CS 5350/6350, DS 4350: Machine Learning Spring 2024

Homework 4

March 30, 2024

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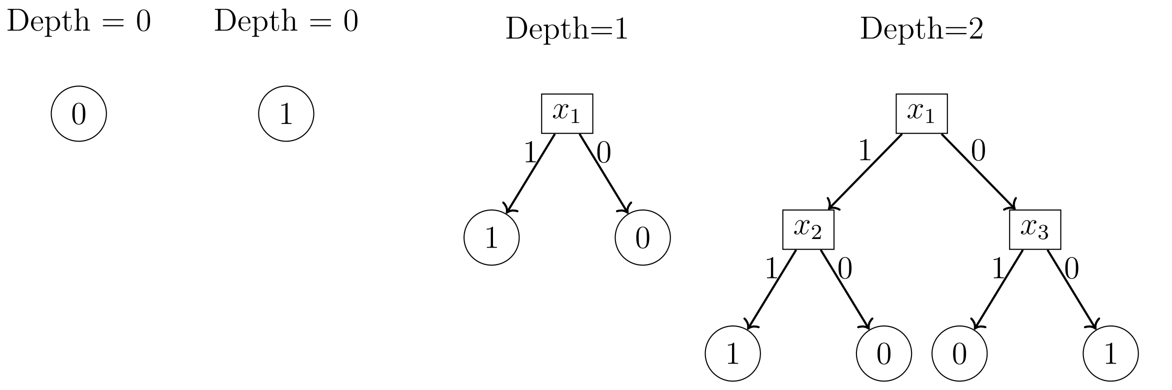
1 PAC Learnability of Depth Limited Decision Trees [30 points]

In this question, you will be showing that depth limited decision trees are PAC learnable.

Suppose we have a binary classification problem with n Boolean features that we seek to solve using decision trees of depth k. For this question assume trees are complete, meaning each node (other than the leaf nodes) has exactly two children. The figure below shows some examples of such trees and their depths.



1. Since decision trees represent a finite hypothesis class, the quantity of interest is the number of such trees—i.e., trees with depth k over n features. Suppose we use $S_n(k)$ to denote the number of the number of trees with depth exactly k if we have n features.

   The following questions guide you through this counting process. Recall that each answer should be accompanied with an explanation.*If you simply write the final answer, you will not get any points.* (**Please see the note at the end of this questions for further clarification**3).

   (a) [2 points] What is $S_n(0)$? That is how many trees of depth 0 exist?

   Response: $S_n(0) = 2$, there are two trees which can be visualized in the figure above for Depth = 0.

(b) [3 points] What is $S_n(1)$? That is, with n features, how many trees of depth 1 exist?

Response: $S_n(1) = n(2^2 - 1) = 3n$, there are exactly n different features that x_i can take; furthermore, there are $2^2 - 1$ different leaf nodes since the binary string $\{01\}$ is structurally the same as $\{10\}$.

(c) [4 points] Suppose you know the number of trees with depth i, for some i. This quantity would be $S_n(i)$ using our notation. Write down a recursive definition for $S_n(i+1)$ in terms of n and $S_n(i)$.

For this expression, you can assume that we are allowed to the use same feature any number of times when the tree is constructed.

Response: We know that $Sn(1) = 3n$. For $i = 2$, we have $2^4 = 16$ different leaf nodes: so 16-1 unique enumerations at the leafs. We can take the permutation at depth 1 to count the different enumerations possible that is count $= {}_nP_2 = \frac{n!}{(n-2)!} = n(n-1)$. At the root we have the same n different enumerations. Recursively this can be written as,

$$S_n(2) = S_n(1) \times 5n(n-1)$$

Following the same pattern for $i = 3$, we obtain,

$$S_n(3) = S_n(2) \times 17\frac{n!}{(n-4)!}$$

And again for $i = 4$:

$$S_n(4) = S_n(3) \times 257\frac{n!}{(n-8)!}$$

Thus, the recursive formula follows,

$$S_n(i+1) = S_n(i) \times \frac{2^{2^{i+1}} - 1}{2^{2^i} - 1}\frac{n!}{(n-2^i)!}$$

(d) [6 points] Recall that the quantity of interest for PAC bounds is the log of the size of the hypothesis class. Using your answer for the previous questions, find a closed form expression representing $\log S_n(k)$ in terms of n and k. Since we are not looking for an exact expression, but just an order of magnitude, so you can write your answer in the big O notation.

