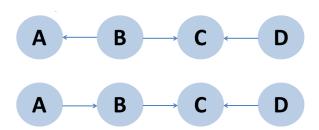
Homework 2 Solutions CS228: Probabilistic Graphical Models

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- 1. [8 points] (I-Maps and P-Maps, Part 1) Consider a probability distribution P over the variables A, B, C, and D that satisfies only the following independencies:
 - 1. $A \perp C \mid B$
 - 2. $A \perp C \mid B, D$
 - 3. $A \perp D \mid B$
 - 4. $A \perp D \mid B, C$
 - 5. $B \perp D$
 - 6. $B \perp D \mid A$
 - 7. $A \perp D$
 - (a) [3 points] Draw a Bayesian network that is a perfect map for P.

Answer: The 2 graphs below are both perfect maps for P. Either of them is valid, and the other is the l-equivalent graph for part (b).



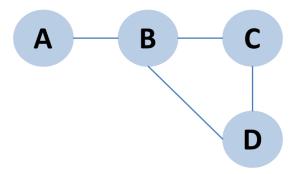
- (b) [2 points] Does this perfect map have any I-equivalent graphs? If so, draw them. If not, explain why not.
 - **Answer:** Yes. See the solution to part (a) for the I-equivalent graphs. Using the theorem shown in lecture

same skeleton + same v-structures \implies l-equivalent

the two graphs are clearly I-equivalent. To show that these are the only I-equivalent graphs, we rely on Theorem 3.8 from the book:

same skeleton + same immoralities \iff I-equivalent.

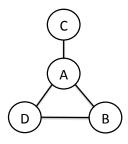
An immorality is defined as a v-structure $X \to Y \leftarrow Z$ where X and Z are not connected. Clearly, there are no other possible graphs with the same A-B-C-D skeleton and the $B \to C \leftarrow D$ immorality.



(c) [3 points] Draw a Markov network that is a minimal I-map for P and explain why the Markov network is or is not also a perfect map.

Answer: A Markov net with these undirected edges and additional B-D edge is a valid I-map. This Markov net is not a perfect map because B and D are not independent in this network, while they are independent in the original probability distribution.

2. [9 points] (I-Maps and P-Maps, Part 2) Consider a distribution P over four binary random variables (A, B, C, D), which gives probability 1/8 to assignments (0, 0, 0, 0) and (1, 1, 0, 0), and gives probability 1/4 to assignments (1, 1, 1, 0), (0, 1, 0, 1), and (1, 0, 1, 1). A skeleton for the Bayesian network G is also provided; the skeleton contains all the nodes and edges, but the directions of the edges are missing.



(a) [2 points] Decide whether the following two independencies are in I(P): $(C \perp D)$, $(C \perp B)$.

Answer: First, compute the marginal distribution on (C, D):

$$P(C=0,D=0) = (1/8) + (1/8) = 1/4;$$
 $P(C=0,D=1) = 1/4;$ $P(C=1,D=0) = 1/4;$ $P(C=1,D=1) = 1/4.$

One can easily check that P(C,D) = P(C)P(D). Then, by definition of independence, $(C \perp D) \in I(P)$.

Second, compute the marginal distribution on (B, C):

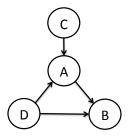
$$P(B=0,C=0)=1/8;$$
 $P(B=0,C=1)=1/4;$ $P(B=1,C=0)=(1/8)+(1/4)=3/8;$ $P(B=1,C=1)=1/4.$

From above, P(B=0)=3/8 and P(C=0)=1/2. So, $P(B=0,C=0)\neq P(B=0)P(C=0)$. Then, again by definition of independence, $(C\perp B)\notin I(P)$.

(b) [5 points] Give a direction to each individual edge in G, such that the resulting Bayesian network is a minimal I-Map of P. Is your solution for this question unique? Briefly state why.

Answer

The only way to have $(C \perp D)$ is to have a V-structure: $D \rightarrow A \leftarrow C$; otherwise there will be an active trail from C to D via A.



Moreover, the only possible direction of the edge between A and B is: $A \to B$; otherwise, we will have a V-structure: $B \to A \leftarrow C$, which contradicts the fact that $(C \perp B) \notin I(P)$.

