

10-601 Machine Learning
Fall 2022
Exam 3 Practice Problems
December 12, 2022
Time Limit: N/A

Name:
AndrewID:

Instructions:

- Fill in your name and Andrew ID above. Be sure to write neatly, or you may not receive credit for your exam.
 - Clearly mark your answers in the allocated space **on the front of each page**. If needed, use the back of a page for scratch space, but you will not get credit for anything written on the back of a page. If you have made a mistake, cross out the invalid parts of your solution, and circle the ones which should be graded.
 - No electronic devices may be used during the exam.
 - Please write all answers in pen.
 - You have N/A to complete the exam. Good luck!
-

Instructions for Specific Problem Types

For “Select One” questions, please fill in the appropriate bubble completely:

Select One: Who taught this course?

- Henry Chai
- Marie Curie
- Noam Chomsky

If you need to change your answer, you may cross out the previous answer and bubble in the new answer:

Select One: Who taught this course?

- Henry Chai
- Marie Curie
- Noam Chomsky

For “Select all that apply” questions, please fill in all appropriate squares completely:

Select all that apply: Which are scientists?

- Stephen Hawking
- Albert Einstein
- Isaac Newton
- I don't know

Again, if you need to change your answer, you may cross out the previous answer(s) and bubble in the new answer(s):

Select all that apply: Which are scientists?

- Stephen Hawking
- Albert Einstein
- Isaac Newton
- I don't know

For questions where you must fill in a blank, please make sure your final answer is fully included in the given space. You may cross out answers or parts of answers, but the final answer must still be within the given space.

Fill in the blank: What is the course number?

10-601

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1 Reinforcement Learning

1.1 Markov Decision Process

Environment Setup (may contain spoilers for Shrek 1)

Lord Farquaad is hoping to evict all fairytale creatures from his kingdom of Duloc, and has one final ogre to evict: Shrek. Unfortunately all his previous attempts to catch the crafty ogre have fallen short, and he turns to you, with your knowledge of Markov Decision Processes (MDP's) to help him catch Shrek once and for all.

Consider the following MDP environment where the agent is Lord Farquaad:

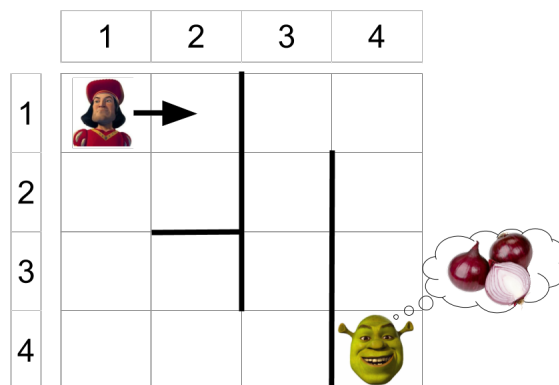


Figure 1: Kingdom of Duloc, circa 2001

Here's how we will define this MDP:

- **S (state space):** a set of states the agent can be in. In this case, the agent (Farquaad) can be in any location (row, col) and also in any orientation $\in \{N, E, S, W\}$. Therefore, state is represented by a three-tuple (row, col, dir) , and $S =$ all possible of such tuples. Farquaad's start state is $(1, 1, E)$.
- **A (action space):** a set of actions that the agent can take. Here, we will have just three actions: turn right, turn left, and move forward (turning does not change row or col , just dir). So our action space is $\{R, L, M\}$. Note that Farquaad is debilitatingly short, so he cannot travel through (or over) the walls. Moving forward when facing a wall results in no change in state (but counts as an action).
- **$R(s, a)$ (reward function):** In this scenario, Farquaad gets a reward of 5 by moving into the swamp (the cell containing Shrek), and a reward of 0 otherwise.
- **$p(s'|s, a)$ (transition probabilities):** We'll use a deterministic environment, so this will be 1 if s' is reachable from s and by taking a , and 0 if not.

1. What are $|S|$ and $|A|$ (size of state space and size of action space)?
2. Why is it called a "Markov" decision process? (Hint: what is the assumption made with p ?)
3. What are the following transition probabilities?

