

The Structure of Hidden Markov Models

- Have N states, states $1 \dots N$
- Without loss of generality, take N to be the final or stop state
- Have an alphabet K . For example $K = \{a, b\}$
- Parameter π_i for $i = 1 \dots N$ is probability of starting in state i
- Parameter $a_{i,j}$ for $i = 1 \dots (N - 1)$, and $j = 1 \dots N$ is probability of state j following state i
- Parameter $b_i(o)$ for $i = 1 \dots (N - 1)$, and $o \in K$ is probability of state i emitting symbol o

An Example

- Take $N = 3$ states. States are $\{1, 2, 3\}$. Final state is state 3.
- Alphabet $K = \{\text{the}, \text{dog}\}$.
- Distribution over initial state is $\pi_1 = 1.0, \pi_2 = 0, \pi_3 = 0$.
- Parameters $a_{i,j}$ are

	j=1	j=2	j=3
i=1	0.5	0.5	0
i=2	0	0.5	0.5

- Parameters $b_i(o)$ are

	o=the	o=dog
i=1	0.9	0.1
i=2	0.1	0.9

A Generative Process

- Pick the start state s_1 to be state i for $i = 1 \dots N$ with probability π_i .
- Set $t = 1$
- Repeat while current state s_t is not the stop state (N):
 - Emit a symbol $o_t \in K$ with probability $b_{s_t}(o)$
 - Pick the next state s_{t+1} as state j with probability $a_{s_t,j}$.
 - $t = t + 1$

Probabilities Over Sequences

- An **output sequence** is a sequence of observations $o_1 \dots o_T$ where each $o_i \in K$
e.g. the dog the dog dog the
- An **state sequence** is a sequence of states $s_1 \dots s_T$ where each $s_i \in \{1 \dots N\}$
e.g. 1 2 1 2 2 1
- HMM defines a probability for each state/output sequence pair

e.g. the/1 dog/2 the/1 dog/2 the/2 dog/1 has probability

$$\pi_1 b_1(\text{the}) a_{1,2} b_2(\text{dog}) a_{2,1} b_1(\text{the}) a_{1,2} b_2(\text{dog}) a_{2,2} b_2(\text{the}) a_{2,1} b_1(\text{dog}) a_{1,3}$$

Formally:

$$P(s_1 \dots s_T, o_1 \dots o_T) = \pi_1 \times \left(\prod_{i=2}^{T-1} P(s_i \mid s_{i-1}) \right) \times \left(\prod_{i=1}^T P(o_i \mid s_i) \right) \times P(N \mid s_T)$$

A Hidden Variable Problem

- We have an HMM with $N = 3, K = \{e, f, g, h\}$
- We see the following **output sequences** in training data

e g
e h
f h
f g

- How would you choose the parameter values for π_i , $a_{i,j}$, and $b_i(o)$?

Another Hidden Variable Problem

- We have an HMM with $N = 3, K = \{e, f, g, h\}$
- We see the following **output sequences** in training data

e g h
e h
f h g
f g g
e h

- How would you choose the parameter values for π_i , $a_{i,j}$, and $b_i(o)$?

A Reminder: Models with Hidden Variables

- Now say we have two sets \mathcal{X} and \mathcal{Y} , and a joint distribution $P(X, Y \mid \Theta)$
- If we had **fully observed data**, (X_i, Y_i) pairs, then

$$L(\Theta) = \sum_i \log P(X_i, Y_i \mid \Theta)$$

- If we have **partially observed data**, X_i examples, then

$$\begin{aligned} L(\Theta) &= \sum_i \log P(X_i \mid \Theta) \\ &= \sum_i \log \sum_{Y \in \mathcal{Y}} P(X_i, Y \mid \Theta) \end{aligned}$$

Hidden Markov Models as a Hidden Variable Problem

- We have two sets \mathcal{X} and \mathcal{Y} , and a joint distribution $P(X, Y | \Theta)$
- In Hidden Markov Models:
 - each $x \in \mathcal{X}$ is an output sequence $o_1 \dots o_T$
 - each $y \in \mathcal{X}$ is an state sequence $s_1 \dots s_T$

