Hidden Markov Models II

Machine Learning 10-601B

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Many of these slides are derived from Tom Mitchell, Ziv Bar-Joseph. Thanks!

Learning HMMs

- Until now we assumed that the emission and transition probabilities are known
- This is usually not the case

  - How is “AI” pronounced by different individuals?

  - What is the probability of hearing “class” after “AI”?

Learning HMM When Hidden States are Observed

- Assume both hidden and observed states are observed
  - Data: $((O^1,Q^1), \ldots, (O^K,Q^K))$ for K sequences, where $O^k = (o_1^k,\ldots,o_T^k)$ $Q^k=(q_1^k,\ldots,q_T^k)$

- MLE for learning!

$$\arg\max \ \log p((O^1,Q^1),\ldots,(O^K,Q^K))$$

$$\arg\max \ \log \prod_k p(q_1^{\ k}) p(o_1^{\ k} \mid q_1^{\ k}) \prod_{t=2}^{T} p(q_t^{\ k} \mid q_{t-1}^{\ k}) p(o_t^{\ k} \mid q_t^{\ k})$$

Learning HMM When Hidden States are Observed

- MLE for HMM

$$\log p((O^1,Q^1),\ldots,(O^K,Q^K))$$

$$= \log \prod_k p(q_1^{\ k}) p(o_1^{\ k} \mid q_1^{\ k}) \prod_{t=2}^{T} p(q_t^{\ k} \mid q_{t-1}^{\ k}) p(o_t^{\ k} \mid q_t^{\ k})$$

$$= \sum_k \log p(q_1^{\ k}) + \sum_k \log\ p(o_1^{\ k} \mid q_1^{\ k}) + \sum_k \sum_t \log\ p(o_t^{\ k} \mid q_t^{\ k}) + \sum_k \sum_t \log\ p(q_t^{\ k} \mid q_{t-1}^{\ k})$$

Involves only initial probabilities

Involves only emission probabilities

Involves only transition probabilities

- Differentiate w.r.t. each parameters and set it to 0 and solve! Closed form solution

Example

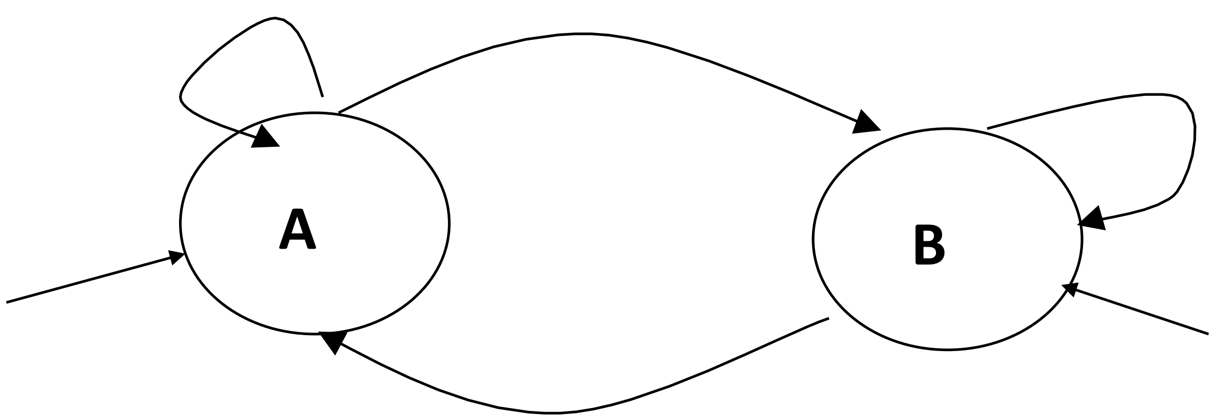
- Assume the model below
- We also observe the following sequence:

  1,2,2,5,6,5,1

  1,3,2,5,6,5,2

  3,2,1,3,6,5,4

- How can we determine the initial, transition and emission probabilities?



Initial probabilities

Q: assume we can observe the following sets of states:

AAABBAA	1,2,2,5,6,5,1
AABBBBB	1,3,2,5,6,5,2
BAABBAB	3,2,1,3,6,5,4

how can we learn the initial probabilities?