$$p((1, 1, N)|(1, 1, N), M) =$$

$$p((1, 1, N)|(1, 1, E), L) =$$

$$p((2, 1, S)|(1, 1, S), M) =$$

$$p((2, 1, E)|(1, 1, S), M) =$$

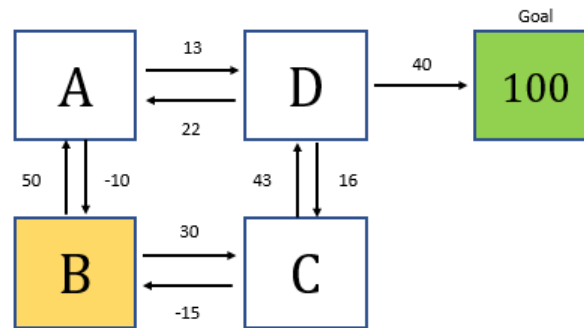
4. Given a start position of $(1, 1, E)$ and a discount factor of $\gamma = 0.5$, what is the expected discounted future reward from $a = R$? For $a = L$? (Fix $\gamma = 0.5$ for following problems).
5. What is the optimal action from each state, given that orientation is fixed at E ? (if there are multiple options, choose any)
6. Farquaad's chief strategist (Vector from Despicable Me) suggests that having $\gamma = 0.9$ will result in a different set of optimal policies. Is he right? Why or why not?
7. Vector then suggests the following setup: $R(s, a) = 0$ when moving into the swamp, and $R(s, a) = -1$ otherwise. Will this result in a different set of optimal policies? Why or why not?

8. Vector now suggests the following setup: $R(s, a) = 5$ when moving into the swamp, and $R(s, a) = 0$ otherwise, but with $\gamma = 1$. Could this result in a different optimal policy? Why or why not?
9. Surprise! Elsa from Frozen suddenly shows up. Vector hypnotizes her and forces her to use her powers to turn the ground into ice. The environment is now stochastic: since the ground is now slippery, when choosing the action M , with a 0.2 chance, Farquaad will slip and move two squares instead of one. What is the expected future-discounted rewards from $s = (2, 4, S)$?

1.2 Value and Policy Iteration

1. **Select all that apply:** Which of the following environment characteristics would increase the computational complexity per iteration for a value iteration algorithm? Choose all that apply:
- Large Action Space
 - A Stochastic Transition Function
 - Large State Space
 - Unknown Reward Function
 - None of the Above
2. **Select all that apply:** Which of the following environment characteristics would increase the computational complexity per iteration for a policy iteration algorithm? Choose all that apply:
- Large Action Space
 - A Stochastic Transition Function
 - Large State Space
 - Unknown Reward Function
 - None of the Above

3. In the image below is a representation of the game that you are about to play. There are 5 states: A, B, C, D, and the goal state. The goal state, when reached, gives 100 points as reward (that is, you can assume $R(\text{D}, \text{right}) = 140$). In addition to the goal's points, you also get points by moving to different states. The amount of points you get are shown next to the arrows. You start at state B. To figure out the best policy, you use asynchronous value iteration with a decay (γ) of 0.9. You should initialize the value of each state to 0.



- (i) When you first start playing the game, what action would you take (up, down, left, right) at state B?

- (ii) What is the total reward at state B at this time?

- (iii) Let's say you keep playing until your total values for each state has converged. What action would you take at state B?

- (iv) What is the total reward at state B at this time?

4. **Select one:** Let $V_k(s)$ indicate the value of state s at iteration k in (synchronous) value iteration. What is the relationship between $V_{k+1}(s)$ and $\sum_{s' \in S} P(s'|s, a)[R(s, a, s') + \gamma V_k(s')]$, for any $a \in A$? Indicate the most restrictive relationship that applies. For example, if $x < y$ always holds, use $<$ instead of \leq . Selecting $?$ means it's not possible to assign any true relationship. Assume $R(s, a, s') \geq 0 \forall s, s' \in S, a \in A$.

$$V_{k+1}(s) \square \sum_{s'} P(s'|s, a)[R(s, a, s') + \gamma V_k(s')]$$

- =
 <
 >
 ≤
 ≥
 ?

1.3 Q-Learning

- For the following true/false, circle one answer and provide a one-sentence explanation:
 - One advantage that Q-learning has over Value and Policy iteration is that it can account for non-deterministic policies.
Circle one: True False
 - You can apply Value or Policy iteration to any problem that Q-learning can be applied to.
Circle one: True False
 - Q-learning is guaranteed to converge to the true value Q^* for a greedy policy.
Circle one: True False
- For the following parts of this problem, recall that the update rule for Q-learning is:

$$\mathbf{w} \leftarrow \mathbf{w} - \alpha \left(q(\mathbf{s}, a; \mathbf{w}) - (r + \gamma \max_{a'} q(\mathbf{s}', a'; \mathbf{w})) \right) \nabla_{\mathbf{w}} q(\mathbf{s}, a; \mathbf{w})$$

- From the update rule, let's look at the specific term $X = (r + \gamma \max_{a'} q(\mathbf{s}', a'; \mathbf{w}))$. Describe in English what is the role of X in the weight update.
- Is this update rule synchronous or asynchronous?
- A common adaptation to Q-learning is to incorporate rewards from more time steps into the term X . Thus, our normal term $r_t + \gamma \max_{a_{t+1}} q(s_{t+1}, a_{t+1}; \mathbf{w})$ would become $r_t + \gamma r_{t+1} + \gamma^2 \max_{a_{t+2}} q(\mathbf{s}_{t+2}, a_{t+2}; \mathbf{w})$. What are the advantages of using more rewards in this estimation?

