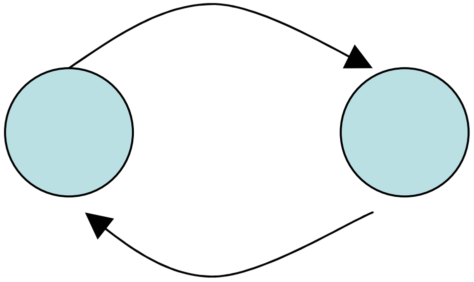
15-780: Graduate Artificial Intelligence

Hidden Markov Models (HMMs)

What's wrong with Bayesian networks

- Bayesian networks are very useful for modeling joint distributions
- But they have their limitations:
  - No mention of time / sequence
  - Dag's (no self or any other loops)

This is not a valid Bayesian network!



Hidden Markov models

- Model a set of observation with a set of hidden states
  - Robot movement
    Observations: range sensor, visual sensor
    Hidden states: location (on a map)
  - Speech processing
    Observations: sound signals
    Hidden states: parts of speech, words
  - Biology
    Observations: DNA base pairs
    Hidden states: Genes

Hidden Markov models

- Model a set of observation with a set of hidden states

  - Robot movement

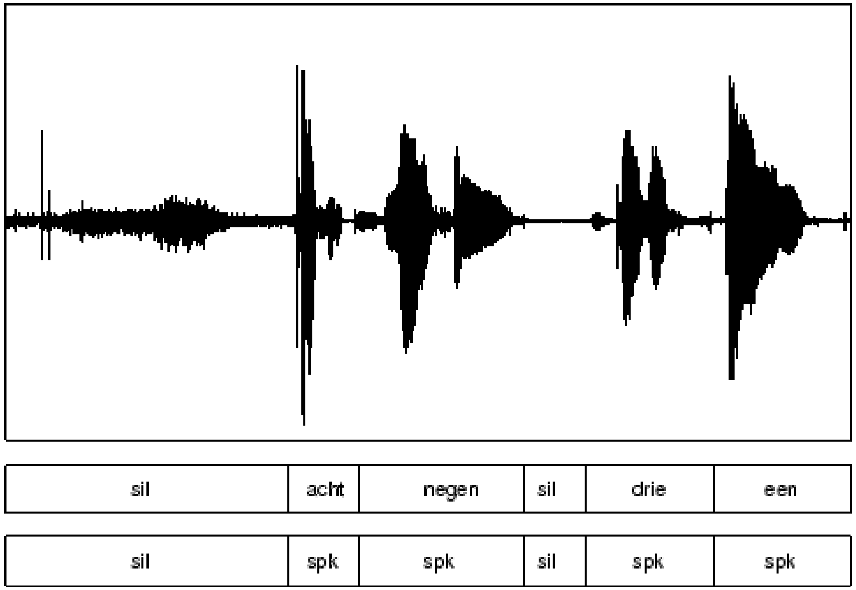
  Observations: range sensor, visual sensor

  Hidden states: location (on a map)

