L13: hidden Markov models

Discrete Markov processes

Hidden Markov models

Forward and Backward procedures

The Viterbi algorithm

Baum-Welch re-estimation

This lecture is based on [Rabiner and Juang, 1993]

Discrete Markov Processes

Consider a system described by the following process

- At any given time, the system can be in one of N possible states $S = \{S_1, S_2 \dots S_N\}$
- At regular times, the system undergoes a transition to a new state
- Transition between states can be described probabilistically

Markov property

- In general, the probability that the system is in state $q_t = S_j$ is a function of the complete history of the system
- To simplify the analysis, however, we will assume that the state of the system depends only on its immediate past

$$P(q_t = S_j | q_{t-1} = S_i, q_{t-2} = S_k \dots) = P(q_t = S_j | q_{t-1} = S_i)$$

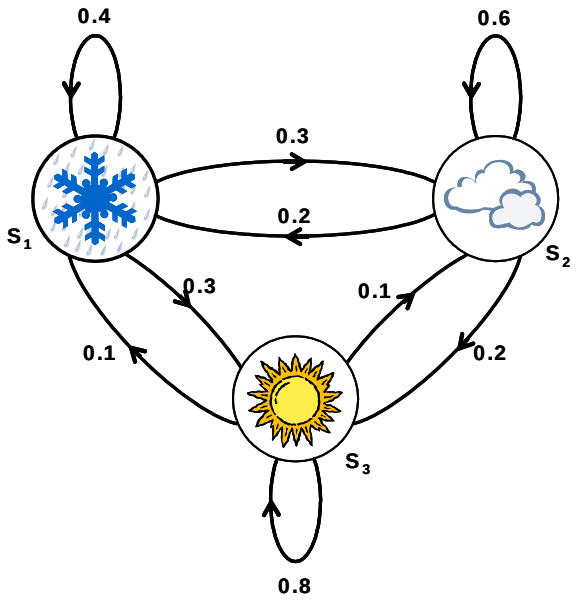
- This is known as a **first-order Markov Process**
- We will also assume that the transition probability between any two states is independent of time

$$a_{ij} = P(q_t = S_j | q_{t-1} = S_i) \;\; s.t. \begin{cases} a_{ij} \geq 0 \\ \sum_{j=1}^{N} a_{ij} = 1 \end{cases}$$

Example

- Consider a simple three-state Markov model of the weather
- Any given day, the weather can be described as being
  - State 1: precipitation (rain or snow)
  - State 2: cloudy
  - State 3: sunny
- Transitions between states are described by the transition matrix

$$A = \{a_{ij}\} = \begin{bmatrix} 0.4 & 0.3 & 0.3 \\ 0.2 & 0.6 & 0.2 \\ 0.1 & 0.1 & 0.8 \end{bmatrix}$$



- Question
  - Given that the weather on day t=1 is sunny, what is the probability that the weather for the next 7 days will be “sun, sun, rain, rain, sun, clouds, sun” ?
  - Answer:

$$
\begin{aligned}
&P(S_3, S_3, S_3, S_1, S_1, S_3, S_2, S_3 | model) \\
&= P(S_3)P(S_3|S_3)P(S_3|S_3)P(S_1|S_3)P(S_1|S_1)P(S_3|S_1)P(S_2|S_3)P(S_3|S_2) \\
&= \pi_3 a_{33} a_{33} a_{13} a_{11} a_{31} a_{23} a_{32} \\
&= 1 \times 0.8 \times 0.8 \times 0.1 \times 0.4 \times 0.3 \times 0.1 \times 0.2
\end{aligned}
$$

- Question
  - What is the probability that the weather stays in the same known state S_i for exactly T consecutive days?
  - Answer:

$$P\left(q_t = S_i, q_{t+1} = S_i \dots q_{t+T} = S_{j \neq i}\right) = a_{ii}^{T-1}(1 - a_{ii})$$