3. **Select one:** Let $Q(s, a)$ indicate the estimated Q-value of state-action pair $(s, a) \in |S| \times |A|$ at some point during Q-learning. Suppose you receive reward r after taking action a at state s and arrive at state s' . Before updating the Q values based on this experience, what is the relationship between $Q(s, a)$ and $r + \gamma \max_{a' \in A} Q(s', a')$? Indicate the most restrictive relationship that applies. For example, if $x < y$ always holds, use $<$ instead of \leq . Selecting ? means it's not possible to assign any true relationship.

$$Q(s, a) \square r + \gamma \max_{a'} Q(s', a')$$

- =
 <
 >
 ≤
 ≥
 ?
4. During standard (not deep) Q-learning, you get reward r after taking action *North* from state *A* and arriving at state *B*. You compute the sample $r + \gamma Q(B, \textit{South})$, where $\textit{South} = \arg \max_a Q(B, a)$.

Which of the following Q-values are updated during this step? (Select all that apply)

- Q(A, North)
 Q(A, South)
 Q(B, North)
 Q(B, South)
 None of the above
5. In general, for Q-Learning (standard/tabular Q-learning, not approximate Q-learning) to converge to the optimal Q-values, which of the following are true?

True or False: It is necessary that every state-action pair is visited infinitely often.

- True
 False

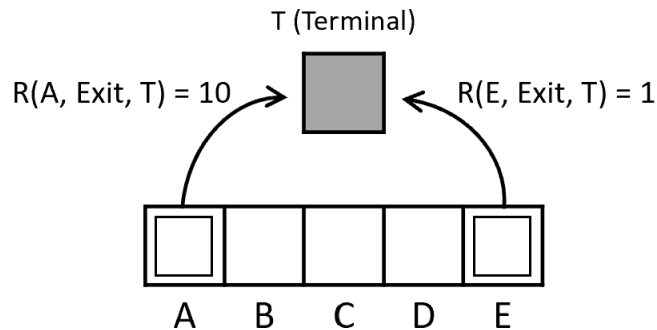
True or False: It is necessary that the discount γ is less than 0.5.

- True
 False

True or False: It is necessary that actions get chosen according to $\arg \max_a Q(s, a)$.

- True
 False

6. Consider training a robot to navigate the following grid-based MDP environment.



- There are six states, A, B, C, D, E, and a terminal state T.
- Actions from states B, C, and D are Left and Right.
- The only action from states A and E is Exit, which leads deterministically to the terminal state

The reward function is as follows:

- $R(A, Exit, T) = 10$
- $R(E, Exit, T) = 1$
- The reward for any other tuple (s, a, s') equals -1

Assume the discount factor is 1. When taking action Left, with probability 0.8, the robot will successfully move one space to the left, and with probability 0.2, the robot will move one space in the opposite direction. When taking action Right, with probability 0.8, the robot will successfully move one space to the right, and with probability 0.2, the robot will move one space in the opposite direction. Run synchronous value iteration on this environment for two iterations. Begin by initializing the value of all states to zero.

Write the value of each state after the first ($k = 1$) and the second ($k = 2$) iterations. Write your values as a comma-separated list of 6 numerical expressions in the alphabetical order of the states, specifically $V(A), V(B), V(C), V(D), V(E), V(T)$. Each of the six entries may be a number or an expression that evaluates to a number. Do not include any max operations in your response.

$V_1(A), V_1(B), V_1(C), V_1(D), V_1(E), V_1(T)$ (Values for 6 states):

$V_2(A), V_2(B), V_2(C), V_2(D), V_2(E), V_2(T)$ (values for 6 states):

What is the resulting policy after this second iteration? Write your answer as a comma-separated list of three actions representing the policy for states, B, C, and D, in that order. Actions may be Left or Right.