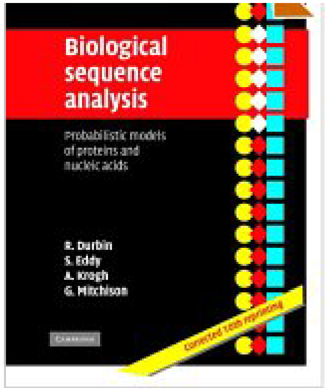
1. Hidden states generate observations

2. Hidden states transition to other hidden states

Examples: Speech processing



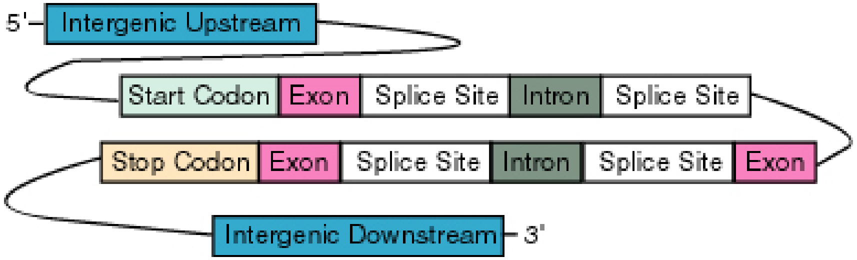
Example: Biological data



Biological sequence analysis

Probabilistic models of proteins and nucleic acids

R. Durbin
S. Eddy
A. Krogh
G. Mitchison

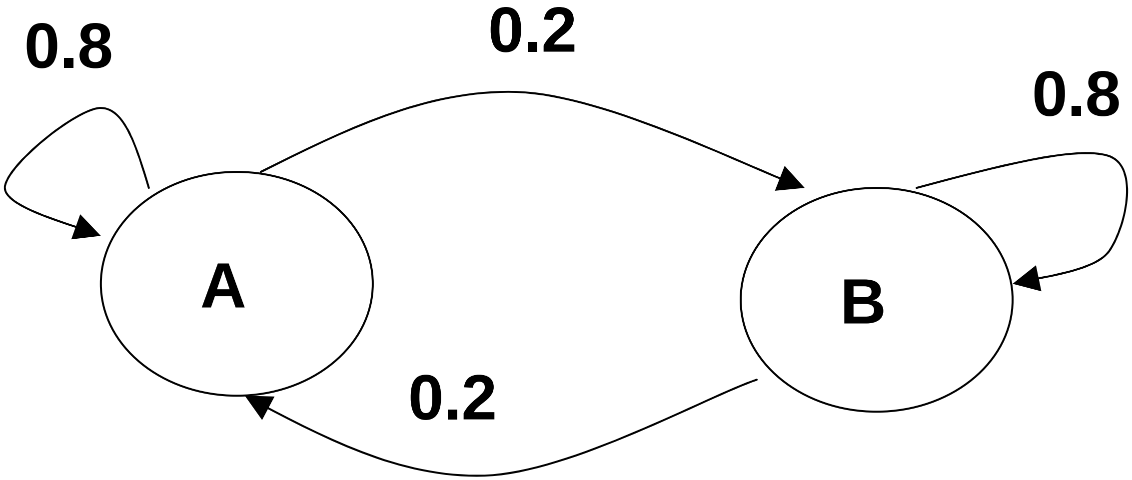


ATGAAGCTACTGTCTTCTATCGAACAAGCATGCG
ATATTTGCCGACTTAAAAAGCTCAAG
TGCTCCAAAGAAAAACCGAAGTGCGCCAAGTGT
CTGAAGAACAACTGGGAGTGTCGCTAC
TCTCCCAAAACCAAAAGGTCTCCGCTGACTAGG
GCACATCTGACAGAAGTGGAATCAAGG
CTAGAAAGACTGGAACAGCTATTTCTACTGATTT
TTCCTCGAGAAGACCTTGACATGATT

Contents

Example: Gambling on dice outcome

- Two dices, both skewed (output model).
- Can either stay with the same dice or switch to the second dice (transition mode).

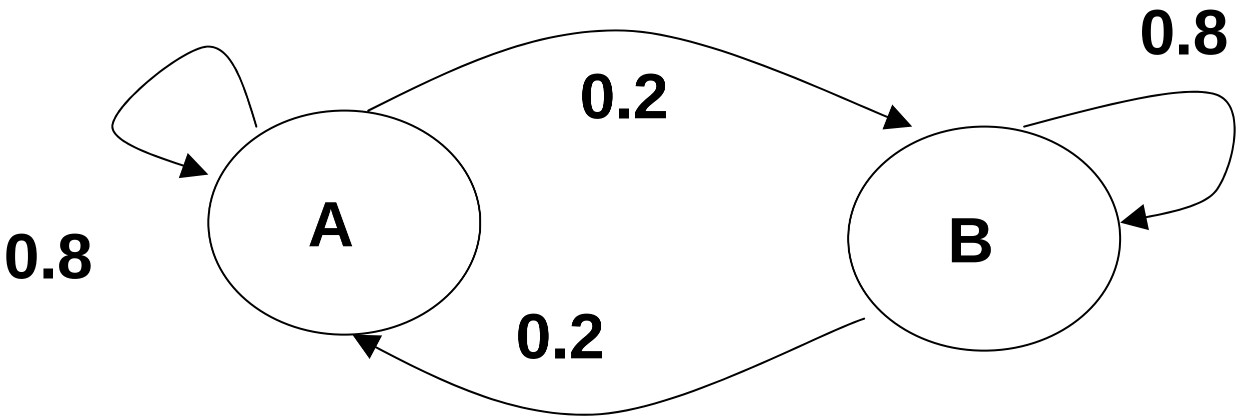


A Hidden Markov model

- 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

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



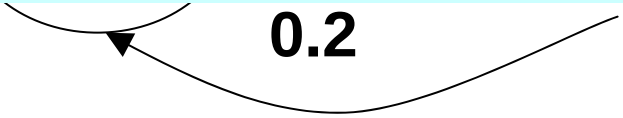
The Markov property

- 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, $P(q_t = s_i \mid q_{t-1} = s_j)$

An important aspect of this definitions is the Markov property: q_{t+1} is conditionally independent of q_{t-1} (and any earlier time points) given q_t

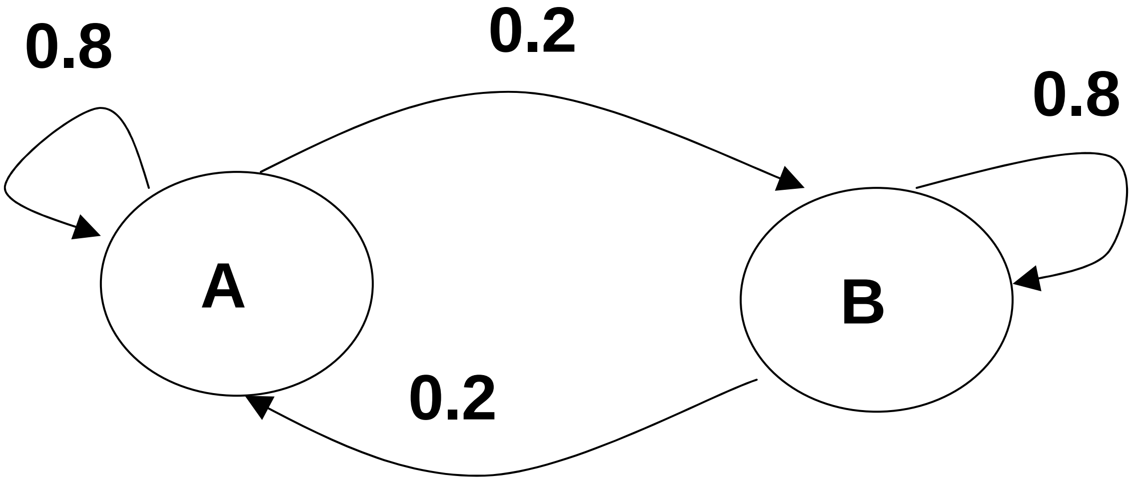
More formally $P(q_{t+1} = s_i \mid q_t = s_j) = P(q_{t+1} = s_i \mid q_t = s_j, q_{t-1} = s_j)$



What can we ask when using a HMM?