Maximum Likelihood Estimates

- We have an HMM with $N = 3, K = \{e, f, g, h\}$
We see the following **paired sequences** in training data

e/1 g/2
e/1 h/2
f/1 h/2
f/1 g/2

- Maximum likelihood estimates:

$$\pi_1 = 1.0, \quad \pi_2 = 0.0, \quad \pi_3 = 0.0$$

		j=1	j=2	j=3
		0	1	0
for parameters $a_{i,j}$:	i=1	0	1	0
	i=2	0	0	1

		o=e	o=f	o=g	o=h
		0.5	0.5	0	0
for parameters $b_i(o)$:	i=1	0.5	0.5	0	0
	i=2	0	0	0.5	0.5

The Likelihood Function for HMMs: Fully Observed Data

- Say $(x, y) = \{o_1 \dots o_T, s_1 \dots s_T\}$, and

$f(i, j, x, y) =$ Number of times state j follows state i in (x, y)

$f(i, x, y) =$ Number of times state i is the initial state in (x, y) (1 or 0)

$f(i, o, x, y) =$ Number of times state i is paired with observation o

- Then

$$P(x, y) = \prod_{i \in \{1 \dots N-1\}} \pi_i^{f(i, x, y)} \prod_{\substack{i \in \{1 \dots N-1\}, \\ j \in \{1 \dots N\}}} a_{i,j}^{f(i, j, x, y)} \prod_{\substack{i \in \{1 \dots N-1\}, \\ o \in K}} b_i(o)^{f(i, o, x, y)}$$

The Likelihood Function for HMMs: Fully Observed Data

- If we have training examples (x_l, y_l) for $l = 1 \dots m$,

$$\begin{aligned} L(\Theta) &= \sum_{l=1}^m \log P(x_l, y_l) \\ &= \sum_{l=1}^m \left(\sum_{i \in \{1 \dots N-1\}} f(i, x_l, y_l) \log \pi_i + \right. \\ &\quad \sum_{\substack{i \in \{1 \dots N-1\}, \\ j \in \{1 \dots N\}}} f(i, j, x_l, y_l) \log a_{i,j} + \\ &\quad \left. \sum_{\substack{i \in \{1 \dots N-1\}, \\ o \in K}} f(i, o, x_l, y_l) \log b_i(o) \right) \end{aligned}$$

- Maximizing this function gives maximum-likelihood estimates:

$$\pi_i = \frac{\sum_l f(i, x_l, y_l)}{\sum_l \sum_k f(k, x_l, y_l)}$$

$$a_{i,j} = \frac{\sum_l f(i, j, x_l, y_l)}{\sum_l \sum_k f(i, k, x_l, y_l)}$$

$$b_i(o) = \frac{\sum_l f(i, o, x_l, y_l)}{\sum_l \sum_{o' \in K} f(i, o', x_l, y_l)}$$

The Likelihood Function for HMMs: Partially Observed Data

- If we have training examples (x_l) for $l = 1 \dots m$,

$$L(\Theta) = \sum_{l=1}^m \log \sum_y P(x_l, y)$$

$$Q(\Theta, \Theta^{t-1}) = \sum_{l=1}^m \sum_y P(y \mid x_l, \Theta^{t-1}) \log P(x_l, y \mid \Theta)$$

$$Q(\Theta, \Theta^{t-1}) = \sum_{l=1}^m \sum_y P(y \mid x_l, \Theta^{t-1}) \left(\sum_{i \in \{1 \dots N-1\}} f(i, x_l, y) \log \pi_i + \right. \\ \left. \sum_{\substack{i \in \{1 \dots N-1\}, \\ j \in \{1 \dots N\}}} f(i, j, x_l, y) \log a_{i,j} + \sum_{\substack{i \in \{1 \dots N-1\}, \\ o \in K}} f(i, o, x_l, y) \log b_i(o) \right)$$

$$= \sum_{l=1}^m \left(\sum_{i \in \{1 \dots N-1\}} g(i, x_l) \log \pi_i + \sum_{\substack{i \in \{1 \dots N-1\}, \\ j \in \{1 \dots N\}}} g(i, j, x_l) \log a_{i,j} + \sum_{\substack{i \in \{1 \dots N-1\}, \\ o \in K}} g(i, o, x_l) \log b_i(o) \right)$$

where each g is an **expected count**:

$$\begin{aligned} g(i, x_l) &= \sum_y P(y \mid x_l, \Theta^{t-1}) f(i, x_l, y) \\ g(i, j, x_l) &= \sum_y P(y \mid x_l, \Theta^{t-1}) f(i, j, x_l, y) \\ g(i, o, x_l) &= \sum_y P(y \mid x_l, \Theta^{t-1}) f(i, o, x_l, y) \end{aligned}$$