$\pi(B), \pi(C), \pi(D)$ based on V_2 :

2 Hidden Markov Models

1. Recall that both the Hidden Markov Model (HMM) can be used to model sequential data with local dependence structures. In this question, let Y_t be the hidden state at time t , X_t be the observation at time t , \mathbf{Y} be all the hidden states, and \mathbf{X} be all the observations.
 - (a) Draw the HMM as a Bayesian network where the observation sequence has length 3 (i.e., $t = 1, 2, 3$), labelling nodes with Y_1, Y_2, Y_3 and X_1, X_2, X_3 .
 - (b) Write out the factorized joint distribution of $P(\mathbf{X}, \mathbf{Y})$ using the independencies/-conditional independencies assumed by the HMM graph, using terms Y_1, Y_2, Y_3 and X_1, X_2, X_3 .
 $P(\mathbf{X}, \mathbf{Y}) =$
 - (c) True or False: In general, we should not include unobserved variables in a graphical model because we cannot learn anything useful about them without observations.
True **False**

2. Consider an HMM with states $Y_t \in \{S_1, S_2, S_3\}$, observations $X_t \in \{A, B, C\}$ and parameters $\boldsymbol{\pi} = [1 \ 0 \ 0]$, transition matrix $\mathbf{B} = \begin{bmatrix} 1/2 & 1/4 & 1/4 \\ 0 & 1/2 & 1/2 \\ 0 & 0 & 1 \end{bmatrix}$, and emission matrix

$$\mathbf{A} = \begin{bmatrix} 1/2 & 1/2 & 0 \\ 1/2 & 0 & 1/2 \\ 0 & 1/2 & 1/2 \end{bmatrix}.$$

- (a) What is $P(Y_5 = S_3)$?

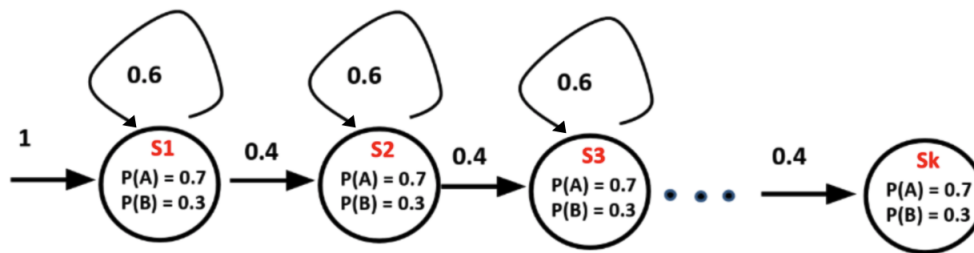
- (b) What is $P(Y_5 = S_3 | X_{1:7} = AABCABC)$?

- (c) Fill in the following table assuming the observation $AABCABC$. The α 's are values obtained during the forward algorithm: $\alpha_t(i) = P(X_1, \dots, X_t, Y_t = i)$.

t	$\alpha_t(1)$	$\alpha_t(2)$	$\alpha_t(3)$
1			
2			
3			
4			
5			
6			
7			

- (d) Write down the sequence of $Y_{1:7}$ with the maximal posterior probability assuming the observation $AABCABC$. What is that posterior probability?

3. Consider the HMM in the figure below.



The HMM has k states (s_1, \dots, s_k) . s_k is the terminal state. All states have the same emission probabilities (shown in the figure). The HMM always starts at s_1 as shown, and can move to either the next greater-number state or stay in the current state. Transition probabilities for all states except s_k are also the same as shown. More formally:

1. $P(Y_i = S_t \mid Y_{i-1} = S_{t-1}) = 0.4$
2. $P(Y_i = S_t \mid Y_{i-1} = S_t) = 0.6$
3. $P(Y_i = S_t \mid Y_{i-1} = S_j) = 0$ for all $j \in [k] \setminus \{t, t-1\}$

Once a run reaches s_k it outputs a symbol based on the s_k state emission probability and terminates.

1. Assume we observed the output AABAABBA from the HMM. Select all answers below that COULD be correct.
 - $k > 8$
 - $k < 8$
 - $k > 6$
 - $k < 6$
 - $k = 7$
2. Now assume that $k = 4$. Let $P('AABA')$ be the probability of observing AABA from a full run of the HMM. For the following equations, fill in the box with $>$, $<$, $=$ or $?$ (? implies it is impossible to tell).

