Aarti Singh Slides courtesy: Eric Xing

Machine Learning 10-701 Apr 10, 2023

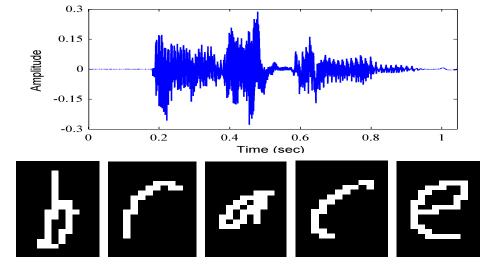




i.i.d to sequential data

- Independent, identically distributed data
- Sequential data
 - Time-series dataE.g. Speech
 - Characters in a sentence

$$\{X_i\}_{i=1}^n \stackrel{iid}{\sim} p(\mathbf{X})$$



Base pairs along a DNA strand



Markov Models

Joint Distribution

$$p(\mathbf{X}) = p(X_1, X_2, \dots, X_n)$$

$$= p(X_1)p(X_2|X_1)p(X_3|X_2, X_1) \dots p(X_i|X_{i-1}, \dots, X_1)$$

$$= \prod_{i=1}^n p(X_i|X_{i-1}, \dots, X_1) \quad \text{Chain rule}$$

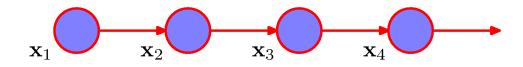
Markov Assumption (mth order)

$$p(\mathbf{X}) = \prod_{i=1}^n p(X_i|X_{i-1},\dots,X_{i-m})$$
 Current observation only depends on past m observations

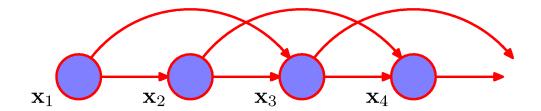
Markov Models

Markov Assumption

$$p(\mathbf{X}) = \prod_{i=1}^{n} p(X_i|X_{i-1})$$



$$p(\mathbf{X}) = \prod_{i=1} p(X_i|X_{i-1}, X_{i-2})$$



Markov Models

Markov Assumption

1st order
$$p(\mathbf{X}) = \prod_{i=1} p(X_i|X_{i-1})$$

parameters in stationary model d-ary variables

 $O(d^2)$

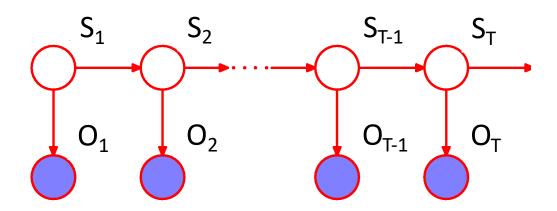
$$\mathbf{m}^{\mathsf{th}} \ \mathsf{order} \qquad p(\mathbf{X}) \quad = \quad \prod_{i=1} p(X_i | X_{i-1}, \dots, X_{i-m}) \ \ \mathsf{O}(\mathsf{d}^{\mathsf{m+1}})$$

$$\mathsf{n-1^{\mathsf{th}}} \ \mathsf{order} \quad p(\mathbf{X}) \quad = \quad \prod_{i=1}^{n} p(X_i|X_{i-1},\ldots,X_1) \qquad \qquad \mathsf{O(d^n)}$$

≡ no assumptions – complete graph

Homogeneous/stationary Markov model (probabilities of transitioning from a particular state value to another value doesn't depend on i)

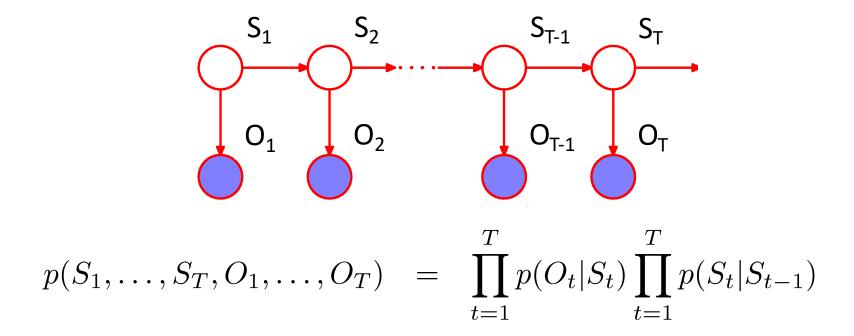
 Distributions that characterize sequential data with few parameters but are not limited by strong Markov assumptions.