Response: From part (c) above:

$$S_n(k) = S_n(k-1) \times \frac{2^{2^k} - 1}{2^{2^{k-1}} - 1}\frac{n!}{(n-2^{k-1})!}$$

Taking the base 2 log of $S_n(k)$ and simplifying,

$$lg(S_n(k)) = lg(S_n(k-1)) + (lg(2^{2^k} - 1) - lg(2^{2^{k-1}} - 1)) + lg(\frac{n!}{(n-2^{k-1})!})$$

Clearly, the first and second terms are not major contributors when taking the limit for a big enough k and n. Thus,

$$lg(S_n(k)) \approxeq lg(\frac{n!}{(n-2^{k-1})!})$$

It is clear by considering properties of the factorial operator that $\frac{n!}{(n-2^{k-1})!} < n^{2^k}$. Therefore, we can declare that,

$$lg(S_n(k)) < lg(n^{2^k})$$

Finally, we can attest that $S_n(k)$ is in the order of $O(2^k\, lg(n))$.

2. Next, you will use your final answer from the previous question to state a sample complexity bound for decision trees of depth k.

   (a) [3 points] With finite hypothesis classes, we saw two Occam's razor results. The first one was for the case of a consistent learner and the second one was for the agnostic setting. For the situation where we are given a dataset and asked to use depth-k decision trees as our hypothesis class, which of these two settings is more appropriate? Why?

   Response: The Agnostic approach to Occam's Razor fits better here. Decision trees with fixed depths might not always capture real-world data complexity. Staying open to the possibility that the true target function lies beyond depth-k trees allows exploring more hypotheses, potentially improving generalization.

   (b) [4 points] Using your answers from questions so far, write the sample complexity bound for the number of examples m needed to guarantee that with probability more than $1-\delta$, we will find a depth-k decision tree whose generalization error is no more than ϵ away from its training error.

   Response: From lecture we know that the number of samples m is lower bounded such that, $m \geq \frac{1}{\epsilon^2}(ln(|H|) + ln(\frac{1}{\sigma}))$, where $|H| = n^{2^k}$. Thus,

$$m \geq \frac{1}{\epsilon^2}(2^k ln(n) + ln(\frac{1}{\sigma}))$$

3. [4 points] Is the set of depth-k decision trees PAC learnable? Is it efficiently PAC learnable?

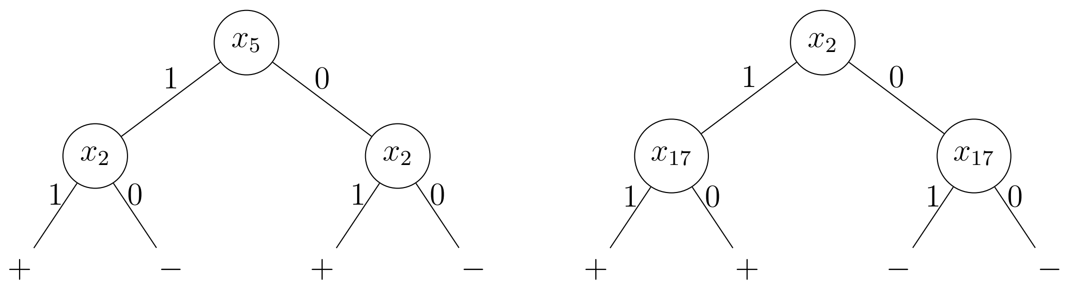
   Response: For depth k decision trees, the hypothesis class is clearly PAC learnable given the big O. Furthermore, the hypothesis class is clearly efficiently PAC learnable since a variety of algorithms exist that solve the problem. For example, the ID3 algorithm is proven to be NP-complete and is in the order of $O(m \times n)$ for n binary features and m examples.

4. [4 points] Suppose the number of features we have is large and the depth limit we are considering is also large (say, in the thousands or more). Will the number of examples

we need be small or large? Discuss the implications of the sample complexity bound from above.

Response: As the feature space and depth limit grow, the hypothesis class size $|H|$ tends to expand, potentially exponentially with tree depth. Consequently, the sample complexity m required by the agnostic bound equation also increases. This suggests that a larger dataset is necessary to effectively learn decision trees with intricate structures and to ensure dependable generalization performance.