(a) $P('AAB')$ $P('BABA')$

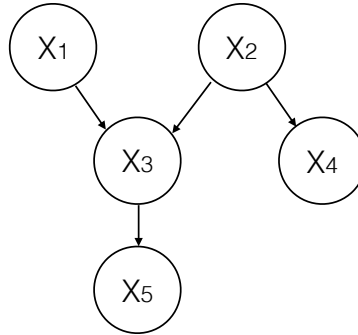
(b) $P('ABAB')$ $P('BABA')$

(c) $P('AAABA')$ $P('BBAB')$

3 Bayesian Networks

1. Consider the following Bayesian network.

(a) Determine whether the following conditional independencies are true.



$$X_1 \perp X_2 \mid X_3?$$

Circle one: Yes No

$$X_1 \perp X_4?$$

Circle one: Yes No

$$X_5 \perp X_2 \mid X_3?$$

Circle one: Yes No

(b) Write out the joint probability in a form that utilizes as many independence/conditional independence assumptions contained in the graph as possible. Answer:

$$P(X_1, X_2, X_3, X_4, X_5) =$$

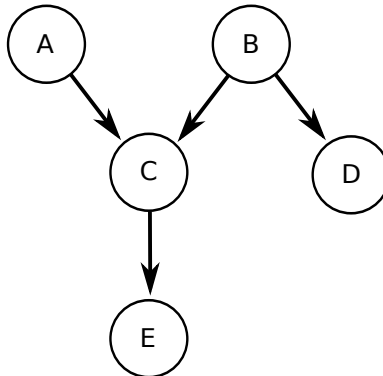
(c) In a Bayesian network, if $X_1 \perp X_2$, then $X_1 \perp X_2 \mid Y$ for every node Y in the graph.

Circle one: True False

(d) In a Bayesian network, if $X_1 \perp X_2 \mid Y$ for some node Y in the graph, it is always true that $X_1 \perp X_2$.

Circle one: True False

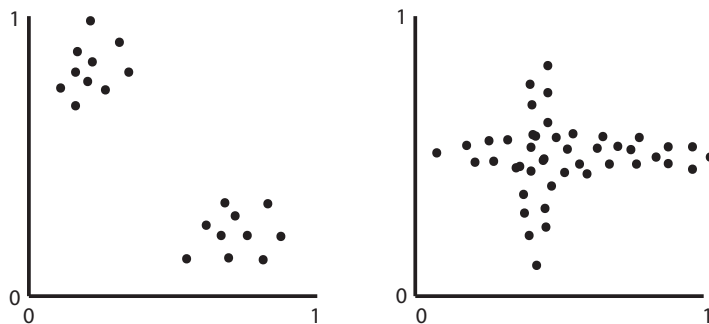
2. Consider the Bayesian network shown below for the following questions (a)-(f). Assume all variables are boolean-valued.



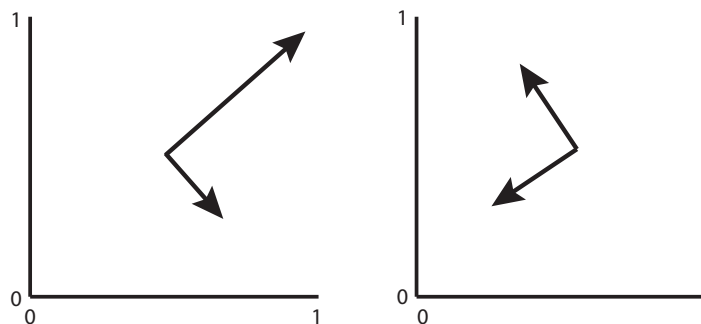
- (a) (Short answer) Write down the factorization of the joint probability $P(A, B, C, D, E)$ for the above graphical model, as a product of the five distributions associated with the five variables.
- (b) **True or False:** Is C conditionally independent of D given B (i.e. is $(C \perp D)|B$)?
- (c) **True or False:** Is A conditionally independent of D given C (i.e. is $(A \perp D)|C$)?
- (d) **True or False:** Is A independent of B (i.e. is $A \perp B$)?
- (e) Write an expression for $P(C = 1|A = 1, B = 0, D = 1, E = 0)$ in terms of the parameters of Conditional Probability Distributions associated with this graphical model.

4 Principal Component Analysis

1. (i) Consider the following two plots of data. Draw arrows from the mean of the data to denote the direction and relative magnitudes of the principal components.



- (ii) Now consider the following two plots, where we have drawn only the principal components. Draw the data ellipse or place data points that could yield the given principal components for each plot. Note that for the right hand plot, the principal components are of equal magnitude.



2. Circle one answer and explain.

In the following two questions, assume that using PCA we factorize $X \in \mathbb{R}^{n \times m}$ as $Z^T U \approx X$, for $Z \in \mathbb{R}^{m \times n}$ and $U \in \mathbb{R}^{m \times m}$, where the rows of X contain the data points, the rows of U are the prototypes/principal components, and $Z^T U = \hat{X}$.

- (i) Removing the last row of U and Z will still result in an approximation of X , but this will never be a better approximation than \hat{X} .

