CSCI567 Machine Learning (Fall 2017)

Prof. Fei Sha

U of Southern California

Lecture on Oct. 26, 2017

Outline

Outline

Schedule change

- Quiz 2 is to be moved to 11/2.
  - If you had written to me about this date, I have finalized and replied to you on 10/25 already
  - If you do not think you have received the email on 10/25 on me, please write to me as soon as possible
- Homework 4 has two deadlines, one for the algorithmic component and the other for programming.

Outline

Generative

- Aim to model the joint distribution $p(x, y)$. For naive Bayes and Gaussian discriminant analysis, this is done by assuming the form

$$p(x, y) = p(y)p(x|y)$$

  and then model $p(x|y)$ and $p(y)$ separately.
- Parameters of the distribution are estimated by maximizing the likelihood

$$\max_{\theta} \sum_{n} \log p(x_n, y_n; \theta)$$

- To classify, compute the posterior probability and identify the latest one

$$\arg\max_y p(y|x) = \arg\max_y p(x, y)$$

Discriminative (such as logistic regression)

- Aim to model the conditional distribution

$$p(y|x)$$

- Parameters of the distribution are estimated by maximizing the conditional likelihood

$$\max_{\theta} \sum_{n} \log p(y_n|x_n;\theta)$$

- To classify, compute the model out

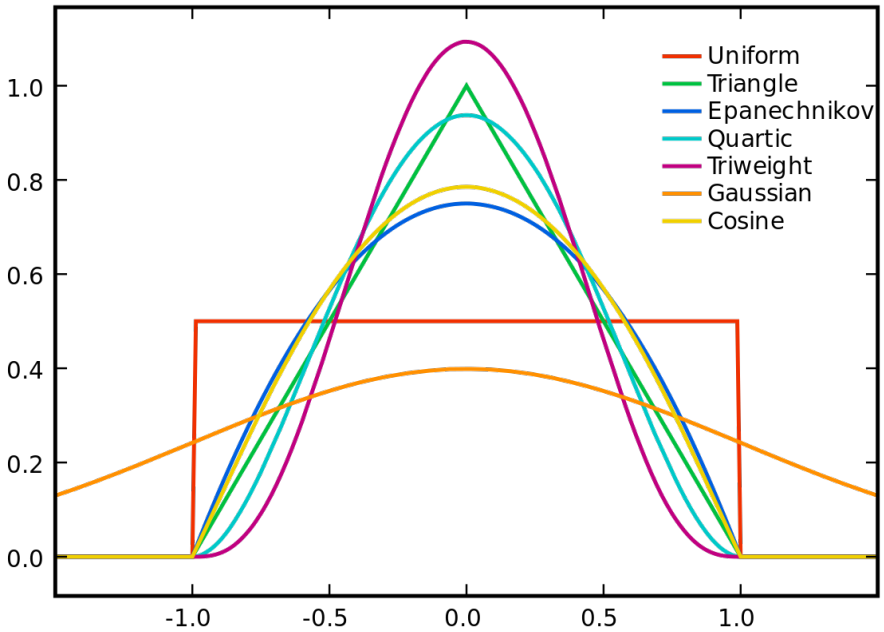
$$\arg\max_y p(y|x) = \arg\max_y p(y|x)$$

Parzen window method

Given a set of data points $x_1, x_2, \cdots, x_n$, the corresponding density estimator is

$$\hat{p}(x) = \sum_{n=1}^{N} \frac{1}{h} K\left(\frac{x - x_n}{h}\right) \frac{1}{N} = \sum_{n=1}^{N} K_h(x - x_n) \frac{1}{N}$$

where $K(\cdot)$ is a kernel function.



Outline

Markov chain

Definition

Given a sequentially ordered random variables $X_1, X_2, \cdots, X_t, \cdots, X_T$, called *states*,

- **Transition probability** for describing how the state at time $t-1$ changes to the state at time t,

$$P(X_t = \text{value}' | X_{t-1} = \text{value})$$

- **Initial probability** for describing the initial state at time $t = 1$.

$$P(X_1 = \text{value})$$

value represents possible values $\{X_t\}$ can take. Note that we will assume that all the random variables (at different times) can take value from the same set and assume that the transition probability does not change with respect to time t, i.e., a stationary Markov chain.

