

6.864: Lecture 5 (September 22nd, 2005)

The EM Algorithm

Overview

- The EM algorithm in general form
- The EM algorithm for hidden markov models (brute force)
- The EM algorithm for hidden markov models (dynamic programming)

An Experiment/Some Intuition

- I have three coins in my pocket,

Coin 0 has probability λ of heads;

Coin 1 has probability p_1 of heads;

Coin 2 has probability p_2 of heads

- For each trial I do the following:

First I toss Coin 0

If Coin 0 turns up **heads**, I toss **coin 1** three times

If Coin 0 turns up **tails**, I toss **coin 2** three times

I don't tell you whether Coin 0 came up heads or tails,
or whether Coin 1 or 2 was tossed three times,

but I do tell you how many heads/tails are seen at each trial

- you see the following sequence:

$\langle HHH \rangle, \langle TTT \rangle, \langle HHH \rangle, \langle TTT \rangle, \langle HHH \rangle$

What would you estimate as the values for λ , p_1 and p_2 ?

Maximum Likelihood Estimation

- We have data points x_1, x_2, \dots, x_n drawn from some (finite or countable) set \mathcal{X}
- We have a parameter vector Θ
- We have a parameter space Ω
- We have a distribution $P(x | \Theta)$ for any $\Theta \in \Omega$, such that

$$\sum_{x \in \mathcal{X}} P(x | \Theta) = 1 \text{ and } P(x | \Theta) \geq 0 \text{ for all } x$$

- We assume that our data points x_1, x_2, \dots, x_n are drawn at random (independently, identically distributed) from a distribution $P(x | \Theta^*)$ for some $\Theta^* \in \Omega$

Log-Likelihood

- We have data points x_1, x_2, \dots, x_n drawn from some (finite or countable) set \mathcal{X}
- We have a parameter vector Θ , and a parameter space Ω
- We have a distribution $P(x \mid \Theta)$ for any $\Theta \in \Omega$

- The likelihood is

$$Likelihood(\Theta) = P(x_1, x_2, \dots, x_n \mid \Theta) = \prod_{i=1}^n P(x_i \mid \Theta)$$

- The log-likelihood is

$$L(\Theta) = \log Likelihood(\Theta) = \sum_{i=1}^n \log P(x_i \mid \Theta)$$

A First Example: Coin Tossing

- $\mathcal{X} = \{\text{H}, \text{T}\}$. Our data points x_1, x_2, \dots, x_n are a sequence of heads and tails, e.g.

HHTTHHHTHH

- Parameter vector Θ is a single parameter, i.e., the probability of coin coming up heads
- Parameter space $\Omega = [0, 1]$
- Distribution $P(x \mid \Theta)$ is defined as

$$P(x \mid \Theta) = \begin{cases} \Theta & \text{If } x = \text{H} \\ 1 - \Theta & \text{If } x = \text{T} \end{cases}$$

Maximum Likelihood Estimation

- Given a sample x_1, x_2, \dots, x_n , choose

$$\Theta_{ML} = \operatorname{argmax}_{\Theta \in \Omega} L(\Theta) = \operatorname{argmax}_{\Theta \in \Omega} \sum_i \log P(x_i | \Theta)$$

- For example, take the coin example:

say $x_1 \dots x_n$ has $Count(H)$ heads, and $(n - Count(H))$ tails

\Rightarrow

$$\begin{aligned} L(\Theta) &= \log \left(\Theta^{Count(H)} \times (1 - \Theta)^{n - Count(H)} \right) \\ &= Count(H) \log \Theta + (n - Count(H)) \log(1 - \Theta) \end{aligned}$$