A few examples:

- “What dice is currently being used?”
- “What is the probability of a 6 in the next role?”
- “What is the probability of 6 in any of the next 3 roles?”



Inference in HMMs

- Computing P(Q) and P($q_t = s_i$)

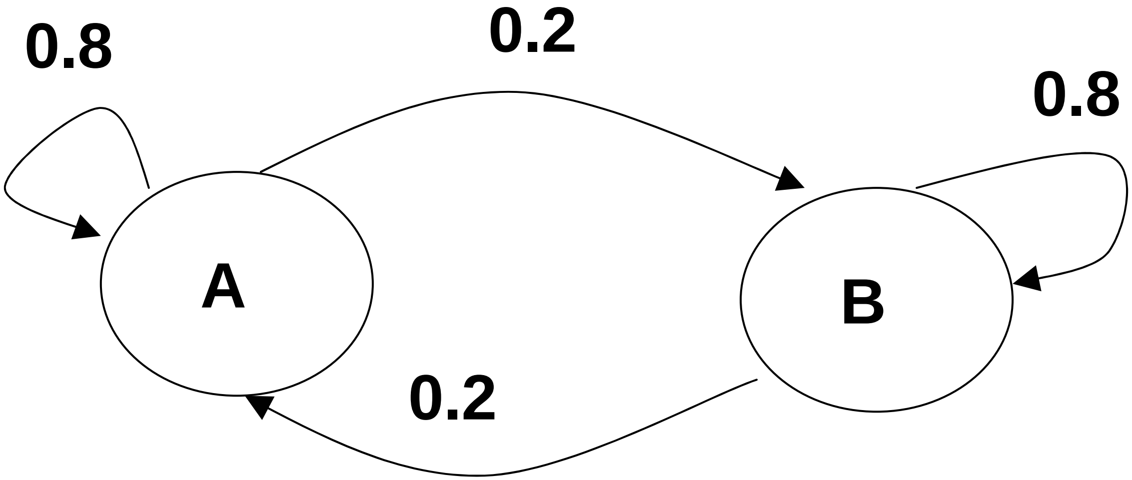
  - If we cannot look at observations
- Computing P(Q | O) and P($q_t = s_i$ |O)

  - When we have observation and care about the last state only
- Computing argmax_QP(Q | O)

  - When we care about the entire path

What dice is currently being used?

- There where t rounds so far
- We want to determine P(q_t = A)
- Lets assume for now that we cannot observe any outputs (we are blind folded)
- How can we compute this?



$P(q_t = A)$?

- Simple answer:

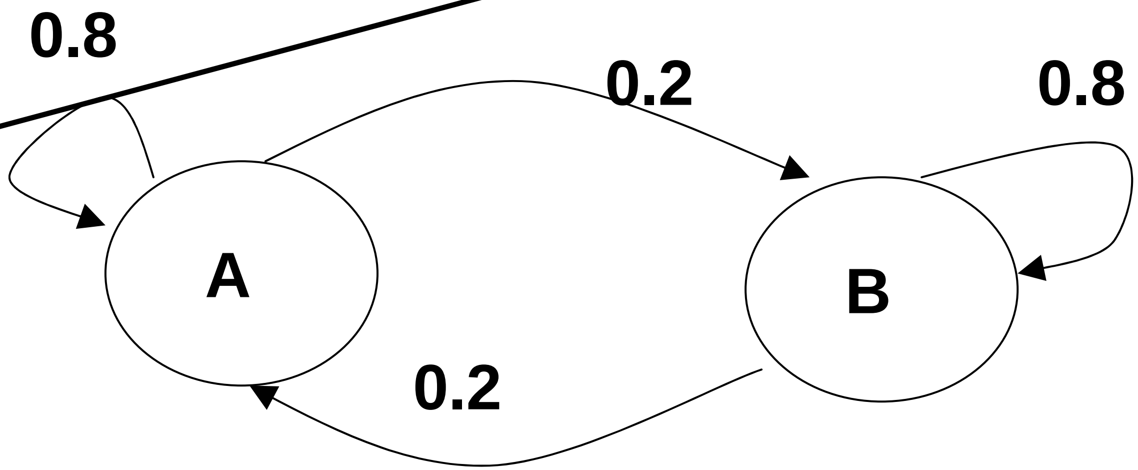
Lets determine P(Q) where Q is any path that ends in A

$Q = q_1, \ldots q_{t-1}, A$

$P(Q) = P(q_1, \ldots q_{t-1}, A) = P(A \mid q_1, \ldots q_{t-1})\, P(q_1, \ldots q_{t-1}) =$
$P(A \mid q_{t-1})\, P(q_1, \ldots q_{t-1}) = \ldots = P(A \mid q_{t-1}) \ldots P(q_2 \mid q_1)\, P(q_1)$

Markov property!

Initial probability



$P(q_t = A)$?

- Simple answer:

1. Lets determine P(Q) where Q is any path that ends in A

$Q = q_1, \dots q_{t-1}, A$

$P(Q) = P(q_1, \dots q_{t-1}, A) = P(A \mid q_1, \dots q_{t-1})\, P(q_1, \dots q_{t-1}) =$
$P(A \mid q_{t-1})\, P(q_1, \dots q_{t-1}) = \dots = P(A \mid q_{t-1}) \dots P(q_2 \mid q_1)\, P(q_1)$

2. $P(q_t = A) = \Sigma P(Q)$

where the sum is over all sets of t
sates that end in A

$P(q_t = A)$?