- Maximizing this function gives EM updates:

$$\pi_i = \frac{\sum_l g(i, x_l)}{\sum_l \sum_k g(k, x_l)} \quad a_{i,j} = \frac{\sum_l g(i, j, x_l)}{\sum_l \sum_k g(i, k, x_l)} \quad b_i(o) = \frac{\sum_l g(i, o, x_l)}{\sum_l \sum_{o' \in K} g(i, o', x_l)}$$

- Compare this to maximum likelihood estimates in fully observed case:

$$\pi_i = \frac{\sum_l f(i, x_l, y_l)}{\sum_l \sum_k f(k, x_l, y_l)} \quad a_{i,j} = \frac{\sum_l f(i, j, x_l, y_l)}{\sum_l \sum_k f(i, k, x_l, y_l)} \quad b_i(o) = \frac{\sum_l f(i, o, x_l, y_l)}{\sum_l \sum_{o' \in K} f(i, o', x_l, y_l)}$$

A Hidden Variable Problem

- We have an HMM with $N = 3, K = \{e, f, g, h\}$
- We see the following **output sequences** in training data

e g
e h
f h
f g

- How would you choose the parameter values for π_i , $a_{i,j}$, and $b_i(o)$?

- Four possible state sequences for the first example:

e/1 g/1

e/1 g/2

e/2 g/1

e/2 g/2

- Four possible state sequences for the first example:

e/1 g/1

e/1 g/2

e/2 g/1

e/2 g/2

- Each state sequence has a different probability:

e/1 g/1 $\pi_1 a_{1,1} a_{1,3} b_1(e) b_1(g)$

e/1 g/2 $\pi_1 a_{1,2} a_{2,3} b_1(e) b_2(g)$

e/2 g/1 $\pi_2 a_{2,1} a_{1,3} b_2(e) b_1(g)$

e/2 g/2 $\pi_2 a_{2,2} a_{2,3} b_2(e) b_2(g)$

A Hidden Variable Problem

- Say we have initial parameter values:

$$\pi_1 = 0.35, \quad \pi_2 = 0.3, \quad \pi_3 = 0.35$$

$a_{i,j}$	j=1	j=2	j=3	$b_i(o)$	o=e	o=f	o=g	o=h
i=1	0.2	0.3	0.5	i=1	0.2	0.25	0.3	0.25
i=2	0.3	0.2	0.5	i=2	0.1	0.2	0.3	0.4

- Each state sequence has a different probability:

e/1 g/1

$$\pi_1 a_{1,1} a_{1,3} b_1(e) b_1(g) = 0.0021$$

e/1 g/2

$$\pi_1 a_{1,2} a_{2,3} b_1(e) b_2(g) = 0.00315$$

e/2 g/1

$$\pi_2 a_{2,1} a_{1,3} b_2(e) b_1(g) = 0.00135$$

e/2 g/2

$$\pi_2 a_{2,2} a_{2,3} b_2(e) b_2(g) = 0.0009$$

A Hidden Variable Problem

- Each state sequence has a different probability:

e/1	g/1	$\pi_1 a_{1,1} a_{1,3} b_1(e) b_1(g) = 0.0021$
e/1	g/2	$\pi_1 a_{1,2} a_{2,3} b_1(e) b_2(g) = 0.00315$
e/2	g/1	$\pi_2 a_{2,1} a_{1,3} b_2(e) b_1(g) = 0.00135$
e/2	g/2	$\pi_2 a_{2,2} a_{2,3} b_2(e) b_2(g) = 0.0009$