A: Maximum likelihood estimation

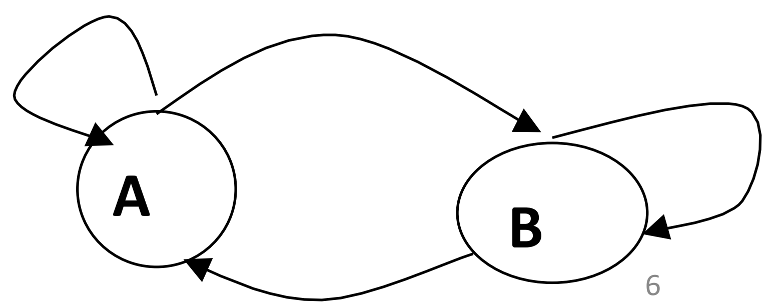
Find the initial probabilities π such that

k is the number of sequences avialable for training

$$\pi^* = \arg\max \ \log \prod_k p(q_1^k) p(o_1^k \mid q_1^k) \prod_{t=2}^{T} p(q_t^k \mid q_{t-1}^k) p(o_t^k \mid q_t^k)$$

$$\pi^* = \arg\max \ \log \prod_k p(q_1^k)$$

$\pi_A = \#A / (\#A + \#B)$



Transition probabilities

Q: assume we can observe the set of states:

AAABBAA 1,2,2,5,6,5,1

AABBBBB 1,3,2,5,6,5,2

BAABBAB 3,2,1,3,6,5,4

how can we learn the transition probabilities?

A: Maximum likelihood estimation

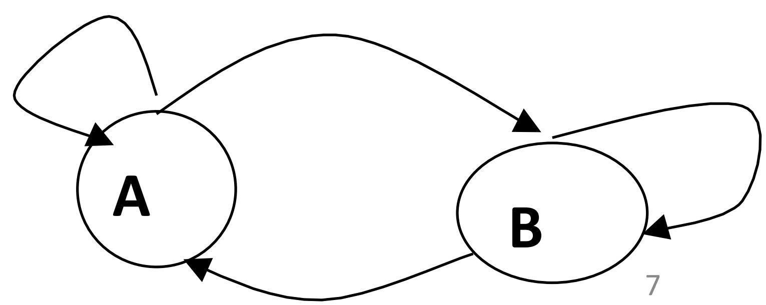
Find a transition matrix *a* such that

remember that we defined $a_{i,j}=p(q_t=s_j | q_{t-1}=s_i)$

$$a^* = \arg\max \ \log \prod_k p(q_1^k) p(o_1^k | q_1^k) \prod_{t=2}^{T} p(q_t^k | q_{t-1}^k) p(o_t^k | q_t^k)$$

$$a^* = \arg\max \ \log \prod_k \prod_{t=2}^{T} p(q_t^k | q_{t-1}^k)$$

$a_{A,B} = \#AB / (\#AB+\#AA)$



Transition probabilities

Q: assume we can observe the set of states:

AAABBAA 1,2,2,5,6,5,1

AABBBBB 1,3,2,5,6,5,2

BAABBAB 3,2,1,3,6,5,4

Moving window of size 2
->#AA, #AB, #BA, #BB

how can we learn the transition probabilities?

remember that we defined
$a_{i,j}=p(q_t=s_j|q_{t-1}=s_i)$

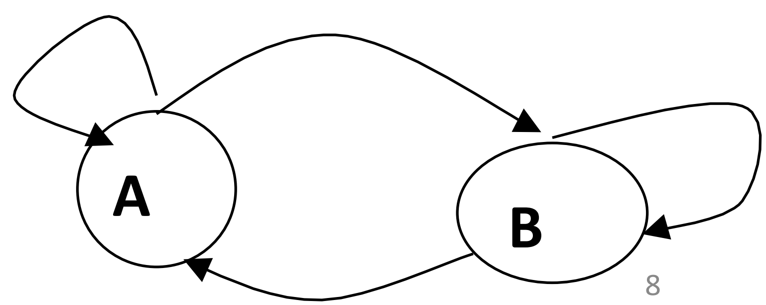
A: Maximum likelihood estimation

Find a transition matrix a such that

$$a^* = \arg\max \log \prod_k p(q_1^k) p(o_1^k | q_1^k) \prod_{t=2}^{T} p(q_t^k | q_{t-1}^k) p(o_t^k | q_t^k)$$

$$a^* = \arg\max \log \prod_k \prod_{t=2}^{T} p(q_t^k | q_{t-1}^k)$$

$$a_{A,B} = \#AB / (\#AB+\#AA)$$



Emission probabilities

Q: assume we can observe the set of states:

AAABBAA   1,2,2,5,6,5,1

AABBBBB   1,3,2,5,6,5,2

BAABBAB   3,2,1,3,6,5,4

how can we learn the transition probabilities?

