HMM: Parameter Estimation

Yuzhen Ye
School of Informatics and Computing
Indiana University, Bloomington
Spring 2013

Content

- Review
  - HMM: three problems
  - The forward & backward algorithms; will be used again for the training of HMM
- When the training sequences are annotated (with known states)—MLE estimations
- When the states are unknown—Baum Welch training
  - An EM algorithm
  - E step—calculate $A_{kl}$ and $E_{k}(b)$
  - M step

Parameters defining a HMM

HMM consists of:
A Markov chain over a set of (hidden) states, and for each state $s$ and observable symbol $x$, an emission probability $p(X_i=x|S_i=s)$.

An HMM model is defined by the parameters: $a_{kl}$ (transition probabilities) and $e_k(b)$ (emission probabilities), for all states $k,l$ and all symbols $b$.

Let $\theta$ denote the collection of these parameters.

Data for HMM learning

To determine the values of (the parameters in) $\theta$, use a training set $\{x^1, x^2, \ldots, x^n\}$, where each $x^i$ is a sequence that is assumed to fit the model.

Given the parameters $\theta$, each sequence $x^i$ has an assigned probability $p(x^i|\theta)$.

Maximum likelihood parameter estimation for HMM

The elements of the training set $\{x^1, x^2, \ldots, x^n\}$, are assumed to be independent,

$$p(x^1, \ldots, x^n|\theta) = \prod_i p(x^i|\theta).$$

ML parameter estimation looks for $\theta$ which maximizes the above.

The exact method for finding or approximating this $\theta$ depends on the nature of the training set used.
Case 1: State paths are fully known

The training set \( \{x_1, \ldots, x_n\} \)

By the ML method, we look for parameters \( \theta^* (a_{kl} \text{ and } e_k(b)) \) which maximize the probability of the sample set:

\[
p(x_1, \ldots, x_n | \theta^*) = \text{MAX}_{\theta} p(x_1, \ldots, x_n | \theta).
\]

For a sequence \( x_j \):

\[
p(x_j | \theta) = a_{kl}^{m_{kl}(k, l)} \prod e_k^{m_k(b)}
\]

\( m_{kl} \) = # transitions from \( k \) to \( l \) in sequence \( x_j \).

\( m_k(b) \) = # emissions of symbol \( b \) from state \( k \) in sequence \( x_j \).

For the entire training set:

\[
A_{kl} = \text{# transitions from } k \text{ to } l \text{ in the training set}.
\]

\( E_k(b) = \text{# emissions of symbol } b \text{ from state } k \) in the training set.

We need to maximize:

\[
\prod_{i=1}^{L} a_{kl}^{A_{kl}(k, l)} \prod e_k^{E_k(b)}
\]

Subject to: for all states \( k \), \( \sum a_{ij} = 1 \), and \( \sum e_k(b) = 1, a_{ij}, e_k(b) \geq 0. \)

MLE for \( n \) outcomes

The MLE is given by the relative frequencies:

\[
\hat{\theta}_i = \frac{n_i}{n}, \quad i = 1, \ldots, k
\]

MLE applied to HMM

We apply the previous technique to get for each \( k \) the parameters \( \{a_{ij}|l=1, \ldots, m\} \text{ and } \{e_k(b)|b\in\Sigma\} \):

\[
a_{ij} = \frac{A_{ij}}{\sum A_{ij}}, \text{ and } e_k(b) = \frac{E_k(b)}{\sum E_k(b)}
\]

Which gives the optimal ML parameters

Adding pseudo counts in HMM

If the sample set is too small, we may get a biased result. In this case we modify the actual count by our prior knowledge/belief:

\( r_{ij} \) is our prior belief and transitions from \( k \) to \( l \).

\( r_k(b) \) is our prior belief on emissions of \( b \) from state \( k \).

\[
a_{ij} = \frac{A_{ij} + r_{ij}}{(A_{ij} + r_{ij})}, \text{ and } e_k(b) = \frac{E_k(b) + r_k(b)}{(E_k(b) + r_k(b))}
\]

Fair casino problem: the sequences are annotated

- Consider the fair casino, where the dealer may use two coins (First and Second).
- HMM: the hidden states are \( \{F(\text{fair}), B(\text{biased})\} \), observation symbols are \( \{H(\text{head}), T(\text{tail})\} \). We want to approximate the HMM parameters, the initial probabilities \( a_0F \) and \( a_0B \), the transition probabilities \( a_{FF}, a_{FB}, a_{BF}, \text{ and } a_{BB} \), the emission probabilities \( e_F(T), e_F(H), e_B(T) \) and \( e_B(H) \).
- When the training set contains annotated sequences, we can simply compute the frequency for each of these cases to estimate the corresponding probabilities, which proved to be the Maximum Likelihood model parameters.
The general process for finding Welch training

For the specific case of HMM, it is the maximization algorithm, which we will meet later.

However, when the states are unknown, the “counting” process is a little trickier; instead, we use averaging. When the states are known, we can simply count.

The sum taken over all hidden state paths $s$!

Finding $\theta^*$ which maximizes $\sum_s p(x,s|\theta)$ is hard.