- Simple answer:

1. Lets determine P(Q) where Q is any path that ends in A

$Q = q_1, \ldots q_{t-1}, A$

$P(Q) = P(q_1, \ldots q_{t-1}, A) = P(A \mid q_1, \ldots q_{t-1})\, P(q_1, \ldots q_{t-1}) =$
$P(A \mid q_{t-1})\, P(q_1, \ldots q_{t-1}) = \ldots = P(A \mid q_{t-1}) \ldots P(q_2 \mid q_1)\, P(q_1)$

2. $P(q_t = A) = \Sigma P(Q)$

where the sum is over all sets of t sates that end in A

Q: How many sets Q are there?

A: A lot! (2^{t-1})

Not a feasible solution

$P(q_t = A)$, the smart way

- Lets define $p_t(i)$ = probability state i at time t = $p(q_t = s_i)$
- We can determine $p_t(i)$ by induction

1. $p_1(i) = \Pi_i$
2. $p_t(i) = ?$

$P(q_t = A)$, the smart way

- Lets define $p_t(i)$ = probability state i at time t = $p(q_t = s_i)$
- We can determine $p_t(i)$ by induction

1. $p_1(i) = \Pi_i$
2. $p_t(i) = \Sigma_j\ p(q_t = s_i \mid q_{t-1} = s_j)p_{t-1}(j)$

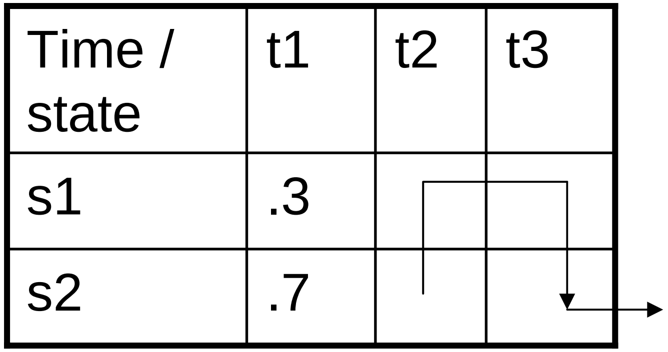
$P(q_t = A)$, the smart way

- Lets define $p_t(i)$ = probability state i at time t = $p(q_t = s_i)$
- We can determine $p_t(i)$ by induction

1. $p_1(i) = \Pi_i$
2. $p_t(i) = \Sigma_j \, p(q_t = s_i \mid q_{t-1} = s_j) p_{t-1}(j)$

This type of computation is called dynamic programming

Complexity: $O(n^2 * t)$



Time / state	t1	t2	t3
s1	.3		
s2	.7		

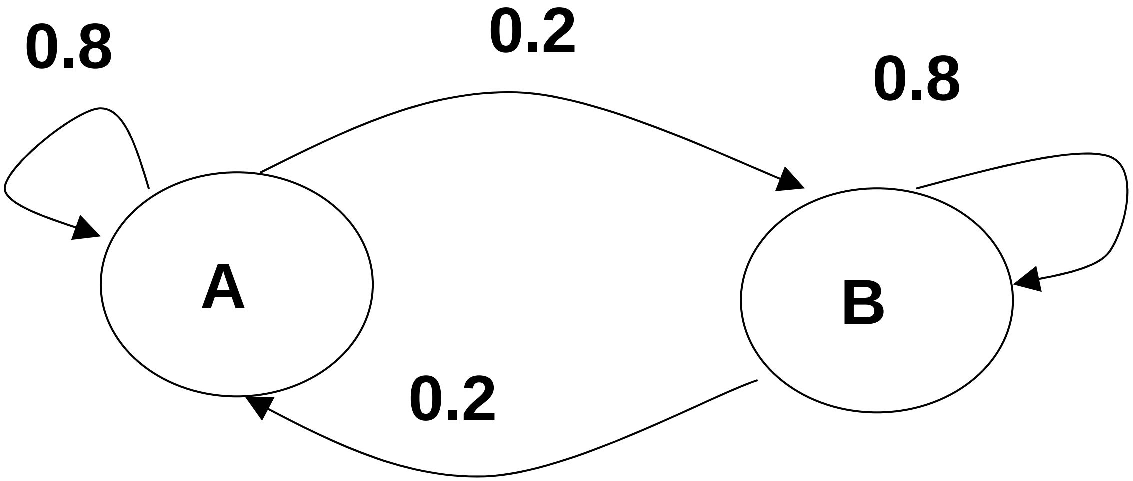
Inference in HMMs

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

But what if we observe outputs?

- So far, we assumed that we could not observe the outputs
- In reality, we almost always can.

v	P(v |A)	P(v |B)
1	.3	.1
2	.2	.1
3	.2	.1
4	.1	.2
5	.1	.2
6	.1	.3



But what if we observe outputs?