Lastly, we must have $D \to B$; otherwise, we'll have a triangular loop (A, B, D), which contradicts the acyclic requirement of Bayesian networks.

From the description above, one can see that such result is unique.

Comment1:

This proof of uniqueness is not rigorous. As some of you have noticed, $(C \perp D)$ is not necessary for an I-map, since all we need for an I-map is $I(G) \subset I(P)$. Without assuming $(C \perp D)$, it takes some computation to present all the conditional independence, and show the uniqueness. We will take special care of similar issues for exam questions.

Comment2:

Some of you show uniqueness by stating that "Equivalent I map has to share same skeleton and v-structure." This is incorrect. See lecture 3 for the original theorem. The converse of the original theorem does not hold.

(c) [2 points] Give the CPDs for each node in your Bayesian network specified in (b).

Answer:

• CPD for variable C:

$$P(C = 0) = P(C = 1) = 1/2.$$

• CPD for variable *D*:

$$P(D=0) = P(D=1) = 1/2.$$

So, both C and D are Bernoulli(1/2). We'll just use tabular CPDs for C, D.

- ullet CPD for variable B: from probability assignments mentioned in the problem description, one can easily be convinced that $B=(A \ {\sf XOR} \ D)$. So a deterministic function (XOR) will be sufficient to characterize this CPD.
- CPD for variable A:

$$\begin{split} P(A=0 \mid C=0,D=0) &= 1/2, \\ P(A=0 \mid C=1,D=0) &= 0, \\ P(A=1 \mid C=0,D=0) &= 1/2; \\ P(A=0 \mid C=0,D=1) &= 1, \\ P(A=1 \mid C=1,D=0) &= 1; \\ P(A=1 \mid C=0,D=1) &= 0; \\ P(A=1 \mid C=1,D=1) &= 0; \\ P(A=1 \mid C=1,D=1) &= 1. \end{split}$$

We'll use the following tree CPD to represent it:

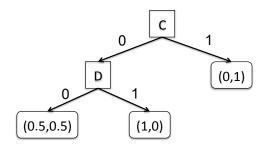
3. [16 points] (Undirected Graphical Models, Inference) The Restricted Boltzmann Machine

Restricted Boltzmann machines (RBMs) have been widely used as a generative model in many fields of machine learning: image processing, speech recognition and collaborative filtering. Concretely, a RBM is an undirected graphical model defined on variables (\mathbf{v}, \mathbf{h}) , $\mathbf{v} \in \{0, 1\}^m$ and $\mathbf{h} \in \{0, 1\}^n$. The joint probability is given by

$$P(\mathbf{v}, \mathbf{h}) = \frac{1}{Z} \exp(\phi(\mathbf{v}, \mathbf{h}))$$

where

$$\phi(\mathbf{v}, \mathbf{h}) = -\alpha^T \mathbf{v} - \beta^T \mathbf{h} - \mathbf{v}^T W \mathbf{h}$$



is a potential function. Here $\alpha \in \mathbb{R}^m$, $\beta \in \mathbb{R}^n$, $W \in \mathbb{R}^{m \times n}$ and Z is the normalizing constant. You can interpret it as a fully connected *bipartite* network with two layers: one for visible variables \mathbf{v} and one for hidden variables \mathbf{h} . In this problem, you will explore inference and learning for RBMs.

(a) [5 points] What is the expression for the marginal conditional distribution of $P(h_i \mid \mathbf{v})$ for a single hidden variable h_i ? Can it be computed tractably, e.g. in polynomial time?

Answer: Let \mathbf{w}_i denote the *i*-th column of W. Then, we have

$$P(h_i \mid v) = \frac{\exp(-h_i(\mathbf{v}^T \mathbf{w}_i) - \beta_i h_i)}{\sum_{h_i} \exp(-h_i(\mathbf{v}^T \mathbf{w}_i) - \beta_i h_i)} = \frac{\exp(-h_i(\mathbf{v}^T \mathbf{w}_i) - \beta_i h_i)}{1 + \exp(-\mathbf{v}^T \mathbf{w}_i - \beta_i)}$$

This computation takes O(m) time due to the dot-product between the m-dimensional vectors \mathbf{v} and \mathbf{w}_i .