Circle one: True False

- (ii) $\hat{X} \hat{X}^T = Z^T Z$.

Circle one: True False

- (iii) The goal of PCA is to interpret the underlying structure of the data in terms of the principal components that are best at predicting the output variable.

Circle one: True False

- (iv) The output of PCA is a new representation of the data that is always of lower dimensionality than the original feature representation.

Circle one: True False

5 Ensemble Methods

1. In Homework 9, we saw the **halving algorithm**, which repeatedly eliminates wrong weak classifiers out of n weak classifiers. However, there must be at least one weak classifier that makes zero mistakes for this algorithm to not terminate prematurely. This is rarely ever guaranteed in real life, and a more realistic algorithm would be to try and match the performance of the best weak classifier in hindsight. Suppose the best weak classifier makes m mistakes. Say we use the same halving algorithm, but we bring back all weak classifiers whenever all of them are eliminated. Derive a bound (big- O) on how many mistakes this algorithm makes in terms of m and n .

2. Recall the Weighted Majority algorithm from lecture. We initially set the weights of all weak classifiers to 1, and take the weighted majority vote for every example to classify. We halve the weight of any weak classifier that makes a mistake. Suppose we have T examples to classify and n weak classifiers. For the t -th example to classify, let $w_i^{(t)}$ be the weight of weak classifier i , and let $W^{(t)} = \sum_{i=1}^n w_i^{(t)}$. Note that the weights here are the weights *before* the weight adjustment for the t -th example; so $W^{(1)} = n$ and the final weight is $W^{(T+1)}$.

- (a) Say weak classifier i makes a total of m_i mistakes. Show that

$$W^{(T+1)} \geq \left(\frac{1}{2}\right)^{m_i}.$$

- (b) Find the smallest constant $0 < c < 1$ such that

$$W^{(t+1)} \leq c \cdot W^{(t)}$$

whenever the algorithm makes a mistake for the t -th example.

- (c) Say the algorithm makes a total of k mistakes. Show that

$$W^{(T+1)} \leq c^k \cdot W^{(1)}$$

for the same c in the previous part.

- (d) Derive a big-O bound on the number of mistakes this algorithm makes in terms of m and n , where m is the number of mistakes the best weak classifier makes.

- (e) Say instead of halving the weights of wrong weak classifiers, we multiply the weights by $1 - \epsilon$ ($0 < \epsilon \leq 1/2$). Mimic this analysis and show that this algorithm makes at most $2(1 + \epsilon)m + \frac{2 \log n}{\epsilon}$ mistakes.

- (f) **True or False:** Say we finished running the algorithm in part (e), and now we are assessing the performance of this algorithm for examples 10, 11, ..., 500. The best weak classifier for these examples makes 20 mistakes, and we have 30 weak classifiers. If $\epsilon = 1/2$, we can use our analysis to estimate at most how many mistakes the algorithm made (either as a big-O bound or some closed form expression).

True

False

3. In the AdaBoost algorithm, if the final hypothesis makes no mistakes on the training data, which of the following is correct?

Select all that apply:

Additional rounds of training can help reduce the errors made on unseen data.

Additional rounds of training have no impact on unseen data.

The individual weak learners also make zero error on the training data.

Additional rounds of training always leads to worse performance on unseen data.

4. **True or False:** In AdaBoost weights of the misclassified examples go up by the same multiplicative factor.

- True
- False

Round	$D_t(A)$	$D_t(B)$	$D_t(C)$	$D_t(D)$	$D_t(E)$	$D_t(F)$
1	?	?	$\frac{1}{6}$?	?	?
2	?	?	?	?	?	?
...						
219	?	?	?	?	?	?
220	$\frac{1}{14}$	$\frac{1}{14}$	$\frac{7}{14}$	$\frac{1}{14}$	$\frac{2}{14}$	$\frac{2}{14}$
221	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{7}{20}$	$\frac{1}{20}$	$\frac{1}{4}$	$\frac{1}{10}$
...						
3017	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{8}$	$\frac{1}{16}$	$\frac{1}{16}$	0
...						
8888	$\frac{1}{8}$	$\frac{3}{8}$	$\frac{1}{8}$	$\frac{2}{8}$	$\frac{3}{8}$	$\frac{1}{8}$

5. In the last semester, someone used AdaBoost to train some data and recorded all the weights throughout iterations but some entries in the table are not recognizable. Clever as you are, you decide to employ your knowledge of Adaboost to determine some of the missing information.

Below, you can see part of table that was used in the problem set. There are columns for the Round # and for the weights of the six training points (A, B, C, D, E, and F) at the start of each round. Some of the entries, marked with “?”, are impossible for you to read.