Special case and our focus for the rest of the course

When X_t are discrete, taking values from $\{1, 2, 3, \cdots, N\}$

- Transition probability becomes a table/matrix $\boldsymbol{A}$ whose elements are

$$a_{ij} = P(X_t = j | X_{t-1} = i)$$

- Initial probability becomes a vector $\boldsymbol{\pi}$ whose elements are

$$\pi_i = P(X_1 = i)$$

where i or j index over from 1 to N. We have the following constraints

$$\sum_j a_{ij} = 1 \quad \sum_i \pi_i = 1$$

Additionally, all those numbers should be non-negative.

Examples

- Example 1 (Language model)

$$P(\text{next\_word} = \text{cream} | \text{current\_word} = \text{ice})$$

is a gigantic matrix of $N \times N$ where N is the number of words in the dictionary. It can be used to inform us what likely the next word(s) is/are.

- Example 2 (Temperature)

$$P(\text{temperature at month } j | \text{temperature at month}(j-1))$$

is a matrix of $N \times N$ where N is the number of possible temperature bucket: extremely cold, very cold, cold, cool, warm, hot, very hot, extremely hot.

High-order Markov

We have assumed the following Markov property

$$P(X_t|X_1, X_2, \cdots, X_{t-1}) = P(X_t|X_{t-1})$$

that is why we are only concerning with ourselves the *immediate* history.

We can extend to use more histories, thus high-order Markov

$$P(X_t|X_1, X_2, \cdots, X_{t-1}) = P(X_t|X_{t-1}, X_{t-2}, \cdots, X_{t-H})$$

For instance, the language model previously is an order-one HMM. Obviously, languages have long-range dependency so the past history (not just a single word) matters.

Parameter estimation for Markov models

Given a training dataset $\mathcal{D}$, how do we estimate the parameters A and π?

$$\mathcal{D} = \{\boldsymbol{x}^1 = (x_1^1, x_2^1, \cdots, x_T^1), \boldsymbol{x}^2 = (x_1^2, x_2^2, \cdots, x_T^2), \cdots$$
$$\boldsymbol{x}^M = (x_1^M, x_2^M, \cdots, x_T^M)\}$$

Note that we have assumed all M *observed* sequences have equal length T — extending to unequal lengths is left as an exercise

Maximum likelihood estimation

$$\boldsymbol{A}^*, \boldsymbol{\pi}^* = \arg\max \log P(\mathcal{D}) = \arg\max \sum_m \log P(\boldsymbol{x}^m)$$

How to compute the probability of a sequence?

We need to compute

$$P(X_1 = x_1, X_2 = x_2, \cdots, X_T = x_T)$$

We use the Markov property to factorize

$$P(X_1 = x_1, X_2 = x_2, \cdots, X_T = x_T) = \tag{1}$$

$$P(X_1 = x_1) \prod_{t=2}^{T} P(X_t = x_t | X_{t-1} = x_{t-1}) \tag{2}$$

How to derive this? Details as an exercise but you should leverage the property in the following way:

$$\begin{aligned} P(X_1, X_2, X_3) &= P(X_3 | X_1, X_2) P(X_1, X_2) \\ &= P(X_3 | X_2) P(X_1, X_2) = P(X_3 | X_2) P(X_2 | X_1) P(X_1) \end{aligned}$$

Maximum likelihood estimation

$$\sum_m \log P(\boldsymbol{x}^m) = \sum_m \log P(x_1^m) + \sum_m \sum_t \log P(x_t^m | x_{t-1}^m)$$
$$= \sum_m \log \pi_{x_1^m} + \sum_m \sum_t \log a_{x_{t-1}^m \, x_t^m}$$