(b) [5 points] What is the conditional distribution $P(\mathbf{h} \mid \mathbf{v})$? Can it be expressed in a compact (factored) form?

Answer: In a RBM, the conditional distribution $P(\mathbf{h} \mid \mathbf{v})$ is the product of the marginals. Let $\mathbf{r}^T = -\beta^T - \mathbf{v}^T W$. Then,

$$P(\mathbf{h} \mid \mathbf{v}) = \frac{P(\mathbf{h}, \mathbf{v})}{P(\mathbf{v})} = \frac{\frac{1}{Z} \exp(-\alpha^T \mathbf{v} + \mathbf{r}^T \mathbf{h})}{\sum_{\mathbf{h}'} \frac{1}{Z} \exp(-\alpha^T \mathbf{v} + \mathbf{r}^T \mathbf{h}')} = \frac{\exp(\mathbf{r}^T \mathbf{h})}{\sum_{\mathbf{h}'} \exp(\mathbf{r}^T \mathbf{h}')}$$
$$= \frac{\prod_{i} \exp(r_i h_i)}{\prod_{i} \sum_{h'_i} \exp(r_i h'_i)} = \prod_{i=1}^{n} P(h_i \mid \mathbf{v})$$

We know from part(a) that $P(h_i \mid v)$ is an O(m) computation, so $P(\mathbf{h} \mid \mathbf{v})$ is an O(mn) computation. Note that this factorization implies $h_i \perp h_j \mid v$ for all $i \neq j$, which matches the interpretation of the RBM as a bipartite graph.

(c) [2 points] Suppose we are given samples for the visible units $\mathcal{D} = \{\mathbf{v}^1, \dots, \mathbf{v}^K\}$ (e.g., the MNSIT digits dataset), and we want to learn the parameters of the RBM to maximize the likelihood of these samples. Since we don't know the values of hidden variables \mathbf{h}^k , a natural approach is to look for parameters that maximize the marginal likelihood of each sample \mathbf{v}^k , given by

$$L(\mathbf{v}) = \sum_{\mathbf{h}} P(\mathbf{h}, \mathbf{v}) = \sum_{\mathbf{h}} \frac{1}{Z} \exp(\phi(\mathbf{v}, \mathbf{h}))$$

For a fixed \mathbf{v} , can

$$\sum_{\mathbf{h} \in \{0,1\}^n} \exp(\phi(\mathbf{v}, \mathbf{h}))$$

be computed efficiently (in time not exponential in n)? Please give a brief justification for full credit.

Answer: Yes, the sum factors because of conditional independency

(d) [2 points] For a fixed h, can

$$\sum_{\mathbf{v} \in \{0,1\}^m} \exp(\phi(\mathbf{v}, \mathbf{h}))$$

be computed efficiently (in time not exponential in m)? Please give a brief justification for full credit.

Answer: Yes, the sum factors because of conditional independency

(e) [2 points] Can the normalization constant

$$Z = \sum_{\mathbf{h}} \sum_{\mathbf{v}} \exp(\phi(\mathbf{v}, \mathbf{h}))$$

be computed efficiently (in time not exponential in m or n)? Please give a brief justification for full credit.

Answer: No

4. [10 points] Maximum Likelihood Learning of Bayes Nets

Let G be a valid Bayes Net structure, and \mathcal{D} be some training data. It can be shown that the log likelihood of \mathcal{D} for a given choice of the parameters θ (specifying the conditional probability tables in G) is

$$\ell_G(\theta; \mathcal{D}) = \sum_{i=1}^n \sum_{\mathbf{u}_i \in Val(Pa(X_i))} \sum_{x_i} M[x_i, \mathbf{u}_i] \log \theta_{x_i | \mathbf{u}_i}$$

We have seen in class that the maximum likelihood estimate $\theta^{ML} = \arg \max_{\theta} \ell_G(\theta; \mathcal{D})$ of the parameters of G can be computed as follows

$$\theta_{x_i|\mathbf{u}_i}^{ML} = \frac{M[x_i, \mathbf{u}_i]}{M[\mathbf{u}_i]} \tag{1}$$

where $M[x_i, u_i]$ is the number of times the tuple $(X_i = x_i, Pa(X_i) = u_i)$ appears in the data \mathcal{D} . Note that u_i is a vector taking on the instantiated values of the parents of X_i .