In the following problems, you may assume that non-consecutive rows are independent of each other, and that a classifier with error less than $\frac{1}{2}$ was chosen at each step.

- (a) The weak classifier chosen in Round 1 correctly classified training points A, B, C, and E but misclassified training points D and F. What should the updated weights have been in the following round, Round 2? Please complete the form below.

Round	$D_2(A)$	$D_2(B)$	$D_2(C)$	$D_2(D)$	$D_2(E)$	$D_2(F)$
2						

- (b) During Round 219, which of the training points (A, B, C, D, E, F) must have been misclassified, in order to produce the updated weights shown at the start of

Round 220? List all the points that were misclassified. If none were misclassified, write 'None'. If it can't be decided, write 'Not Sure' instead.

(c) You observe that the weights in round 3017 or 8888 (or both) cannot possibly be right. Which one is incorrect? Why? Please explain in one or two short sentences.

- Round 3017 is incorrect.
- Round 8888 is incorrect.
- Both rounds 3017 and 8888 are incorrect.

6. What condition must a weak learner satisfy in order for boosting to work?

Short answer:

7. After an iteration of training, AdaBoost more heavily weights which data points to train the next weak learner? (Provide an intuitive answer with no math symbols.)

Short answer:

8. **Extra credit** Do you think that a deep neural network is nothing but a case of boosting? Why or why not? Impress us.

Answer:

6 Recommender Systems

1. Applied to the Netflix Prize problem, which of the following methods does NOT always require side information about the users and the movies?

Select all that apply:

- Neighborhood methods
- Content filtering
- Latent factor methods
- Collaborative filtering
- None of the above

2. **Select all that apply:**

- Using matrix factorization, we can embed both users and items in the same space
- Using matrix factorization, we can embed either solely users or solely items in the same space, as we cannot combine different types of data
- In a rating matrix of users by books that we are trying to fill up, the best-known solution is to fill the empty values with 0s and apply PCA, allowing the dimensionality reduction to make up for this lack of data
- Alternating minimization allows us to minimize over two variables
- Alternating minimization avoids the issue of getting stuck in local minima
- If the data is multidimensional, then overfitting is extremely rare
- Nearest neighbor methods in recommender systems are restricted to using euclidian distance for their distance metric
- None of the above

3. Your friend Duncan wants to build a recommender system for his new website DuncanTube, where users can like and dislike videos that are posted there. In order to build his system using collaborative filtering, he decides to use Non-Negative Matrix Factorization. What is an issue with Duncan's approach, and what could he change about the website *or* the algorithm in order to fix it?

4. You and your friends want to build a movie recommendation system based on collaborative filtering. There are three websites (A, B and C) that you decide to extract users rating from. On website A, the rating scale is from 1 to 5. On website B, the rating scale is from 1 to 10. On website C, the rating scale is from 1 to 100. Assume you will have enough information to identify users and movies on one website with users and movies on another website. Would you be able to build a recommendation system? And briefly explain how would you do it?

5. What is the difference between collaborative filtering and content filtering?

7 K-Means

1. For **True or False** questions, circle your answer and justify it; for **QA** questions, write down your answer.

(i) For a particular dataset and a particular k , k -means always produce the same result, if the initialized centers are the same. Assume there is no tie when assigning the clusters.

True

False

Justify your answer:

(ii) k -means can always converge to the global optimum.

True

False

Justify your answer:

(iii) k -means is not sensitive to outliers.

True

False

Justify your answer:

(iv) k in k -nearest neighbors and k -means have the same meaning.

True

False

Justify your answer:

(v) What's the biggest difference between k -nearest neighbors and k -means?

Write your answer in one sentence:

2. In k-means, random initialization could possibly lead to a local optimum with very bad performance. To alleviate this issue, instead of initializing all of the centers completely randomly, we decide to use a smarter initialization method. This leads us to k-means++.

The only difference between k-means and k-means++ is the initialization strategy, and all of the other parts are the same. The basic idea of k-means++ is that instead of simply choosing the centers to be random points, we sample the initial centers iteratively, each time putting higher probability on points that are far from any existing center. Formally, the algorithm proceeds as follows.