ML Parameter Estimation for HMM

The general process for finding $\theta$ in this case is
1. Start with an initial value of $\theta$.
2. Find $\theta'$ so that $p(x|\theta') > p(x|\theta)$
3. set $\theta = \theta'$. 
4. Repeat until some convergence criterion is met.

A general algorithm of this type is the Expectation Maximization algorithm, which we will meet later. For the specific case of HMM, it is the Baum-Welch training.

When the states are known, we can simply count. However, when the states are unknown, the “counting” process is a little trickier; instead, we use averaging process.

For each edge $s_i \rightarrow s$, we compute the average number of “$k$ to $l$” transitions, for all possible pairs $(k,l)$, over this edge. Then, for each $k$ and $l$, we take $A_{kl}$ to be the sum over all edges.

Case 2: State paths are unknown

For a given $\theta$ we have:
$p(x^1, ..., x^n|\theta) = p(x^1|\theta) \cdots p(x^n|\theta)$

(since the $x^i$ are independent)

For each sequence $x$: $p(x|\theta) = \sum_s p(x,s|\theta)$

We start with some values of $a_{kl}$ and $e_{kl}(b)$, which define prior values of $\theta$.

Then we use an iterative algorithm which attempts to replace $\theta$ by a $\theta^*$ s.t.
$p(x|\theta^*) > p(x|\theta)$

This is done by “imitating” the algorithm for Case 1, where all states are known:

Computing $P(s_{L-1} = k, s_L = l | x, \theta)$

$$P(x_1, ..., x_L, s_{L-1} = k, s_L = l | \theta) = \frac{a_{kl} \cdot e_{kl}(b) \cdot \prod_{i=1}^{L-1} P(x_i, x_{i+1} | \theta)}{p(x|\theta)}$$

Fair casino problem: learning

<table>
<thead>
<tr>
<th>Seq1</th>
<th>Seq2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Obs: THHTHHHTHH</td>
<td>Obs: THHTHHHTHH</td>
</tr>
<tr>
<td>Hid: FFFFFFFFFBFFFF</td>
<td>Hid: FFFFFFFFFBFFFF</td>
</tr>
</tbody>
</table>

MLE

$a_{tt} = \#(T,T)/\#T = 10/12 = 0.83; a_{tb} = \#(T,B)/\#(T) = 2/12 = 0.17$

$a_{bt} = \#(B,T)/\#B = 1/10 = 0.10; a_{tt} = \#(T,T)/\#(T) = 9/10 = 0.9$

Fx means the di-hidden states with $F$ as the first state.

$a_{0T}(T) = \#(T,F)/\#(F) = 7/13 = 0.53; a_{0H}(H) = \#(H,F)/\#(F) = 6/13 = 0.47$

$a_{0B}(T) = \#(T,B)/\#(B) = 2/11 = 0.18; a_{0H}(H) = \#(H,B)/\#(B) = 9/11 = 0.82$
Compute $A_{kl}$ for one sequence

For each pair $(k,l)$, compute the expected number of state transitions from $k$ to $l$ as the sum of the expected number of $k$ to $l$ transitions over all $L$ edges:

$$A_{kl} = \frac{1}{\rho(x|\theta)} \sum_{j=1}^{L} p(s_{j-1} = k, s_{j} = l, x_j | \theta)$$

$$A_{kl} = \frac{1}{\rho(x|\theta)} \sum_{j=1}^{L} f_j^l (x_j - 1) a_{kl} e_j^l (x_j) b_j^l (x_j)$$

Compute expected number of symbol emissions

for state $k$ and each symbol $b$, for each $i$, compute the expected number of times that $X_i = b, E_i^b(k)$

One edge

$p(s_i = k) \mid x_1, \ldots, x_i = \frac{p(x_i \ldots x_n, s_i = k)}{p(x_i \ldots x_n)}$

One sequence

$E_i^b(k) = \frac{1}{\rho(x_i^l | \theta)} \sum_{j=1}^{L} f_j^l (x_j - 1) a_{kl} e_j^l (x_j) b_j^l (x_j)$

Summary of the E step

Task: compute the expected numbers $A_{kl}$ of $k,l$ transitions for all pairs of states $k$ and $l$, and the expected numbers $E_i^b(k)$ of transitions of symbol $b$ from state $k$, for all states $k$ and symbols $b$.

The next step is the M step, which is identical to the computation of optimal ML parameters when all states are known.

Baum Welch: M step

Use the $A_{ij}$'s, $E_i^b(k)$'s to compute the new values of $a_{ij}$ and $e_i^b$. These values define $\theta'$.

$$a_{ij} = \frac{A_{ij}}{\sum_{i} A_{ij}}$$  ,  and  $$e_i^b = \frac{E_i^b}{\sum_{i} E_i}$$

The correctness of the EM algorithm implies that:

$p(x_i^l \ldots x_n | \theta') \geq p(x_i^l \ldots x_n | \theta)$

i.e, $\theta'$ increases the probability of the data

This procedure is iterated, until some convergence criterion is met. Be aware of the local maximum (minimum) problem!