Let G' be a valid Bayes net structure obtained by adding an edge to G. Show that

$$\max_{\theta'} \ell_{G'}(\theta'; \mathcal{D}) \ge \max_{\theta} \ell_{G}(\theta; \mathcal{D})$$

Note that G' is strictly more expressive than G (G' makes less conditional independence assumptions). This is confirmed by the fact that to specify a Bayes Net with structure G' we need more parameters, i.e., the vector θ' has more components than θ . The goal of this exercise is to show directly that the more "complex" a Bayesian Network is, the better we can fit it to data.

You may assume that G and G' are identical, except for an extra $x_1 \to x_n$ edge in G'.

Hint: There are several ways to show this. You may find Jensen's inequality or properties of KL divergence useful.

Answer: Let $Pa(X_i)$ refer to the parents of X_i in graph G, and let $Pa'(X_i)$ refer to the parents of X_i in graph G'. Thus, we have

$$Pa'(X_i) = \begin{cases} Pa(X_n) \cup \{X_1\} & i = n \\ Pa(X_i) & \text{otherwise} \end{cases}$$

$$\begin{split} & \left\{ \mathcal{C}(\theta_{G'}^{ML}; \mathcal{D}) - \ell_{G}(\theta_{G'}^{ML}; \mathcal{D}) \right. \\ & = \left[\sum_{i=1}^{n} \sum_{\tilde{u}_{i} \in Val(Pa'(X_{i}))} \sum_{x_{i}} M[x_{i}, \hat{u}_{i}] \log \theta_{x_{i}}|_{\tilde{u}_{i}} \right] - \left[\sum_{i=1}^{n} \sum_{u_{i} \in Val(Pa(X_{i}))} \sum_{x_{i}} M[x_{i}, u_{i}] \log \theta_{x_{i}}|_{u_{i}} \right] \\ & = \sum_{i=1}^{n} \sum_{x_{i}} \left[\sum_{\tilde{u}_{i} \in Val(Pa'(X_{i}))} M[x_{i}, \hat{u}_{i}] \log \theta_{x_{i}}|_{\tilde{u}_{i}} - \sum_{u_{i} \in Val(Pa(X_{i}))} M[x_{i}, u_{i}] \log \theta_{x_{i}}|_{u_{i}} \right] \\ & = \sum_{x_{n}} \left[\sum_{\tilde{u}_{n} \in Val(Pa(X_{n}) \cup \{X_{1}\})} M[x_{n}, u_{n}] \log \frac{M[x_{n}, \hat{u}_{n}]}{M[\hat{u}_{n}]} - \sum_{u_{n} \in Val(Pa(X_{n}))} M[x_{n}, u_{n}] \log \frac{M[x_{n}, u_{n}]}{M[u_{n}]} \right] \\ & = \sum_{x_{n}} \left[\sum_{u_{n} \in Val(Pa(X_{n}))} \sum_{x_{1}} M[x_{n}, u_{n}, x_{1}] \log \frac{M[x_{n}, u_{n}, x_{1}]}{M[u_{n}, x_{1}]} - \sum_{u_{n} \in Val(Pa(X_{n}))} M[x_{n}, u_{n}] \log \frac{M[x_{n}, u_{n}]}{M[u_{n}]} \right] \\ & = \sum_{x_{n}} \sum_{u_{n} \in Val(Pa(X_{n}))} \sum_{x_{1}} M[x_{n}, u_{n}, x_{1}] \log \frac{M[x_{n}, u_{n}, x_{1}]}{M[u_{n}, x_{1}]} - \log \frac{M[x_{n}, u_{n}]}{M[u_{n}]} \right] \\ & = \sum_{x_{n}} \sum_{u_{n} \in Val(Pa(X_{n}))} \sum_{x_{1}} M[x_{n}, u_{n}, x_{1}] \log \frac{M[x_{n}, u_{n}, x_{1}]}{M[u_{n}, x_{1}]} - \log \frac{M[x_{n}, u_{n}]}{M[u_{n}]} \right) \quad \text{using } M[u_{n}, x_{1}] \\ & = |\mathcal{D}| \sum_{x_{n}} \sum_{u_{n} \in Val(Pa(X_{n}))} \sum_{x_{1}} \frac{M[x_{n}, u_{n}, x_{1}]}{|\mathcal{D}|} \log \left(\frac{M[x_{n}, u_{n}, x_{1}]}{M[u_{n}, x_{1}]} \frac{M[u_{n}]}{M[x_{n}, u_{n}]} \right) \\ & = |\mathcal{D}| \sum_{x_{n}} \sum_{u_{n} \in Val(Pa(X_{n}))} \sum_{x_{1}} \sum_{x_{1}} \hat{P}(x_{n}, x_{1}, u_{n}) \log \frac{\hat{P}(x_{n} \mid u_{n}, x_{1})}{\hat{P}(x_{n} \mid u_{n})} \\ & = |\mathcal{D}| \sum_{u_{n} \in Val(Pa(X_{n}))} \sum_{x_{1}} \sum_{x_{n}} \hat{P}(x_{n}, x_{1}, u_{n}) \log \frac{\hat{P}(x_{n} \mid u_{n}, x_{1})}{\hat{P}(x_{1} \mid u_{n})} \\ & = |\mathcal{D}| I_{p}(X_{n}; X_{1} \mid Pa(X_{n})) \end{aligned}$$

