Problem Set 5

10-601 Fall 2012

Due: Friday Nov 30th, by 4pm

Please write both your Andrew ID and name on the assignment.

TAs: Selen and Brendan

1 Bayes Net questions [Brendan]

1.a Legal Bayes Nets [10 points]

Prove that in every Bayesian network there is at least one node with **no** incoming edge.

[Solution:

By definition, a Bayes Net is a directed acyclic graph. If every node had an incoming edge, we could construct a cycle: start at one node, proceed to one of its parents, and repeat. If all nodes have incoming edges, this process could be repeated infinitely; but if it is repeated more times than the number of nodes, it is necessary to visit some node twice, thus a cycle. Therefore, in a BN it cannot be the case that every node has at least one incoming edge.

End solution]

1.b Stochastic inference [10 points]

Prove that when performing stochastic inference, if not all nodes have been sampled then there is always at least one **unsampled node** that either

- Does not have any parent, or
- All its parents have been already sampled

[Solution:

Simplest solution: Consider the set of unsampled nodes. They and all edges connecting them must form a DAG, since it is a subgraph of the overall BN which is a DAG. By the previous question, it must contain a node without a parent (in the subgraph). This node must have had all its parent been sampled, by definition of the subgraph. (Or this condition vacuously holds because it has no parents in the original DAG.)

Another view: here is pseudo-code for the sampling algorithm.

Input: a query, which is a set of nodes (random variables). Goal is to create a single sample: values for those query nodes.

Maintain a data structure S: a to-be-sampled set of nodes. (And also a set of already-been-sampled nodes)

Procedure:

1. Initialize $S :=$ all roots (i.e. nodes without parents)
2. Sample values for all variables in S.
3. Let $S := \{$ all nodes, that haven't been sampled yet, for whom all their parents have been sampled $\}$
4. Go to step (2). Terminate when all nodes involved in the query have been sampled.

So when S is non-empty there are several possible cases. First, it could be one of the root variables (that have no parent). Otherwise, a variable is added to S only when all its parents have already been sampled. (Because you can't sample a variable until its parents have been sampled). Those are the two possibilities the question asked us to verify.

Another popular way to solve this problem was proof by contradiction.

End solution]

2 Hidden Markov Models [30 points] [Selen]

Hidden Markov Models (HMMs) are probabilistic models that are used in a wide variety of sequence analysis problems. We define an HMM for K classes of hidden states and T data points. Let the data set be $\mathbf{X} = \{x_1, \ldots, x_T\}$, where each x_i a discrete observed variable. Hidden state variables are $\mathbf{Z} = \{z_1, \ldots, z_T\}$, where each hidden state is $z_t \in \{1..K\}$.

The transition probabilities are given by a $K \times K$ matrix $\mathbf{A}$, where $a_{kj} = P(z_t = k|z_{t-1} = j)$. The initial state variable z_1 is special since it does not have a parent node. Its distribution can be represented by a vector of probabilities π where $P(z_1) = \pi_{z_1}$. Finally, the emission distribution for a hidden state class k is parametrized by $\vec{\phi}_{.k}$, where $\phi_{xk} = P(x_i = x|z_i = k)$. Let $\mathbf{\Theta} = \{\mathbf{A}, \pi, \phi\}$.

2.a The full likelihood of a data set

If we have a data set $\mathbf{X} = \{x_1, \ldots, x_T\}$, write the following expressions in terms of the parameters.