Hidden Markov models

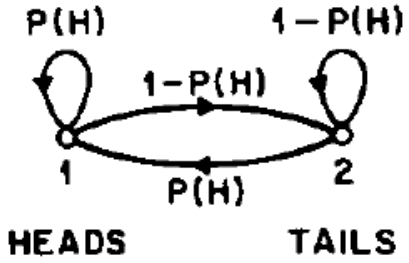
Introduction

- The previous model assumes that each state can be uniquely associated with an observable event
  - Once an observation is made, the state of the system is then trivially retrieved
  - This model, however, is too restrictive to be of practical use for most realistic problems
- To make the model more flexible, we will assume that the outcomes or observations of the model are a probabilistic function of each state
  - Each state can produce a number of outputs according to a unique probability distribution, and each distinct output can potentially be generated at any state
  - These are known a *Hidden Markov Models* (HMM), because the state sequence is not directly observable, it can only be approximated from the sequence of observations produced by the system

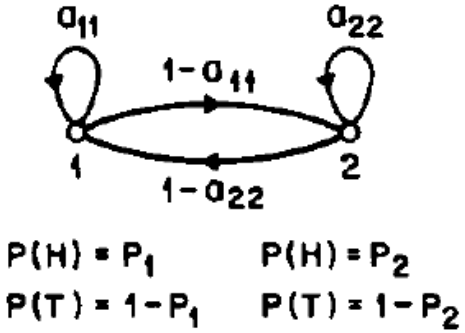
The coin-toss problem

- To illustrate the concept of an HMM, consider the following scenario
  - You are placed in a room with a curtain
  - Behind the curtain there is a person performing a coin-toss experiment
  - This person selects one of several coins, and tosses it: heads (H) or tails (T)
  - She tells you the outcome (H,T), but not which coin was used each time
- Your goal is to build a probabilistic model that best explains a sequence of observations $O = \{o_1, o_2, o_3 \ldots\} = \{H, T, T, H \ldots\}$
  - The coins represent the states; these are hidden because you do not know which coin was tossed each time
  - The outcome of each toss represents an observation
  - A "likely" sequence of coins may be inferred from the observations, but this state sequence will not be unique
- If the coins are hidden, how many states should the HMM have?

- One-coin model
  - In this case, we assume that the person behind the curtain only has one coin
  - As a result, the Markov model is observable since there is only one state
  - In fact, we may describe the system with a deterministic model where the states are the actual observations (see figure)
  - In either case, the model parameter P(H) may be found from the ratio of heads and tails

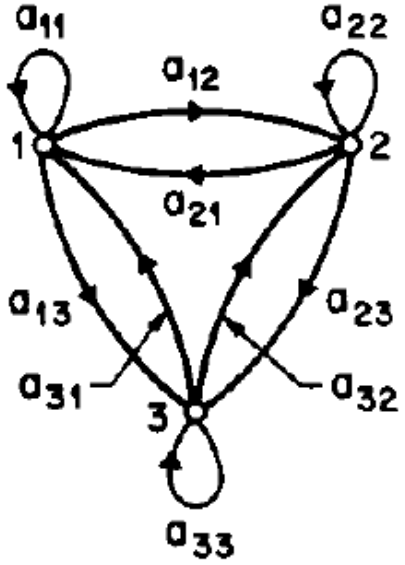


- Two-coin model
  - A more sophisticated HMM would be to assume that there are two coins
    - Each coin (state) has its own distribution of heads and tails, to model the fact that the coins may be biased
    - Transitions between the two states model the random process used by the person behind the curtain to select one of the coins
  - The model has 4 free parameters



[Rabiner, 1989]

- Three-coin model
  - In this case, the model would have three separate states
    - This HMM can be interpreted in a similar fashion as the two-coin model
  - The model has 9 free parameters



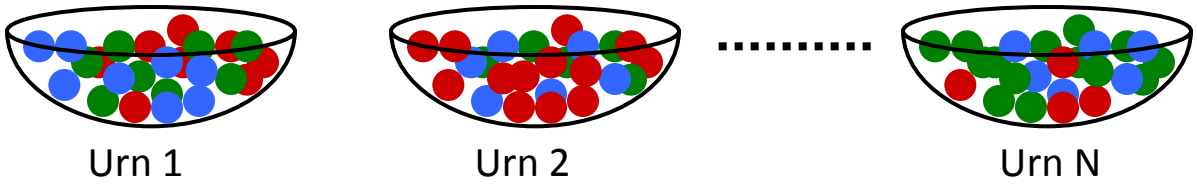
- Which of these models is best?
  - Since the states are not observable, the best we can do is select the model that best explains the data (e.g., using a Maximum Likelihood criterion)
  - Whether the observation sequence is long and rich enough to warrant a more complex model is a different story, though