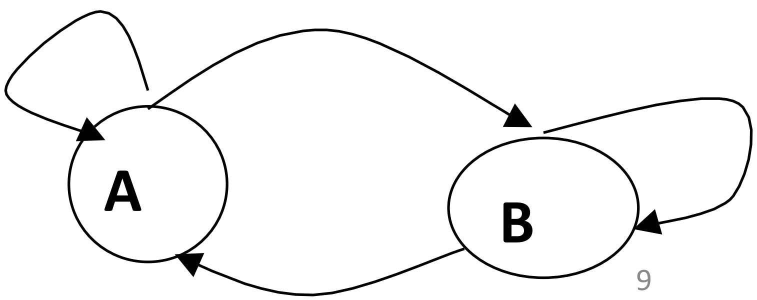
remember that we defined $b_i(o_t) = P(o_t \mid s_i)$

A: Maximum likelihood estimation

Find an emission matrix *b* such that

$$b^* = \arg\max \log \prod_k p(q_1^k) p(o_1^k \mid q_1^k) \prod_{t=2}^{T} p(q_t^k \mid q_{t-1}^k) p(o_t^k \mid q_t^k)$$

$$b^* = \arg\max \log \prod_k p(o_1^k \mid q_1^k) \prod_{t=2}^{T} p(o_t^k \mid q_t^k)$$



$b_A(5)$= #A5 / (#A1+#A2 + … +#A6)

Learning HMMs

- In most case we do not know what states generated each of the outputs (hidden states are unobserved)
  - … but had we known, it would be very easy to determine an emission and transition model!
  - On the other hand, if we had such a model we could determine the set of states using the inference methods we discussed

Expectation Maximization (EM)

- Appropriate for problems with 'missing values' for the variables.
- For example, in HMMs we usually do not observe the states
- Assume complete data log likelihood and maximize expected log likelihood

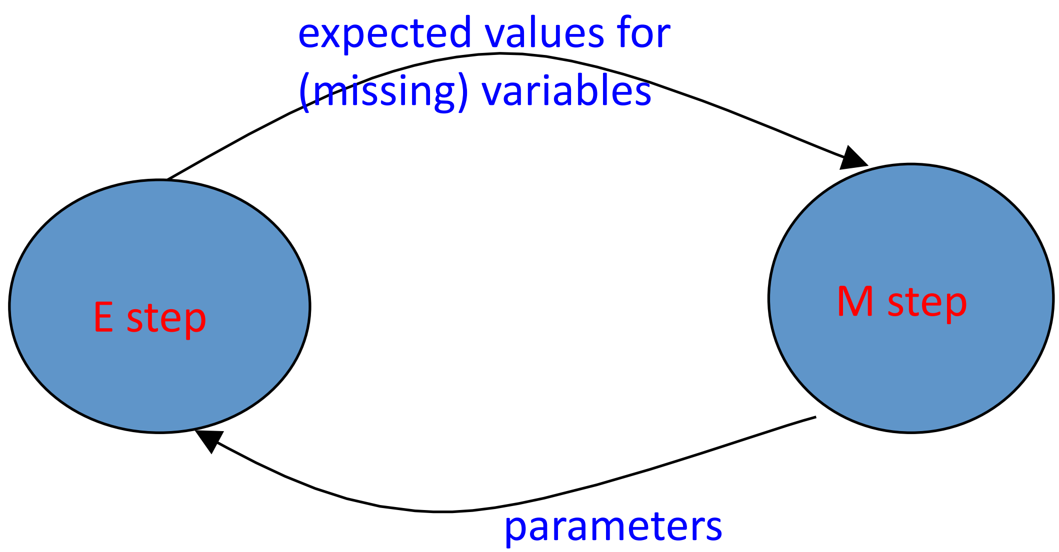
$$\arg\max \; E[\log p((O^1,Q^1),\ldots,(O^K,Q^K))]$$

$$\arg\max \; E[\log \prod_k p(q_1^{\,k})\, p(o_1^{\,k} \mid q_1^{\,k}) \prod_{t=2}^{T} p(q_t^{\,k} \mid q_{t-1}^{\,k})\, p(o_t^{\,k} \mid q_t^{\,k})]$$

where the expectation is taken with respect to p(Q|O, parameters)

Expectation Maximization (EM): Quick reminder

- Two steps
  - E step: Fill in the missing variables with the expected values
  - M step: Regular maximum likelihood estimation (MLE) using the values computed in the E step and the values of the other variables
- Guaranteed to converge (though only to a local minima).



