10-701
Machine Learning

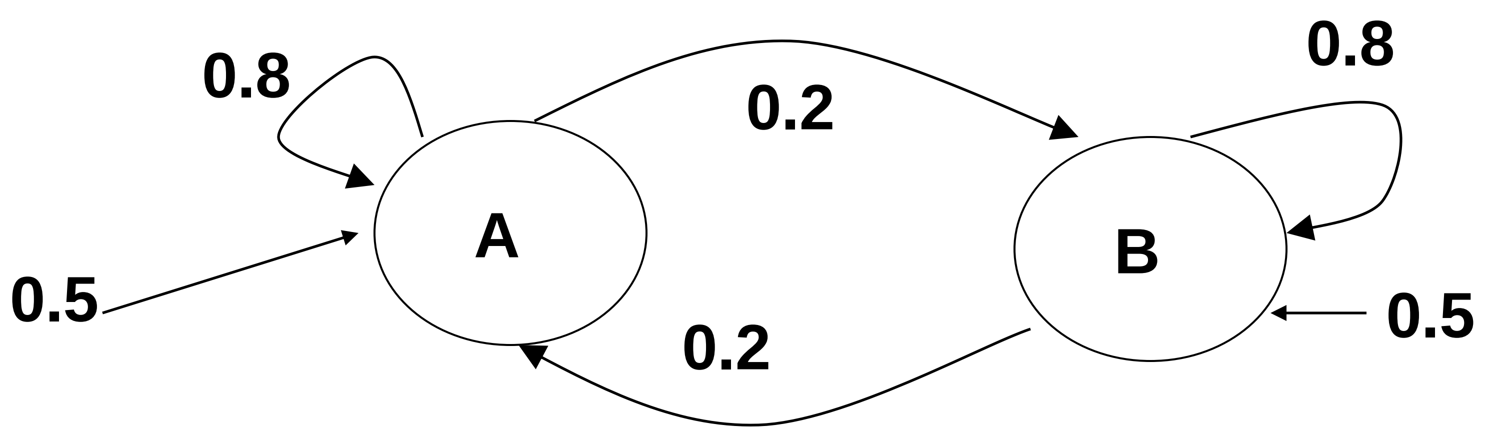
Learning HMMs

A Hidden Markov model

- A set of states $\{s_1 \ldots s_n\}$

  - In each time point we are in exactly one of these states denoted by q_t
- Π_i, the probability that we *start* at state s_i
- A transition probability model, $P(q_t = s_i \mid q_{t-1} = s_j)$
- A set of possible outputs Σ

  - At time *t* we emit a symbol $\sigma \in \Sigma$
- An emission probability model, $p(o_t = \sigma \mid s_i)$



Inference in HMMs

- Computing $P(Q)$ and $P(q_t = s_i)$ √
- Computing $P(Q \mid O)$ and $P(q_t = s_i \mid O)$ √
- Computing $\text{argmax}_Q P(Q)$ √

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”?

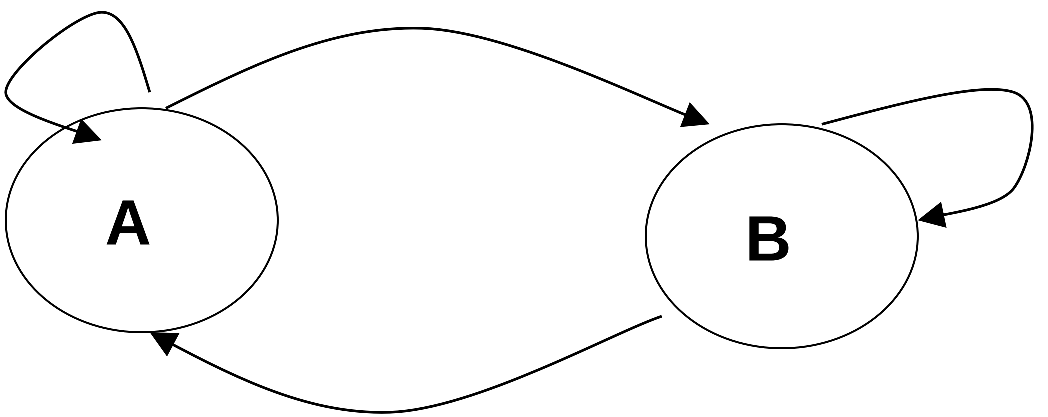
While we will discuss learning the transition and emission models, we will not discuss selecting the states.