	STATE 1	2	3
P(H)	P_1	P_2	P_3
P(T)	$1-P_1$	$1-P_2$	$1-P_3$

[Rabiner, 1989]

The urn-ball problem

- To further illustrate the concept of an HMM, consider this scenario
  - You are placed in the same room with a curtain
  - Behind the curtain there are N urns, each containing a large number of balls from M different colors
  - The person behind the curtain selects an urn according to an internal random process, then randomly grabs a ball from the selected urn
  - He shows you the ball, and places it back in the urn
  - This process is repeated over and over
- Questions
  - How would you represent this experiment with an HMM? What are the states? Why are the states hidden? What are the observations?



Elements of an HMM

- An HMM is characterized by the following set of parameters
  - N, the number of states in the model $S = \{S_1, S_2 \dots S_N\}$
  - M, the number of discrete observation symbols $V = \{v_1, v_2 \dots v_M\}$
  - $A = \{a_{ij}\}$, the state transition probability
    $$a_{ij} = P(q_{t+1} = S_j | q_t = S_i)$$
  - $B = \{b_j(k)\}$, the observation or emission probability distribution
    $$b_j(k) = P(o_t = v_k | q_t = S_j)$$
  - π, the initial state distribution
    $$\pi_j = P(q_1 = S_j)$$
- Therefore, an HMM is specified by two scalars (N and M) and three probability distributions (A,B, and π)
  - In what follows, we will represent an HMM by the compact notation
    $$\lambda = (A, B, \pi)$$

HMM generation of observation sequences

- Given a completely specified HMM $\lambda = (A, B, \pi)$, how can an observation sequence $O = \{o_1, o_2, o_3, o_4, \dots\}$ be generated?
  1. Choose an initial state S_1 according to the initial state distribution π
  2. Set $t = 1$
  3. Generate observation o_t according to the emission probability $b_j(k)$
  4. Move to a new state S_{t+1} according to state-transition at that state a_{ij}
  5. Set $t = t + 1$ and return to 3 until $t \geq T$
- Example
  - Generate an observation sequence with $T = 5$ for a coin tossing experiment with three coins and the following probabilities

	$\boldsymbol{S_1}$	$\boldsymbol{S_2}$	$\boldsymbol{S_3}$
$\boldsymbol{P(H)}$	0.5	0.75	0.25
$\boldsymbol{P(T)}$	0.5	0.25	0.75

$$A = \{a_{ij}\} = \frac{1}{3} \forall i, j \qquad \pi = \{\pi_i\} = \frac{1}{3} \ \forall i$$

The three basic HMM problems

- Problem 1: Probability Evaluation
  - Given observation sequence $O = \{o_1, o_2, o_3 \dots\}$ and model $\lambda = \{A, B, \pi\}$, how do we efficiently compute $P(O|\lambda)$, the likelihood of the observation sequence given the model?
    - The solution is given by the Forward and Backward procedures
- Problem 2: Optimal State Sequence
  - Given observation sequence $O = \{o_1, o_2, o_3 \dots\}$ and model λ, how do we choose a state sequence $Q = \{q_1, q_2, q_3 \dots\}$ that is optimal (i.e., best explains the data)?
    - The solution is provided by the Viterbi algorithm
- Problem 3: Parameter Estimation
  - How do we adjust the parameters of the model $\lambda = \{A, B, \pi\}$ to maximize the likelihood $P(O|\lambda)$
    - The solution is given by the Baum-Welch re-estimation procedure