Maximizing this, we will get (derivation is left as an exercise)

$$\pi_i = \frac{\#\text{of sequences starting with } i}{\#\text{of sequences}}$$

and

$$a_{ij} = \frac{\#\text{of transitions starting with } i \text{ but ending with } j}{\#\text{of transitions starting with } i}$$

Example

Suppose we have two possible states $X_t \in \{0, 1\}$, and we have observed the following 3 sequences

$$1\ 0\ 0\ 1$$
$$0\ 1\ 1\ 1$$
$$1\ 1\ 1\ 1$$

Thus

$$\pi_0 = \frac{1}{3}, \quad \pi_1 = \frac{2}{3}$$

and

$$a_{00} = \frac{1}{3}, \quad a_{01} = \frac{2}{3}$$
$$a_{10} = \frac{1}{6}, \quad a_{11} = \frac{5}{6}$$

Example

If its rainy one day, theres a 0.5 chance it will be rainy the next day, a 0.5 chance it will be sunny.
If its sunny one day, theres a 0.8 chance it will be sunny the next day, a 0.2 chance it will be rainy.
Let rainy be state zero, sunny state one, and write the transition matrix:

$$\begin{bmatrix} 0.5 & 0.5 \\ 0.2 & 0.8 \end{bmatrix}$$

If today (Oct 26th) is rainy, what is the probability that after 10 days (Nov 5th) we will have a rainy day?

Outline

Motivation example

Underlying process is Markov chain

Say, the temperature fluctuation in each month:
cold, cold, hot, hot, cold, hot, ...

But we observe only indirectly, through a related quantity

Say, we can measure how many scoops of ice creams that have been consumed
1, 3, 3, 2, 1, 1, ...

Question

How do we infer the trace of the temperatures from how much we have eaten the ice creams?

Hidden Markov Models

Brief History:

- The foundations that we know today were laid down in three papers by LE Baum and colleagues in 1966, 1970 and 1972.
- A bit earlier than this (1960-61), the foundations of what we now call (linear) state-space models were being developed by R Kalman, RS Bucy and others.
- In the mid-1970s, it was realized that HMMs are discrete non-linear state-space models; equivalently, linear state space models are linear continuous HMMs. Soon afterwards, hybrid forms appeared.
- Applications: first in finance, later in text modeling and speech recognition, in 80s genetics and molecular biology, and now everywhere.

Formal definition of Hidden Markov Models (HMMs)

What are the variables?

- Underlying Markov chain, i.e., a set of random variables
  1. $Z_1, Z_2, \cdots, Z_t, \cdots Z_T$
  2. $Z_t \in \{s_1, s_2, s_3, \cdots, s_S\}$, a discrete set of S values
- Observed variable, i.e, a set of random variables
  1. $X_1, X_2, \cdots, X_t, \cdots X_T$
  2. $X_t \in \{o_1, o_2, o_3, \cdots, o_N\}$, a discrete set of N values

Key difference: Zs are never observed. However, their values can be inferred from the observed values Xs.

Explanation of notations

To avoid confusion, we will use

- Capitalized letter such as Z_t represents a random variable
- Lower-case letter such as z_t represents the value Z_t has taken
- Lower-case letter such as s_1, s_2 represent the value Z_t could take, i.e., its domain.

In other words, we can have

- $P(Z_t)$ mean probability of the random variable (of taking some value)
- $P(Z_t = z_t)$ or $P(z_t)$ mean probability taking value z_t
- $P(Z_t = s_1)$ mean probability take value s_1