This is usually a function of domain knowledge.

Example

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

  1,2,2,5,6,5,1,2,3,3,5,3,3,2 …..
- How can we determine the initial, transition and emission probabilities?



MLE when states are observed

- We will initially assume that we can observe the states themselves
- Obviously, this is not the case. We will relax this assumption to both, infer the states and learn the parameters.

Initial probabilities

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

AAABBAA

AABBBBB

BAABBAB

how can we learn the initial probabilities?

A: Maximum likelihood estimation

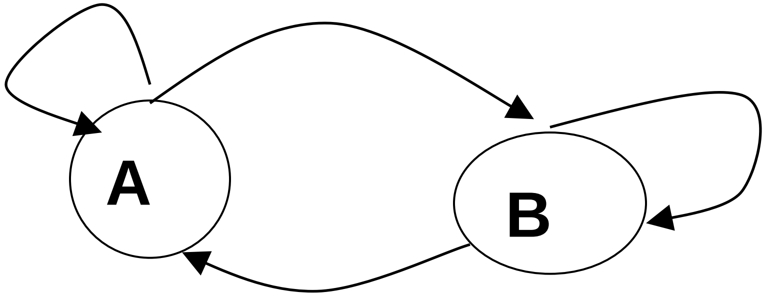
Find the initial probabilities π such that

k is the number of sequences avialable for training

$$\pi^* = \arg\max_{\pi} \prod_{k} \pi(q_1) \prod_{t=2}^{T} p(q_t \mid q_{t-1}) \Rightarrow$$

$$\pi^* = \arg\max_{\pi} \prod_{k} \pi(q_1)$$

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



Transition probabilities

Q: assume we can observe the set of states:

AAABBAAAABBBBBAAAABBBB

how can we learn the transition probabilities?

A: Maximum likelihood estimation

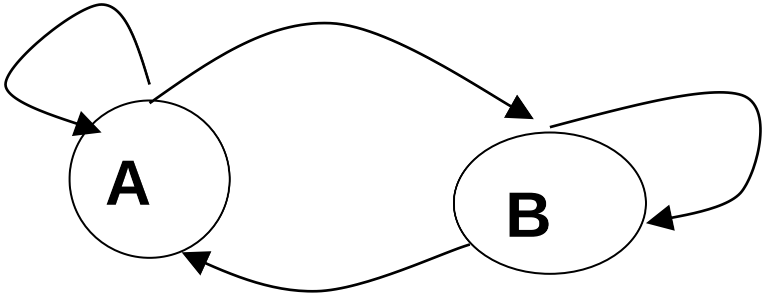
Find a transition matrix *a* such that

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

$$a^* = \operatorname{argmax}_a \prod_k \pi(q_1) \prod_{t=2}^{T} p(q_t \mid q_{t-1}) \Rightarrow$$

$$a^* = \operatorname{argmax}_a \prod_{t=2}^{T} p(q_t \mid q_{t-1})$$

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



Emission probabilities

Q: assume we can observe the set of states:

A A A B B A A A A B B B B B A A

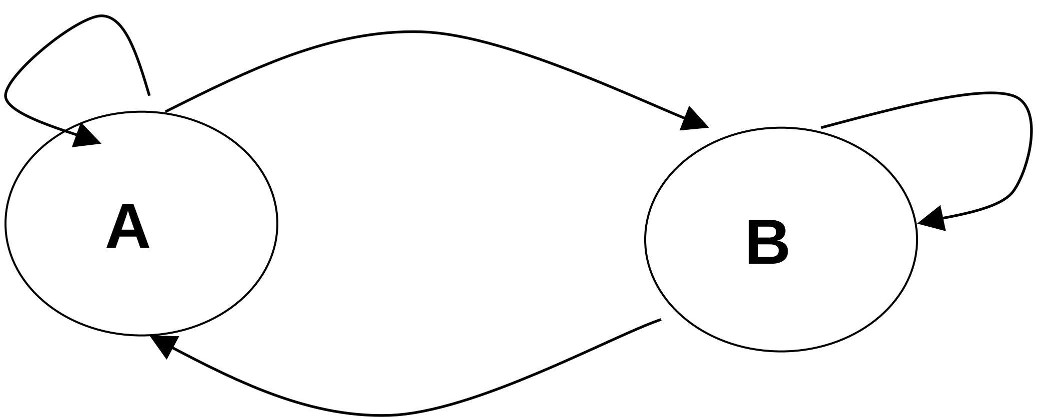
and the set of dice values

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

how can we learn the emission probabilities?

