CS 475 Machine Learning: Homework 5 Analytical (60 points)

Assigned: Friday, November 15, 2024 Due: Friday, November 29, 2024, 11:59 pm US/Eastern

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Instructions

We have provided this LATEX document for turning in this homework. We give you one or more boxes to answer each question. The question to answer for each box will be noted in the title of the box. You can change the size of the box if you need more space.

Other than your name, do not type anything outside the boxes. Leave the rest of the document unchanged.

Do not change any formatting in this document, or we may be unable to grade your work. This includes, but is not limited to, the font sizes, and the spacing of text. Additionally, do not add text outside of the answer boxes. Entering your answers are the only changes allowed.

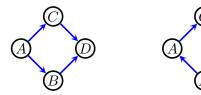
We strongly recommend you review your answers in the generated PDF to ensure they appear correct. We will grade what appears in the answer boxes in the submitted PDF, NOT the original latex file.

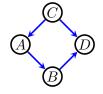
Observational Equivalence of DAGs and the GES Algorithm

Question 1. (20 pts)

Two DAGs \mathcal{G}_1 and \mathcal{G}_2 are said to be *observationally equivalent* if the list of conditional independences implied by the d-separation criterion in both graphs is the same. In other words, \mathcal{G}_1 and \mathcal{G}_2 are observationally equivalent if they imply the same statistical model.

A result by Thomas Verma and Judea Pearl states that \mathcal{G}_1 and \mathcal{G}_2 are observationally equivalent if and only if they agree on edge adjacencies (in other words, if V_i and V_j share an edge in \mathcal{G}_1 , then V_i and V_j share an edge in \mathcal{G}_2 , and vice versa – ignoring edge orientation), and agree on unshielded colliders. An unshielded collider is a structure of the form $V_i \to V_k \leftarrow V_j$ such that V_i and V_j do not share an edge. As an example, the following three graphs are observationally equivalent:





The above three DAGs give the same model: $(B \perp\!\!\!\perp C \mid A)$, $(D \perp\!\!\!\perp A \mid B, C)$.

(a) Write out all equivalence classes for DAGs with three vertices. How many equivalence classes are there?

Eq. class 1: $A \to B \to C$

Eq. class 2: $A \to B \leftarrow C$

Eq. class 3: $A \to B \to C, A \to C$

All other DAGs produce the same equivalence classes as these three base ones, so there are a total of three equivalence classes.

(b) Assume all data is binary. Write down the dimension of each model corresponding to each equivalence class in (a).

The dimension of each model is 2^k for k parents of the node. In the order presented, their dimensions are 5, 6, and 7.

(c) Create an undirected graph representing the discrete state space for structure learning, where vertices represent equivalence classes in (a), and there is an edge connecting any two classes where a DAG in one class differs from a DAG in another class by addition or deletion precisely one → edge.

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(d) Assume the GES algorithm performs the following sequence of edge additions and deletions (starting from the empty graph): add $A \to B$, add $B \to C$, add $A \to C$, remove $B \to C$. Write down all sequences of equivalence classes consistent with this set of edge additions and removals. Note: there could be more than one such sequence.

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 \begin{cases} \{A \to B\} \\ \{A \to B \to C\} \\ \{A \to B \to C, A \to C\} \\ \{A \to B, A \to C\} \end{cases}
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(e) Consider a DAG $V_1 \rightarrow V_2 \rightarrow V_3 \rightarrow V_4 \rightarrow V_k$. How many DAGs are observationally equivalent to this DAG? Explain.

Directed and split triplets function the same when evaluating the independence statements. Collider triplets, however, do not. This DAG consists only of directed triplets, so altering the relationships so long as they do not create collider triplets will produce observationally equivalent DAGs. No edges can be removed or added as well. This leaves 4 possible alternative DAGs (or k-1 for arbitrary length k), as each edge can be flipped, but all edges to the left of it must also be flipped so that no collider triplet is present.

