PROBABILISTIC MODELS FOR STRUCTURED DATA

03: Hidden Markov Models

Instructor: Yizhou Sun

yzsun@cs.ucla.edu

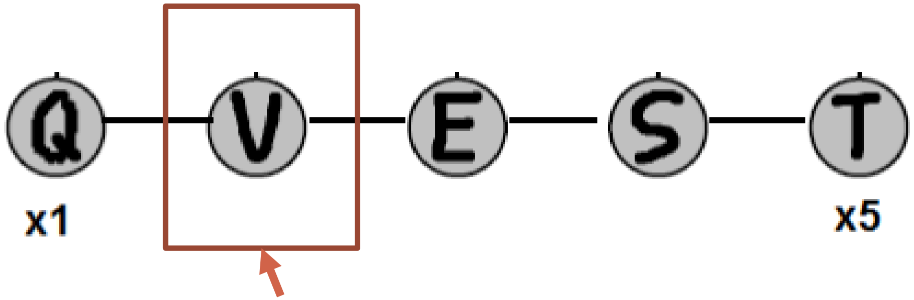
January 17, 2019

Content

- Preliminary: Markov Chains
- The Hidden Markov Model
- Inference
  - Likelihood Computation: The Forward Algorithm
  - Decoding: The Viterbi Algorithm
- Learning
  - The Forward-Backward Algorithm
- Summary

From I.I.D. Data to Sequence

- Dependency exists among data points, which form a sequence
- Examples
  - Speech recognition
  - Handwriting recognition



Is it a V or a U?

Note: this is a data model, not a graphical model

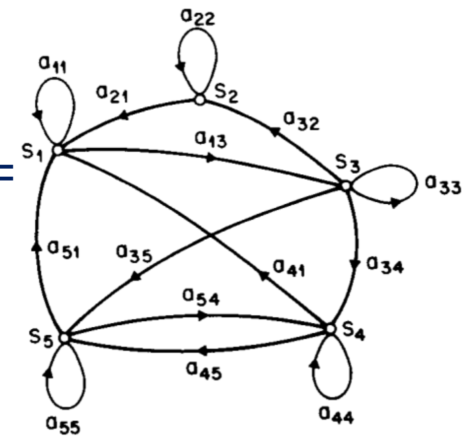
  - Named-entity recognition (NER)

(Discrete) Markov Chain

- Sequence
  - Ordered elements or events
    - $< x_1, x_2, \cdots, x_T >$
  - Examples:
    - A word, where each element is a letter
    - A sequence of text, where each element is a word
- Markov chain (also called observed Markov chain)
  - A probabilistic graphical model
  - Model how an observed sequence is generated

Definition of a First-Order Markov Chain

- N States: $S = \{S_1, S_2, \dots, S_N\}$
  - Sometimes, a start state S_0 and an end state S_F are included
  - Examples:
    - For a word sequence, 26 states are 26 letters
    - For a text sequence, |V| states are |V| words in the dictionary
- Transition probability matrix: $A = \{a_{ij}\}_{i,j=1}^{N}$
  - First order: $P(x_t = S_j | x_{t-1} = S_i, x_{t-2} = S_k, \dots) = P(x_t = S_j | x_{t-1} = S_i)$ *(Markov Assumption)*
  - $a_{ij} = P(x_t = S_j | x_{t-1} = S_i)$
    - $a_{ij} \geq 0$ and $\sum_j a_{ij} = 1$
- Initial distribution: $\pi = \{\pi_1, \pi_2, \dots, \pi_N\}$
  - $\pi_i = P(x_1 = S_i)$, the probability that the Markov chain starts with state S_i
    - $\pi_i \geq 0$ *and* $\sum_i \pi_i = 1$



Generation of a Sequence

- To generate an observed sequence: $\boldsymbol{x} = (x_1 x_2 \dots x_T)$
  - $For\ t = 1$, sample $x_1 \sim \pi$
  - $For\ t = 2{:}T$
    - Sample a new state $x_t | x_{t-1} \sim a_{x_{t-1}}$.