Forward and Backward procedures

Problem 1: Probability Evaluation

- Our goal is to compute the likelihood of an observation sequence $O = \{o_1, o_2, o_3 \dots\}$ given a particular HMM model $\lambda = \{A, B, \pi\}$
- Computation of this probability involves enumerating every possible state sequence and evaluating the corresponding probability

$$P(O|\lambda) = \sum_{\forall Q} P(O|Q,\lambda)P(Q|\lambda)$$

- For a particular state sequence $Q = \{q_1, q_2, q_3 \dots\}$, $P(O|Q,\lambda)$ is

$$P(O|Q,\lambda) = \prod_{t=1}^{T} P(o_t|q_t,\lambda) = \prod_{t=1}^{T} b_{q_t}(o_t)$$

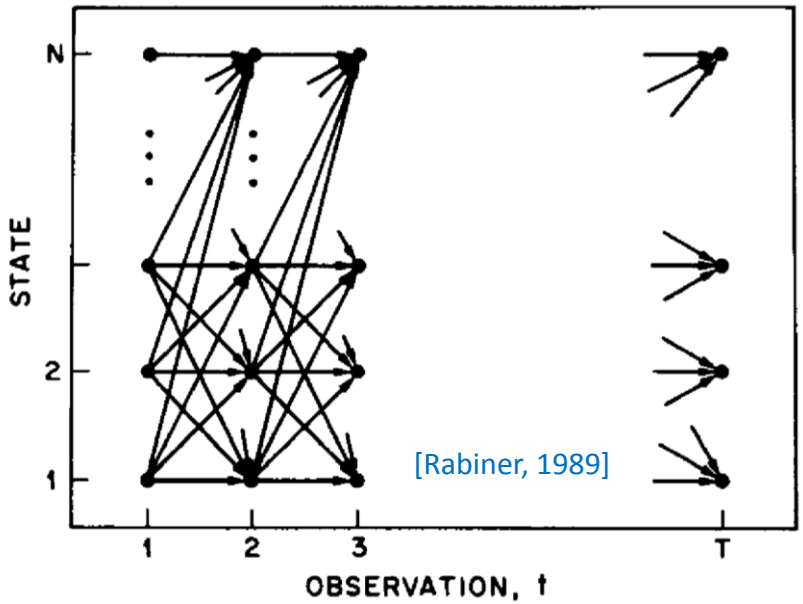
- The probability of the state sequence Q is

$$P(Q|\lambda) = \pi_{q_1} a_{q_1 q_2} a_{q_2 q_3} \dots a_{q_{T-1} q_T}$$

- Merging these results, we obtain

$$P(O|\lambda) = \sum_{q_1, q_2 \dots q_T} \pi_{q_1} b_{q_1}(o_{q_1})\, a_{q_1 q_2} b_{q_2}(o_{q_2}) \dots a_{q_{T-1} q_T} b_{q_T}(o_{q_T})$$

- Computational complexity
  - With N^T possible state sequences, this approach becomes unfeasible even for small problems… sound familiar?
    - For $N = 5$ and $T = 100$, the order of computations is in the order of 10^7
  - Fortunately, the computation of $P(O|\lambda)$ has a lattice (or trellis) structure, which lends itself to a very efficient implementation known as the *Forward procedure*



The Forward procedure

– Consider the following variable $\alpha_t(i)$ defined as

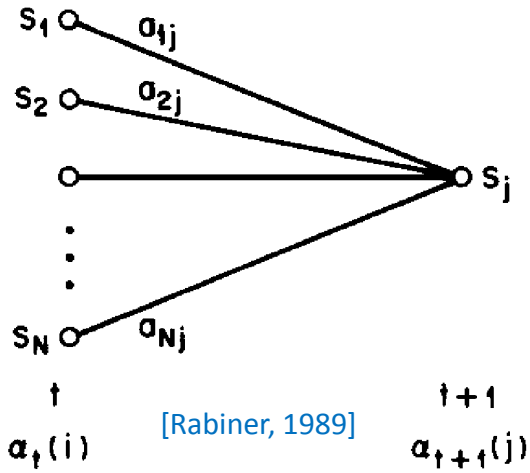
$$\alpha_t(i) = P(o_1, o_2 \dots o_t, q_t = S_i|\lambda)$$

