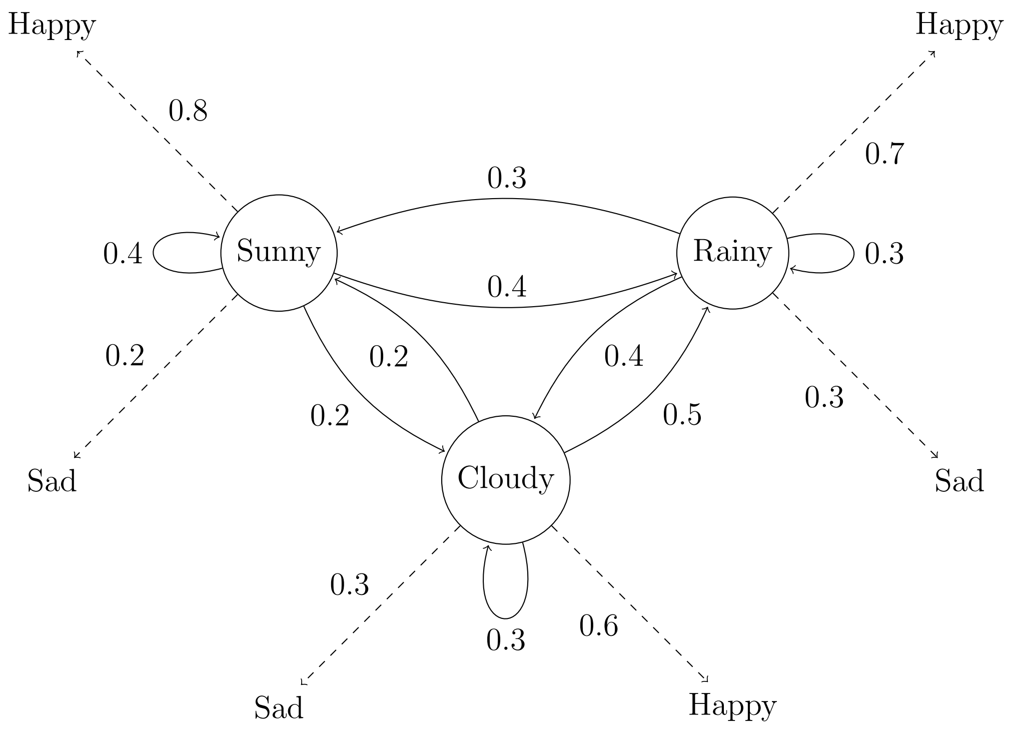
4.2.1 Predictive Model

We can use HMM to generate a sequence of potential observations. Given a a hidden markov model, lets call it H = $\{N, M, A, B, \pi\}$, to generate a sequence of T observations O we do the following steps:

1. Using π as a probability measure, set $t = 1$ and randomly select a state as the first $q_1 = s_i$.
2. Using $b_i(k)$ as a probability measure, randomly select the observation $O_t = v_k$.
3. Using a_{ij} as a probability measures, set $t = t + 1$ and randomly select a the next state $q_{t+1} = s_j$.
4. Repeat steps 2 and 3 until $t = T$

To demonstrate this method, we will use an adapted version of 3.5. This version will have the Markov chain from before as the underlying hidden process and another process with state-space {Happy, Sad}, which we can observe.

Example 4.2. Suppose Alice is hidden away from the world and has no access to information regarding the weather. She meets Bob every day and knows how weather affects his mood. For simplicity, assume Bob only has two moods, happy and sad. Given matrix A, B and vector π can she predict his mood for three consecutive days?
From context we can deduce the following: enumerate



The solid lines represent hidden probabilities, and the dashed represent observable.

N = 3, number of hidden states

M = 2, number of possible observations

$$A = \begin{bmatrix} 0.4 & 0.4 & 0.2 \\ 0.3 & 0.3 & 0.4 \\ 0.2 & 0.5 & 0.3 \end{bmatrix} \tag{4.1}$$

$$B = \begin{bmatrix} 0.8 & 0.2 \\ 0.7 & 0.3 \\ 0.6 & 0.4 \end{bmatrix} \tag{4.2}$$

$$\pi = \begin{bmatrix} 0.5 \\ 0.3 \\ 0.2 \end{bmatrix} \tag{4.3}$$

enumerate

We can now use 4.2.1 to create an observation sequence $O = \{o_1, o_2, o_3\}$. We will require multiple random variables generated using various probability measures. We will these through python using the "rand.py" file. We will use a uniform random variable. We will label this r.v. We select the state that corresponds to the region on the cumulative probability distribution that the random variable lies on.