NOTE: In this question we are counting trees that are structurally different instead of functionally different. As an exercise, you can confirm that the following two trees are structurally different but equal in terms of the label they assign to any example, namely the trees are functionally equivalent.



2 Shattering [15 points, for 6350 students]

Suppose we have a set X_n consists of all binary sequences of a length n. For example, if $n = 3$, the set would consist of the eight elements {`000, 001, 010, 011, 100, 101, 110, 111`}.

Consider a set of functions H_n that we will call the set of *templates*. Each template is a sequence of length n that is constructed using `0`, `1` or `-` and returns $+1$ for input binary sequences that match it and -1 otherwise. While checking whether a template matches an input, a `-` can match both a `0` and a `1`.

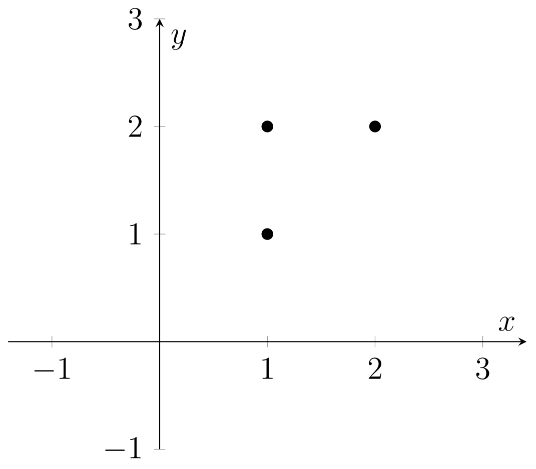
For example, the template `-10` matches the binary strings `010` and `110`, while `-1-` matches all strings that have a `1` in the middle position, namely `010`, `011`, `110` and `111`.

Does the set of templates H_n shatter the set X_n? Prove your answer.

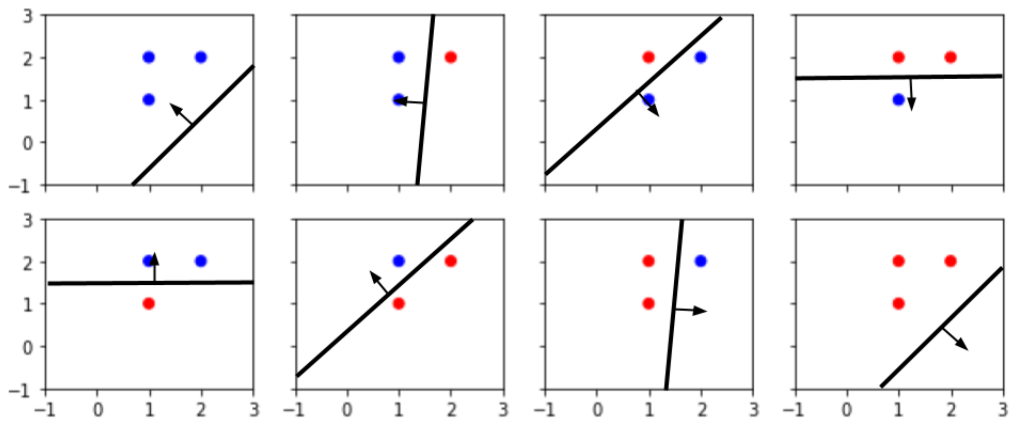
Response: Suppose set X_3 consists of all binary strings of length n=3. Then, $X_3 = \{\{000\}, \{001\}, ..., \{111\}\}$ and $|X_3| = 8$. As stated in the example above $\{-1-\}$ matches 010, 011, 110, and 111. This can be generalized to state that a template w/ k unique dashes can match 2^k different binary strings in X_n. Lets assume that H_n has at least as many elements as X_n. The maximum size $|H_n|$ is 3^n which is larger than the length of X_n or 2^n. Because one template can match 2^k different binary strings of length n, we can realistically ensure that the set of templates H_n can shatter the set X_n.

3 VC Dimension [45 points]

1. [5 points] Assume that the three points below can be labeled in any way. Show with pictures how they can be shattered by a linear classifier. Use filled dots to represent positive classes and unfilled dots to represent negative classes.



Response: Refer to figure below for a visualization of a linear classifier shattering this dataset.