- which represents the probability of the observation sequence up to time t AND the state S_i at time t, given model λ

– Computation of this variable can be efficiently performed by induction

- **Initialization:** $\alpha_1(i) = \pi_i b_i(o_1)$
- **Induction:** $\alpha_{t+1}(j) = \left[\sum_{i=1}^{N} \alpha_t(i) a_{ij}\right] b_j(o_{t+1}) \quad \begin{cases} 1 \le t \le \mathrm{T} - 1 \\ 1 \le j \le N \end{cases}$
- **Termination:** $P(O|\lambda) = \sum_{i=1}^{N} \alpha_T(i)$

- As a result, computation of $P(O|\lambda)$ can be reduced from $2T \times N^T$ down to $N^2 \times \mathrm{T}$ operations (from 10^{72} to 3000 for $N = 5, T = 100$)



[Rabiner, 1989]

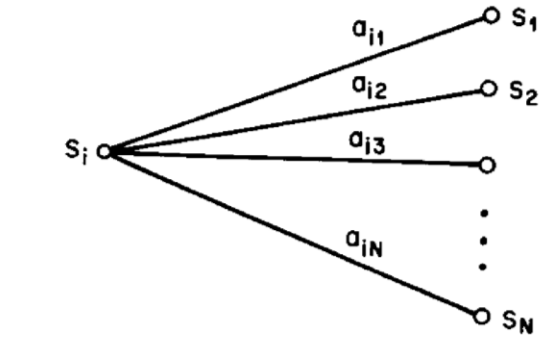
The Backward procedure

- Analogously, consider the backward variable $\beta_t(i)$ defined as

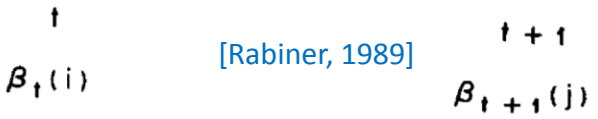
$$\beta_t(i) = P(o_{t+1}, o_{t+2} \dots o_T | q_t = S_i | \lambda)$$

- $\beta_t(i)$ represents the probability of the partial observation sequence from $t+1$ to the end, given state S_i at time t and model λ
  - As before, $\beta_t(i)$ can be computed through induction
  - **Initialization:** $\beta_T(i) = 1$ (arbitrarily)
  - **Induction:** $\beta_t(i) = \sum_{j=1}^{N} a_{ij} b_j(o_{t+1}) \beta_{t+1}(j)$ $\begin{cases} t = T-1, T-2 \dots 1 \\ 1 \le i \le N \end{cases}$

- Similarly, this computation can be effectively performed in the order of $N^2 \times T$ operations



[Rabiner, 1989]



The Viterbi algorithm

Problem 2: Optimal State Sequence

- Finding the optimal state sequence is more difficult problem that the estimation of $P(O|\lambda)$
- Part of the issue has to do with defining an optimality measure, since several criteria are possible
  - Finding the states q_t that are *individually* more likely at each time t
  - Finding the *single best* state sequence path (i.e., maximize the posterior $P(O|Q,\lambda)$
- The second criterion is the most widely used, and leads to the well-known Viterbi algorithm
  - However, we first optimize the first criterion as it allows us to define a variable that will be used later in the solution of Problem 3

- As in the Forward-Backward procedures, we define a variable $\gamma_t(i)$

$$\gamma_t(i) = P(q_t = S_i|O, \lambda)$$

  - which represents the probability of being in state S_i at time t, given the observation sequence O and model λ

- Using the definition of conditional probability, we can write

$$\gamma_t(i) = P(q_t = S_i|O, \lambda) = \frac{P(O, q_t = S_i|\lambda)}{P(O|\lambda)} = \frac{P(O, q_t = S_i|\lambda)}{\sum_{i=1}^{N} P(O, q_t = S_i|\lambda)}$$

- Now, the numerator of $\gamma_t(i)$ is equal to the product of $\alpha_t(i)$ and $\beta_t(i)$

$$\gamma_t(i) = \frac{P(O, q_t = S_i|\lambda)}{\sum_{i=1}^{N} P(O, q_t = S_i|\lambda)} = \frac{\alpha_t(i)\beta_t(i)}{\sum_{i=1}^{N} \alpha_t(i)\beta_t(i)}$$