i We generate a r.v. $= 0.0058$. Using Pi as the probaility distribution, we select Sunny. We can now set $q_1 = s_1$.

ii We generate a r.v. $= 0.1947$. Using $b_1(k)$ as the probability distribution we select Happy as the observation. We can now set $o_1 = v_1$.

iii we generate a r.v. $= 0.7168$. Using a_{1j} as the probability distribution we select Rainy as the next state. We now set $q_2 = s_2$.

iv We generate a r.v. $= 0.1060$. Using $b_2(k)$ as the probability distribution we select Happy as the observation. We can now set $o_2 = v_1$.

v we generate a r.v. $= 0.8977$. Using a_{2j} as the probability distribution we select Cloudy as the next state. We now set $q_3 = s_3$.

vi We generate a r.v. $= 0.1369$. Using $b_3(k)$ as the probability distribution we select Happy as the observation. We can now set $o_2 = v_1$.

Finally, we can look back on our prediction O and see that it is equal to $\{v_1, v_1, v_1\}$, i.e. we predict three consecutive Happy days.

4.2.2 Three Key Problems

There are many interesting questions one may pose regarding the HMM but there are three famous ones, highlighted in Rabiner and Juang, 1986 which we will focus on.

1. Evaluation
   Given model H $= \{N, M, A, B, \pi\}$ what is the probability that it generated the sequence of observations $O = \{o_1, o_2, ..., o_T\}$? i.e. $\mathbb{P}(O \mid H)$

2. Decoding
   What sequence of states $Q = \{q_1, q_2, ..., q_3\}$ best explains a sequence of observations $O = \{o_1, o_2, ..., o_T\}$?

3. Learning
   Given a set of observation $O = \{o_1, o_2, ..., o_T\}$, how can we learn the model H $= \{N, M, A, B, \pi\}$ that would generate them?

In the coming sections, we will be motivating uses and developing solutions for each problem.

4.3 Problem 1: Evaluation

Lets start by addressing question 1. Informally, we are looking for the probability that a given model generated a sequence of observations, i.e. $\mathbb{P}(O|\lambda)$.

This probability has many useful applications. For example, we may have multiple potential models λ_i and cannot decide which one is the most suitable. In this case, we can now calculate this probability for each λ_i and the largest.

To find this probability, we must consider the hidden internal states of the model. Since our probability of observations $\{b_j(k)\}$ is conditioned on the hidden state, we can start by calculating this probability conditioned on these states. Lets assume we know what the state sequence $Q = \{q_1, q_2, ..., q_t\}$ is. To $\mathbb{P}(O|Q, \lambda)$ we can find the product of all the probabilities of an observation given the models state at all times t. In essence, this breaks the $\mathbb{P}(O|Q, \lambda)$ into T parts.

$$\mathbb{P}(O|Q, \lambda) = \prod_{t=1}^{T} \mathbb{P}(O_t|q_t, \lambda) \tag{4.4}$$

An observation one may make is that these probabilities are simply taken from the matrix B.

$$\mathbb{P}(O_t|q_t, \lambda) = b_{q_t}(O_t), \quad \forall t \in [0, T] \tag{4.5}$$

Thus we can rewrite 4.4 as:

$$\mathbb{P}(O|Q, \lambda) = b_{q_1}(O_1)b_{q_2}(O_2)...b_{q_T}(O_T) \tag{4.6}$$

Our next objective is to remove Q from the conditioned part of the probability. To do this, we must first calculate $\mathbb{P}(Q|\lambda)$. This is simply the probability of transitioning from q_1 to q_2, q_2 to q_3 etc. More formally we can use matrix A to find the probability of each of these transitions, and since we are finding the total for the entire sequence, we multiply them all together. We start with π_{q_1} as we also need the probability of starting at q_1.

$$\mathbb{P}(Q|\lambda) = \pi_{q_1} a_{q_1 q_2} a_{q_2 q_3} ... a_{q_{T-1} q_T} \tag{4.7}$$