A: Maximum likelihood estimation

$b_A(5) = \#A5 / (\#A1 + \#A2 + \ldots + \#A6)$



Learning HMMs

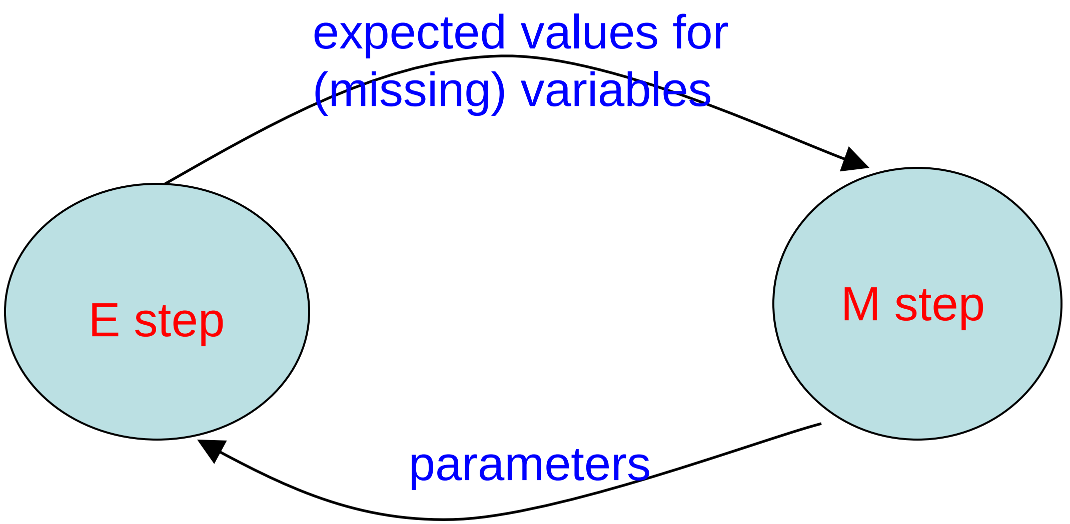
- In most case we do not know what states generated each of the outputs (fully unsupervised)
- … but had we known, it would be very easy to determine an emission and transition model!
- On the other hand, if we had such a model we could determine the set of states using the inference methods we discussed

Expectation Maximization (EM)

- Appropriate for problems with ‘missing values’ for the variables.
- For example, in HMMs we usually do not observe the states

Expectation Maximization (EM): Quick reminder

- Two steps
- E step: Fill in the expected values for the missing variables
- 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).



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

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

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

Forward-Backward

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- Using these two definitions we can show

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

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

State and transition probabilities

- Probability of a state

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

- We can also derive a transition probability

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

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

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 $O_1 \ldots O_T$
  2. Number of states, model