- We now have

$$\Theta_{ML} = \frac{Count(H)}{n}$$

A Second Example: Probabilistic Context-Free Grammars

- \mathcal{X} is the set of all parse trees generated by the underlying context-free grammar. Our sample is n trees $T_1 \dots T_n$ such that each $T_i \in \mathcal{X}$.
- R is the set of rules in the context free grammar
 N is the set of non-terminals in the grammar
- Θ_r for $r \in R$ is the parameter for rule r
- Let $R(\alpha) \subset R$ be the rules of the form $\alpha \rightarrow \beta$ for some β
- The parameter space Ω is the set of $\Theta \in [0, 1]^{|R|}$ such that

$$\text{for all } \alpha \in N \quad \sum_{r \in R(\alpha)} \Theta_r = 1$$

- We have

$$P(T \mid \Theta) = \prod_{r \in R} \Theta_r^{\text{Count}(T, r)}$$

where $\text{Count}(T, r)$ is the number of times rule r is seen in the tree T

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

Maximum Likelihood Estimation for PCFGs

- We have

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

where $\text{Count}(T, r)$ is the number of times rule r is seen in the tree T

- And,

$$L(\Theta) = \sum_i \log P(T_i \mid \Theta) = \sum_i \sum_{r \in R} \text{Count}(T_i, r) \log \Theta_r$$

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

$$\Theta_r = \frac{\sum_i \text{Count}(T_i, r)}{\sum_i \sum_{s \in R(\alpha)} \text{Count}(T_i, s)}$$

where r is of the form $\alpha \rightarrow \beta$ for some β

Multinomial Distributions

- \mathcal{X} is a finite set, e.g., $\mathcal{X} = \{\text{dog, cat, the, saw}\}$
- Our sample x_1, x_2, \dots, x_n is drawn from \mathcal{X}
e.g., $x_1, x_2, x_3 = \text{dog, the, saw}$
- The parameter Θ is a vector in \mathbb{R}^m where $m = |\mathcal{X}|$
e.g., $\Theta_1 = P(\text{dog}), \Theta_2 = P(\text{cat}), \Theta_3 = P(\text{the}), \Theta_4 = P(\text{saw})$
- The parameter space is

$$\Omega = \left\{ \Theta : \sum_{i=1}^m \Theta_i = 1 \text{ and } \forall i, \Theta_i \geq 0 \right\}$$

- If our sample is $x_1, x_2, x_3 = \text{dog, the, saw}$, then

$$L(\Theta) = \log P(x_1, x_2, x_3 = \text{dog, the, saw}) = \log \Theta_1 + \log \Theta_3 + \log \Theta_4$$

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

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

- The **EM (Expectation Maximization) algorithm** is a method for finding

$$\Theta_{ML} = \operatorname{argmax}_{\Theta} \sum_i \log \sum_{y \in \mathcal{Y}} P(x_i, y \mid \Theta)$$

The Three Coins Example

- e.g., in the three coins example:

$$\mathcal{Y} = \{H, T\}$$

$$\mathcal{X} = \{HHH, TTT, HTT, THH, HHT, TTH, HTH, THT\}$$

$$\Theta = \{\lambda, p_1, p_2\}$$

- and

$$P(x, y | \Theta) = P(y | \Theta)P(x | y, \Theta)$$

where

$$P(y | \Theta) = \begin{cases} \lambda & \text{If } y = H \\ 1 - \lambda & \text{If } y = T \end{cases}$$

and

$$P(x | y, \Theta) = \begin{cases} p_1^h (1 - p_1)^t & \text{If } y = H \\ p_2^h (1 - p_2)^t & \text{If } y = T \end{cases}$$

where h = number of heads in x , t = number of tails in x

The Three Coins Example

- Various probabilities can be calculated, for example:

$$P(x = \text{THT}, y = \text{H} \mid \Theta) = \lambda p_1 (1 - p_1)^2$$

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$$P(x = \text{THT}, y = \text{H} \mid \Theta) = \lambda p_1 (1 - p_1)^2$$

$$P(x = \text{THT}, y = \text{T} \mid \Theta) = (1 - \lambda) p_2 (1 - p_2)^2$$

$$\begin{aligned} P(x = \text{THT} \mid \Theta) &= P(x = \text{THT}, y = \text{H} \mid \Theta) \\ &\quad + P(x = \text{THT}, y = \text{T} \mid \Theta) \\ &= \lambda p_1 (1 - p_1)^2 + (1 - \lambda) p_2 (1 - p_2)^2 \end{aligned}$$