We can now successfully remove Q from the condition using 4.6 and 4.7:

$$\begin{aligned} \mathbb{P}(O, Q|\lambda) &= \mathbb{P}(O|Q, \lambda)\mathbb{P}(Q|\lambda) && (4.8) \\ &= \pi_{q_1} b_{q_1}(O_1) a_{q_1 q_2} b_{q_2}(O_2) a_{q_2 q_3} ... a_{q_{T-1} q_T} b_{q_T}(O_T) && (4.9) \end{aligned}$$

This gives us the joint probability of observations and the internal states. In other words, it provides the probabilty that given observations O and internal state sequence Q was generated by model λ. To achieve our desired probablity all we need to do is get rid of the Q. Since it is another input, all we must do is sum each value of 4.8. As we have accounted for every possible Q, we no longer need to worry about its particular value. This leaves us with:

$$\begin{aligned} \mathbb{P}(O|\lambda) &= \sum_{allQ} \mathbb{P}(O|Q, \lambda) P(Q|\lambda) && (4.10) \\ &= \sum_{q_1, q_2, \ldots, q_T} \pi_{q_1} b_{q_1}(O_1) a_{q_1 q_2} b_{q_2}(O_2) a_{q_2 q_3} ... a_{q_{T-1} q_T} b_{q_T}(O_T) && (4.11) \end{aligned}$$

Although this solution is correct, calculating this is infeasible because it requires too many computations. For T timesteps and N states, to find every possible Q, we must sum over N^T state sequences. For each timestep we require a multiplication to $a_{q_{i-1} q_i}$ and $b_{q_i}(O_i)$, except the last where there are no transitions, which leads to $2T - 1$ multiplications for each state sequence. Lastly, we require N^T addition operations to sum the result for each state sequence. Our final total number of operations of $(2T - 1)N^T + (N^T - 1)$.

Example 4.3. Lets refer back to 4.2. Suppose we would like to find the probability of a string of 10 observations using model H. Here $N = 3$ and $T = 10$.

$$\begin{aligned} operations &= (2T - 1)N^T + (N^T - 1) && (4.12) \\ &= (20 - 1)3^1 0 + (3^1 0 - 1) && (4.13) \\ &= 1180979 && (4.14) \end{aligned}$$

We have a problem as even with a smaller model 4.4 we require a considerable number of calculations. For a moderate to large-sized model, we would require an infeasible amount of calculations. To overcome this problem, we look for a more efficient method, the Forward-Backward algorithm.

4.3.1 Forward-Backward Algorithm

The Forward-Backward algorithm (F-B) comprises two helper functions α and β. We will start by discussing the former.

$$\alpha_t(i) = \mathbb{P}(O_1, O_2, O_3, ..., O_t, q_t = S_i|\lambda) \tag{4.15}$$

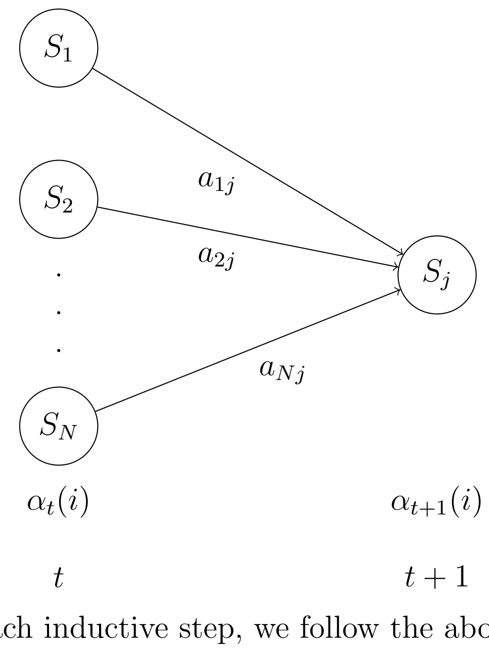
α is an extremly powerful tool in reducing the number of calculations. As given by 4.3.1, it providse the probability that at time t we have seen a sequence of observations and are currently at state $q_t = S_i$. This is not quite $\mathbb{P}(O|\lambda)$ but it represents a part of it. Instead of the probability of the whole sequence, it breaks it into a chunk of size t, commits to end at a particular state and then calculates the same proabbility for this.