1. **[2 points]** Write down the the full likelihood of observed and latent variables, $P(\mathbf{X}, \mathbf{Z}|\mathbf{\Theta})$.
   [Solution:

$$
\begin{aligned}
P(\mathbf{X}, \mathbf{Z}|\theta) &= P(\mathbf{X}|\mathbf{Z}, \theta)P(\mathbf{Z}|\theta) \\
&= \prod_{t=1}^{T} P(x_t|z_t)P(z_1)\prod_{t=2}^{T} P(z_t|z_{t-1}) \\
&= \prod_{t=1}^{T} \phi^t_{x_{tk}} \pi_{z_1} \prod_{t=2}^{T} a^t_{kj} \\
&= \prod_{k=1}^{K} \pi_{z_1}^{\delta(z_{1k})} \prod_{t=1}^{T}\prod_{k=1}^{K}\prod_{j=1}^{K} a_{jk}^{\delta(z_{tk}z_{t-1j})} \prod_{t=1}^{T}\prod_{k=1}^{K} \phi_{x_t k}^{\delta(z_{tk})}
\end{aligned}
$$

   End solution]

2. **[2 points]** Write down the the likelihood of the data set, $P(\mathbf{X}|\mathbf{\Theta})$.
   [Solution:
   $P(\mathbf{X}|\theta) = \sum_{\mathbf{Z}} P(\mathbf{X}, \mathbf{Z}|\theta)$
   End solution]

2.b Expectation-Maximization (EM) for Maximum Likelihood Learning

Our goal is to estimate $\mathbf{A}$ and ϕ that maximizes the likelihood of the data set $P(\mathbf{X}|\mathbf{\Theta})$.

1. **[3 points]** We can use the EM algorithm to compute $P(\mathbf{X}|\mathbf{\Theta})$:

- In the E step, we use the current parameters and compute the posterior distribution of the latent variables $P(\mathbf{Z}|\mathbf{X}, \mathbf{\Theta}^{\text{old}})$.
- In the M step, we find the new parameter values by solving an optimization problem:

$$\Theta^{\text{new}} = \text{argmax}_{\mathbf{\Theta}} Q(\mathbf{\Theta}, \mathbf{\Theta}^{\text{old}}) \tag{1}$$

  where

$$Q(\Theta, \Theta^{\text{old}}) = \sum_{\mathbf{Z}} P(\mathbf{Z}|\mathbf{X}, \mathbf{\Theta}^{\text{old}}) \ln P(\mathbf{X}, \mathbf{Z}|\mathbf{\Theta}) \tag{2}$$

Assume that we can compute $P(\mathbf{X}, \mathbf{Z}|\mathbf{\Theta})$ in $O(1)$. What is the time complexity of $P(\mathbf{X}|\mathbf{\Theta})$ if we use the above procedure?
[Solution:

The runtime of the E step is $O(K^2T)$ and the run time of the M step is $O(K^T)$. Since $O(K^T)$ dominates $O(K^2T)$, the run time of the algorithm will be $O(K^T)$.

End solution]

2. **[8 points]** In class, we learned how to compute:

$$\alpha(z_t) = P(x_1, \ldots, x_t, z_t) \tag{3}$$
$$\beta(z_t) = P(x_{t+1}, \ldots, x_T|z_t) \tag{4}$$

Show that

$$\xi(z_{t-1}, z_t) = P(z_{t-1}, z_t|\mathbf{X}) \tag{5}$$
$$= \frac{\alpha(z_{t-1})P(x_t|z_t)P(z_t|z_{t-1})\beta(z_t)}{p(\mathbf{X})} \tag{6}$$

How can you use one of the α or β definitions to compute $P(\mathbf{X})$?
[Solution:

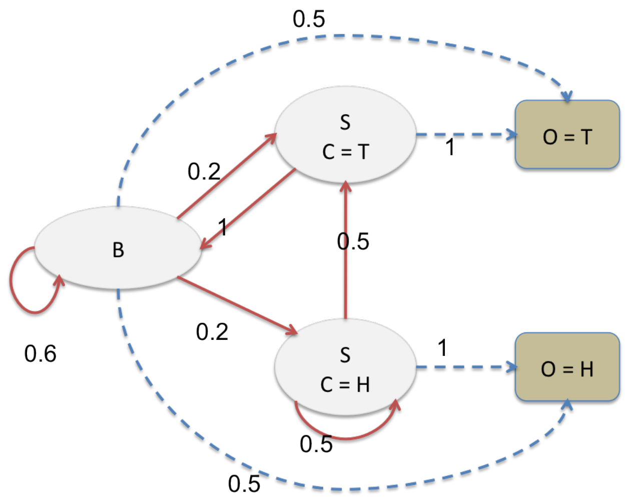
$$\begin{aligned}\xi(z_{t-1}, z_t) =& P(z_{t-1}, z_t|\mathbf{X})\\ =& \frac{P(\mathbf{X}|z_{t-1}, z_t)P(z_{t-1}, z_n)}{P(\mathbf{X})} \text{(Bayes rule)}\\ =& \frac{P(x_1, ..., x_{t-1}|z_{t-1})P(x_t|z_t)P(x_{t+1}, \ldots, x_T|z_t)P(z_t|z_{t-1})P(z_{t-1})}{P(\mathbf{X})} \text{from d-seperation}\\ =& \frac{\alpha(z_{t-1})P(x_t|z_t)P(z_t|z_{t-1})\beta(z_t)}{P(\mathbf{X})}\end{aligned}$$

$P(\mathbf{X}) = \sum_{z_T} \alpha(z_T)$
End solution]

3. **[5 points]** Can we say that if any elements of the parameters π or $\mathbf{A}$ for a hidden Markov model are initially set to 0, then they will remain zero in all subsequent updates of the EM algorithm? If yes, show your steps. If no, explain.
[Solution:

π and $\mathbf{A}$ updated based on the following update rules

$$\begin{aligned}\pi_k =& \frac{\gamma(z_{1k})}{\sum_{j=1}^{K} \gamma(z_{1j})}\\ A_{jk} =& \frac{\sum_{t=1}^{T} \xi(z_{t-1,j} z_{tk})}{\sum_{m=1}^{K} \sum_{t=2}^{T} \xi(z_{t-1,j} z_{tm})}\end{aligned}$$



We found in the previous question that $\xi(z_{t-1}, z_t) == \frac{\alpha(z_{t-1})P(x_t|z_t)P(z_t|z_{t-1})\beta(z_t)}{P(\mathbf{X})}$. If A_{jk} is 0, then $\xi(z_{t-1}, z_t)$ is also 0, which makes the subsequent updates in the EM algorithm 0.

End solution]

2.c A coin game [10 points]

TA's Brendan and Selen play a coin toss game to illustrate how we can use HMMs for sequence analysis problems. Brendan starts tossing first, and they take turns. The game finishes when "THT" appears, and the winner is the one who last flips the coin. At each timestep, they can flip the coin many times, and the stopping rules are as follows:
a. At his turn, each time Brendan flips the coin, he also flips an extra biased coin ($P(H) = 0.4$.) He stops only if the extra coin lands H, otherwise he keeps flipping the fair and extra coins. The flips of the extra biased coin are not recorded.
b. At her turn, Selen flips the (fair) coin until T appears (all of her flips are recorded).
You are given a sequence of recorded coin flips, you would like to infer the winner and the flips of each player.

1. **[5 points]** Describe an HMM to model this game.

2. **[5 points]** How would you use this HMM model to infer the (most probable) winner and the (most probable) flips of each player?

[Solution:

Please see the Figure below.

End solution]

3 HMM Programming [Brendan]

Anthropologists in the future are trying to study global warming in our present day, but have lost all temperature records. However, they have my diary of how many ice cream cones I've eaten every day, and want to reconstruct the temperatures from that.[1] (Note that, compared to Problem 2, we now include an explicit STOP state to make the stochastic process well-defined.)

We model this as a Hidden Markov Model, with three latent states {COLD, HOT, STOP} and three discrete observation types {ONEIC, TWOIC, THREEIC}. (I only eat 1, 2, or 3 cones.) Cold days tend to follow cold days, and hot days tend to follow hot days; and we eat more ice cream on hot days.