The Probability of a Sequence

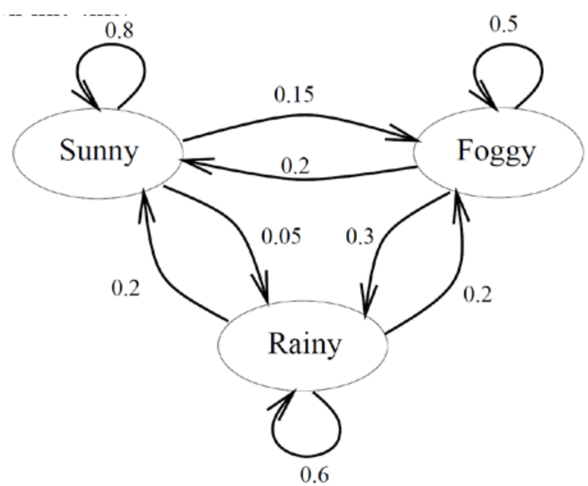
- Under first-order Markov chain model
  - $$P(x_1, x_2, \cdots, x_T) \\ = P(x_1)P(x_2|x_1) \ldots P(x_T|x_{T-1}, x_{T-2}, \ldots, x_1) \\ = P(x_1) \prod_{t=2} P(x_t|x_{t-1}) = \pi_{x_1} \prod_{t=2} a_{x_{t-1}x_t}$$

The Weather Example

- Three states: Sunny, Rainy, and Foggy
- Transition probability matrix

		Tomorrow's Weather		
		Sunny	Rainy	Foggy
Today's Weather	Sunny	0.8	0.05	0.15
	Rainy	0.2	0.6	0.2
	Foggy	0.2	0.3	0.5

represented as a table



represented as a graph

The Weather Example (Continued)

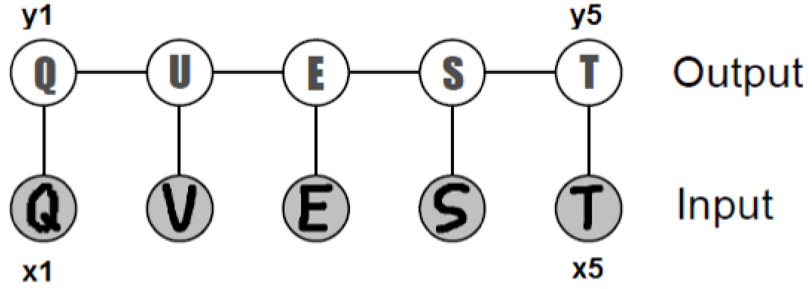
- Question 1: What's the probability that tomorrow is sunny and the day after is rainy, given today is sunny?
  - $P(x_2 = Sunny, x_3 = Rainy | x_1 = Sunny) = P(x_2 = Sunny | x_1 = Sunny) \times P(x_3 = Rainy | x_2 = Sunny) = 0.8 \times 0.05 = 0.04$
- Question 2: What's the probability it will be rainy two days from now, given today is foggy?
  - $P(x_3 = Rainy | x_1 = Foggy) = \sum_i P(x_3 = Rainy, x_2 = S_i | x_1 = Foggy) = P(x_3 = Rainy, x_2 = Sunny | x_1 = Foggy) + P(x_3 = Rainy, x_2 = Rainy | x_1 = Foggy) + P(x_3 = Rainy, x_2 = Foggy | x_1 = Foggy) = 0.34$

Content

- Preliminary: Markov Chains
- The Hidden Markov Model
- Inference
  - Likelihood Computation: The Forward Algorithm
  - Decoding: The Viterbi Algorithm
- Learning
  - The Forward-Backward Algorithm
- Summary

Hidden Markov Model

- States are not observable, observations are generated from a hidden state
  - Hidden state sequence
    - $< y_1, y_2, \ldots, y_T >$
  - Observation sequence
    - $< x_1, x_2, \ldots, x_T >$
- Examples
  - Speech recognition
  - Handwriting recognition



  - Named-entity recognition (NER)