We can combine with induction to produce an iterative process that can calculate **??**.

i Base case
For the base case we require the probability of the q_1 being equal to S_1 and giving us observation O_1. The former is addressed by π_i and the later by $b_i(O_1)$. This gives us:

$$\alpha_1(i) = \pi_i b_i(O_1), \quad i \in [1, N] \tag{4.16}$$

ii Inductive step:



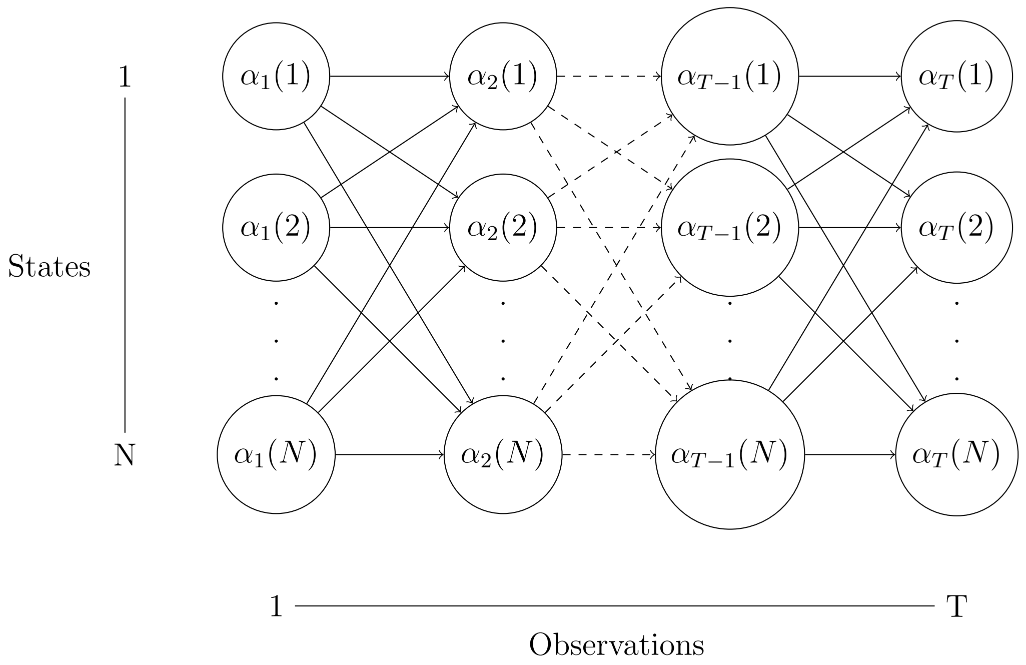
For each state j, for each inductive step, we follow the above method. Each$\alpha_t(i)$ is multiplied by each a_{ij} and then summed up. This resultmultipled by $b_j(O_{t+1}$ gives us $\alpha_{t+1}(j)$.

For the inductive step we must consider how to approach the next timestep. We will again be calculating for all $j \in [1, N]$ and as such must take into consideration, for each j, every possible i. This is again the same set of $[1, N]$. Therefore, to account for all possible previous states and their transition to the current state, we must sum over 1 to N the product of $\alpha_t(i)$ and a_{ij}. For the given observation, as before, we compute $b_j(O_{t+1})$. Additionally, we must stop before reaching the final step as there is no outward transition and thus this would not be applicable. This gives us:

$$\alpha_{t+1}(j) = \left[\sum_{i=1}^{N} \alpha_t(i)a_{ij}\right] b_j(O_{t+1}), \quad j \in [1, N], t \in [1, T-1] \tag{4.17}$$

iii Termination step:
For the termination step, we sum over all alpha at the final time T. Each alpha represents the probability of being in that given state at that particular time, through all possible sequences that it may have followed.

$$\mathbb{P}(O|\lambda) = \sum_{i=1}^{N} \alpha_T(i) \tag{4.18}$$



For each α at time t, we require all α at time $t-1$. Thus werequire N^2 calculations for each timestep.

One can see that this method is far more efficient than 4.10. It requires N^2 multiplications for $\alpha_t(i)$ and a_{ij} for T time periods. At each T there are N addition operations for the summation and N multiplication for the $b_j(O_{t+1})$, which is true for all but the first and last timestep, where there are N multiplications and N additions respectively. This gives us $(T-2)(N^2+N+1)+2N$ calculations. Considering the order, we see that the previous method had order $O(TN^T)$ whereas F-B gives us an order of $O(TN^2)$. It is now feasible to compute $\mathbb{P}(O|\lambda)$.