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- Various probabilities can be calculated, for example:

$$P(x = \text{THT}, y = \text{H} \mid \Theta) = \lambda p_1 (1 - p_1)^2$$

$$P(x = \text{THT}, y = \text{T} \mid \Theta) = (1 - \lambda) p_2 (1 - p_2)^2$$

$$\begin{aligned} P(x = \text{THT} \mid \Theta) &= P(x = \text{THT}, y = \text{H} \mid \Theta) \\ &\quad + P(x = \text{THT}, y = \text{T} \mid \Theta) \\ &= \lambda p_1 (1 - p_1)^2 + (1 - \lambda) p_2 (1 - p_2)^2 \end{aligned}$$

$$\begin{aligned} P(y = \text{H} \mid x = \text{THT}, \Theta) &= \frac{P(x = \text{THT}, y = \text{H} \mid \Theta)}{P(x = \text{THT} \mid \Theta)} \\ &= \frac{\lambda p_1 (1 - p_1)^2}{\lambda p_1 (1 - p_1)^2 + (1 - \lambda) p_2 (1 - p_2)^2} \end{aligned}$$

The Three Coins Example

- Fully observed data might look like:

$(\langle HHH \rangle, H), (\langle TTT \rangle, T), (\langle HHH \rangle, H), (\langle TTT \rangle, T), (\langle HHH \rangle, H)$

- In this case maximum likelihood estimates are:

$$\lambda = \frac{3}{5}$$

$$p_1 = \frac{9}{9}$$

$$p_2 = \frac{0}{6}$$

The Three Coins Example

- Partially observed data might look like:

$\langle HHH \rangle, \langle TTT \rangle, \langle HHH \rangle, \langle TTT \rangle, \langle HHH \rangle$

- How do we find the maximum likelihood parameters?

The Three Coins Example

- Partially observed data might look like:

$$\langle HHH \rangle, \langle TTT \rangle, \langle HHH \rangle, \langle TTT \rangle, \langle HHH \rangle$$

- If current parameters are λ, p_1, p_2

$$\begin{aligned} P(y = H \mid x = \langle HHH \rangle) &= \frac{P(\langle HHH \rangle, H)}{P(\langle HHH \rangle, H) + P(\langle HHH \rangle, T)} \\ &= \frac{\lambda p_1^3}{\lambda p_1^3 + (1 - \lambda) p_2^3} \end{aligned}$$

$$\begin{aligned} P(y = H \mid x = \langle TTT \rangle) &= \frac{P(\langle TTT \rangle, H)}{P(\langle TTT \rangle, H) + P(\langle TTT \rangle, T)} \\ &= \frac{\lambda(1 - p_1)^3}{\lambda(1 - p_1)^3 + (1 - \lambda)(1 - p_2)^3} \end{aligned}$$

The Three Coins Example

- If current parameters are λ, p_1, p_2

$$P(y = \text{H} \mid x = \langle \text{HHH} \rangle) = \frac{\lambda p_1^3}{\lambda p_1^3 + (1 - \lambda) p_2^3}$$

$$P(y = \text{H} \mid x = \langle \text{TTT} \rangle) = \frac{\lambda(1 - p_1)^3}{\lambda(1 - p_1)^3 + (1 - \lambda)(1 - p_2)^3}$$

- If $\lambda = 0.3, p_1 = 0.3, p_2 = 0.6$:

$$P(y = \text{H} \mid x = \langle \text{HHH} \rangle) = 0.0508$$

$$P(y = \text{H} \mid x = \langle \text{TTT} \rangle) = 0.6967$$

The Three Coins Example

- After filling in hidden variables for each example, partially observed data might look like:

$$(\langle \text{HHH} \rangle, H) \quad P(y = \text{H} \mid \text{HHH}) = 0.0508$$

$$(\langle \text{HHH} \rangle, T) \quad P(y = \text{T} \mid \text{HHH}) = 0.9492$$

$$(\langle \text{TTT} \rangle, H) \quad P(y = \text{H} \mid \text{TTT}) = 0.6967$$

$$(\langle \text{TTT} \rangle, T) \quad P(y = \text{T} \mid \text{TTT}) = 0.3033$$

$$(\langle \text{HHH} \rangle, H) \quad P(y = \text{H} \mid \text{HHH}) = 0.0508$$

$$(\langle \text{HHH} \rangle, T) \quad P(y = \text{T} \mid \text{HHH}) = 0.9492$$

$$(\langle \text{TTT} \rangle, H) \quad P(y = \text{H} \mid \text{TTT}) = 0.6967$$

$$(\langle \text{TTT} \rangle, T) \quad P(y = \text{T} \mid \text{TTT}) = 0.3033$$

$$(\langle \text{HHH} \rangle, H) \quad P(y = \text{H} \mid \text{HHH}) = 0.0508$$

$$(\langle \text{HHH} \rangle, T) \quad P(y = \text{T} \mid \text{HHH}) = 0.9492$$