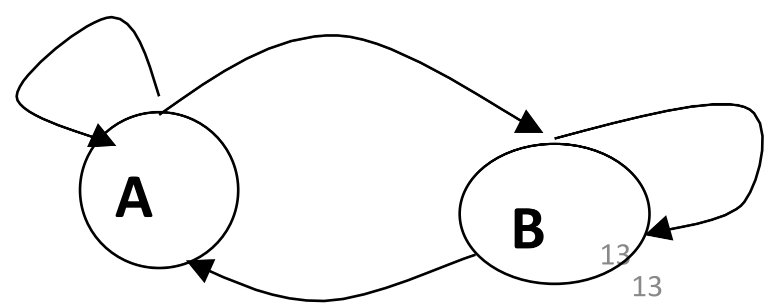
E Step

- In our example, with complete data, we needed
  - #A, #B to estimate initial probabilities
  - #AA, #AB, #BA, #BB to estimate transition probabilities

- When hidden states are not observed, we need "expected counts" in E step

$$P(q_t = s_i \mid O_1, \cdots, O_T) = S_t(i)$$

$$P(q_t = s_i, q_{t+1} = s_j \mid o_1, \cdots, o_T) = S_t(i, j)$$



13

Forward-Backward

- We already defined a *forward* looking variable

$$\alpha_t(i) = P(O_1 \ldots O_t \wedge q_t = s_i)$$

- We also need to define a *backward* looking variable

$$\beta_t(i) = P(O_{t+1}, \cdots, O_T \mid s_t = i)$$

Forward-Backward Algorithm

- We already defined a *forward* looking variable

$$\alpha_t(i) = P(O_1 \ldots O_t \wedge q_t = s_i)$$

- We also need to define a *backward* looking variable

Forward-Backward Algorithm

- Backward step

$$\beta_t(i) = P(O_{t+1},\cdots,O_T \mid q_t = s_i)$$

$$= \sum_j P(O_{t+1},\cdots,O_T, q_{t+1} = s_j \mid q_t = s_i)$$

$$= \sum_j P(q_{t+1} = s_j \mid q_t = s_i) P(O_{t+1},\cdots,O_T \mid q_{t+1} = s_j, q_t = s_i)$$

$$= \sum_j P(q_{t+1} = s_j \mid q_t = s_i) P(O_{t+1},\cdots,O_T \mid q_{t+1} = s_j)$$

$$= \sum_j P(q_{t+1} = s_j \mid q_t = s_i) P(O_{t+1} \mid q_{t+1} = s_j) P(O_{t+2},\cdots,O_T \mid q_{t+1} = s_j)$$

$$= \sum_j a_{i,j} b_j(O_{t+1}) \beta_{t+1}(j)$$

Forward-Backward

- We already defined a *forward* looking variable

$$\alpha_t(i) = P(O_1 \ldots O_t \wedge q_t = s_i)$$

- We also need to define a *backward* looking variable

$$\beta_t(i) = P(O_{t+1}, \cdots, O_T \mid q_t = s_i)$$

- Using these two definitions we can show

P(A|B)=P(A,B)/P(B)

$$P(q_t = s_i \mid O_1, \cdots, O_T) = \frac{\alpha_t(i)\beta_t(i)}{\sum_j \alpha_t(j)\beta_t(j)} \stackrel{def}{=} S_t(i)$$

Forward-Backward

- *forward* looking variable $\alpha_t(i) = P(O_1 \ldots O_t \wedge q_t = s_i)$
- *backward* looking variable $\beta_t(i) = P(O_{t+1}, \cdots, O_T \mid q_t = s_i)$
- Using these two definitions we can show

$$P(q_t = s_i \mid O_1, \cdots, O_T) = \frac{P(q_t = s_i, O_1, \cdots, O_T)}{P(O_1, \cdots, O_T)}$$

$$= \frac{P(O_1, \ldots, O_t, q_t = s_i \mid O_{t+1}, \ldots, O_T) P(O_{t+1}, \cdots, O_T \mid q_t = s_i)}{P(O_1, \cdots, O_T)}$$

$$= \frac{\alpha_t(i)\beta_t(i)}{\sum_j \alpha_t(j)\beta_t(j)} \overset{def}{=} S_t(i)$$

State and transition probabilities

- Probability of a state given observations

$$P(q_t = s_i \mid O_1, \cdots, O_T) = \frac{\alpha_t(i)\beta_t(i)}{\sum_j \alpha_t(j)\beta_t(j)} \stackrel{def}{=} S_t(i)$$

- We can also derive a transition probability given observations

$$P(q_t = s_i, q_{t+1} = s_j \mid o_1, \cdots, o_T)$$
$$= \frac{\alpha_t(i)P(q_{t+1} = s_j \mid q_t = s_i)P(o_{t+1} \mid q_{t+1} = s_j)\beta_{t+1}(j)}{\sum_j \alpha_t(j)\beta_t(j)} \stackrel{def}{=} S_t(i,j)$$