Missing Data

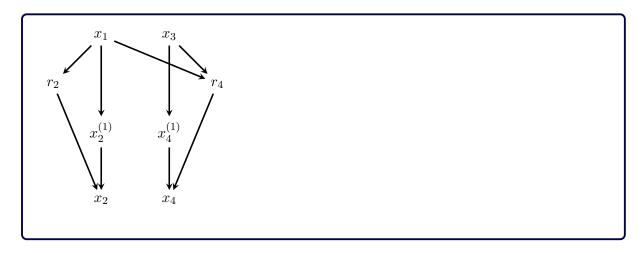
Question 2. (24 pts)

(a) Consider the following observed data likelihood:

$$\mathcal{L}_{[D]}(\beta) = \prod_{i=1}^{n} \sum_{x_{2i}^{(1)} \text{ if } r_{2i}=0} \sum_{x_{4i}^{(1)} \text{ if } r_{4i}=0} p(x_{1i}, x_{3i}) p(r_{4i} \mid x_{1i}, x_{3i}) p(r_{2i} \mid x_{1i}) p(x_{2i}^{(1)} \mid x_{1i}) p(x_{4i}^{(1)} \mid x_{3i})$$

$$p(x_{2i} \mid r_{2i}, x_{2i}^{(1)}) p(x_{4i} \mid r_{4i}, x_{4i}^{(1)})$$

Draw the missing data graph for this model.



(b) Does this likelihood represent a missing at random (MAR) model or missing not at random (MNAR) model?

It is MAR because the r values depend only on observed variables and not on the values of the missing data itself.

(c) Express $p(x_1, x_2^{(1)}, x_3, x_4^{(1)})$ as a function $p(x_1, x_2, x_3, x_4, r_2, r_4)$.

Expanded form: $p(x_1, x_2, x_3, x_4, r_2, r_4) = p(x_1)p(x_3)p(r_2|x_1)p(r_4|x_1, x_3)p(x_2^{(1)}|x_1)p(x_4^{(1)}|x_3)p(x_2|x_2^{(1)}, r_2)$ $p(x_4|x_4^{(1)}, r_4)$ Handle $x_2^{(1)}$ and $x_4^{(1)}$: $p(x_1, x_2^{(1)}, x_3, x_4^{(1)}) = \sum_{r_2, r_4} \int_{x_2} \int_{x_4} p(x_1, x_2, x_3, x_4, r_2, r_4) dx_2 dx_4$. Substituting and simplifying results in: $p(x_1, x_2^{(1)}, x_3, x_4^{(1)}) = p(x_1)p(x_3)\sum_{r_2} p(r_2|x_1)\sum_{r_4} p(r_4|x_1, x_3)p(x_2^{(1)}|x_1)p(x_4^{(1)}|x_3)$

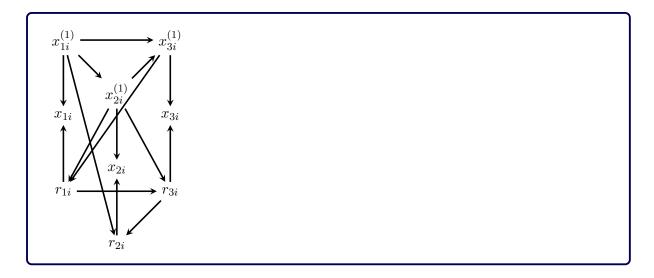
(d) Consider the following observed data likelihood:

$$\mathcal{L}_{[D]}(\beta) = \prod_{i=1}^{n} \sum_{x_{1i}^{(1)} \text{ if } r_{1i}=0} \sum_{x_{2i}^{(1)} \text{ if } r_{2i}=0} \sum_{x_{3i}^{(1)} \text{ if } r_{3i}=0} p(x_{1i}^{(1)}) p(x_{2i}^{(1)} \mid x_{1i}^{(1)}) p(x_{3i}^{(1)} \mid x_{2i}^{(1)}, x_{1i}^{(1)})$$

$$p(r_{1i} \mid x_{2i}^{(1)}, x_{3i}^{(1)}) p(r_{2i} \mid x_{1i}^{(1)}, r_{3i}) p(r_{3i} \mid x_{2i}^{(1)}, r_{1i})$$

$$p(x_{1i} \mid r_{1i}, x_{1i}^{(1)}) p(x_{2i} \mid r_{2i}, x_{2i}^{(1)}) p(x_{3i} \mid r_{3i}, x_{3i}^{(1)})$$

Draw the missing data graph for this model.



(e) Does this likelihood represent a missing at random (MAR) model or missing not at random (MNAR) model?

It is MNAR because some of the r values depend on unobserved variables and not on the values of the missing data itself.