Example 4.4. We attempt to solve the problem 4.4 again but this time using the F-B algorithm. Suppose we would like to find the probability of a string of 10 observations using model H. Here $N = 3$ and $T = 10$.

$$\begin{aligned} operations &= (T-2)(N^2+N+1)+2N && (4.19)\\ &= (10-2)(3^2+10+1)+6 && (4.20)\\ &= 118 && (4.21) \end{aligned}$$

118 is many orders of magnitude smaller than 1180979, which was the requirement without F-B algorithm. Thus it is a significant improvement. The improvement against the base method will be even more drastic for larger models, as F-B has a fixed N^2 instead of the N^T term.

For question 1 this is sufficient. However, we will later require the β, the backward component and as such we will describe it now. Logically it is the same principle as the forward component except this time instead of moving forward step by step we are moving backwards.

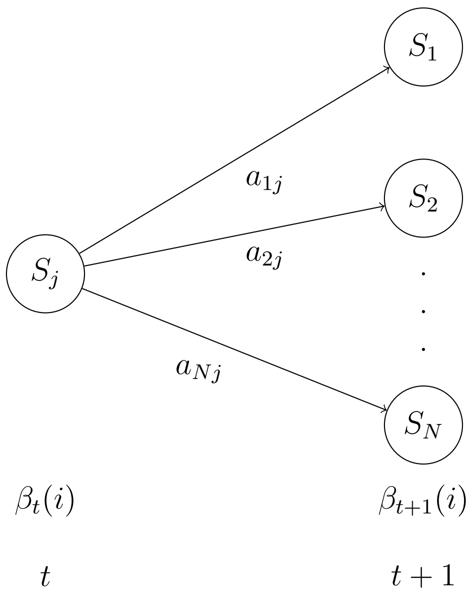
$$\beta_t(i) = \mathbb{P}(O_{t+1}, O_{t+2}, , ..., O_T | q_t = S_i, \lambda) \tag{4.22}$$

This represents the probability of seeing the observations O_{t+1} up to O_T given that at time t the model λ is at state S_i. We again calculate this inductively.

1. Base case
   For each state we must assume that it is the final state in order to iterate from it. This gives us:

$$\beta_T(i) = 1, \quad i \in [1, N] \tag{4.23}$$

2. Inductive step:



Similar to α, we use induction. However, this time we look into the future of the sequence and take steps backwards.

Each inductive step we move back by one timestep. As before, we will be calculating for all N states except this time i will be varying instead of j. This makes sense as we are stepping backward and we want to see which previous state is the most likely previous state. At each step, we the transaction probability of having coming from i, a_{ij} to the probability of seeing the given observation at state S_j, $b_j(O_{t+1})$ and the liklihood of being at that state based on future states $\beta_{t+1}(i)$. This gives us:

$$\beta_t(i) = \sum_{j=1}^{N} a_{ij} b_j(O_{t+1}) \beta_{t+1}(i), \quad i \in [1, N], t \in [1, T-1] \tag{4.24}$$

4.4 Problem 2: Decoding

We now turn our attention to 2. This problem is somewhat more difficult, as the definition of 'best' is quite vague and open to interpretations. An obvious appraoch would be to look for the states that are individually most likely for each state for a set time t given all observations and the model. Lets define this probaility as γ.