E step

- Compute $S_t(i)$ and $S_t(i,j)$ for all t, i, and j ($1 \le t \le n$, $1 \le i \le k$, $2 \le j \le k$)

$$P(q_t = s_i \mid O_1, \cdots, O_T) = S_t(i)$$

$$P(q_t = s_i, q_{t+1} = s_j \mid o_1, \cdots, o_T) = S_t(i, j)$$

M step (1)

Compute transition probabilities:

$$a_{i,j} = \frac{\hat{n}(i,j)}{\sum_k \hat{n}(i,k)}$$

where

$$\hat{n}(i,j) = \sum_t S_t(i,j)$$

M step (2)

Compute emission probabilities (here we assume a multinomial distribution):

define:

$$B_k(j) = \sum_{t|o_t=j} S_t(k)$$

then

$$b_k(j) = \frac{B_k(j)}{\sum_i B_k(i)}$$

Complete EM algorithm for learning the parameters of HMMs (Baum-Welch)

- Inputs: 1 .Observations $O_1 \dots O_T$

  2. Number of states, model

1. Guess initial transition and emission parameters
2. Compute E step: $S_t(i)$ and $S_t(i,j)$
3. Compute M step
4. Convergence?
5. Output complete model

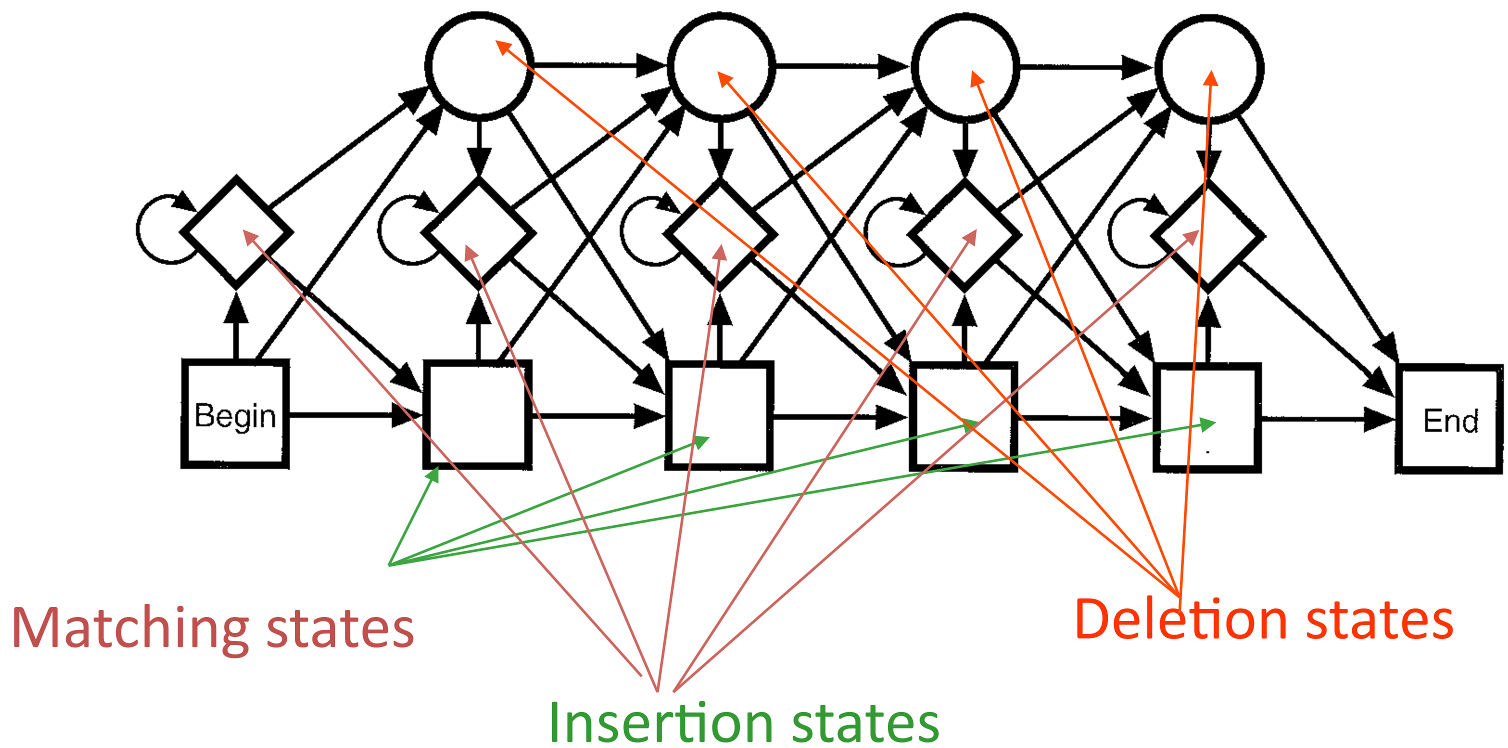
No

We did not discuss initial probability estimation. These can be deduced from the 1st observation in each of the multiple sequences of observations