- The individually most likely state q_t^* at each time is then

$$q_t^* = \arg\max_{1 \le i \le N}[\gamma_t(i)] \quad \forall t = 1 \dots T$$

- The problem with choosing the individually most likely states is that the overall state sequence may not be valid
  - Consider a situation where the individually most likely states are $q_t = S_i$ and $q_{t+1} = S_j$, but the transition probability $a_{ij} = 0$

- Instead, and to avoid this problem, it is common to look for the *single best* state sequence, at the expense of having sub-optimal individual states
- This is accomplished with the *Viterbi algorithm*

The Viterbi algorithm

- To find the single best state sequence we define yet another variable

$$\delta_t(i) = \max_{q_1 q_2 \ldots q_{t-1}} P(q_1 q_2 \ldots q_t = S_i, o_1 o_2 \ldots o_t | \lambda)$$

  - which represents the highest probability along a single path that accounts for the first t observations and ends at state S_i

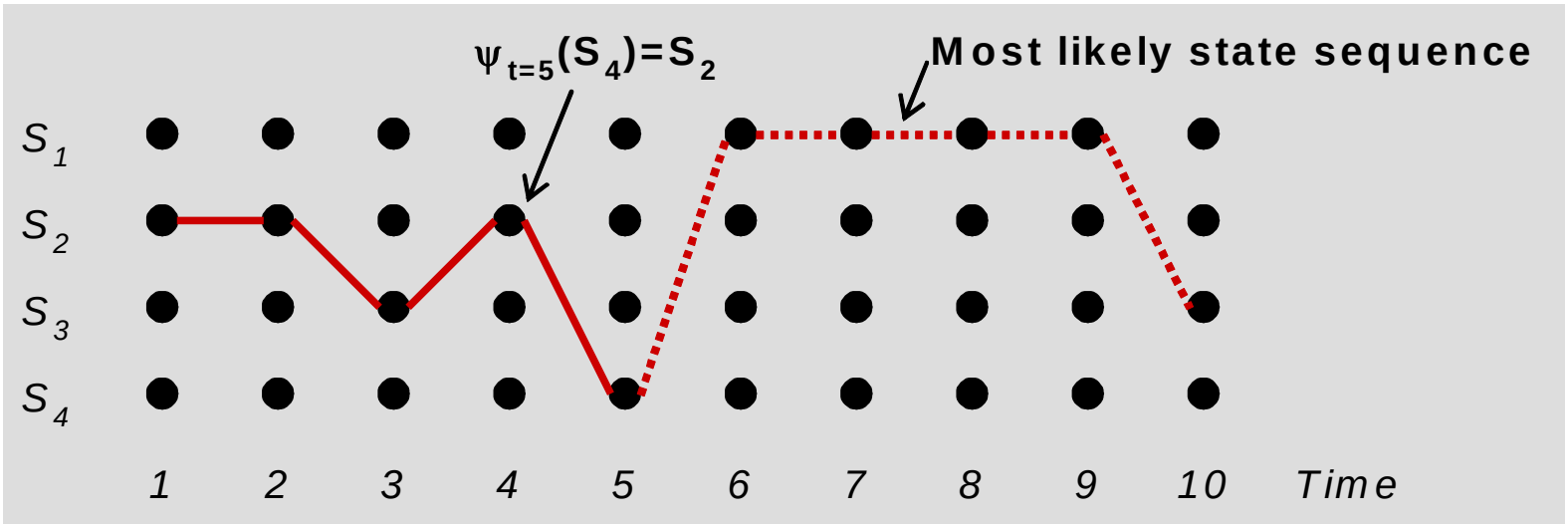
- By induction, $\delta_{t+1}(j)$ can be computed as

$$\delta_{t+1}(j) = \max_i \left[\delta_t(i) a_{ij}\right] b_j(o_{t+1})$$

- To retrieve the state sequence, we also need to keep track of the state that maximizes $\delta_t(i)$ at each time t, which is done by constructing an array

$$\Psi_{t+1}(j) = \arg\max_{1 \le i \le N} \left[\delta_t(i) a_{ij}\right]$$

  - $\Psi_{t+1}(j)$ is the state at time t from which a transition to state S_j maximizes the probability $\delta_{t+1}(j)$