$$\gamma_t(i) = \mathbb{P}(q_t = S_i | O, \lambda) \tag{4.25}$$

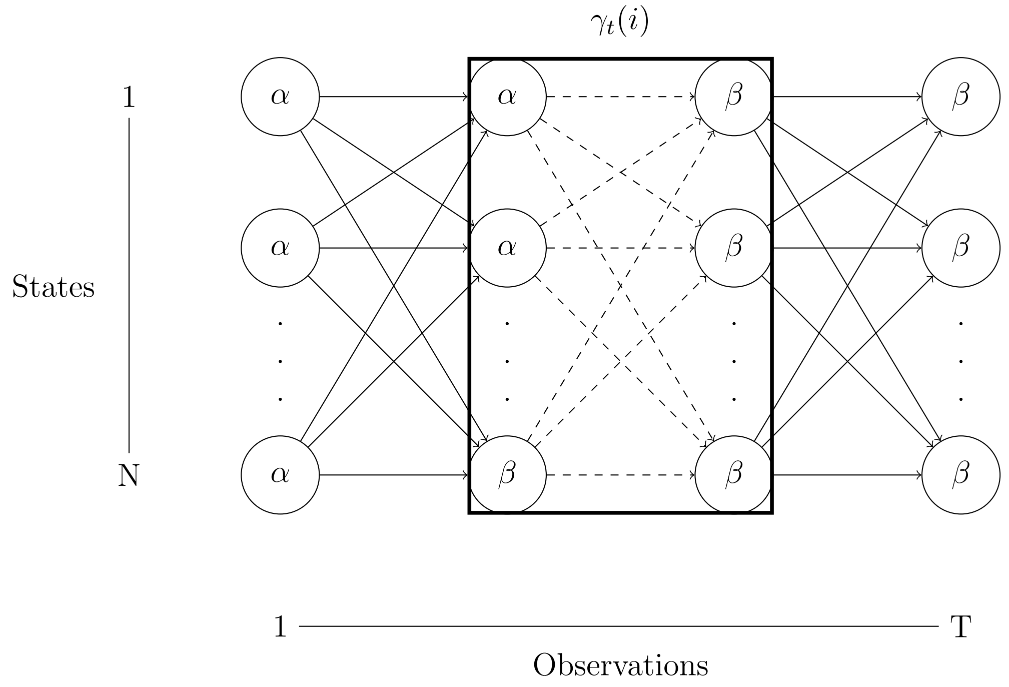
Using 4.3.1 and 4.22 we can solve for γ quite quickly. If we recall, $\alpha_t(i)$ provides us with the probability of being in state i after seeing all the previous observations and $\beta_t(i)$ gives us the probability of being in state i see all the remaining observations in the future. This gives us $\alpha_t(i)\beta_t(i)$. We now normalise this to get a probability, which is possible by dividing by the probability of getting this particular observation given all possible observation sequences $\mathbb{P}(O|\lambda)$. This is equivalent to dividing by the sum of $\alpha_t(j)\beta_t(j)$ over all possible states j.

$$\gamma_t(i) = \frac{\alpha_t(i)\beta_t(i)}{\mathbb{P}(O|\lambda)} \tag{4.26}$$

$$= \frac{\alpha_t(i)\beta_t(i)}{\sum_{j=1}^{N} \alpha_t(j)\beta_t(j)} \tag{4.27}$$

This ensures that:

$$\sum_{i=1}^{N} \gamma_t(i) = 1 \tag{4.28}$$



Each dashed line represents a calculation for $\gamma_t(i)$. For each time step, we calculate these and then find the maximum. We select the state corresponding to the maximum and add it to the state sequence.

As such this ensures all $\gamma_t(i)$ are probabilities. We can now go through each timestep t calculating $\gamma_t(i)$ and selecting state i corresponding to the largest $\gamma_t(i)$.

This method will maximise the number of correct states and give the correct answer if the model is completely connected, i.e. each state can reach every other state. If this is not the case, we may get a state sequence that is not possible. e.g. At time t the model is in state i and at time $t+1$ it is in j, but $a_{ij} = 0$, thus is not possible.

In the scenario given, we must redefine 'best' to the path that maximises $\mathbb{P}(Q|O, \lambda)$. Since we are maximising this, we can equivalently maximise $\mathbb{P}(Q, O|\lambda)$. To solve this problem, we require the Viterbi Algorithm.

4.4.1 Viterbi Algorithm

The Viterbi Algorithm Viterbi, 1967, explored in depth in Forney, 1973 follows a similar lattice structure of the F-B algorithm. Similar to how we broke 1 into smaller pieces, we do the same to $\mathbb{P}(Q|O, \lambda)$.

$$\delta_t(i) = max_{q_1,q_2,...,q_t-1}\mathbb{P}(\{q_1, q_2, ...q_t = i\}, O_1, O_2, ..., O_t|\lambda) \tag{4.29}$$

An important point to note is $\delta_t(i)$ does not store the sequence. Thus we must introduce a new variable that will be responsible for doing so. We can call this $\psi_t(i)$, where it is equal to the state we have come from given we are at time t and state i. We will once again use induction. The process is as follows.