Observation space Hidden states

$$O_t \in \{y_1, y_2, ..., y_K\}$$

 $S_t \in \{1, ..., S\}$



 1^{st} order Markov assumption on hidden states $\{S_t\}$ t = 1, ..., T (can be extended to higher order).

Note: O_t depends on all previous observations $\{O_{t-1},...O_1\}$

 Parameters – stationary/homogeneous markov model (independent of time t)

Initial probabilities

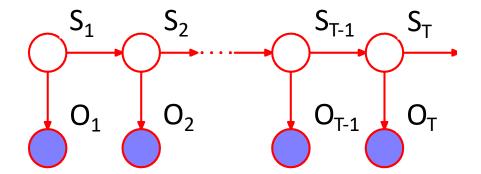
$$p(S_1 = i) = \pi_i$$

Transition probabilities

$$p(S_t = j | S_{t-1} = i) = p_{ij}$$

Emission probabilities

$$p(O_t = y | S_t = i) = q_i^y$$



$$p(\{S_t\}_{t=1}^T, \{O_t\}_{t=1}^T) = p(S_1) \prod_{t=2}^T p(S_t|S_{t-1}) \prod_{t=1}^T p(O_t|S_t)$$

HMM Example

The Dishonest Casino

A casino has two die:

Fair dice

$$P(1) = P(2) = P(3) = P(5) = P(6) = 1/6$$

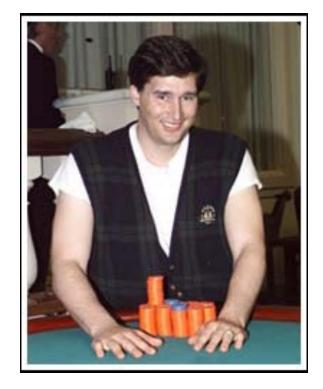
Loaded dice

$$P(1) = P(2) = P(3) = P(5) = 1/10$$

$$P(6) = \frac{1}{2}$$

Casino player switches back-&forth between fair and loaded die once every 20 turns





HMM Problems

GIVEN: A sequence of rolls by the casino player

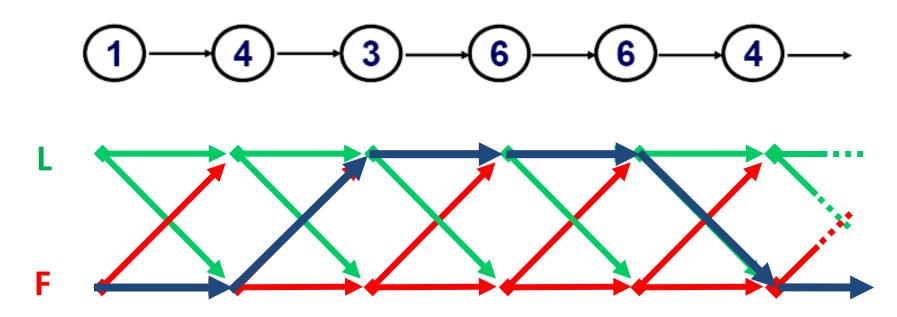
1245526462146146136136661664661636616366163616515615115146123562344

QUESTION

- How likely is this sequence, given our model of how the casino works?
 - This is the EVALUATION problem in HMMs
- What portion of the sequence was generated with the fair die, and what portion with the loaded die?
 - This is the **DECODING** question in HMMs
- How "loaded" is the loaded die? How "fair" is the fair die? How often does the casino player change from fair to loaded, and back?
 - This is the **LEARNING** question in HMMs

HMM Example

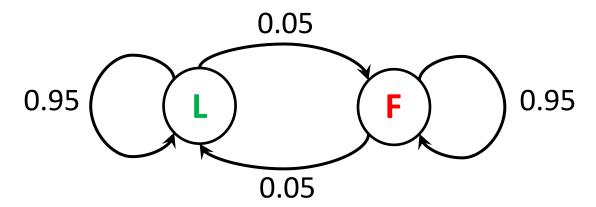
• Observed sequence: $\{O_t\}_{t=1}^T$



• Hidden sequence $\{S_t\}_{t=1}^T$ or segmentation):