Alternative solution: It is possible to avoid rigorous math in the proof. The key idea is that if we apply the ML estimation θ^{ML} of the original graph to the new graph, we will obtain the same maximum log likelihood as in the original graph $\ell_{G'}(\theta^{ML};\mathcal{D}) = \ell_G(\theta^{ML};\mathcal{D}) = \max_{\theta} \ell_G(\theta;\mathcal{D})$. Since $\max_{\theta'} \ell_{G'}(\theta';\mathcal{D}) \geq \ell_{G'}(\theta^{ML};\mathcal{D})$ (the maximum log likelihood is larger than log likelihood with any given θ), we derive the inequality.

It takes some insights to find this alternative solution. If you figure this out yourself, you have a very deep understanding of the problem and strong intuition towards the quantities! However, working through the math will also be helpful.

5. [47 points] (Programming Assignment) Tree Augmented Naive Bayes

Naive Bayes (NB) classifiers are often competitive classifiers even though their strong independence assumptions may be unrealistic. We will explore an extension of this classification framework, Tree Augmented Naive Bayes (TANB), which will aim to improve the results of NB by modelling correlations between attributes while still being computationally tractable. If C denotes the class variable and (A_1, \ldots, A_N) the attributes, then a NB model can be represented as a directed graph with these variables as nodes and edges $\{(C, A_j) : 1 \le j \le n\}$. A TANB model extends this graph structure by allowing each child A_j to have one additional node A_i as a parent with the restriction that these additional edges (A_i, A_j) must form a tree. Figure 1 illustrates the difference in the graph structure.

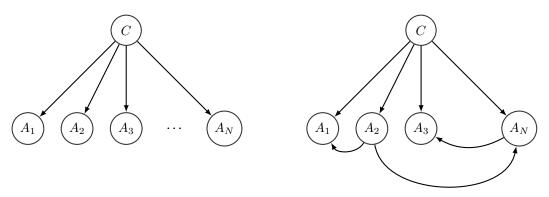


Figure 1: A Naive Bayes model and Tree Augmented Naive Bayes model

In general, learning the structure of this graph can be hard, but we will cover this topic later in the course. For now we have supplied starter code necessary to learn the structure of the graph for the dataset.

In this problem, you will implement the parameter learning for both NB and TANB classifiers and explore the trade-offs of both. You will apply these classifiers to predict the party affiliation of either Democrat or Republican of US Congressmen (the class variable) based on their votes for 16 different measures (the attribute variables) shown in Table 1. Not all Congressmen voted on all 16 measures so sometimes entries in this dataset will have missing attributes, however, we will still be able to utilize our Bayes Network to accurately classify these examples. To keep things simple, the class and attribute variables are all binary with 0, 1 corresponding to a no, yes vote respectively. Missing attributes will have a value of -1 assigned in the raw data (appears only during evaluation).

When training the models, some of the parameters may not have enough examples for accurate estimation. To mitigate this, we will perform Laplace smoothing with a pseudocount of $\alpha = 0.1$ for every value of an attribute given its parents when learning the parameters.