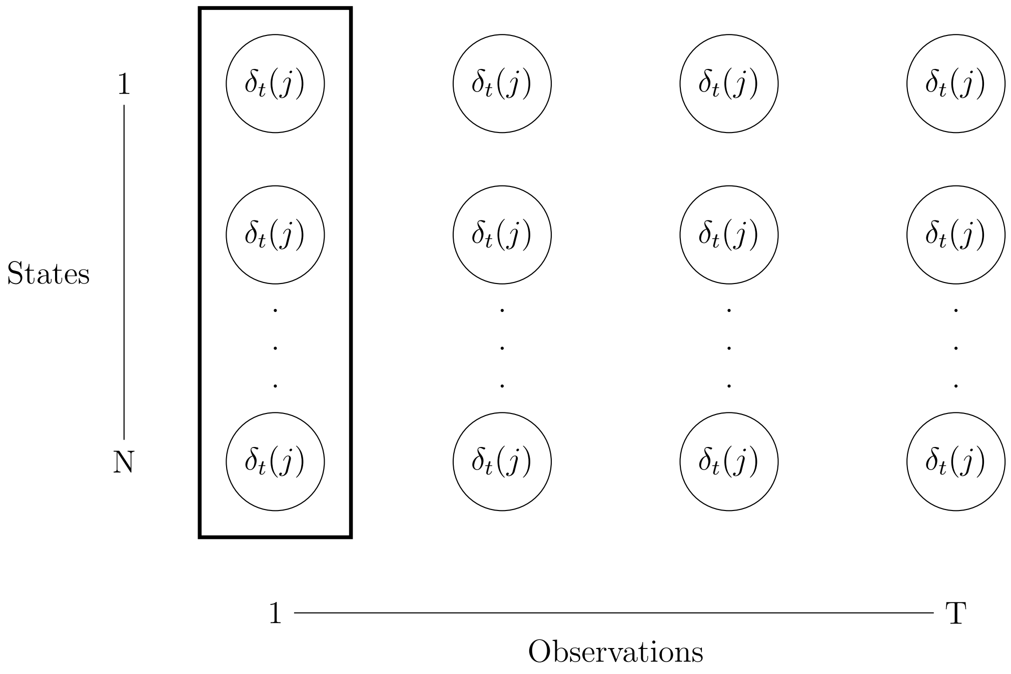
1. Base case
   For each state we must calculate $\pi_i b_i(O_1)$ to determine which intial state is most likely.

We also must set $\psi_1(i) = 0$ as there have not been any states until now.

$$\begin{aligned} \delta_1(i) &= \pi_i b_i(O_1) \qquad (4.30) \\ \psi_1(i) &= 0 \qquad (4.31) \end{aligned}$$

2. Inductive step:
For each state we calculate the $\delta_{t-1}(i)$ times a_{ij} to find the most likely next state based on previous state liklihood and the transition probability. We maximize this term and the multiply by $b_j(O_t)$ to include a bias based on the observation probabilities. As before we store the argument of the maximum in ψ. This gives us:

$$\begin{aligned} \delta_t(j) &= max_{1\le i\le N}[\delta_{t-1}(i)a_{ij}]b_j(O_t), t \in [2,T] \qquad (4.32) \\ \psi_t(j) &= argmax_{1\le i\le N}[\delta_{t-1}(i)a_{ij}], j \in [1,N] \qquad (4.33) \end{aligned}$$



Once $\delta_t(j)$ is calculated for a particular t, we find the maximum, which is the state we add to our state sequence. Since $\delta_t(j)$ accounts for transition probability a_{ij}, impossible transitions will always be equal to 0. Thus unless all transitions are equal to 0, they cannot be the maximum.

3. Termination step:
To terminate this recursion, we need to find the maximum $\delta_T(i)$. Here we maximise, as the values we already calculated the values in the induction. We will store this probability in $\mathbb{P}*$. Similarly, we need to find the argument corresponding to this max for the final state, and we set this to the final state q_T^*.

$$\begin{aligned} \mathbb{P}^* &= max_{1\le i\le N}[\delta_T(i)] \qquad (4.34) \\ q_T^* &= argmax_{1\le i\le N}[\delta_T(i)] \qquad (4.35) \end{aligned}$$

To find any particular states that we may be interseted in q_t^*, we use $q_t^* = \psi_{t+1}(q_{t+1}^*)$.

4.5 Problem 3: Learning

The third problem 3 addresses learning. How can we learn a model from given data of observations? This problem is critical as we often do not have the model, and calculating it is not simple. In these cases, we must derive the model from the data we have, a set of observations. Given the set of observations $O = \{O_1, O_2, ..., O_T\}$ we want to find the most suitable $\lambda = (A, B, \pi)$. To do this, we use the Baum-Welch algorithm.