- Each state sequence has a different **conditional** probability,
e.g.:

$$P(1\ 1 \mid e\ g, \Theta) = \frac{0.0021}{0.0021 + 0.00315 + 0.00135 + 0.0009} = 0.28$$

e/1	g/1	$P(1\ 1 \mid e\ g, \Theta) = 0.28$
e/1	g/2	$P(1\ 2 \mid e\ g, \Theta) = 0.42$
e/2	g/1	$P(2\ 1 \mid e\ g, \Theta) = 0.18$
e/2	g/2	$P(2\ 2 \mid e\ g, \Theta) = 0.12$

fill in hidden values for (e g), (e h), (f h), (f g)

$$e/1 \quad g/1 \quad P(1 \ 1 \mid e \ g, \Theta) = 0.28$$

$$e/1 \quad g/2 \quad P(1 \ 2 \mid e \ g, \Theta) = 0.42$$

$$e/2 \quad g/1 \quad P(2 \ 1 \mid e \ g, \Theta) = 0.18$$

$$e/2 \quad g/2 \quad P(2 \ 2 \mid e \ g, \Theta) = 0.12$$

$$e/1 \quad h/1 \quad P(1 \ 1 \mid e \ h, \Theta) = 0.211$$

$$e/1 \quad h/2 \quad P(1 \ 2 \mid e \ h, \Theta) = 0.508$$

$$e/2 \quad h/1 \quad P(2 \ 1 \mid e \ h, \Theta) = 0.136$$

$$e/2 \quad h/2 \quad P(2 \ 2 \mid e \ h, \Theta) = 0.145$$

$$f/1 \quad h/1 \quad P(1 \ 1 \mid f \ h, \Theta) = 0.181$$

$$f/1 \quad h/2 \quad P(1 \ 2 \mid f \ h, \Theta) = 0.434$$

$$f/2 \quad h/1 \quad P(2 \ 1 \mid f \ h, \Theta) = 0.186$$

$$f/2 \quad h/2 \quad P(2 \ 2 \mid f \ h, \Theta) = 0.198$$

$$f/1 \quad g/1 \quad P(1 \ 1 \mid f \ g, \Theta) = 0.237$$

$$f/1 \quad g/2 \quad P(1 \ 2 \mid f \ g, \Theta) = 0.356$$

$$f/2 \quad g/1 \quad P(2 \ 1 \mid f \ g, \Theta) = 0.244$$

$$f/2 \quad g/2 \quad P(2 \ 2 \mid f \ g, \Theta) = 0.162$$

Calculate the expected counts:

$$\sum_l g(1, x_l) = 0.28 + 0.42 + 0.211 + 0.508 + 0.181 + 0.434 + 0.237 + 0.356 = 2.628$$

$$\sum_l g(2, x_l) = 1.372$$

$$\sum_l g(3, x_l) = 0.0$$

$$\sum_l g(1, 1, x_l) = 0.28 + 0.211 + 0.181 + 0.237 = 0.910$$

$$\sum_l g(1, 2, x_l) = 1.72$$

$$\sum_l g(2, 1, x_l) = 0.746$$

$$\sum_l g(2, 2, x_l) = 0.626$$

$$\sum_l g(1, 3, x_l) = 1.656$$

$$\sum_l g(2, 3, x_l) = 2.344$$

Calculate the expected counts:

$$\sum_l g(1, e, x_l) = 0.28 + 0.42 + 0.211 + 0.508 = 1.4$$

$$\sum_l g(1, f, x_l) = 1.209$$

$$\sum_l g(1, g, x_l) = 0.941$$

$$\sum_l g(1, h, x_l) = 0.827$$

$$\sum_l g(2, e, x_l) = 0.6$$

$$\sum_l g(2, f, x_l) = 0.385$$

$$\sum_l g(2, g, x_l) = 1.465$$

$$\sum_l g(2, h, x_l) = 1.173$$

Calculate the new estimates:

$$\pi_1 = \frac{\sum_l g(1, x_l)}{\sum_l g(1, x_l) + \sum_l g(2, x_l) + \sum_l g(3, x_l)} = \frac{2.628}{2.628 + 1.372 + 0} = 0.657$$

$$\pi_2 = 0.343 \quad \pi_3 = 0$$

$$a_{1,1} = \frac{\sum_l g(1, 1, x_l)}{\sum_l g(1, 1, x_l) + \sum_l g(1, 2, x_l) + \sum_l g(1, 3, x_l)} = \frac{0.91}{0.91 + 1.72 + 1.656} = 0.212$$