[1]This example is adapted from Jason Eisner: `http://cs.jhu.edu/~jason/papers/#eisner-2002-tnlp`

Generation proceeds until it reaches a STOP state. Let T be the number of observations (same thing as the number of state variables, not including the STOP state). For example, one possible generated chain, three timesteps long, consists of latent states $(z_1...z_4) = (\text{COLD}, \text{HOT}, \text{HOT}, \text{STOP})$ and observations $(x_1...x_3) = (\text{ONEIC}, \text{THREEIC}, \text{TWOIC})$. Note the output space is discrete: the numbers don't matter; they could just as well be meaningless symbols.

$$\begin{tikzcd}
\text{z1 = COLD} \arrow[r] \arrow[d] & \text{z2 = HOT} \arrow[r] \arrow[d] & \text{z3 = HOT} \arrow[r] \arrow[d] & \text{z4 = STOP} \\
\text{x1 = 1} & \text{x2 = 3} & \text{x3 = 2} &
\end{tikzcd}$$

Given a dataset of $x_1 \dots x_T$, and known transition and emission parameters, we are interested in inferring the most likely path $z_1 \dots z_T$, which we'll explicitly write out for clarity:

$$\arg\max_{z_1 \dots z_T} P(x_1 \dots x_T, z_t \dots z_T, z_{T+1} = \text{STOP}) \tag{7}$$

$$= P(z_1)P(x_1 \mid z_1) \left(\prod_{t=2}^{T} p(z_t \mid z_{t-1}) p(x_t \mid z_t) \right) p(z_{T+1} = \text{STOP} \mid z_T) \tag{8}$$

The transition and emission parameters A and ϕ are provided in the starter code on the website. See below for submission details.

1. **[5 points]** Implement an exhaustive best-path algorithm: enumerate every possible path, compute its log-probability, and choose the highest-scoring one.

   [Debugging hint: check the examples $x = \{1, 2, 1\}$ and $x = \{3, 2, 3\}$. The second datapoint is equally likely under either state, but the most likely path states are different due to the HMM chain dependencies: the HMM gives you temporal smoothing, where you consider both past and future for a better estimate of the present.]

   Report the most-likely path for this example dataset (*smallX* in the starter code):

   $$\vec{x} = [1, 1, 3, 1, 2, 3, 3]$$

   [Solution:

   Actually, there are three paths tied at equal probability, log-prob -11.639,

   $$\begin{aligned} &[1, 1, 1, 1, 1, 2, 2] \quad (A) \\ &[1, 1, 1, 1, 2, 2, 2] \quad (B) \\ &[1, 1, 2, 2, 2, 2, 2] \quad (C) \end{aligned}$$

   This is because of the symmetries in the transition and emission distributions. It's simple why (A) and (B) are tied. They only disagree on the 5th timestep, which is a two-icecream-day; two-icecream days are equally likely under either hot or cold days. While the model does care about the transition from cold to hot, it doesn't have an opinion whether it happened on the 5th or 6th timestep.

   (C) is more complex. The third and fourth timesteps have highly differing amounts of ice cream (1 then 3 scoops), which by the emission distribution alone would imply a cold then hot day. But transition stickiness disprefers this sort of flip-flopping, so it wants to pick a run. Thinking they're both cold isn't a great explanation because it's bad for the three-icecream day, but thinking they're both hot isn't good either for the one-icecream day. In fact, they're both equally bad because of the symmetries in the emissions matrix; thus (B) and (C) are tied.

   End solution]

2. **[2 points]** Find and report a dataset for which the most-likely path is all HOT's, that differs from *smallX* to the minimal extent possible.

   [Solution:

   There are many possibilities, but here is one answer that differs by smallX on only one day: flips the first day to 3.

   $$\vec{x} = [3, 1, 3, 1, 2, 3, 3], \quad \log p(\vec{x}, \vec{y}) = -12.8921$$

   This illustrates the joint smoothing inferences done by the HMM. Contrast to the (A-C) solution, which has a string of colds then transitions in the middle to hot. Using a '3' on the first day flips all the initial cold states to hot. Since the HMM likes to be sticky, sufficiently changing the evidence on just one day persuades the model that it must have been hot that day, and that it's better to use the stickiness assumption (that temperature shifts are unlikely) to explain all the middle days as hot, rather than assuming hot days in the middle bookended by cold ones.