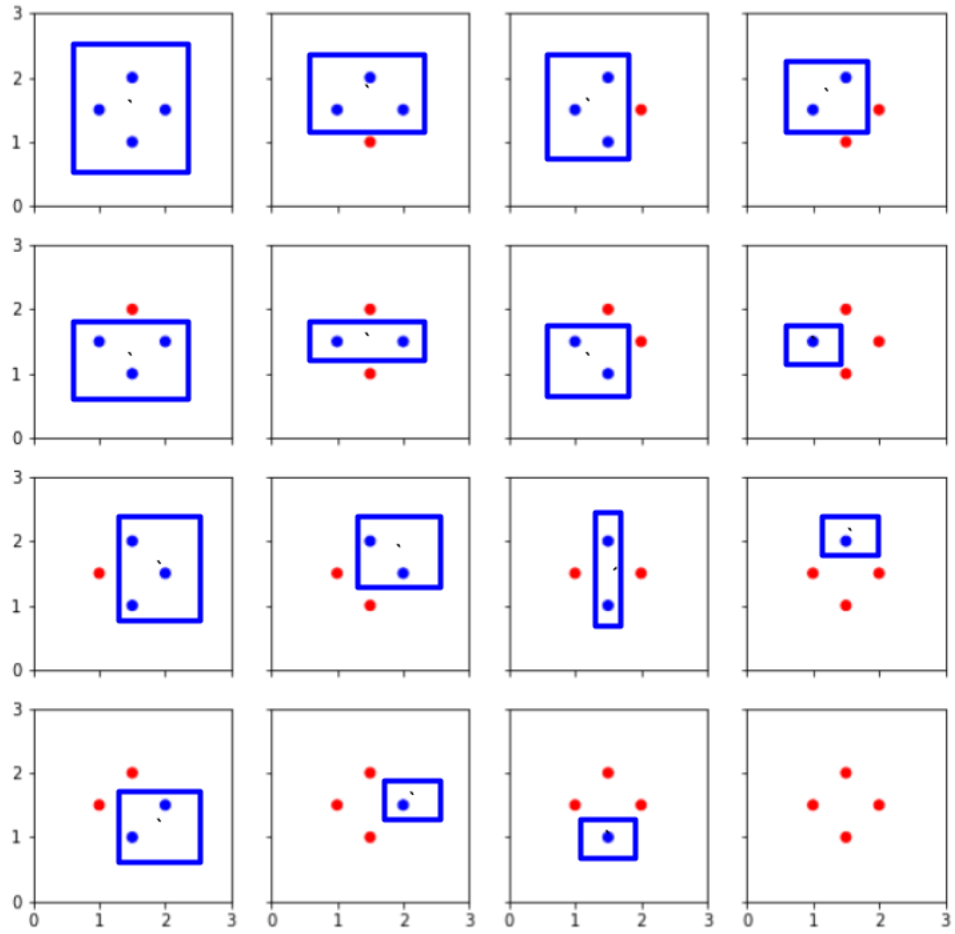
2. **VC-dimension of axis aligned rectangles in $\mathbb{R}^d$:** Let H^d_{rec} be the class of axis-aligned rectangles in $\mathbb{R}^d$. When $d = 2$, this class simply consists of rectangles on the plane, and labels all points strictly outside the rectangle as negative and all points on or inside the rectangle as positive. In higher dimensions, this generalizes to d-dimensional

boxes, with points outside the box labeled negative.

(a) [10 points] Show that the VC dimension of H^2_{rec} is 4.

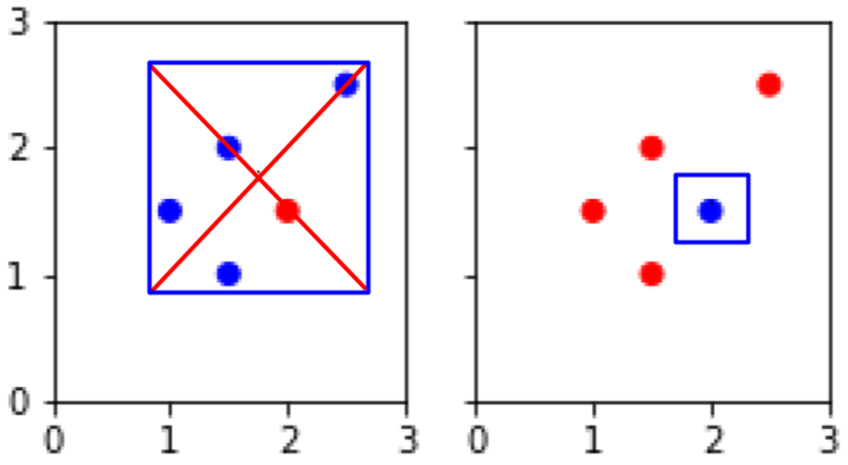
Response: To prove that the VC dimension of H^2_{rec} is 4, H^2_{rec} must shatter at least one subset of size 4 (ie, $VC(H^2_{rec}) \geq 4$) but there must not exist a single subset of size 5 that $VC(H^2_{rec})$ can shatter so $VC(H^2_{rec}) < 5$.