Definition of a Discrete Hidden Markov Model

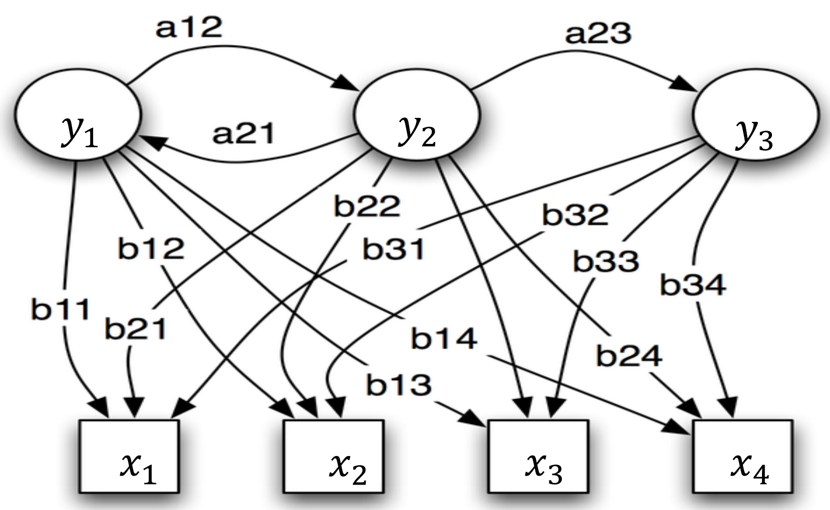
- N States: $S = \{S_1, S_2, \dots, S_N\}$
- M observation symbols: $V = \{v_1, v_2, \dots, v_M\}$
- Transition probability matrix: $A = \{a_{ij}\}_{i,j=1}^{N}$
  - $a_{ij} = P(y_t = S_j | y_{t-1} = S_i)$
    - $a_{ij} \geq 0$ and $\sum_j a_{ij} = 1$
- Observation symbol probability distribution: $B = \{b_{ik}\}, 1 \leq i \leq N, 1 \leq k \leq M$
  - $b_{ik} = P(x_t = v_k | y_t = S_i)$
    - $b_{ik} \geq 0$ and $\sum_k b_{ik} = 1$
- Initial distribution: $\pi = \{\pi_1, \pi_2, \dots, \pi_N\}$
  - $\pi_i = P(y_1 = S_i)$
    - $\pi_i \geq 0$ and $\sum_i \pi_i = 1$

Can be extended to numerical values

Multinoulli: Can be extended to other probabilistic distribution

Generation of a Sequence

- To generate an observed sequence: $\boldsymbol{x} = (x_1 x_2 \dots x_T)$
  - For $t = 1$, sample $y_1 \sim \pi$, sample $x_1 | y_1 \sim b_{y_1}$.
  - $For\ t = 2{:}T$
    - Sample a new state $y_t | y_{t-1} \sim a_{y_{t-1}}$.
    - Sample an observation $x_t | y_t \sim b_{y_t}$.



Three Basic Questions

- [**Likelihood Computation**] How likely is a given sequence?
  - The Forward algorithm
- [**Decoding**] What is the most probable "path" for generating a given sequence?
  - The Viterbi algorithm
- [**Learning**] How can we learn the HMM parameters given a set of sequences?
  - The Forward-Backward (Baum-Welch) algorithm

Content

- Preliminary: Markov Chains
- The Hidden Markov Model
- Inference
  - Likelihood Computation: The Forward Algorithm
  - Decoding: The Viterbi Algorithm
- Learning
  - The Forward-Backward Algorithm
- Summary

Likelihood Computation

- Given an HMM $\lambda = (A, B, \pi)$ and an observation sequence $\boldsymbol{x} = (x_1 x_2 \dots x_T)$, determine the likelihood $P(\boldsymbol{x}|\lambda)$
  - $P(\boldsymbol{x}|\lambda) = \sum_{\boldsymbol{y}} P(\boldsymbol{x}, \boldsymbol{y}|\lambda) = \sum_{\boldsymbol{y}} P(\boldsymbol{x}|\boldsymbol{y}, \lambda)\, P(\boldsymbol{y}|\lambda)$
    - $P(\boldsymbol{x}|\boldsymbol{y}, \lambda)$: the conditional probability of observation sequence when a state sequence known
      - $P(\boldsymbol{x}|\boldsymbol{y}, \lambda) = \prod_t P(x_t|y_t, \lambda) = \prod_t b_{y_t x_t}$
    - $P(\boldsymbol{y}|\lambda)$: the probability of a state sequence $\boldsymbol{y}$
      - $P(\boldsymbol{y}|\lambda) = P(y_1) \prod_{t=2} P(y_t|y_{t-1}) = \pi_{y_1} \prod_{t=2} a_{y_{t-1} y_t}$