The Three Coins Example

- New Estimates:

$$(\langle \text{HHH} \rangle, H) \quad P(y = H \mid \text{HHH}) = 0.0508$$

$$(\langle \text{HHH} \rangle, T) \quad P(y = T \mid \text{HHH}) = 0.9492$$

$$(\langle \text{TTT} \rangle, H) \quad P(y = H \mid \text{TTT}) = 0.6967$$

$$(\langle \text{TTT} \rangle, T) \quad P(y = T \mid \text{TTT}) = 0.3033$$

...

$$\lambda = \frac{3 \times 0.0508 + 2 \times 0.6967}{5} = 0.3092$$

$$p_1 = \frac{3 \times 3 \times 0.0508 + 0 \times 2 \times 0.6967}{3 \times 3 \times 0.0508 + 3 \times 2 \times 0.6967} = 0.0987$$

$$p_2 = \frac{3 \times 3 \times 0.9492 + 0 \times 2 \times 0.3033}{3 \times 3 \times 0.9492 + 3 \times 2 \times 0.3033} = 0.8244$$

The Three Coins Example: Summary

- Begin with parameters $\lambda = 0.3, p_1 = 0.3, p_2 = 0.6$
- Fill in hidden variables, using

$$P(y = \text{H} \mid x = \langle \text{HHH} \rangle) = 0.0508$$

$$P(y = \text{H} \mid x = \langle \text{TTT} \rangle) = 0.6967$$

- Re-estimate parameters to be $\lambda = 0.3092, p_1 = 0.0987, p_2 = 0.8244$

Iteration	λ	p_1	p_2	\tilde{p}_1	\tilde{p}_2	\tilde{p}_3	\tilde{p}_4
0	0.3000	0.3000	0.6000	0.0508	0.6967	0.0508	0.6967
1	0.3738	0.0680	0.7578	0.0004	0.9714	0.0004	0.9714
2	0.4859	0.0004	0.9722	0.0000	1.0000	0.0000	1.0000
3	0.5000	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000

The coin example for $\mathbf{y} = \{\langle HHH \rangle, \langle TTT \rangle, \langle HHH \rangle, \langle TTT \rangle\}$. The solution that EM reaches is intuitively correct: the coin-tosser has two coins, one which always shows up heads, the other which always shows tails, and is picking between them with equal probability ($\lambda = 0.5$). The posterior probabilities \tilde{p}_i show that we are certain that coin 1 (tail-biased) generated y_2 and y_4 , whereas coin 2 generated y_1 and y_3 .

Iteration	λ	p_1	p_2	\tilde{p}_1	\tilde{p}_2	\tilde{p}_3	\tilde{p}_4	\tilde{p}_5
0	0.3000	0.3000	0.6000	0.0508	0.6967	0.0508	0.6967	0.0508
1	0.3092	0.0987	0.8244	0.0008	0.9837	0.0008	0.9837	0.0008
2	0.3940	0.0012	0.9893	0.0000	1.0000	0.0000	1.0000	0.0000
3	0.4000	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000

The coin example for $\{\langle HHH \rangle, \langle TTT \rangle, \langle HHH \rangle, \langle TTT \rangle, \langle HHH \rangle\}$. λ is now 0.4, indicating that the coin-tosser has probability 0.4 of selecting the tail-biased coin.