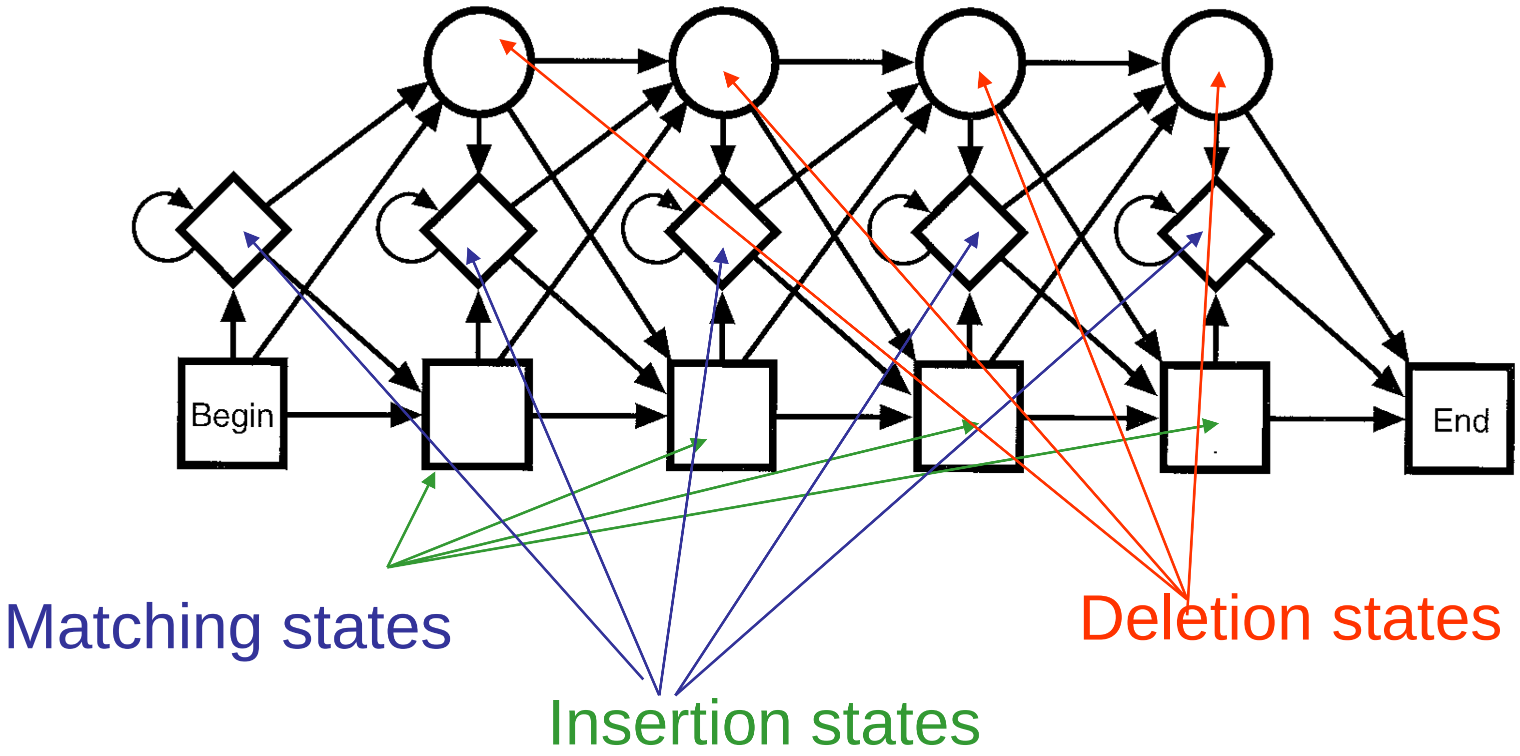
1. Guess initial transition and emission parameters
2. Compute E step: $S_t(i)$ and $S_t(i,j)$
3. Compute M step
4. Convergence? No
5. Output complete model

We did not discuss initial probability estimation. These can be deduced from multiple sets of observation (for example, several recorded customers for speech processing)