$\psi_{t=5}(S_4)=S_2$
Most likely state sequence
S_1
S_2
S_3
S_4
1
2
3
4
5
6
7
8
9
10
Time

– The Viterbi algorithm for finding the optimal state sequence becomes

- **Initialization:**

$$\begin{cases} \delta_1(i) = \pi_i b_i(o_1) & 1 \le i \le N \\ \Psi_1(i) = 0 & \text{(no previous states)} \end{cases}$$

- **Recursion:**

$$\left.\begin{aligned} \delta_t(j) &= \max_{1 \le i \le N} \left[\delta_{t-1}(i) a_{ij}\right] b_j(o_t) \\ \Psi_t(j) &= \arg\max_{1 \le i \le N} \left[\delta_{t-1}(i) a_{ij}\right] \end{aligned}\right\} 2 \le t \le T; \;\; 1 \le j \le N$$

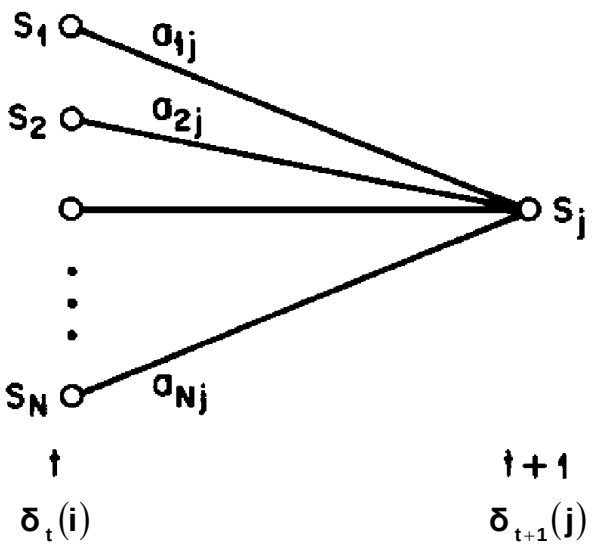
- **Termination:**

$$\begin{cases} P^* = \max_{1 \le i \le N} [\delta_T(i)] \\ q_T^* = \arg\max_{1 \le i \le N} [\delta_T(i)] \end{cases}$$

– And the optimal state sequence can be retrieved by backtracking

$$q_t^* = \Psi_{t+1}(q_{t+1}^*) \quad t = T-1, T-2 \ldots 1$$

– Notice that the Viterbi algorithm is similar to the Forward procedure, except that it uses a maximization over previous states instead of a summation



[Rabiner, 1989]