Parameters for specifying the probabilistic structures

- For the Markov chain
  1. Transition probability: $a_{ij} = P(Z_t = s_j | Z_{t-1} = s_i)$ for $1 \leq i, j \leq S$
  2. Initial probability: $\pi_i = P(Z_1 = s_i)$ for $1 \leq i \leq S$.
- For observation model

$$b_i(k) = P(X_t = o_k | Z_t = s_i)$$

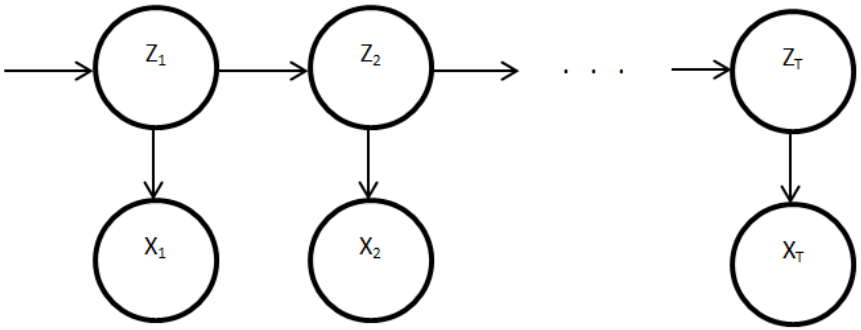
for $1 \leq k \leq N$ and $1 \leq i \leq S$.

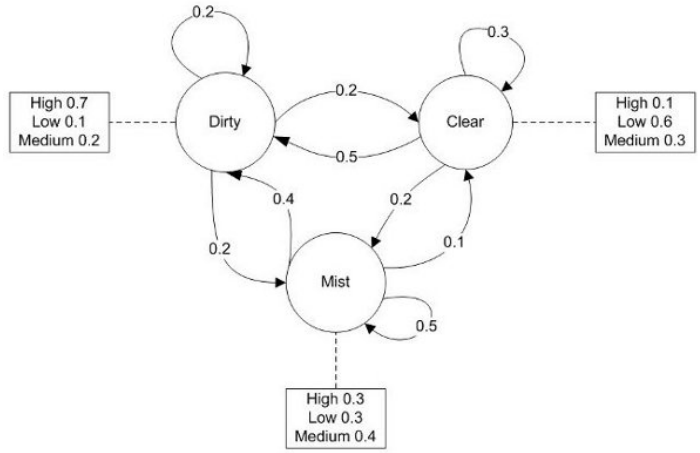
Collectively, $\lambda = (\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{\pi})$

The ice cream example

- States: $s_1 =$ cold and $s_2 =$ hot with $S = 2$
- Observed variables: $o_1 = 1$, $o_2 = 2$, and $o_3 = 3$ with $N = 3$

Graphical Model Representation of HMM





HMM defines a joint probability

$$P(X_1, X_2, \cdots, X_T, Z_1, Z_2, \cdots, Z_T)$$
$$= P(Z_1, Z_2, \cdots, Z_T) P(X_1, X_2, \cdots, X_T | Z_1, Z_2, \cdots, Z_T)$$

- Markov assumption simplifies the first term

$$P(Z_1, Z_2, \cdots, Z_T) = P(Z_1) \prod_{t=2}^{T} P(Z_t | Z_{t-1})$$

- The *independence* assumption simplifies the second term

$$P(X_1, X_2, \cdots, X_T | Z_1, Z_2, \cdots, Z_T) = \prod_{t=1}^{T} P(X_t | Z_t)$$

Namely, each X_t is conditionally independent of anything else, if conditioned on Z_t.

Intuition of these assumptions

Ice cream example

- How hot every month is governed by a physical process whose current state depends on the previous state.
  For example, how far we are from the Sun
- How much ice cream you like to eat depends on the temperature of that day.
  - If I tell you what the temprature today is, then you know how much ice cream you will eat
  - If I tell you only what the temperature yesterday is, then how much ice cream you eat is correlated with that
  - If I tell you what you have eaten yesterday, then how much ice cream you eat yesterday correlates with how much you eat today
  - If I tell you what you have eaten yesterday, or yesterday's temperature and today's temperature, then the information is a bit redundant since you have known today's temperature

In HMMs, we are often interested in the following problems

- Total probability of observing a whole sequence

$$P(x_1, x_2, \cdots, x_T)$$

- The most likely path of the Markov chain's states

$$(z_1^*, z_2^*, \cdots, z_T^*) = \arg\max P(z_1, z_2, \cdots, z_T | x_1, x_2, \cdots, x_T)$$

- The likelihood of a state at a given time

$$P(z_t | x_1, x_2, \cdots, x_T)$$

- The likelihood of two consecutive states at a given time

$$P(z_{t-1}, z_t | x_1, x_2, \cdots, x_T)$$

They are all related to how HMMs is to be used, as well as how to estimate parameters of HMMs from data.