$a_{i,j}$	j=1	j=2	j=3
i=1	0.212	0.401	0.387
i=2	0.201	0.169	0.631

$b_i(o)$	o=e	o=f	o=g	o=h
i=1	0.320	0.276	0.215	0.189
i=2	0.166	0.106	0.404	0.324

Iterate this 3 times:

$$\pi_1 = 0.9986, \quad \pi_2 = 0.00138 \quad \pi_3 = 0$$

$a_{i,j}$	j=1	j=2	j=3
i=1	0.0054	0.9896	0.00543
i=2	0.0	0.0013627	0.9986

$b_i(o)$	o=e	o=f	o=g	o=h
i=1	0.497	0.497	0.00258	0.00272
i=2	0.001	0.000189	0.4996	0.4992

Overview

- The EM algorithm in general form
(more about the 3 coin example)
- The EM algorithm for hidden markov models (brute force)
- The EM algorithm for hidden markov models (dynamic programming)

The Forward-Backward or Baum-Welch Algorithm

- Aim is to (efficiently!) calculate the expected counts:

$$g(i, x_l) = \sum_y P(y | x_l, \Theta^{t-1}) f(i, x_l, y)$$

$$g(i, j, x_l) = \sum_y P(y | x_l, \Theta^{t-1}) f(i, j, x_l, y)$$

$$g(i, o, x_l) = \sum_y P(y | x_l, \Theta^{t-1}) f(i, o, x_l, y)$$

The Forward-Backward or Baum-Welch Algorithm

- Suppose we could calculate the following quantities, given an input sequence $o_1 \dots o_T$:

$$\alpha_i(t) = P(o_1 \dots o_{t-1}, s_t = i \mid \Theta) \quad \text{forward probabilities}$$

$$\beta_i(t) = P(o_t \dots o_T \mid s_t = i, \Theta) \quad \text{backward probabilities}$$

- The probability of being in state i at time t , is

$$p_t(i) = P(s_t = i \mid o_1 \dots o_T, \Theta)$$

$$= \frac{P(s_t = i, o_1 \dots o_T \mid \Theta)}{P(o_1 \dots o_T \mid \Theta)}$$

$$= \frac{\alpha_t(i)\beta_t(i)}{P(o_1 \dots o_T \mid \Theta)}$$

also,

$$P(o_1 \dots o_T \mid \Theta) = \sum_i \alpha_t(i)\beta_t(i) \text{ for any } t$$

Expected Initial Counts

- As before,

$g(i, o_1 \dots o_T) = \text{expected number of times state } i \text{ is state 1}$

- We can calculate this as

$$g(i, o_1 \dots o_T) = p_1(i)$$

Expected Emission Counts

- As before,

$g(i, o, o_1 \dots o_T) = \text{expected number of times state } i \text{ emits the symbol } o$

- We can calculate this as

$$g(i, o, o_1 \dots o_T) = \sum_{t: o_t = o} p_t(i)$$

The Forward-Backward or Baum-Welch Algorithm

- Suppose we could calculate the following quantities, given an input sequence $o_1 \dots o_T$:

$$\alpha_i(t) = P(o_1 \dots o_{t-1}, s_t = i \mid \Theta) \quad \text{forward probabilities}$$

$$\beta_i(t) = P(o_t \dots o_T \mid s_t = i, \Theta) \quad \text{backward probabilities}$$

- The probability of being in state i at time t , and in state j at time $t + 1$, is

$$p_t(i, j) = P(s_t = i, s_{t+1} = j \mid o_1 \dots o_T, \Theta)$$

$$= \frac{P(s_t = i, s_{t+1} = j, o_1 \dots o_T \mid \Theta)}{P(o_1 \dots o_T \mid \Theta)}$$

$$= \frac{\alpha_t(i) a_{i,j} b_i(o_t) \beta_{t+1}(j)}{P(o_1 \dots o_T \mid \Theta)}$$

also,

$$P(o_1 \dots o_T \mid \Theta) = \sum_i \alpha_t(i) \beta_t(i) \text{ for any } t$$