In order to evaluate the performance of our classifiers on the dataset, we will use 10-fold cross-validation. Under 10-fold cross-validation, the dataset is first partitioned into 10 equally sized partitions. Of these 10 partitions, one of them is used for the test set while the rest of the data are used as the training set to compute test error on this partition. This process is repeated for the other nine partitions, and we can take the average of the resulting test errors to obtain the 10-fold CV test error. We have implemented this procedure for you in the function evaluate.

(a) [8 points] Implement a NB classifier that both learns the parameters from the training data and can use these parameters to score and classify examples in the training data. What is your test error rate using 10-fold cross-validation?

Note: you can use the evaluate function in the starter code, but leave the optional argument train_subset to its default value until part (d).

Answer: 10-fold cross validation total test accuracy 0.9181 on 232 examples

(b) [12 points] We have provided starter code that implements the Chow-Liu algorithm (see Friedman et al. 1997) to learn the tree structure from the training data for a TANB. Using this tree, implement

Name	Incomplete Entry 1
handicapped infants	1
water project cost sharing	1
adoption of the budget resolution	0
physician fee freeze	0
El Salvador aid	0
religious groups in schools	0
anti satellite test ban	0
aid to Nicaraguan Contras	?
mx missile	?
immigration	0
synfuels corporation cutback	0
education spending	?
superfund right to sue	?
crime	?
duty free exports	0
export administration act south Africa	0
	handicapped infants water project cost sharing adoption of the budget resolution physician fee freeze El Salvador aid religious groups in schools anti satellite test ban aid to Nicaraguan Contras mx missile immigration synfuels corporation cutback education spending superfund right to sue crime duty free exports

Table 1: Attribute names for Congressional Voting Records together with an incomplete example that has some voting records missing for a particular Congressman.

a TANB classifier that learns the parameters from the training data and uses these to score examples. What is your test error rate using 10-fold cross-validation?

Answer: 10-fold cross validation total test accuracy 0.9526 on 232 examples

(c) [15 points] In general, working with data where the values of attributes and labels are missing is difficult when learning model parameters. However, we can still use our generative model from a fully trained Bayes Network to classify examples in which some of the attributes may be unobserved. Suppose A_i is unobserved. We can still compute $P(C \mid A_1, \ldots, A_{i-1}, A_{i+1}, \ldots, A_N)$ by computing $P(C, A_i \mid A_1, \ldots, A_{i-1}, A_{i+1}, \ldots, A_N)$ and marginalizing over A_i .

Update your TANB implementation to handle the case where some attributes may have missing values and use this new implementation to classify Incomplete Entry 1 in Table 1¹. Given the observed attributes/votes, what is the marginal probability that this Congressman is Democrat (C = 1)? What is the marginal probability that this Congressman voted on education spending $(A_{12} = 1)$?

Notice the power of a generative model. It can easily handle missing data and can be used to answer all sorts of probabilistic queries. In contrast, this would *not* be possible with a discriminative model, e.g., if you trained a logistic regression or a random forest classifier to directly predict the affiliation of a Congressman (C), because these models would only provide you with the conditional distribution $P(C \mid A_1, \ldots, A_N)$.

Hint: If you're having trouble marginalizing out multiple variables at once, itertools.product() may help.

Answer: TANB Classifier on missing data

 $P(C=1 \mid A_{\text{observed}}) = 0.9899$

 $P(A_{12} = 1 \mid A_{\text{observed}}) = 0.1022$

¹Your implementation does not have to be fully general. It's fine as long as it works on that particular example.

Note: You should train your classifier on the full dataset. You can use the function <code>evaluate_incomplete_entry</code>, which both trains on the full dataset and loads Incomplete Entry 1 for classification.

(d) [12 points] What is the test error when you train both classifiers on a smaller subset of the training data? Notice the different gap of the two classifiers. Explain why the test error for the TANB may not strictly be better than NB.

Note: set the arguments train_subset=True when calling evaluate so that the classifiers are trained on a much smaller subset of the data.

Answer: Naive Bayes

10-fold cross validation total test accuracy 0.9009 on 232 examples

TANBClassifier

10-fold cross validation total test accuracy 0.8922 on 232 examples

Training on a smaller subset of the data could lead to the TANB overfitting and learning dependencies present in the training data that do not hold across the dataset.