Challenge of Brute-force Computation

- $P(\boldsymbol{x}|\lambda) = \sum_{\boldsymbol{y}} P(\boldsymbol{x}, \boldsymbol{y}|\lambda) = \sum_{\boldsymbol{y}} P(\boldsymbol{x}|\boldsymbol{y}, \lambda)\, P(\boldsymbol{y}|\lambda)$
  - Sum over all the possible state sequences
  - How many of them?
    - N^T (why?)

The Forward Algorithm

A special case of variable elimination

- A dynamic programming algorithm
  - Use table to store intermediate results
- Define forward variable $\alpha_t(j)$ as the probability of seeing the first *t* observations and the t-th state is *j*
  - $\alpha_t(j) = P(x_1, x_2, \dots, x_t, y_t = j|\lambda)$

$$= \sum_{y_1, y_2, \dots, y_{t-1}} P(y_1, y_2, \dots, y_{t-1}, y_t = j, x_1, x_2, \dots, x_t|\lambda)$$

- $\alpha_t(j)$ can be recursively defined as
  - $\alpha_t(j) = \sum_i \alpha_{t-1}(i) a_{ij} b_{jx_t}$ $(when\ 1 < t \leq T)$

$\alpha_{t-1}(i)$: $P(x_1, x_2, \dots, x_{t-1}, y_{t-1} = i)$

a_{ij}: $P(y_t = j|y_{t-1} = i)$

b_{jx_t}: $P(x_t|y_t = j)$

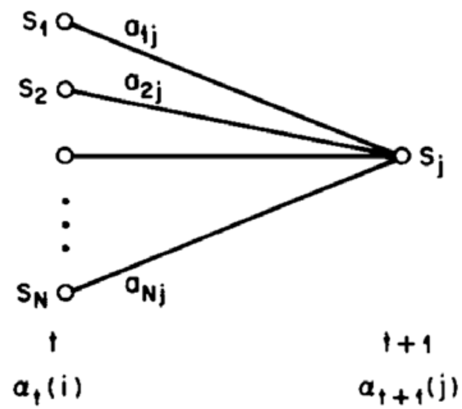
Major Steps

1. Initialization ($when\ t = 1$):
   - $\alpha_1(j) = \pi_j b_{jx_1},\ for\ 1 \le j \le N$
2. Recursion ($when\ 1 < t \le T$):
   - $\alpha_t(j) = \sum_i \alpha_{t-1}(i) a_{ij} b_{jx_t},\ for\ 1 \le j \le N$
3. Termination:
   - $P(\boldsymbol{x}|\lambda) = \sum_j \alpha_T(j)$