(f) Does the observed data likelihood have a unique global maximum? In other words, is $p(x_1^{(1)}, x_2^{(1)}, x_3^{(1)}, r_1, r_2, r_3)$ a function of the observed data distribution $p(x_1, x_2, x_3, r_1, r_2, r_3)$? Why? (This is a yes/no question with an explanation: if such a function exists, you don't have to give it)

No. This is because $p(x_1^{(1)}, x_2^{(1)}, x_3^{(1)}, r_1, r_2, r_3)$ involves summation over missing data. This heavily complicates things as multiple values for these missing data points can provide different maxima.

Reinforcement Learning.

Question 3. (16 pts)

(a) We run policy π in a MDP and obtain a sequence of state and action T timesteps:

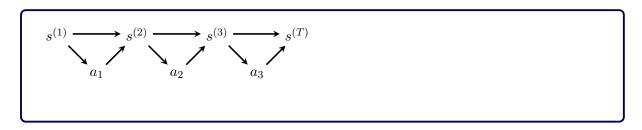
$$\tau = \{s^{(1)}, a_1, s^{(2)}, a_2, s^{(3)}, a_3, \cdots, a_{T-1}, s^{(T)}\}\$$

Assume that a stationary policy π : $a_t \sim \pi(\cdot \mid s^{(t)}), \forall t \in [T]$, write the loglikehood of this trajectory: $\log p(\tau)$.

Likelihood:
$$p(\tau) = p(s^{(1)}, a_1, s^{(2)}, a_2, ..., a^{T-1}, s^{(T)})$$

 $\implies p(\tau) = p(s^{(1)}) \prod_{t=1}^{T-1} p(a_t | s^{(t)}) p(s^{(t+1)} | s^{(t)}, a_t)$ Log-likelihood: $\log p(\tau) = \log p(s^{(1)}) + \sum_{t=1}^{T-1} \log p(a_t | s^{(t)}) + \log p(s^{(t+1)} | s^{(t)}, a_t)$
Replace $p(a_t | s^{(t)})$ with $\pi(a_t | s^{(t)})$ due to policy being stationary $\log p(\tau) = \log p(s^{(1)}) + \sum_{t=1}^{T-1} \log \pi(a_t | s^{(t)}) + \log p(s^{(t+1)} | s^{(t)}, a_t)$

(b) Draw a DAG for $p(\tau)$ in question (a)



- (c) As we've seen in class that the discount factor $0 \le \gamma \le 1$ represents how much weight is placed on future rewards compared to immediate rewards. Assume the rewards are bounded, $R_a(s^{(t)}, s^{(t+1)}) \in [0, 1]$.
 - Give a brief explanation of why the value function V(s) could be unbounded for $\gamma = 1$ in the **infinite horizon** setting, even if we assume the reward is bounded.
 - Show that $V(s) \leq \frac{1}{1-\gamma}$, and $Q(s,a) \leq \frac{1}{1-\gamma}$, for $\gamma \in [0,1)$?

There is no discounting in future rewards, so even if rewards are bounded, there is no limit to the total reward accumulated over.

If the discount factor is less than one, $V(s) = \sum_{t=1}^{\infty} \gamma^t R_a \leq \sum_{t=1}^{\infty} \gamma^t$ because R_a is either 0 or 1. Because it is a geometric series, it can then be represented as $\frac{1}{1-\gamma}$, so $V(s) \leq \frac{1}{1-\gamma}$. Since the policy is stationary, Q(s,a) is likewise bounded.

(d) Remind that the update rule for the value function is:

$$V_Q(s) = \max_a Q(s, a),$$

(the value function update of Value Iteration algorithm in the lecture is simply $V^{(t)} = V_{Q^{(t)}}$). Show that for any two Q, Q' state-action value functions:

$$\left| V_Q(s) - V_{Q'}(s) \right| \le \max_{a \in \mathcal{A}} \left| Q(s, a) - Q'(s, a) \right|.$$

Difference between value functions (and plug in above definition):

 $|V_Q(s) - V_{Q'}(s)| = |\max_{a \in A} Q(s, a) - \max_{a \in A} Q'(s, a)|$ Because the maximum difference between Q(s, a) and Q'(s, a) is $\max_{a \in A} |Q(s, a) - Q'(s, a)|$, we get the final inequality: $|V_Q(s) - V_{Q'}(s)| \le \max_{a \in A} |Q(s, a) - Q'(s, a)|$