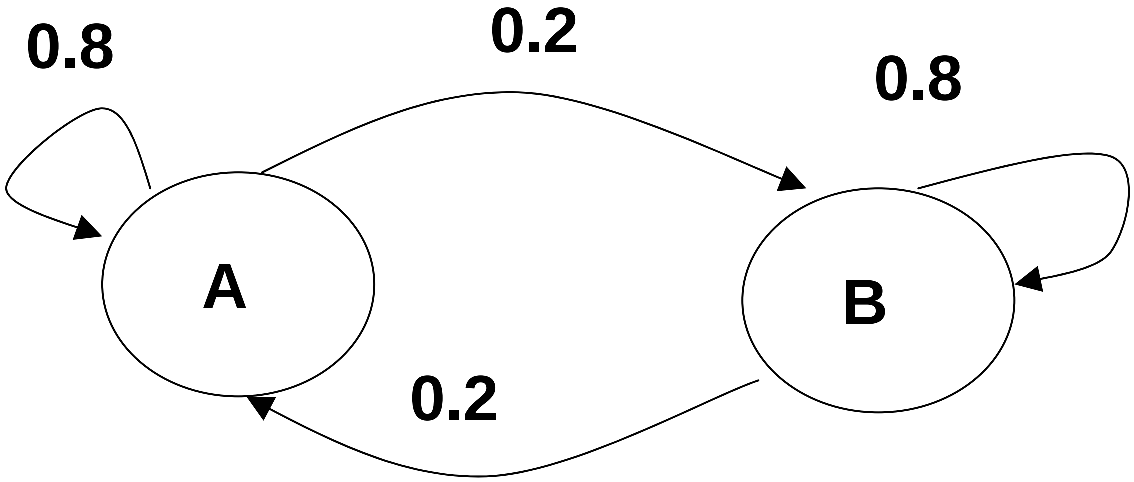
- So far, we assumed that we could not observe the outputs
- In reality, we almost a

v	P(v |A)	P(v |B)
1	.3	.1
2	.2	.1
3	.2	.1
4	.1	.2
5	.1	.2
6	.1	.3

Does observing the sequence

5, 6, 4, 5, 6, 6

Change our belief about the state?



But what if we observe outputs?

- So far, we assumed that we could not observe the outputs
- In reality, we almost a

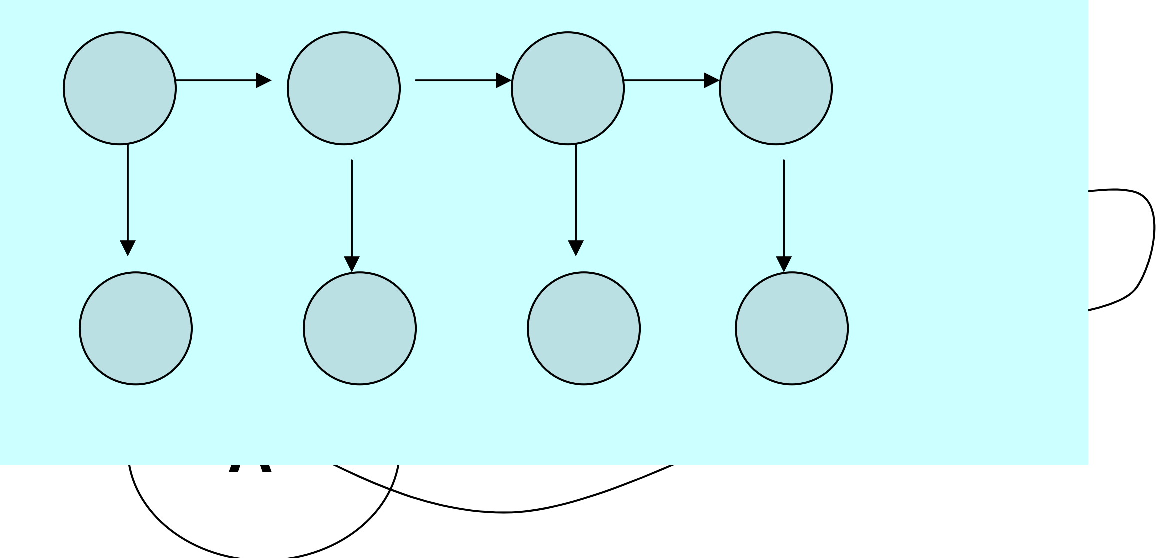
Does observing the sequence

5, 6, 4, 5, 6, 6

Change our belief about the state?

v	P(v |A)	P(v |B)
1	.3	.1
2	.2	.1
6	.1	.3

HMMs are often represented by the following structure:



$P(q_t = A)$ when outputs are observed

- We want to compute $P(q_t = A \mid O_1 \ldots O_t)$
- For ease of writing we will use the following notations (common in literature)
- $a_{i,j} = P(q_t = s_i \mid q_{t-1} = s_j)$
- $b_i(o_t) = P(o_t \mid s_i)$

$P(q_t = A)$ when outputs are observed

- We want to compute $P(q_t = A \mid O_1 \ldots O_t)$
- Lets start with a simpler question. Given a sequence of states Q, what is $P(Q \mid O_1 \ldots O_t) = P(Q \mid O)$

  - We already know how to move from P(Q) to $P(q_t = A)$

  - In some cases P(Q) is the more important question

    - Speech processing

    - NLP

$P(Q \mid O)$

- We can use Bayes rule:

$$P(Q|O) = \frac{P(O \mid Q)P(Q)}{P(O)}$$

Easy, $P(O \mid Q) = P(o_1 \mid q_1)\, P(o_2 \mid q_2) \ldots P(o_t \mid q_t)$

P(Q | O)

- We can use Bayes rule:

$$P(Q|O) = \frac{P(O \mid Q)P(Q)}{P(O)}$$

Easy, $P(Q) = P(q_1)\ P(q_2 \mid q_1)\ \ldots\ P(q_t \mid q_{t-1})$

P(Q | O)

- We can use Bayes rule:

$$P(Q|O) = \frac{P(O \mid Q)P(Q)}{P(O)}$$

Hard!

$P(O)$

- What is the probability of seeing a set of observations:
  - An important question in it own rights, for example classification using two HMMs
- Define $\alpha_t(i) = P(o_1, o_2 \ldots, o_t \wedge q_t = s_i)$
- $\alpha_t(i)$ is the probability that we:
  1. Observe $o_1, o_2 \ldots, o_t$
  2. End up at state i

How do we compute $\alpha_t(i)$?