   End solution]

3. **[5 points]** Report the log joint probability (natural logarithm, please!) that these two data-path pairs attain; i.e. for each, where $\hat{z}$ is the max-likely path, report:

   $$\log p(x_1 \ldots x_T, \hat{z}_1 \ldots \hat{z}_T, z_{T+1} = \text{STOP})$$

4. **[20 points]** Implement the Viterbi algorithm to compute the best-path. Test it on small examples; it should always agree with the exhaustive solution. (Corner case: for certain inputs, there may be multiple paths that tie for the highest probability; in that case, they may give different solutions, but the solutions should both have the same probability.)

   [Hint: *simdata.m* will simulate new examples for more thorough testing, if you like. You will not of course always recover the correct path, but should be reasonably close, especially if A is sharper. In any case, both Viterbi and the exhaustive algorithm should agree. We will test your implementations with similar simulated data.]

   Report the Viterbi algorithm's solution to the the dataset *bigX*. Is it feasible to run the exhaustive algorithm on this dataset?

   [Solution:

   No, it is not feasible: exhaustive takes exponential time in the sequence length! By contrast, Viterbi is linear.

   Exhaustive runtime: $O(K^N)$

   Viterbi runtime: $O(K^2 N)$

   End solution]

3.a Submitting your code

Write your solution in either Matlab or Python, and fill out the stubs given (we provide starter code for both languages). Submit both hardcopy and electronically:

- Print out your implementation. **Your code must be 2 or fewer pages long, in 10-point font.** It should be fewer than 100 lines, and certainly less than 200.

- Copy your code to Andrew AFS, e.g. by using *scp* or an SFTP program to *unix.andrew.cmu.edu*, to the directory:

  ```
  /afs/andrew.cmu.edu/usr10/brendano/10601/ps5_submit/YOURANDREWID/
  ```

Only copy the files you need: if you write in Matlab, don't copy the Python files, and vice versa. Please copy all the individual files so that it is directly runnable.

Try copying a file into the directory before the deadline to make sure everything is working. You should be able to delete the file as well.

Make sure your implementations have filled out the three given functions *logjointprob*, *exhaustive_bestpath*, and *viterbi_bestpath*.We will use automated scripts to call those functions.

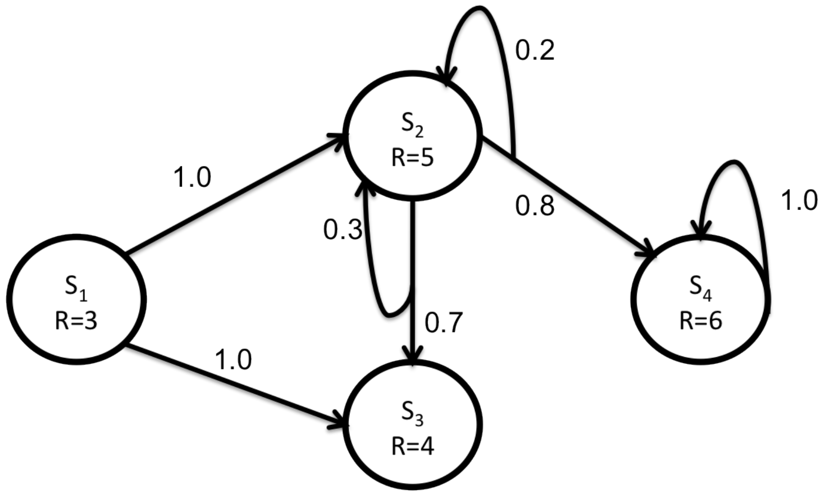
Your code must be runnable on *unix.andrew.cmu.edu*, and is not allowed to use any external libraries (so we can run it reliably).