Expected Transition Counts

- As before,

$g(i, j, o_1 \dots o_T)$ = expected number of times state j follows state i

- We can calculate this as

$$g(i, j, o_1 \dots o_T) = \sum_t p_t(i, j)$$

Recursive Definitions for Forward Probabilities

- Given an input sequence $o_1 \dots o_T$:

$$\alpha_i(t) = P(o_1 \dots o_{t-1}, s_t = i \mid \Theta) \quad \text{forward probabilities}$$

- Base case:**

$$\alpha_i(1) = \pi_i \quad \text{for all } i$$

- Recursive case:**

$$\alpha_j(t+1) = \sum_i \alpha_i(t) a_{i,j} b_i(o_t) \quad \text{for all } j = 1 \dots N \text{ and } t = 2 \dots T$$

Recursive Definitions for Backward Probabilities

- Given an input sequence $o_1 \dots o_T$:

$$\beta_i(t) = P(o_t \dots o_T \mid s_t = i, \Theta) \quad \text{backward probabilities}$$

- Base case:**

$$\beta_i(T+1) = 1 \quad \text{for } i = N$$

$$\beta_i(T+1) = 0 \quad \text{for } i \neq N$$

- Recursive case:**

$$\beta_i(t) = \sum_j a_{i,j} b_i(o_t) \beta_j(t+1) \quad \text{for all } j = 1 \dots N \text{ and } t = 1 \dots T$$

Overview

- The EM algorithm in general form
(more about the 3 coin example)
- The EM algorithm for hidden markov models (brute force)
- The EM algorithm for hidden markov models (dynamic programming)
- Briefly: The EM algorithm for PCFGs

EM for Probabilistic Context-Free Grammars

- A PCFG defines a distribution $P(S, T \mid \Theta)$ over tree/sentence pairs (S, T)
- If we had tree/sentence pairs (**fully observed data**) then

$$L(\Theta) = \sum_i \log P(S_i, T_i \mid \Theta)$$

- Say we have sentences only, $S_1 \dots S_n$
⇒ trees are hidden variables

$$L(\Theta) = \sum_i \log \sum_T P(S_i, T \mid \Theta)$$

EM for Probabilistic Context-Free Grammars

- Say we have sentences only, $S_1 \dots S_n$
⇒ trees are hidden variables

$$L(\Theta) = \sum_i \log \sum_T P(S_i, T \mid \Theta)$$

- EM algorithm is then $\Theta^t = \text{argmax}_\Theta Q(\Theta, \Theta^{t-1})$, where

$$Q(\Theta, \Theta^{t-1}) = \sum_i \sum_T P(T \mid S_i, \Theta^{t-1}) \log P(S_i, T \mid \Theta)$$

- Remember:

$$\log P(S_i, T \mid \Theta) = \sum_{r \in R} Count(S_i, T, r) \log \Theta_r$$

where $Count(S, T, r)$ is the number of times rule r is seen in the sentence/tree pair (S, T)

$$\begin{aligned}\Rightarrow Q(\Theta, \Theta^{t-1}) &= \sum_i \sum_T P(T \mid S_i, \Theta^{t-1}) \log P(S_i, T \mid \Theta) \\ &= \sum_i \sum_T P(T \mid S_i, \Theta^{t-1}) \sum_{r \in R} Count(S_i, T, r) \log \Theta_r \\ &= \sum_i \sum_{r \in R} Count(S_i, r) \log \Theta_r\end{aligned}$$

where $Count(S_i, r) = \sum_T P(T \mid S_i, \Theta^{t-1}) Count(S_i, T, r)$
the expected counts

- Solving $\Theta_{ML} = \operatorname{argmax}_{\Theta \in \Omega} L(\Theta)$ gives

$$\Theta_{\alpha \rightarrow \beta} = \frac{\sum_i Count(S_i, \alpha \rightarrow \beta)}{\sum_i \sum_{s \in R(\alpha)} Count(S_i, s)}$$

- There are efficient algorithms for calculating

$$Count(S_i, r) = \sum_T P(T \mid S_i, \Theta^{t-1}) Count(S_i, T, r)$$

for a PCFG. See (Baker 1979), called “The Inside Outside Algorithm”. See also Manning and Schuetze section 11.3.4.