States in HMM

- How to decide on the number of states in HMM
  - More states means a more complex model, overfitting!
  - Cross validation
  - Nonparametric Bayesian model

Building HMMs–*Topology*

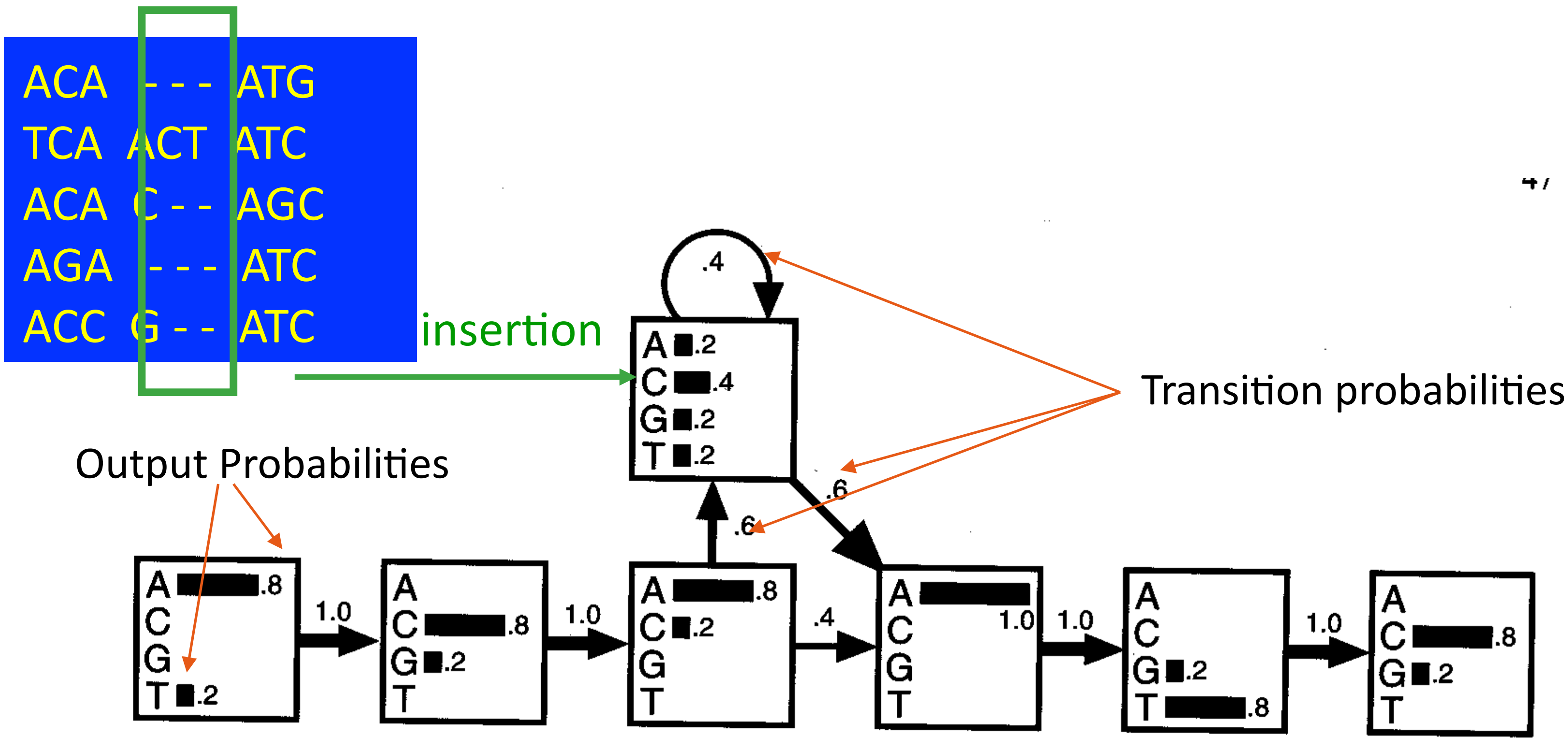


No of matching states = average sequence length in the family

PFAM Database - of Protein families

(**http://pfam.wustl.edu**)

Building – *from an existing alignment*



A HMM model for a DNA motif alignments, The transitions are shown with arrows whose thickness indicate their probability. In each state, the histogram shows the probabilities of the four bases.