Computing $\alpha_t(i)$

- $\alpha_1(i) = P(o_1 \wedge q_t = i) = P(o_1 \mid q_t = s_i)\Pi_I$

We must be at a state in time t

chain rule

Markov property

Example: Computing $\alpha_3(B)$

- We observed 2,3,6

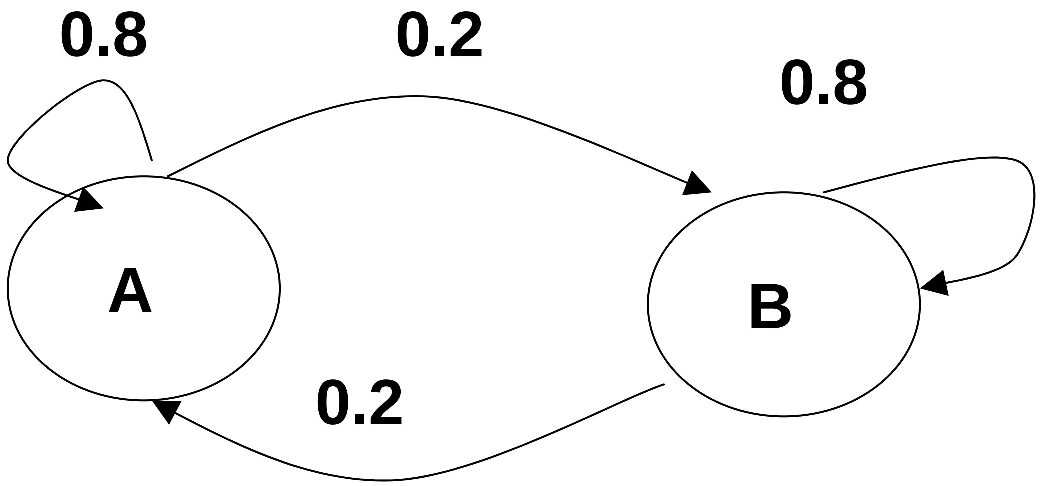
$\alpha_1(A) = P(2 \wedge\ q_1 = A) = P(2 \mid q_1 = A)\Pi_A = .2*.7 = .14,\ \alpha_1(B) = .1*.3 = .03$

$\alpha_2(A) = \Sigma_{j=A,,B} b_A(3) a_{j,A}\ \alpha_1(\ j) = .2*.8*.14 + .2*.2*.03 = 0.0236,\ \alpha_2(B) = 0.0052$

$\alpha_3(B) = \Sigma_{j=A,,B} b_B(6) a_{j,B}\ \alpha_2(\ j) = .3*.2*.0236 + .3*.8*.0052 = 0.00264$

$\Pi_A = 0.7$
$\Pi_b = 0.3$

v	P(v |A)	P(v |B)
1	.3	.1
2	.2	.1
3	.2	.1
4	.1	.2
5	.1	.2
6	.1	.3



Where we are

- We want to compute $P(Q \mid O)$
- For this, we only need to compute $P(O)$
- We know how to compute $\alpha_t(i)$

From now its easy

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

so

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

note that

$$p(q_t = s_i \mid o_1, o_2 \ldots, o_t) = \frac{\alpha_t(i)}{\sum_j \alpha_t(j)}$$

$P(A \mid B) = P(A \wedge B) / P(B)$

Complexity

- How long does it take to compute $P(Q \mid O)$?
- $P(Q)$: $O(n)$
- $P(O|Q)$: $O(n)$
- $P(O)$: $O(n^2 t)$

Inference in HMMs

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

Most probable path

- We are almost done …
- One final question remains

  How do we find the most probable path, that is Q* such that

  $$P(Q^* \mid O) = \text{argmax}_Q P(Q|O)?$$

- This is an important path

  - The words in speech processing
  - The set of genes in the genome
  - etc.

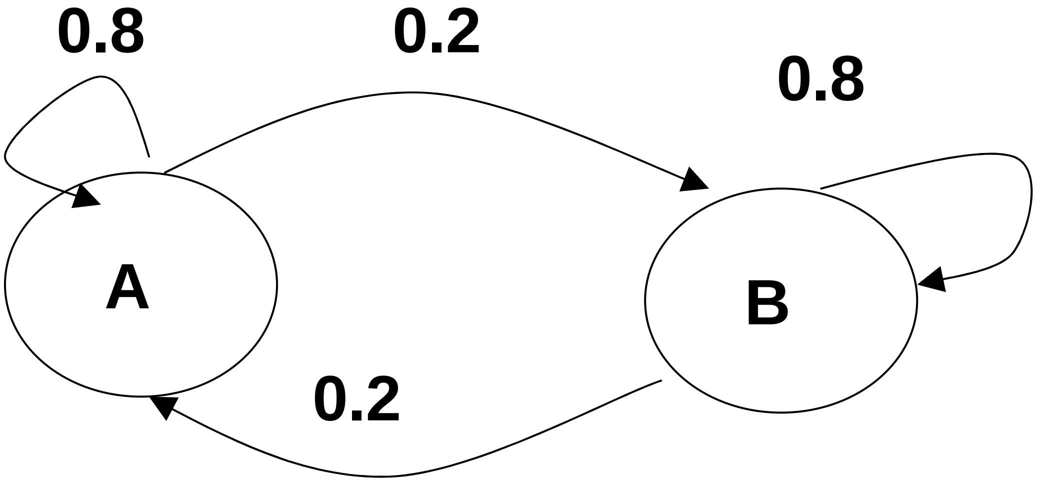
Example

- What is the most probable set of states leading to the sequence:

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

Π_A=0.7
Π_b=0.3

v	P(v |A)	P(v |B)
1	.3	.1
2	.2	.1
3	.2	.1
4	.1	.2
5	.1	.2
6	.1	.3



Most probable path

$$\arg\max_Q P(Q \mid O) = \arg\max_Q \frac{P(O \mid Q)P(Q)}{P(O)}$$

$$= \arg\max_Q P(O \mid Q)P(Q)$$

We will use the following definition:

$$\delta_t(i) = \max_{q_1 \ldots q_{t-1}} p(q_1 \ldots q_{t-1} \wedge q_t = s_i \wedge O_1 \ldots O_t)$$

In other words we are interested in the most likely path from 1 to t that:

1. Ends in S_i
2. Produces outputs O_1 … O_t

Computing $\delta_t(i)$

$$\delta_t(i) = \max_{q_1 \ldots q_{t-1}} p(q_1 \ldots q_{t-1} \wedge q_t = s_i \wedge O_1 \ldots O_t)$$

$$\begin{aligned}\delta_1(i) &= p(q_1 = s_i \wedge O_1) \\ &= p(q_1 = s_i) p(O_1 \mid q_1 = s_i) \\ &= \pi_i b_i(O_1)\end{aligned}$$

Q: Given $\delta_t(i)$, how can we compute $\delta_{t+1}(i)$?

A: To get from $\delta_t(i)$ to $\delta_{t+1}(i)$ we need to

1. Add an emission for time t+1 (O_{t+1})
2. Transition to state s_i

$$\begin{aligned}\delta_{t+1}(i) &= \max_{q_1 \ldots q_t} p(q_1 \ldots q_t \wedge q_{t+1} = s_i \wedge O_1 \ldots O_{t+1}) \\ &= \max_j \delta_t(j) p(q_{t+1} = s_i \mid q_t = s_j) p(O_{t+1} \mid q_{t+1} = s_i) \\ &= \max_j \delta_t(j) a_{j,i} b_i(O_{t+1})\end{aligned}$$

The Viterbi algorithm

$$
\begin{aligned}
\delta_{t+1}(i) &= \max_{q_1 \ldots q_t} p(q_1 \ldots q_t \wedge q_{t+1} = s_i \wedge O_1 ... O_{t+1}) \\
&= \max_j \delta_{t+1}(j)\, p(q_{t+1} = s_i \mid q_t = s_j)\, p(O_{t+1} \mid q_{t+1} = s_i) \\
&= \max_j \delta_{t+1}(j)\, a_{j,i} b_i(O_{t+1})
\end{aligned}
$$

- Once again we use dynamic programming for solving $\delta_t(i)$
- Once we have $\delta_t(i)$, we can solve for our P(Q*|O)

By:

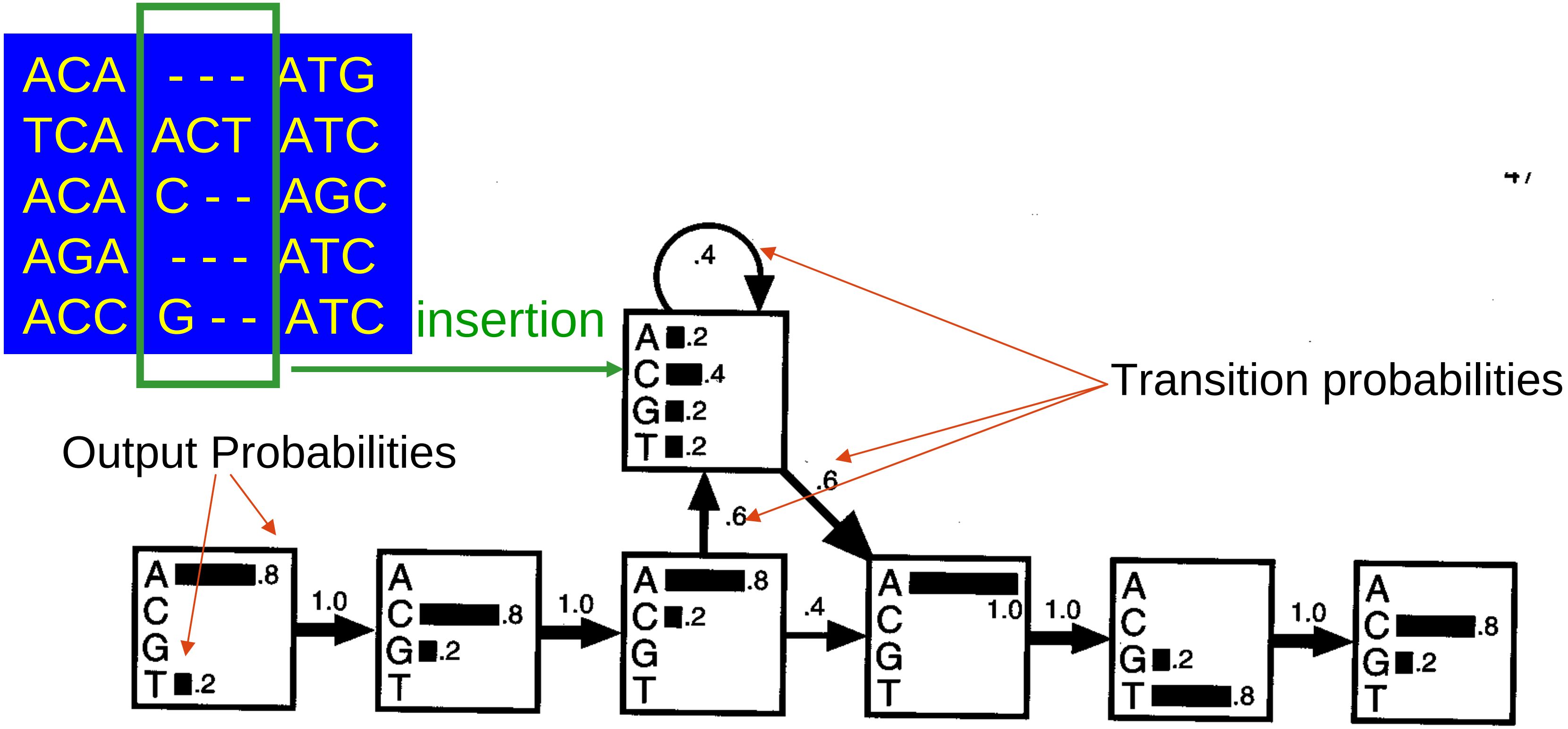
P(Q* | O) = argmax_QP(Q|O) = P(Q* | O) =