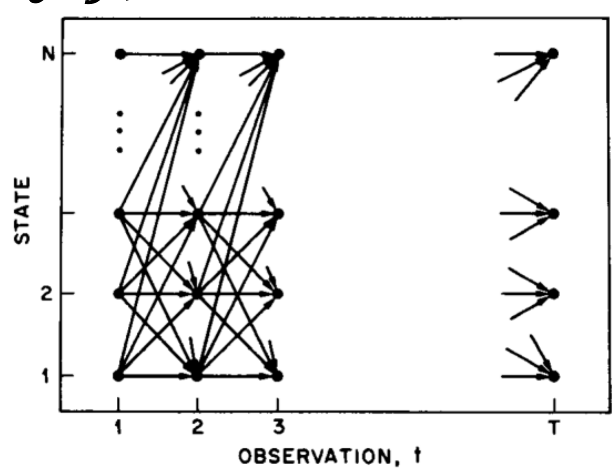
- Time complexity
  - $O(N^2T)$

Illustration

- Operations for computing $\alpha_{t+1}(j)$ from $\alpha_t(j)$



- Computing $\alpha_t(j)$ as a lattice



The Decoding Problem

- Given an HMM $\lambda = (A, B, \pi)$ and an observation sequence $\boldsymbol{x} = (x_1 x_2 \dots x_T)$, find the most probable sequence of states $\boldsymbol{y} = (y_1 y_2 \dots y_T)$
  - $\boldsymbol{y} = argmax_{\boldsymbol{y}} P(\boldsymbol{y}|\boldsymbol{x}, \lambda) = argmax_{\boldsymbol{y}} P(\boldsymbol{x}, \boldsymbol{y}|\lambda)$
- Brute-force computation
  - Enumerate all the possible state sequences, and pick the one with the maximum likelihood
  - Challenge: the same as before, N^T possible sequences!

The Viterbi Algorithm

- Also a dynamic programming algorithm

A special case of max product

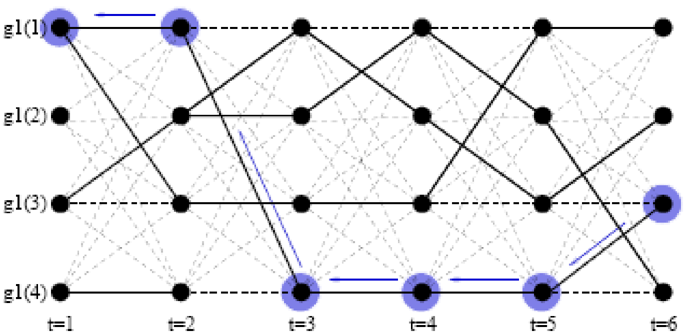
- Define $v_t(j)$ as the probability of the most probable path accounting for the first t observations and ending in state j

Almost identical to the forward algorithm, except replacing sum with max

  - $v_t(j) = \max_{y_1, y_2, \dots, y_{t-1}} P(y_1, y_2, \dots, y_{t-1}, y_t = j, x_1, x_2, \dots, x_t | \lambda)$
- $v_t(j)$ can be recursively defined as
  - $v_t(j) = \max_{\mathrm{i}} v_{t-1}(i) a_{ij} b_{jx_t} \; (1 < t \leq T)$
- Backtracking the best path
  - Keep the maximizing argument for each t and j

Major Steps

1. Initialization ($when\ t = 1$):
   - $v_1(j) = \pi_j b_{jx_1},\ for\ 1 \le j \le N$
2. Recursion ($when\ 1 < t \le T$):
   - $v_t(j) = \max_i v_{t-1}(i) a_{ij} b_{jx_t},\ for\ 1 \le j \le N$
   - $ptr_t(j) = argmax_i\ v_{t-1}(i) a_{ij} b_{jx_t},,\ for\ 1 \le j \le N$
   - Termination:
   - $P^* = maxP(\boldsymbol{y}|\boldsymbol{x},\lambda) = \max_j v_T(j)$
   - Backtracking from $argmax_j v_T(j)$



- Time complexity
  - $O(N^2T)$

Content

- Preliminary: Markov Chains
- The Hidden Markov Model
- Inference
  - Likelihood Computation: The Forward Algorithm
  - Decoding: The Viterbi Algorithm
- Learning
  - The Forward-Backward Algorithm
- Summary

Learning the Parameters of an HMM

- Given an observation sequence ***x*** and the set of possible states in the HMM, learn the HMM parameters $\lambda = (A, B, \pi)$
  - Find $\lambda = (A, B, \pi)$ that locally maximizes $P(\boldsymbol{x}|\lambda)$ (Maximum Likelihood Estimation, MLE)
    - Gradient techniques
    - Forward-backward algorithm (Baum-Welch algorithm)
      - A special case of EM (Expectation-Maximization) algorithm

How to Estimate Parameters for an Observed Markov Chain Model?