Dynamic Bayesian Networks (DBNs)

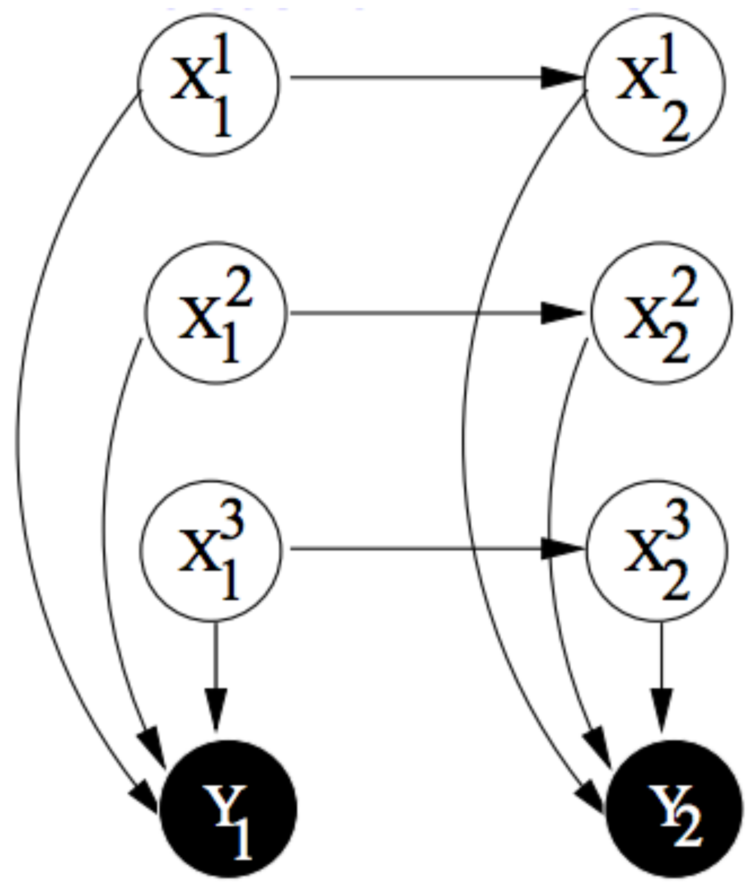
- Bayesian networks for modeling dynamic process. HMM is a special case of DBN
  - HMM represents the state with a single random variable: $P(Q_t|Q_{t-1})$
  - DBN represents the state with a set of random variables: $P(Q_t|Q_{t-1})$, where Q_t is a set of variables

- DBN often has a compact representation of HMM representations
  - DBN may have exponentially fewer parameters than its corresponding HMM
  - Faster inference and learning

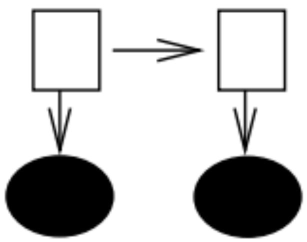
Factorial HMMs

- DBN with D chains, each with K states
  - Three $O(K^2 D)$ transition probabilities
  - 12 parameters

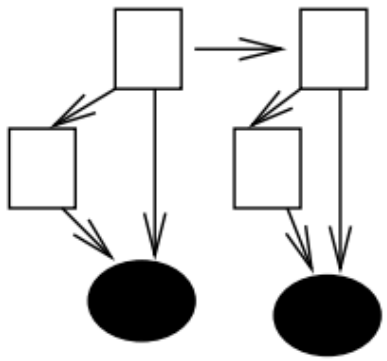
- HMM representations?
  - K^D states
  - $O(K^{2D})$ transition probabilities