How to compute $P(x_1, x_2, \cdots, x_T)$?

We need to marginalize all the hidden variables

$$P(x_1, x_2, \cdots, x_T) = \sum_{Z_1} \sum_{Z_2} \cdots \sum_{Z_T} P(x_1, x_2, \cdots, x_T, Z_1, Z_2, \cdots, Z_T)$$

and there are exponential number of sums. But the structure of HMMs will enable an efficient way of computing it.

We will start with an auxiliary quantity[1]

$$\alpha_t(j) = P(Z_t = s_j | x_{1:t})$$

where $x_{1:t}$ represents $x_1, x_2, \cdots, x_t$. This quantity is called "forward message". The intuition is, if we observe up to time t, what is the likelihood of the Markov chain in state s_j?

Note that, this quantity can be defined differently, resulting slightly different algorithms.

Forward message can be computed recursively

$$
\begin{aligned}
\alpha_t(j) &= \frac{P(Z_t = s_j, x_{1:t-1}, x_t)}{P(x_{1:t})} \\
&= \frac{P(x_t | Z_t = s_j, x_{1:t-1}) P(Z_t = s_j, x_{1:t-1})}{P(x_{1:t})} \\
&\underset{\text{due to independence}}{=} \frac{P(x_t | Z_t = s_j) P(Z_t = s_j, x_{1:t-1})}{P(x_{1:t})} \\
&= \frac{P(x_t | Z_t = s_j) \sum_i P(Z_t = s_j, Z_{t-1} = s_i, x_{1:t-1})}{P(x_{1:t})} \\
&= \frac{P(x_t | Z_t = s_j) \sum_i P(Z_t = s_j | Z_{t-1} = s_i, x_{1:t-1}) P(Z_{t-1} = s_i, x_{1:t-1})}{P(x_{1:t})} \\
&= \frac{P(x_t | Z_t = s_j) \sum_i P(Z_t = s_j | Z_{t-1} = s_i) P(Z_{t-1} = s_i, x_{1:t-1})}{P(x_{1:t})} \\
&= \frac{P(x_t | Z_t = s_j) \sum_i P(Z_t = s_j | Z_{t-1} = s_i) P(Z_{t-1} = s_i | x_{1:t-1})}{P(x_{1:t}) / P(x_{1:t-1})}
\end{aligned}
$$

Recursion

$$\alpha_t(j) = \frac{P(x_t|Z_t = s_j) \sum_i a_{ij}\alpha_{t-1}(i)}{\text{something}_t}$$

Do we need to compute something$_t$? There is an easy way:

$$\text{something}_t = \sum_j P(x_t|Z_t = s_j) \sum_i a_{ij}\alpha_{t-1}(i)$$

because we need to make sure $\sum_j \alpha_t(j) = 1$ (because $\alpha_t(j)$ is a probability).

Base case

When $t = 1$

$$\alpha_1(j) = P(Z_1 = s_1|x_1) = \frac{P(x_1|Z_1 = s_j)P(Z_1 = s_j)}{P(x_1)} = \frac{\pi_j P(x_1|Z_1 = s_j)}{P(x_1)}$$

where $P(x_1)$ is

$$\sum_j \pi_j P(x_1|Z_1 = s_j)$$

So what is $P(x_{1:T})$?

$$P(x_{1:T}) = P(x_1)\frac{P(x_{1:2})}{P(x_1)}\frac{P(x_{1:3})}{P(x_{1:2})}\cdots\frac{P(x_{1:t})}{P(x_{1:t-1})}\cdots\frac{P(x_{1:T})}{P(x_{1:T-1})}$$

which is

$\text{something}_1 \times \text{something}_2 \times \text{something}_3 \cdots \times \text{something}_t \times \cdots \times \text{something}_T$

Note that this is the formula given in the textbook by Kevin Murphy.