HMM for DNA / Protein alignment

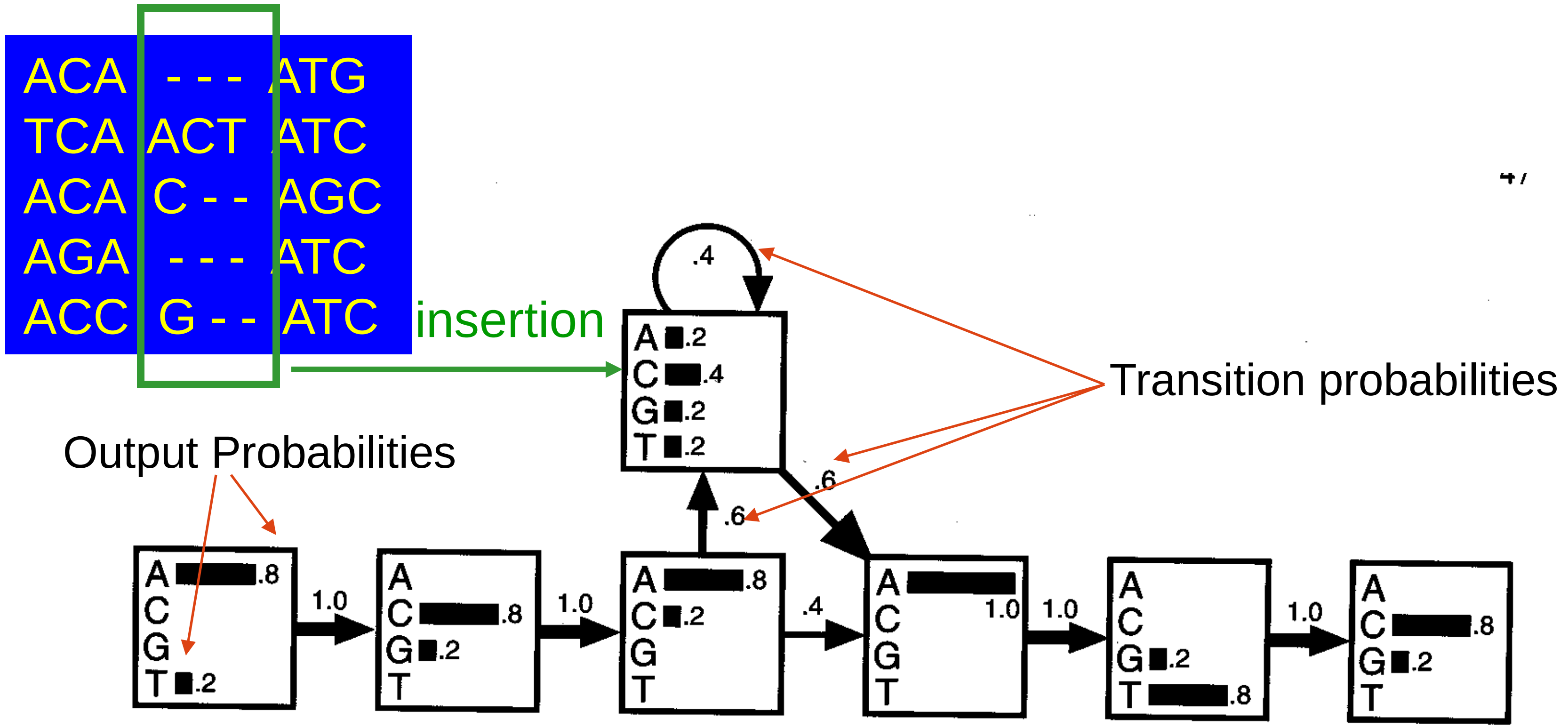
ACA	- - -	ATG
TCA	ACT	ATC
ACA	C - -	AGC
AGA	- - -	ATC
ACC	G - -	ATC

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.

Computing $\alpha_t(i)$

$\alpha_t(i) = P(o_1, o_2 \ldots, o_t \wedge q_t = s_i)$

- $\alpha_1(i) = P(o_1 \wedge q_1 = i) = P(o_1 \mid q_1 = s_i)\Pi_i$

We must be at a state in time t

chain rule

Markov property

$$\alpha_{t+1}(i) = P(O_1 \ldots O_{t+1} \wedge q_{t+1} = s_i) =$$

$$\sum_j P(O_1 \ldots O_t \wedge q_t = s_j \wedge O_{t+1} \wedge q_{t+1} = s_i) =$$

$$\sum_j P(O_{t+1} \wedge q_{t+1} = s_i \mid O_1 \ldots O_t \wedge q_t = s_j) P(O_1 \ldots O_t \wedge q_t = s_j) =$$

$$\sum_j P(O_{t+1} \wedge q_{t+1} = s_i \mid O_1 \ldots O_t \wedge q_t = s_j) \alpha_t(j) =$$

$$\sum_j P(O_{t+1} \mid q_{t+1} = s_i) P(q_{t+1} = s_i \mid q_t = s_j) \alpha_t(j) =$$

$$\sum_j b_i(O_{t+1}) a_{j,i} \alpha_t(j)$$