- MLE estimation
  - Find $\lambda = (A, \pi)$ that locally maximizes $P(\boldsymbol{y}|\lambda)$
    - $L(\lambda; \boldsymbol{y}) = P(\boldsymbol{y}|\lambda) = \pi_{y_1} \prod_{t=2} a_{y_{t-1}y_t}$
    - Constraints:
      - $\pi_i \geq 0 \; and \; \sum_i \pi_i = 1$
      - $a_{ij} \geq 0$ and $\sum_j a_{ij} = 1$
    - Lagrange multiplier method
      - $\widehat{\pi_i} = 1 \; if \; y_1 = i$
      - $\widehat{a_{ij}} = \frac{C(i \to j)}{\sum_{k \in S} C(i \to k)}$, where $C(i \to j)$ is the number of times state *i* transits to state *j*

How to Estimate Parameters *B* If Both *y* and *x* are observed?

- MLE estimation
  - Find B that maximizes $P(\boldsymbol{x}, \boldsymbol{y}|B)$
  - Equivalently find B that maximizes $P(\boldsymbol{x}|\boldsymbol{y}, B)$

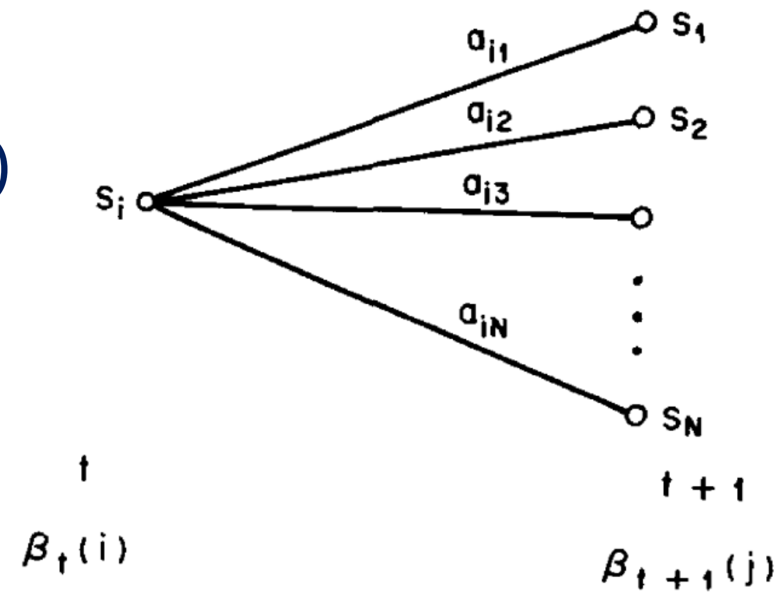
Backward Procedure

- Define backward probability $\beta_t(i)$ as the probability of seeing the observations from time $t+1$ to the end, given state at time t is *i*
  - $\beta_t(i) = P(x_{t+1}, x_{t+2}, \dots, x_T | y_t = i, \lambda)$
- $\beta_t(i)$ can be recursively defined as
  - $\beta_t(i) = \sum_j a_{ij} b_{j x_{t+1}} \beta_{t+1}(j)$
    - $P(x_{t+1}, x_{t+2}, \dots, x_T | y_t = i, \lambda) =$
      $\sum_j P(x_{t+1}, x_{t+2}, \dots, x_T, y_{t+1} = j | y_t = i, \lambda) =$
      $\sum_j P(x_{t+1}, x_{t+2}, \dots, x_T \, | \cancel{y_t = i}, y_{t+1} = j, \lambda) P(y_{t+1} = j | y_t = i, \lambda) =$

$= \sum_j P(x_{t+1} | y_{t+1} = j, \lambda) \, P(x_{t+2}, \dots, x_T | \cancel{x_{t+1}}, y_{t+1} = j, \lambda)$
$P(y_{t+1} = j | y_t = i, \lambda)$

Major Steps

1. Initialization $(when\ t = T)$:
   - $\beta_T(j) = 1, for\ 1 \leq j \leq N$
2. Recursion $(when\ 1 < t \leq T)$:
   - $\beta_t(i) = \sum_j a_{ij} b_{jx_{t+1}} \beta_{t+1}(j)\ , for\ 1 \leq j \leq N$
3. Termination:
   - $P(\boldsymbol{x}|\lambda) = \sum_j \pi_j b_{jx_1} \beta_1(j)$