4.5.1 Baum-Welch Algorithm

For the Baum-Welch algorithm we will need all three parameters intrudced earlier; α 4.3.1, β 4.22 and γ 4.25. We will also need a new parameter $\xi_t(i,j)$. This will capture the probability of being in some state S_i at time t and then S_j at time $t+1$ given the observations and the model.

$$\xi_t(i,j) = \mathbb{P}(q_t = S_i, q_{t+1} = S_j | O, \lambda) \tag{4.36}$$

To solve this problem we can refer back to 4.3.1 for the left hand side (including q_t) and 4.22 for the right hand side (indlucing q_{t+1}). To get from state i to j we use $a_{ij}b_j(O_{t+1})$. Putting this all togther we get a liklihood. To normalize this into a probabiltiy we once more use $\mathbb{P}(O|\lambda)$. This gives us:

$$\xi_t(i,j) = \frac{\alpha_t(i)a_{ij}b_j(O_{t+1})\beta_{t+1}(j)}{\mathbb{P}(O|\lambda)} \tag{4.37}$$

Since we are interested in the probability of going from one i to one j, for the denominator we use the sum of all i and all j.

$$\xi_t(i,j) = \frac{\alpha_t(i)a_{ij}b_j(O_{t+1})\beta_{t+1}(j)}{\sum_{i=1}^{N}\sum_{j=1}^{N}\alpha_t(i)a_{ij}b_j(O_{t+1})\beta_{t+1}(j)} \tag{4.38}$$

One may find it helpful to compare $\xi_t(i,j)$ with $\gamma_t(i)$. $\gamma_t(i)$ represents the probability of being at state i at timestep t. Summing over j for $\xi_t(i,j)$ leaves us with $\xi_t(i)$ which represents the probability of being at state i at timestep t. This is identical to $\gamma_t(i)$. We can now state:

$$\gamma_t(i) = \sum_{j=1}^{N} \xi_t(i,j) \tag{4.39}$$

For $\gamma_t(i)$, if we sum over t we can get a number that can be used as the expected number of times S_i is visited. Thus the expected number of transitions from S_i can be calculated by:

$$\sum_{t=1}^{T-1} \gamma_t(i) \tag{4.40}$$

Similarly for $\xi_t(i)$, if we sum over t we can get a number that can be used as the expected number of times S_i transitions to S_j.Thus the expected number of transitions from S_i to S_j can be calculated by:

$$\sum_{t=1}^{T-1} \xi_t(i,j) \tag{4.41}$$

Now that we have created a set of tools, we will need to tackle the learning problem itself. To build a improved λ, $\bar{\lambda}$, we need to find $\bar{\pi}$, $\bar{A}$ and $\bar{B}$.

i $\bar{\pi}$
Since $\gamma_t(i)$ represents the expected frequency in S_i at time t, if we let t=1 this now is equvialent to $\bar{\pi}$

$$\bar{\pi} = \gamma_1(i) \tag{4.42}$$

ii $\bar{a_{ij}}$
Here we can use the expected number of transitions from state i to j divided by expected number of transitions from i in total. This will provide the appropriate transition probability.

$$\bar{a_{ij}} = \frac{\sum_{t=1}^{T-1} \xi_t(i,j)}{\sum_{t=1}^{T-1} \gamma_t(i)} \tag{4.43}$$

iii $\bar{b_j(k)}$
For the B matrix, we will need to divide the expected number of times the model is in state j and observes v_k by the expected number of times it is j.

$$\bar{b_j(k)} = \frac{\sum_{t=1, s.t. O_t = v_k}^{T} \gamma_t(j)}{\sum_{t=1}^{T-1} \gamma_t(j)} \tag{4.44}$$

We have used our λ and O to produce our parameters: $\alpha_t(i)$, $beta_t(i)$, $\gamma_t(i)$, $\xi_t(i,j)$. This is called parameter re-estimation. We have then used these parameters to produce our $\bar{\lambda}$ = $\{\bar{\pi}, \bar{a_{ij}}, \bar{b_j(k)}\}$. This is called expectation maximization. This method can be iterated and each iteration should provide an improvement for lambda or worst case senario be equvialent. Proof of this can be found in Leonard E Baum et al., n.d. Once lambda stabalizes and is no longer changing, we can assume a local optimumum has been reached.

4.6 Modified HMM

4.6.1 GMM

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