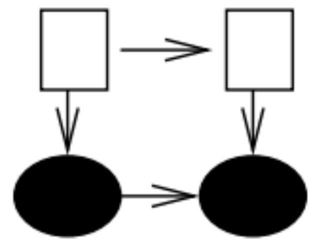
Other Variants of HMMs as DBNs



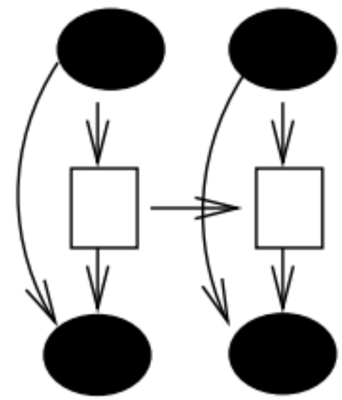
HMM



Mixture of Gaussian HMM



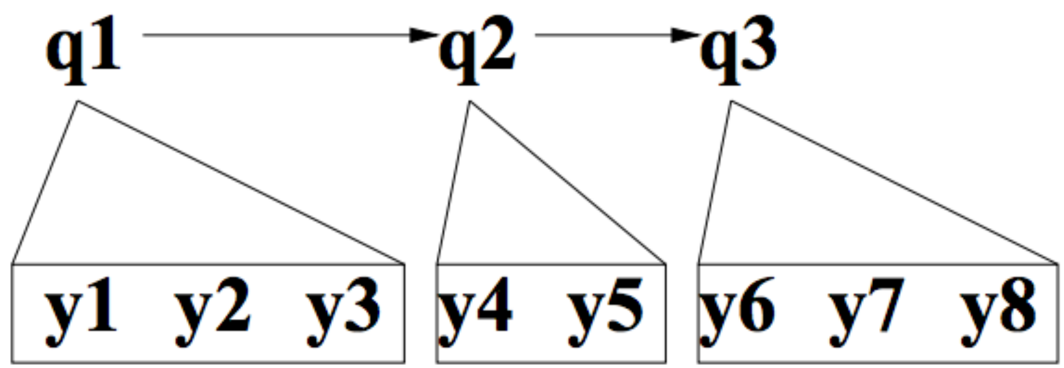
Autoregressive HMM



Input-output HMM

Semi-Markov HMM

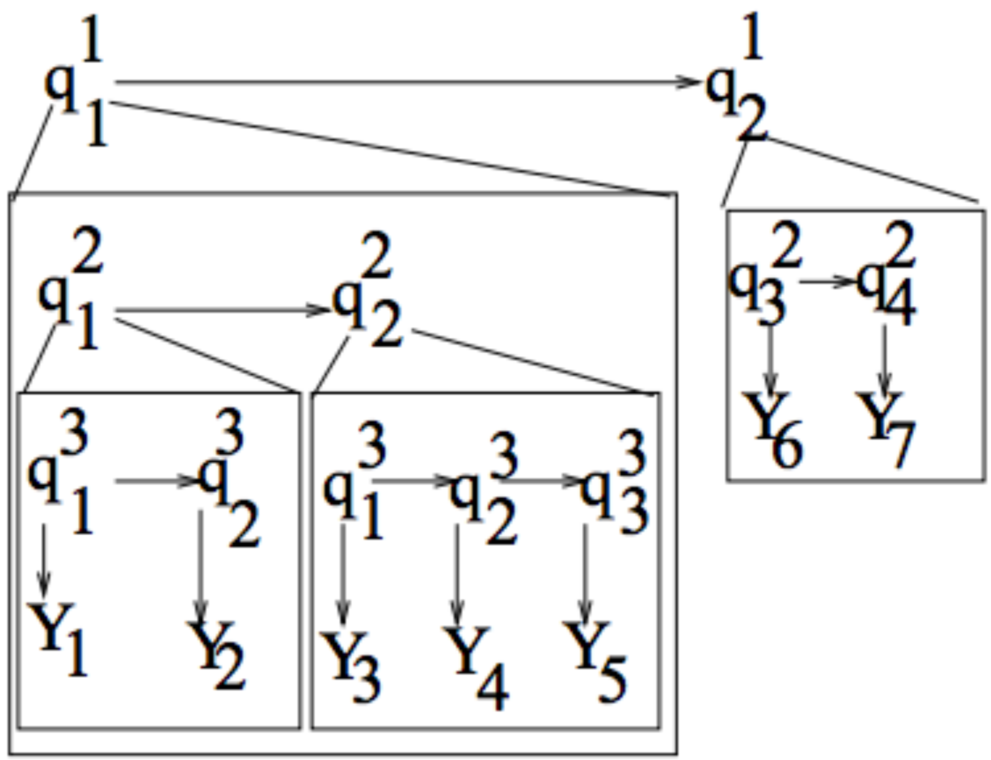
- Relax the Markov constraint to allow staying in the current state for an explicit duration of time L_t



$$P(Y_{t-l+1:l} | Q_t, L_t = l) = \prod_{i=1}^{l} P(Y_i | Q_t)$$

Hierarchical HMM

- Each state can emit another HMM that generate sequences



What you should know

- Why HMMs? Which applications are suitable?
- Inference in HMMs

  - No observations

  - Probability of next state w. observations

  - Maximum scoring path (Viterbi)
- Learning in HMMs
  - EM algorithm with inference as a subroutine