- Time complexity
  - $O(N^2T)$

The Forward-Backward Algorithm

- Also called Baum-Welch algorithm
- A special case of EM algorithm
  - Repeat until converge
    - E-step:
      - Expected state occupancy count $\gamma_t(j) = P(y_t = j | \boldsymbol{x}, \lambda)$
        - Probability of being in state j at time t
      - Expected state transition count $\xi_t(i,j) = P(y_t = i, y_{t+1} = j | \boldsymbol{x}, \lambda)$
        - Probability of being in state i at time t and in state j at time t+1
    - M-step:
      - Estimate π_i, a_{ij}, b_{ik}

E-Step: Compute $\gamma_t(j)$

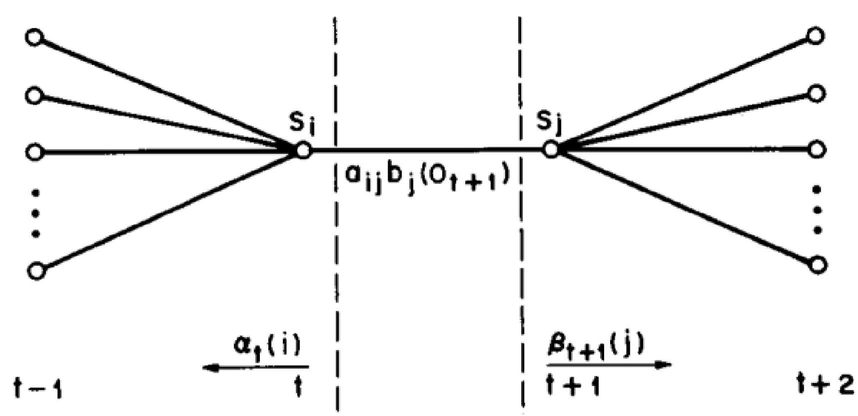
- $\gamma_t(j) = P(y_t = j|\boldsymbol{x}, \lambda) = \frac{P(y_t=j,\boldsymbol{x}|\lambda)}{P(\boldsymbol{x}|\lambda)}$
  - $P(y_t = j, \boldsymbol{x}|\lambda) =$
    $P(x_1, \dots, x_t, y_t = j|\lambda)P(x_{t+1}, \dots, x_T|\cancel{x_1, \dots, x_t,}\, y_t = j, \lambda)$
    $= \alpha_t(j)\beta_t(j)$
  - $P(\boldsymbol{x}|\lambda) = \sum_j \alpha_t(j)\beta_t(j)$

- Therefore, $\gamma_t(j) = \frac{\alpha_t(j)\beta_t(j)}{\sum_i \alpha_t(i)\beta_t(i)}$

E-Step: Compute $\xi_t(i,j)$

- $\xi_t(i,j) = P(y_t = i, y_{t+1} = j | \boldsymbol{x}, \lambda) = \frac{P(y_t = i, y_{t+1} = j, \boldsymbol{x} | \lambda)}{P(\boldsymbol{x}|\lambda)}$
  - $P(y_t = i, y_{t+1} = j, \boldsymbol{x}|\lambda) =$
    $P(x_1, \ldots, x_t, y_t = i|\lambda) P(y_{t+1} = j, x_{t+1}, \ldots x_T |$ ~~$x_1, \ldots, x_t,$~~ $y_t = i, \lambda)$
    $= P(x_1, \ldots, x_t, y_t = i|\lambda) P(y_{t+1} = j | y_t = i, \lambda) P(x_{t+1}, \ldots x_T | y_{t+1} = j)$
    $= \alpha_t(i) a_{ij} b_{j x_{t+1}} \beta_{t+1}(j)$
  - $P(\boldsymbol{x}|\lambda) = \sum_i \sum_j \alpha_t(i) a_{ij} b_{j x_{t+1}} \beta_{t+1}(j)$