State Space Representation

Switch between F and L once every 20 turns (1/20 = 0.05)



HMM Parameters

Initial probs
Transition probs

Emission probabilities

$$P(S_1 = L) = 0.5 = P(S_1 = F)$$

 $P(S_t = L/F | S_{t-1} = L/F) = 0.95$
 $P(S_t = F/L | S_{t-1} = L/F) = 0.05$
 $P(O_t = y | S_t = F) = 1/6$ $y = 1,2,3,4,5,6$
 $P(O_t = y | S_t = L) = 1/10$ $y = 1,2,3,4,5$
 $= 1/2$ $y = 6$

Three main problems in HMMs

- Evaluation Given HMM parameters & observation seqn $\{O_t\}_{t=1}^T$ find $p(\{O_t\}_{t=1}^T)$ prob of observed sequence
- Decoding Given HMM parameters & observation seqn $\{O_t\}_{t=1}^T$ find $\arg\max_{s_1,\dots,s_T}p(\{S_t\}_{t=1}^T|\{O_t\}_{t=1}^T)$ most probable sequence of hidden states
- Learning Given HMM with unknown parameters and $\{O_t\}_{t=1}^T$ observation sequence

find $\arg\max_{\theta} p(\{O_t\}_{t=1}^T | \theta)$ parameters that maximize likelihood of observed data

HMM Algorithms

 Evaluation – What is the probability of the observed sequence? Forward Algorithm

- Decoding What is the probability that the third roll was loaded given the observed sequence? Forward-Backward Algorithm
 - What is the most likely die sequence given the observed sequence? Viterbi Algorithm
- Learning Under what parameterization is the observed sequence most probable? Baum-Welch Algorithm (EM)

Evaluation Problem

Given HMM parameters $p(S_1), p(S_t|S_{t-1}), p(O_t|S_t)$ & observation sequence $\{O_t\}_{t=1}^T$

find probability of observed sequence
$$p(\{O_t\}_{t=1}^T) = \sum_{S_1,...,S_T} p(\{O_t\}_{t=1}^T, \{S_t\}_{t=1}^T)$$

$$= \sum_{S_1,...,S_T} p(S_1) \prod_{t=2}^T p(S_t|S_{t-1}) \prod_{t=1}^T p(O_t|S_t)$$

requires summing over all possible hidden state values at all times – S^T exponential # terms!

Instead:
$$p(\{O_t\}_{t=1}^T) = \sum_k p(\{O_t\}_{t=1}^T, S_T = k)$$

$$\alpha_{\mathsf{T}}^{\mathsf{k}} \quad \textit{Compute recursively}$$

Forward Probability

$$p(\{O_t\}_{t=1}^T) = \sum_k p(\{O_t\}_{t=1}^T, S_T = k) = \sum_k \alpha_T^k$$

Compute forward probability α_t^k recursively over t

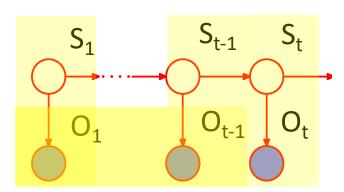
$$\alpha_t^k := p(O_1, \dots, O_t, S_t = k)$$

Introduce S_{t-1}

Chain rule

Markov assumption

$$= p(O_t|S_t = k) \sum_{i} \alpha_{t-1}^i p(S_t = k|S_{t-1} = i)$$



Forward Algorithm

Can compute α_t^k for all k, t using dynamic programming:

• Initialize:
$$\alpha_1^k = p(O_1 | S_1 = k) p(S_1 = k)$$
 for all k

• Iterate: for t = 2, ..., T

$$\alpha_t^k = p(O_t | S_t = k) \sum_i \alpha_{t-1}^i p(S_t = k | S_{t-1} = i)$$
 for all k