path defined by $\text{argmax}_j\ \delta_t(j)$,

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 $\text{argmax}_Q P(Q)$ √

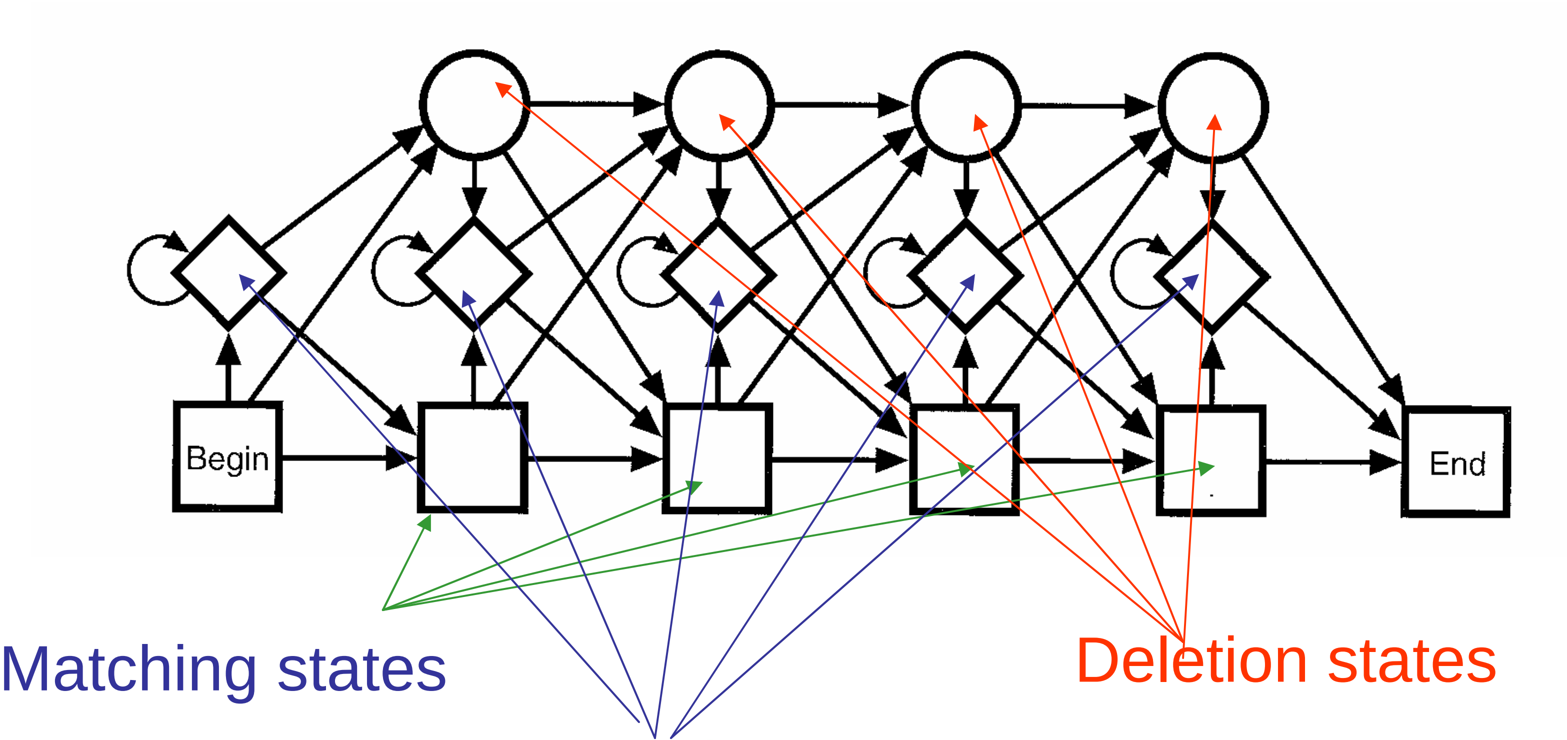
Building – *from an existing alignment*



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

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.

Building – *Final Topology*



Matching states

Deletion states

Insertion states

No of matching states = average sequence length in the family

PFAM Database - of Protein families

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

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)

Computing $\alpha_t(i)$

- $\alpha_1(i) = P(o_1 \wedge q_t = i) = P(o_1 \mid q_t = s_i)\Pi_I$

We must be at a state in time t

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

chain rule

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

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

Markov property

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

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

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