Forward procedure

- Compute $\alpha_1(j)$ for all $1 \leq j \leq S$.
- Compute something$_1 = P(x_1)$.
- Use the recursion to compute $\alpha_t(j)$ and make sure you keep something$_t$ for $2 \leq t \leq T$
- Compute $P(x_{1:T})$ using all the accumulated something$_t$

Alternative method

This is somewhat simpler and more stable numerically

- Define $\alpha_t(j) = P(Z_t = s_j, x_{1:t})$ — note that this is not a conditional probability
- Base case: $\alpha_1(j) = P(x_1|Z_1 = s_j)P(Z_1 = s_j) = \pi_j P(x_1|Z_1 = s_j)$
- Use recursion

$$\alpha_t(j) = P(x_t|Z_t = s_j) \sum_i a_{ij}\alpha_{t-1}(i)$$

- Compute

$$P(x_{1:T}) = \sum_j \alpha_T(j)$$

Showing the correctness of this procedure is left as an exercise. This procedure has one advantage: we do not have to keep something$_t$ along the way.

Backward algorithm

We can define backward messages

$$\beta_t(j) = P(x_{t+1:T}|Z_t = s_j)$$

The interpretation is: if we are told that the Markov chain at time t is in the state s_j, then what are the likelihood of observing *future* observations from $t+1$ to T?

Recursion

$$\beta_{t-1}(i) = \sum_j \beta_t(j) a_{ij} p(x_t|z_t = s_j)$$

with the base case of $\beta_T(j) = 1$ for any j.

Derivation on overhead projector!

Why we need both forward and backward?

How to compute $P(x_{1:T})$ from backward messages?

$$P(x_{1:T}) = \sum_i \beta_1(i)\pi_i P(x_1|Z_1 = s_i)$$

This is a good trick to check whether your forward/backward code is implemented correctly!

How to compute the likelihood of a state at a given time?

$$\gamma_t(j) = P(Z_t = s_j|x_{1:T}) = \frac{\alpha_t(j)\beta_t(j)}{\sum_{j'} \alpha_t(j')\beta_t(j')}$$

How to compute the likelihood of two consecutive states at a given time?

$$\xi_{t,t+1}(i,j) = p(Z_t = s_i, Z_{t+1} = s_j|x_{1:T}) = \frac{\alpha_t(i)p(x_{t+1}|z_{t+1} = s_j)\beta_{t+1}(j)a_{ij}}{something}$$

Making the most likely path

Yet another recursion!

Define the most likely path ending with j at time t

$$\delta_t(j) = \max_{z_1, z_2, \cdots z_{t-1}} P(Z_1 = z_1, Z_2 = z_2, \cdots Z_{t-1} = z_{t-1}, Z_t = s_j, x_{1:t})$$

It relates to

$$\delta_t(j) = \max_i \delta_{t-1}(i) a_{ij} P(x_t | Z_t = s_j)$$

The probability of the most likely path is then

$$\arg\max_j \delta_T(j)$$

Derivation on overhead projector!

Central Techniques: EM Algorithm

Therefore maximizing $F(q, \theta)$ is equivalent to maximizing the expected complete log-likelihood $Q(\theta|\theta_n) = \sum_z q(z|x, \theta_n) \log p(x, z|\theta)$. We can reexpress the EM algorithm as follows:

E-step: compute $Q(\theta|\theta_n) = E_{q(z|x,\theta_n)}[\log p(x, z|\theta)]$

M-step: $\theta_{n+1} = \arg\max_\theta Q(\theta|\theta_n)$.

Estimating HMM parameters

Can you guess what the parameter estimation formulae looks like?

Hint. Check the parameter estimation formulae for Markov model. Imagine the "#" there should be replaced with soft-counts (when we derive EM for Gaussian mixture models), i.e., the probabilities of states as well as state pairs.