- Therefore, $\xi_t(i,j) = \frac{\alpha_t(i) a_{ij} b_{j x_{t+1}} \beta_{t+1}(j)}{\sum_i \sum_j \alpha_t(i) a_{ij} b_{j x_{t+1}} \beta_{t+1}(j)}$

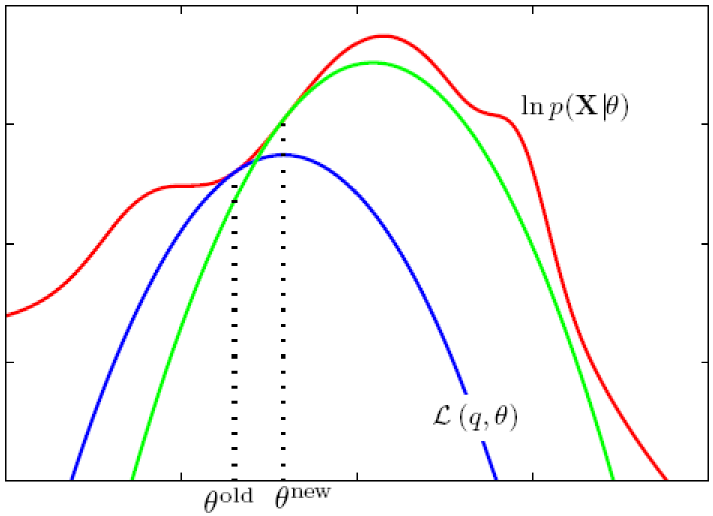


M-Step

- π_i
  - $\widehat{\pi_i} = \gamma_1(i)$
- a_{ij}
  - $\widehat{a_{ij}} = \frac{\sum_{t=1}^{T-1} \xi_t(i,j)}{\sum_k \sum_{t=1}^{T-1} \xi_t(i,k)}$
- b_{ik}
  - $\widehat{b_{ik}} = \frac{\sum_{x_t = v_k} \gamma_t(i)}{\sum_{t=1}^{T} \gamma_t(i)}$

More on EM Algorithm

- E-Step: computing a **tight** lower bound L of the original objective function l at θ_{old}
- M-Step: find θ_{new} to maximize the lower bound
- $l(\theta_{new}) \geq L(\theta_{new}) \geq L(\theta_{old}) = l(\theta_{old})$



How to Find Tight Lower Bound?

- $$\begin{aligned} \ell(\theta) &= \log \sum_h p(d,h;\theta) \\ &= \log \sum_h \frac{q(h)}{q(h)} p(d,h;\theta) \\ &= \log \sum_h q(h) \frac{p(d,h;\theta)}{q(h)} \end{aligned}$$

$q(h)$: a distribution function over h, the key to tight lower bound we want to get

- Jensen's inequality
  - $$\log \sum_h q(h) \frac{p(d,h;\theta)}{q(h)} \geq \sum_h q(h) \log \frac{p(d,h;\theta)}{q(h)}$$

the tight lower bound

- When "=" holds to get a tight lower bound?
  - $q(h) = p(h|d,\theta)$ (why?)

Content

- Preliminary: Markov Chains
- The Hidden Markov Model
- Inference
  - Likelihood Computation: The Forward Algorithm
  - Decoding: The Viterbi Algorithm
- Learning
  - The Forward-Backward Algorithm
- Summary

Summary

- Preliminary: Markov Chains
  - Generative model for observed state sequence
- The Hidden Markov Model
  - Generative model for sequence where states are unseen
- Inference
  - Likelihood Computation: The Forward Algorithm
    - Dynamic programming; Forward variable: $\alpha_t(i)$
  - Decoding: The Viterbi Algorithm
    - $v_t(j)$
- Learning
  - The Forward-Backward Algorithm
    - Backward variable: $\beta_t(i)$

References

- Matlab Code: https://www.mathworks.com/help/stats/hidden-markov-models-hmm.html
- Lawrence R. Rabiner. A Tutorial on Hidden Markov Models. 2009
- Daniel Jurafsky & James H. Martin. Speech and Language Processing, Chapter 9. 2017