Given: Data set $x^{(i)}, i = 1, \dots, N$

Initialize:

$$\mu^{(1)} \sim \text{Uniform}(\{x^{(i)}\}_{i=1}^N)$$

For $j = 2, \dots, k$

Computing probabilities of selecting each point

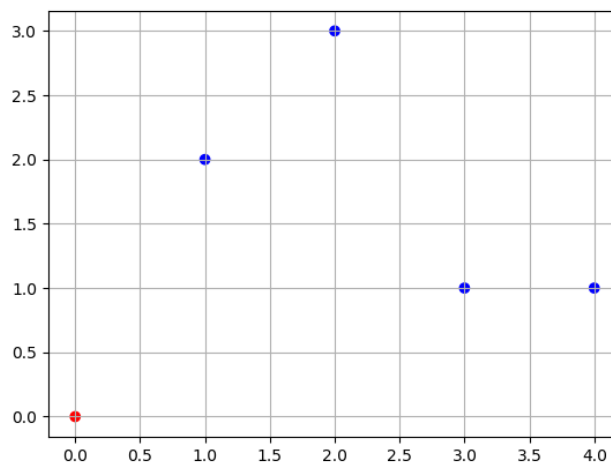
$$p_i = \frac{\min_{j' < j} \|\mu^{(j')} - x^{(i)}\|_2^2}{\sum_{i'=1}^N \min_{j' < j} \|\mu^{(j')} - x^{(i')}\|_2^2}$$

Select next center given the appropriate probabilities

$$\mu^{(j)} \sim \text{Categorical}(\{x^{(i)}\}_{i=1}^N, \mathbf{p}_{1:N})$$

Note: n is the number of data points, k is the number of clusters. For cluster 1's center, you just randomly choose one data point. For the following centers, every time you initialize a new center, you will first compute the distance between a data point and the center closest to this data point. After computing the distances for all data points, perform a normalization and you will get the probability. Use this probability to sample for a new center.

Now assume we have 5 data points (n=5): (0, 0), (1, 2), (2, 3), (3, 1), (4, 1). The number of clusters is 3 (k=3). The center of cluster 1 is randomly chosen as (0, 0). These data points are shown in the figure below.



- (i) What is the probability of every data point being chosen as the center for cluster 2? (The answer should contain 5 probabilities, each for every data point)

- (ii) Which data point is mostly likely chosen as the center for cluster 2?

- (iii) Assume the center for cluster 2 is chosen to be the most likely one as you computed in the previous question. Now what is the probability of every data point being chosen as the center for cluster 3? (The answer should contain 5 probabilities, each for every data point)

- (iv) Which data point is mostly likely chosen as the center for cluster 3?

- (v) Assume the center for cluster 3 is also chosen to be the most likely one as you computed in the previous question. Now we finish the initialization for all 3 centers. List the data points that are classified into cluster 1, 2, 3 respectively.

(vi) Based on the above clustering result, what's the new center for every cluster?



(vii) According to the result of (ii) and (iv), explain how does k-means++ alleviate the local optimum issue due to initialization?



8 Clustering and k -means (Lloyd's Algorithm)

8.1 True/False

Circle True or False for the questions below. **If your answer is False, provide a one line justification.**

1. In k -means, the cost always drops after one update step.

Circle one: True False

2. k -means is more likely to pick the wrong centers when number of clusters k increases.

Circle one: True False

3. Recall the k -means++ algorithm from lecture. Here we provide the generalized version of k -means++:

- Choose \mathbf{c}_1 at random.
- For $j = 2, \dots, K$
 - Pick \mathbf{c}_j among $\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(N)}$ according to the distribution

$$P(\mathbf{c}_j = \mathbf{x}^{(i)}) \propto \min_{j' < j} \|\mathbf{x}^{(i)} - \mathbf{c}_{j'}\|^\alpha$$

The lecture version uses $\alpha = 2$.

Circle one: True False

4. When α in k -means++ becomes 0, it means random sampling.

Circle one: True False

8.2 k -Means

Consider a dataset with seven points $\{x_1, \dots, x_7\}$. Given below are the distances between all pairs of points.

	x_1	x_2	x_3	x_4	x_5	x_6	x_7
x_1	0	5	3	1	6	2	3
x_2	5	0	4	6	1	7	8
x_3	3	4	0	4	3	5	6
x_4	1	6	4	0	7	1	2
x_5	6	1	3	7	0	8	9
x_6	2	7	5	1	8	0	1
x_7	3	8	6	2	9	1	0

Assume that $k = 2$, and the cluster centers are initialized to x_3 and x_6 . Which of the following shows the two clusters formed at the end of the first iteration of k -means? Circle the correct option.

- (a) $\{x_1, x_2, x_3, x_4\}, \{x_5, x_6, x_7\}$
- (b) $\{x_2, x_3, x_5\}, \{x_1, x_4, x_6, x_7\}$
- (c) $\{x_1, x_2, x_3, x_5\}, \{x_4, x_6, x_7\}$
- (d) $\{x_2, x_3, x_4, x_7\}, \{x_1, x_5, x_6\}$