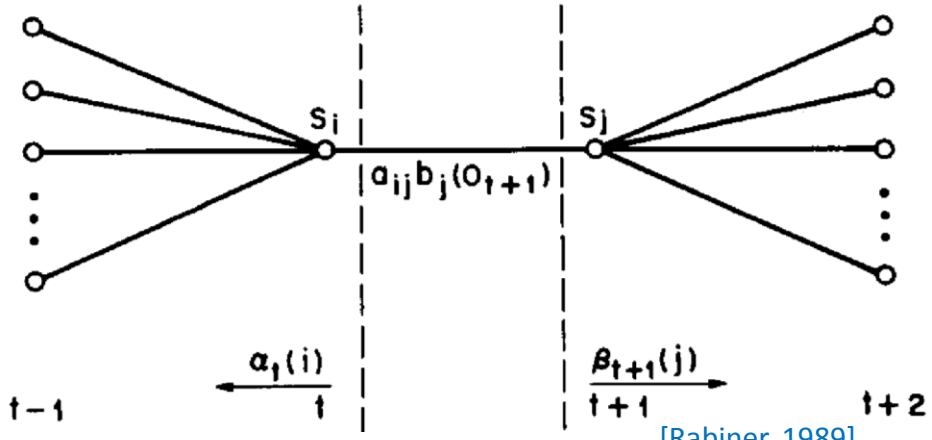
Baum-Welsh re-estimation

Problem 3: Parameter estimation

- The most important and difficult problem in HMMs is to estimate model parameters $\lambda = \{A, B, \pi\}$ from data
  - HMMs are trained with a Maximum Likelihood criterion: seek model parameters λ that best explain the observations, as measured by $P(O|\lambda)$
  - This problem is solved with an iterative procedure known as *Baum-Welch*, which is an implementation of the EM algorithm we discussed earlier
- As usual, we begin by defining a new variable, $\xi_t(i,j)$

$$\xi_t(i,j) = P(q_t = S_i, q_{t+1} = S_j | O, \lambda)$$

  - which is the probability of being in S_i at time t, and S_j at time $t+1$



[Rabiner, 1989]

- From the definition of $\alpha_t(i)$, $\beta_t(i)$ and conditional probability:

$$\xi_t(i,j) = \frac{P(q_t = S_i, q_{t+1} = S_j, O|\lambda)}{P(O|\lambda)} = \frac{\alpha_t(i)\, a_{ij}\, b_j(o_{t+1})\, \beta_{t+1}(j)}{P(O|\lambda)}$$
$$= \frac{\alpha_t(i)\, a_{ij}\, b_j(o_{t+1})\, \beta_{t+1}(j)}{\sum_{i=1}^{N}\sum_{j=1}^{N} \alpha_t(i)\, a_{ij}\, b_j(o_{t+1})\, \beta_{t+1}(j)}$$

- Intuitive interpretation of $\gamma_t(i)$ and $\xi_t(i,j)$
  - First note that, since $\gamma_t(i)$ is the probability of being in state S_i at time t given observation sequence O and model λ, $\xi_t(i,j)$ can be related to $\gamma_t(i)$ by

$$\gamma_t(i) = \sum_{j=1}^{N} \xi_t(i,j)$$

  - The sum of $\gamma_t(i)$ over time may be interpreted as the expected number of times that state S_i is visited or, excluding time $t = T$, the number of transitions from S_i

$$\sum_{t=1}^{T-1} \gamma_t(i) = \text{"expected number of transitions from state } S_i \text{ in O"}$$

  - Similarly, summation of $\xi_t(i,j)$ from $t = 1$ to $t = T - 1$ may be interpreted as the expected number of transitions from state S_i to state S_j

$$\sum_{t=1}^{T-1} \xi_t(i,j) = \text{"expected number of transitions from state } S_i \text{ to state } S_j\text{"}$$

Re-estimation procedure

- Using this line of reasoning, we can produce a method to iteratively update the parameters of an HMM by simply "counting events"

$$\hat{\pi}_i = \text{"expected frequency (number of times) in state } \mathrm{S_i} \text{ at time } (t=1)\text{"} = \gamma_1(i)$$

$$\hat{a}_{ij} = \frac{\text{"expected number of transitions from } \mathrm{S_i} \text{ to } \mathrm{S_j}\text{"}}{\text{"expected number of transitions from } \mathrm{S_i}\text{"}} = \frac{\sum_{t=1}^{T-1} \xi_t(i,j)}{\sum_{t=1}^{T-1} \gamma_t(i)}$$

$$\hat{b}_j(k) = \frac{\text{"expected number of times in } \mathrm{S_j} \text{ and obseving } \mathrm{v_k}\text{"}}{\text{"expected number of times in } \mathrm{S_j}\text{"}} = \frac{\sum_{\substack{t=1 \\ s.t. o_t = v_k}}^{T} \gamma_t(j)}{\sum_{t=1}^{T} \gamma_t(j)}$$

  - where the rhs of the equations is computed from the "old" parameter values, and the lhs are the re-estimated "new" parameters

- It can be shown that each iteration of this procedure increases the likelihood of the data until a local minimum is found

$$P\left(O|\lambda^{(new)}\right) \geq P\left(O|\lambda^{(old)}\right)$$

  - This property is due to the fact that Baum-Welch is an implementation of the Expectation-Maximization algorithm