• Termination:
$$p(\{O_t\}_{t=1}^T) = \sum_{k} \alpha_T^k$$

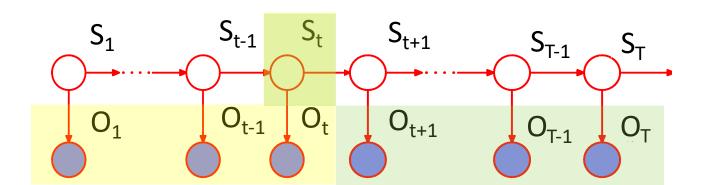
Decoding Problem 1

• Given HMM parameters $p(S_1), p(S_t|S_{t-1}), p(O_t|S_t)$ & observation sequence $\{O_t\}_{t=1}^T$

find probability that hidden state at time t was k $p(S_t = k | \{O_t\}_{t=1}^T)$

$$p(S_t=k,\{O_t\}_{t=1}^T) = p(O_1,\ldots,O_t,S_t=k,O_{t+1},\ldots,O_T)$$

$$= p(O_1,\ldots,O_t,S_t=k)p(O_{t+1},\ldots,O_T|S_t=k)$$
 Compute recursively
$$\alpha_t^k$$



Backward Probability

$$p(S_t = k, \{O_t\}_{t=1}^T) = p(O_1, \dots, O_t, S_t = k) p(O_{t+1}, \dots, O_T | S_t = k) = \alpha_t^k \beta_t^k$$

Compute forward probability β_t^k recursively over t

Chain rule

Markov assumption

$$= \sum_{i} p(S_{t+1} = i | S_t = k) p(O_{t+1} | S_{t+1} = i) \beta_{t+1}^{i}$$

Backward Algorithm

Can compute β_t^k for all k, t using dynamic programming:

- Initialize: $\beta_T^k = 1$ for all k
- Iterate: for t = T-1, ..., 1

$$\beta_t^k = \sum_i p(S_{t+1} = i | S_t = k) p(O_{t+1} | S_{t+1} = i) \beta_{t+1}^i$$
 for all k

• Termination: $p(S_t = k, \{O_t\}_{t=1}^T) = \alpha_t^k \beta_t^k$

$$p(S_t = k | \{O_t\}_{t=1}^T) = \frac{p(S_t = k, \{O_t\}_{t=1}^T)}{p(\{O_t\}_{t=1}^T)} = \frac{\alpha_t^k \beta_t^k}{\sum_i \alpha_t^i \beta_t^i}$$

Most likely state vs. Most likely sequence

Most likely state assignment at time t

$$\arg\max_{k} p(S_t = k | \{O_t\}_{t=1}^T) = \arg\max_{k} \alpha_t^k \beta_t^k$$

E.g. Which die was most likely used by the casino in the third roll given the observed sequence?

Most likely assignment of state sequence

$$\arg\max_{\{S_t\}_{t=1}^T} p(\{S_t\}_{t=1}^T | \{O_t\}_{t=1}^T)$$

E.g. What was the most likely sequence of die rolls used by the casino given the observed sequence?

Not the same solution!

MLA of x? MLA of (x,y)? P(x,y)

0.05

0.3 0.3

Decoding Problem 2

• Given HMM parameters $p(S_1), p(S_t|S_{t-1}), p(O_t|S_t)$ & observation sequence $\{O_t\}_{t=1}^T$

find most likely assignment of state sequence

$$\arg\max_{\{S_t\}_{t=1}^T} p(\{S_t\}_{t=1}^T | \{O_t\}_{t=1}^T) = \arg\max_{\{S_t\}_{t=1}^T} p(\{S_t\}_{t=1}^T, \{O_t\}_{t=1}^T)$$

$$= \arg\max_{k} \max_{\{S_t\}_{t=1}^{T-1}} p(S_T = k, \{S_t\}_{t=1}^{T-1}, \{O_t\}_{t=1}^T)$$

$$\bigvee_{\mathsf{T}}^{\mathsf{K}}$$

Compute recursively

 V_T^k - probability of most likely sequence of states ending at state $S_T = k$

Viterbi Decoding

$$\max_{\{S_t\}_{t=1}^T} p(\{S_t\}_{t=1}^T, \{O_t\}_{t=1}^T) = \max_k V_T^k$$

Compute probability V_t recursively over t

$$V_t^k := \max_{S_1, \dots, S_{t-1}} p(S_t = k, S_1, \dots, S_{t-1}, O_1, \dots, O_t)$$

Chain rule

Markov assumption

O₁

O_{t-1}

$$= p(O_t|S_t = k) \max_{i} p(S_t = k|S_{t-1} = i)V_{t-1}^i$$

Viterbi Algorithm

Can compute V_t^k for all k, t using dynamic programming:

• Initialize:
$$V_1^k = p(O_1|S_1=k)p(S_1=k)$$
 for all k

• Iterate: for t = 2, ..., T

$$V_t^k = p(O_t|S_t = k) \max_i p(S_t = k|S_{t-1} = i)V_{t-1}^i$$
 for all k

• Termination:
$$\max_{\{S_t\}_{t=1}^T} p(\{S_t\}_{t=1}^T, \{O_t\}_{t=1}^T) = \max_k V_T^k$$

Traceback:
$$S_T^* = \arg\max_k V_T^k$$

$$S_{t-1}^* = \arg\max_i p(S_t^*|S_{t-1}=i)V_{t-1}^i$$

Computational complexity

 What is the running time for Forward, Forward-Backward, Viterbi?

$$\alpha_t^k = q_k^{O_t} \sum_i \alpha_{t-1}^i p_{i,k}$$

$$\beta_t^k = \sum_i p_{k,i} q_i^{O_{t+1}} \beta_{t+1}^i$$

$$V_t^k = q_k^{O_t} \max_i p_{i,k} V_{t-1}^i$$

O(S²T) linear in T instead of O(S^T) exponential in T!

Learning Problem

• Given HMM with unknown parameters $\theta = \{\{\pi_i\}, \{p_{ij}\}, \{q_i^k\}\}$ and observation sequence $\mathbf{O} = \{O_t\}_{t=1}^T$

find parameters that maximize likelihood of observed data

$$\arg\max_{\theta} p(\{O_t\}_{t=1}^T | \theta)$$

But likelihood doesn't factorize since observations not i.i.d.

hidden variables – state sequence $\{S_t\}_{t=1}^T$

EM (Baum-Welch) Algorithm:

E-step – Fix parameters, find expected state assignments

M-step – Fix expected state assignments, update parameters

Baum-Welch (EM) Algorithm

- Start with random initialization of parameters
- E-step Fix parameters, find expected state assignments

$$\gamma_i(t) = p(S_t = i|O, \theta) = \frac{\alpha_t^i \beta_t^i}{\sum_j \alpha_t^j \beta_t^j}$$

Forward-Backward algorithm

$$\xi_{ij}(t) = p(S_{t-1} = i, S_t = j | O, \theta)$$

$$= \frac{p(S_{t-1} = i | O, \theta) p(S_t = j, O_t, \dots, O_T | S_{t-1} = i, \theta)}{p(O_t, \dots, O_T | S_{t-1} = i, \theta)}$$

$$= \frac{\gamma_i(t-1) p_{ij} q_j^{O_t} \beta_t^j}{\beta_{t-1}^i}$$

Baum-Welch (EM) Algorithm

- Start with random initialization of parameters
- E-step

$$\gamma_i(t) = p(S_t = i|O,\theta)$$

$$\xi_{ij}(t) = p(S_{t-1} = i, S_t = j | O, \theta)$$

$$\sum_{t=1}^{T} \gamma_i(t) = \text{expected \# times}$$
 in state i
$$\sum_{t=1}^{T-1} \gamma_i(t) = \text{expected \# transitions}$$

$$\sum_{t=1}^{T-1} \xi_{ij}(t) = \text{expected \# transitions}$$
 from state i to j

from state i

M-step

$$\pi_i = \gamma_i(1)$$

$$p_{ij} = \frac{\sum_{t=1}^{T-1} \xi_{ij}(t)}{\sum_{t=1}^{T-1} \gamma_i(t)}$$

$$q_i^k = \frac{\sum_{t=1}^T \delta_{O_t = k} \gamma_i(t)}{\sum_{t=1}^T \gamma_i(t)}$$

HMMs.. What you should know

- Useful for modeling sequential data with few parameters using discrete hidden states that satisfy Markov assumption
- Representation initial prob, transition prob, emission prob,
 State space representation
- Algorithms for inference and learning in HMMs
 - Computing marginal likelihood of the observed sequence: forward algorithm
 - Predicting a single hidden state: forward-backward
 - Predicting an entire sequence of hidden states: viterbi
 - Learning HMM parameters: an EM algorithm known as Baum-Welch