Iteration	λ	p_1	p_2	\tilde{p}_1	\tilde{p}_2	\tilde{p}_3	\tilde{p}_4
0	0.3000	0.3000	0.6000	0.1579	0.6967	0.0508	0.6967
1	0.4005	0.0974	0.6300	0.0375	0.9065	0.0025	0.9065
2	0.4632	0.0148	0.7635	0.0014	0.9842	0.0000	0.9842
3	0.4924	0.0005	0.8205	0.0000	0.9941	0.0000	0.9941
4	0.4970	0.0000	0.8284	0.0000	0.9949	0.0000	0.9949

The coin example for $\mathbf{y} = \{\langle HHT \rangle, \langle TTT \rangle, \langle HHH \rangle, \langle TTT \rangle\}$. EM selects a tails-only coin, and a coin which is heavily heads-biased ($p_2 = 0.8284$). It's certain that y_1 and y_3 were generated by coin 2, as they contain heads. y_2 and y_4 could have been generated by either coin, but coin 1 is far more likely.

Iteration	λ	p_1	p_2	\tilde{p}_1	\tilde{p}_2	\tilde{p}_3	\tilde{p}_4
0	0.3000	0.7000	0.7000	0.3000	0.3000	0.3000	0.3000
1	0.3000	0.5000	0.5000	0.3000	0.3000	0.3000	0.3000
2	0.3000	0.5000	0.5000	0.3000	0.3000	0.3000	0.3000
3	0.3000	0.5000	0.5000	0.3000	0.3000	0.3000	0.3000
4	0.3000	0.5000	0.5000	0.3000	0.3000	0.3000	0.3000
5	0.3000	0.5000	0.5000	0.3000	0.3000	0.3000	0.3000
6	0.3000	0.5000	0.5000	0.3000	0.3000	0.3000	0.3000

The coin example for $\mathbf{y} = \{\langle HHH \rangle, \langle TTT \rangle, \langle HHH \rangle, \langle TTT \rangle\}$, with p_1 and p_2 initialised to the same value. EM is stuck at a saddle point

Iteration	λ	p_1	p_2	\tilde{p}_1	\tilde{p}_2	\tilde{p}_3	\tilde{p}_4
0	0.3000	0.7001	0.7000	0.3001	0.2998	0.3001	0.2998
1	0.2999	0.5003	0.4999	0.3004	0.2995	0.3004	0.2995
2	0.2999	0.5008	0.4997	0.3013	0.2986	0.3013	0.2986
3	0.2999	0.5023	0.4990	0.3040	0.2959	0.3040	0.2959
4	0.3000	0.5068	0.4971	0.3122	0.2879	0.3122	0.2879
5	0.3000	0.5202	0.4913	0.3373	0.2645	0.3373	0.2645
6	0.3009	0.5605	0.4740	0.4157	0.2007	0.4157	0.2007
7	0.3082	0.6744	0.4223	0.6447	0.0739	0.6447	0.0739
8	0.3593	0.8972	0.2773	0.9500	0.0016	0.9500	0.0016
9	0.4758	0.9983	0.0477	0.9999	0.0000	0.9999	0.0000
10	0.4999	1.0000	0.0001	1.0000	0.0000	1.0000	0.0000
11	0.5000	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000

The coin example for $\mathbf{y} = \{\langle HHH \rangle, \langle TTT \rangle, \langle HHH \rangle, \langle TTT \rangle\}$. If we initialise p_1 and p_2 to be a small amount away from the saddle point $p_1 = p_2$, the algorithm diverges from the saddle point and eventually reaches the global maximum.

Iteration	λ	p_1	p_2	\tilde{p}_1	\tilde{p}_2	\tilde{p}_3	\tilde{p}_4
0	0.3000	0.6999	0.7000	0.2999	0.3002	0.2999	0.3002
1	0.3001	0.4998	0.5001	0.2996	0.3005	0.2996	0.3005
2	0.3001	0.4993	0.5003	0.2987	0.3014	0.2987	0.3014
3	0.3001	0.4978	0.5010	0.2960	0.3041	0.2960	0.3041
4	0.3001	0.4933	0.5029	0.2880	0.3123	0.2880	0.3123
5	0.3002	0.4798	0.5087	0.2646	0.3374	0.2646	0.3374
6	0.3010	0.4396	0.5260	0.2008	0.4158	0.2008	0.4158
7	0.3083	0.3257	0.5777	0.0739	0.6448	0.0739	0.6448
8	0.3594	0.1029	0.7228	0.0016	0.9500	0.0016	0.9500
9	0.4758	0.0017	0.9523	0.0000	0.9999	0.0000	0.9999
10	0.4999	0.0000	0.9999	0.0000	1.0000	0.0000	1.0000
11	0.5000	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000

The coin example for $y = \{\langle HHH \rangle, \langle TTT \rangle, \langle HHH \rangle, \langle TTT \rangle\}$. If we initialise p_1 and p_2 to be a small amount away from the saddle point $p_1 = p_2$, the algorithm diverges from the saddle point and eventually reaches the global maximum.