4 Markov Decision Processes [20 points] [Selen]

1. [10 points] A standard (first-order) MDP is described by a set of states S, a set of actions A, a transition function T, and a reward function R where $T(s; a; s')$ gives the probability of transitioning to s' after taking action a in state s, and $R(s)$ gives the immediate reward of being in state s. In a k-order MDP, probability of transitioning into a state s' given that an action a was taken in state s depends on the previous $k-1$ states. Formally, the transition function T is described as $T(s_{k-1}, ..., s_1, s, a, s') = P(s', a, s, s_1, ..., s_{k-1})$ where $P(s', a, s, s_1, ..., s_{k-1})$ is the probability of transitioning to state s' given that action a was taken in state s, and the previous $k-1$ states are $(s_{k-1}, ..., s_1)$.

Given a k-order MDP M = (S; A; T; R) describe how to construct a standard (first-order) MDP $M' = (S'; A'; T'; R')$ that is equivalent to M, meaning that a solution to M' can be easily converted into a solution to M. Describe S', A', T', R' and give a brief justification for your construction.

2. [10 points] Consider the MDP given in the figure below. R denotes rewards, and the numbers next to arrows denote probabilities of outcomes. The discount factor is $\gamma = 0.8$.



[Solution:

A k-order MDP M depends on the current state s, and the previous k-1 states. Denoting the current and previous states as a k-tuple, i.e. $(s, s_1, s_2, \dots s_{k-1})$ we can construct S^k states in the new MDP M', each state assigned to a k-tuple. Therefore, each state in M' corresponds to a state and its history in M. Note that $|S'| = |S|^k$, the number of states in M' is exponential in k.
Actions are the same in both MDPs, i.e. A' = A. This is given in the description.
Reward function depends on the current state only, so $R'((s, s_1, s_2, \dots s_k)) = R(s)$. Note the tuple notation in R'.

Transitions in M′ is defined as follows:

$$\begin{aligned} T'((s_{k-1},...,s_1,s),a,s^*) &= P(s',a,s,s_1,....,s_{k-1}) && \text{if} s^* = (s',s,s_1,s_2,\ldots s_{k-2}) \\ &= 0 \end{aligned}$$

This enforces that the history is maintained correctly after each state transitions: a transition to a state that does not update the history correctly has 0 probability. The correct transition to the new state s′ has the same probability given by M, and this transition involves shifting the history in the current state s by one step.

End solution]

a. [5 points] Write down the numerical value of $J(S_2)$ after the first and second iterations of Value Iteration (in other words compute $J^1(S_2)$ and $J^2(S_2)$).
Initial value functions are $J^0(S_1) = 0, J^0(S_2) = 0, J^0(S_3) = 0, J^0(S_4) = 0.$

[Solution:

$$\begin{aligned} J^1(S_2) =& 5 \text{ immediate reward} \\ J^2(S_2) =& \max(5 + \gamma(0.7J^1(S3) + 0.3J^1(S2)), 5 + \gamma(0.8J^1(S4) + 0.2J^1(S2))) \\ J^2(S_2) =& \max(5 + 0.8(0.7 * 4 + 0.3 * 5), 5 + 0.8(0.8 * 6 + 0.2 * 5)) \\ J^2(S_2) =& \max(8.44, 9.64) \\ J^2(S_2) =& 9.64 \end{aligned}$$

End solution]

b. [5 points] Write down $J^*(S_2)$, the optimal value of state S_2.

[Solution:

Optimal policy from S_2 will try to transition to S_4, since it is the state with the largest reward. Lets first compute the optimal value of S_4

$$\begin{aligned} J^*(S4) =& 6 + 0.8J^*(S4) \\ J^*(S4) =& 30 \end{aligned}$$

Using $J^*(S4)$ we can compute $J^*(S2)$:

$$\begin{aligned} J^*(S2) =& 5 + 0.8(0.8J^*(S4) + 0.2J^*(S2)) \\ J^*(S2) =& 5 + 0.8(24 + 0.2J^*(S2)) \\ J^*(S2) =& \frac{24.2}{0.84} \\ J^*(S2) =& 28.8 \end{aligned}$$

End solution]