The EM Algorithm

- Θ^t is the parameter vector at t 'th iteration
- Choose Θ^0 (at random, or using various heuristics)
- Iterative procedure is defined as

$$\Theta^t = \operatorname{argmax}_{\Theta} Q(\Theta, \Theta^{t-1})$$

where

$$Q(\Theta, \Theta^{t-1}) = \sum_i \sum_{y \in \mathcal{Y}} P(y | x_i, \Theta^{t-1}) \log P(x_i, y | \Theta)$$

The EM Algorithm

- Iterative procedure is defined as $\Theta^t = \operatorname{argmax}_{\Theta} Q(\Theta, \Theta^{t-1})$, where

$$Q(\Theta, \Theta^{t-1}) = \sum_i \sum_{y \in \mathcal{Y}} P(y | x_i, \Theta^{t-1}) \log P(x_i, y | \Theta)$$

- Key points:

- Intuition: fill in hidden variables y according to $P(y | x_i, \Theta)$
- EM is guaranteed to converge to a local maximum, or saddle-point, of the likelihood function
- In general, if

$$\operatorname{argmax}_{\Theta} \sum_i \log P(x_i, y_i | \Theta)$$

has a simple (analytic) solution, then

$$\operatorname{argmax}_{\Theta} \sum_i \sum_y P(y | x_i, \Theta) \log P(x_i, y | \Theta)$$

also has a simple (analytic) solution.

Overview

- The EM algorithm in general form
- The EM algorithm for hidden markov models (brute force)
- The EM algorithm for hidden markov models (dynamic programming)

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 $K = \{the, dog\}$.
- 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 $b_{s_t}(o_t)$
 - 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**
- A **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:

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

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 $P(x, y \mid \Theta)$
- In Hidden Markov Models:
 - each $x \in \mathcal{X}$ is an output sequence $o_1 \dots o_T$
 - each $y \in \mathcal{Y}$ is a 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
for parameters $a_{i,j}$:	i=1	0	1	0
	i=2	0	0	1

		o=e	o=f	o=g	o=h
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 $l = 1 \dots m$,

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

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

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

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

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

- 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
i=1	0.2	0.3	0.5
i=2	0.3	0.2	0.5

$b_i(o)$	o=e	o=f	o=g	o=h
i=1	0.2	0.25	0.3	0.25
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
- 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

$$\begin{aligned} p_t(i) &= P(s_t = i \mid o_1 \dots o_T, \Theta) \\ &= \frac{P(s_t = i, o_1 \dots o_T \mid \Theta)}{P(o_1 \dots o_T \mid \Theta)} \\ &= \frac{\alpha_t(i)\beta_t(i)}{P(o_1 \dots o_T \mid \Theta)} \end{aligned}$$

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,

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

- We can calculate this as

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

Expected Emission Counts

- As before,

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

$$\begin{aligned} p_t(i, j) &= P(s_t = i, s_{t+1} = j \mid o_1 \dots o_T, \Theta) \\ &= \frac{P(s_t = i, s_{t+1} = j, o_1 \dots o_T \mid \Theta)}{P(o_1 \dots o_T \mid \Theta)} \\ &= \frac{\alpha_t(i) a_{i,j} b_i(o_t) \beta_{t+1}(j)}{P(o_1 \dots o_T \mid \Theta)} \end{aligned}$$

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:**

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

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, $S_1 \dots S_n$
 \Rightarrow 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 $\Theta^t = \operatorname{argmax}_{\Theta} Q(\Theta, \Theta^{t-1})$, 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:

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

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

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

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

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

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

- There are efficient algorithms for calculating

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

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