i. Direct proof for $VC(H^2_{rec}) \geq 4$: Below is a visualization showcasing how there exists at least one subset of size 4 that is shattered by H^2_{rec}.

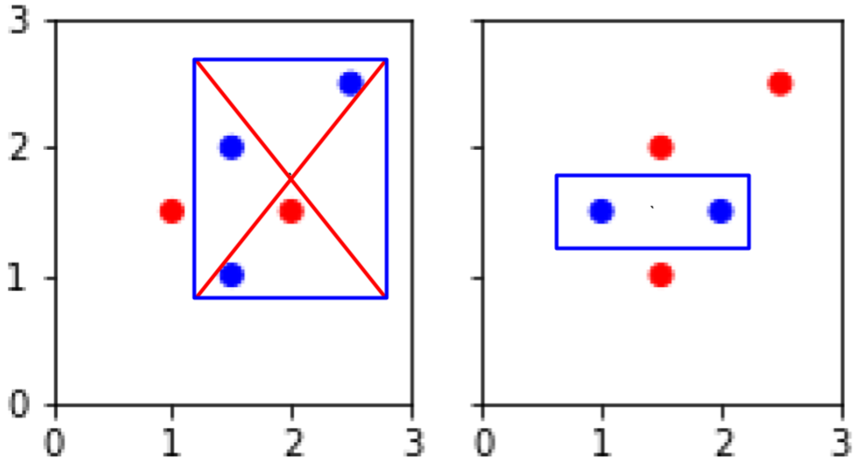


ii. Proof by contradiction for $VC(H^2_{rec}) < 5$: For $VC(H^2_{rec}) >= 5$, there must exist at least one subset of size 5 that is shattered by H^2_{rec}. Let there be a set of four points p_1, p_2, p_3, p_4, and p_5. Now consider two cases, case 1 where four points are enclosed and case 2 where only three points are within the rectangle.

1. **Case 1:** Let's assume that an axis-aligned rectangle correctly classifies p_1, p_2, p_3 and p_4 as positive and leaves p_5 outside the rectangle (labeled as negative). However, we can relabel the points such that p_5 is inside the rectangle, while the other four points are outside. This contradicts the assumption that the rectangle correctly classifies the points.



2. **Case 2:** If an axis-aligned rectangle correctly classifies three points (p_1, p_3, and p_5) as positive and two points as negative (remaining points), we can rearrange the points such that p_2 and p_4 are inside the rectangle while the rest are outside. Again, this contradicts the assumption.



Since no single rectangle can correctly classify all possible labelings of these five points, it's impossible to shatter a set of five points in $\mathbb{R}^2$.

(b) [10 points] Generalize your argument from the previous proof to show that for d dimensions, the VC dimension of H^d_{rec} is $2d$.

Response: To generalize on d-dimensions H^d_{rec} must shatter at least one subset of size $2d$ (ie, $VC(H^d_{rec}) \geq 2d$) but there must not exist a single subset of size $2d + 1$ that $VC(H^d_{rec})$ can shatter so $VC(H^d_{rec}) < 2d + 1$.
Consider a set of points, each characterized by d attributes. Each attribute can be positively or negatively labeled for each point. When we examine any subset of these points, we can always identify a rectangle that exclusively encompasses those points and not others. This observation establishes that the VC-dimension is at least $2d$. Now, let's establish that the VC-dimension is less than $2d + 1$. Visualize another set of points, this time focusing on the smallest rectangle that encompasses all these points. Given that we have more than $2d$ points, at least

one point must reside within this rectangle. If we designate this interior point as "negative," no rectangle can effectively isolate it from the other points outside the rectangle. Hence, this demonstrates that the VC-dimension is less than $2d + 1$. Combining these insights, we conclude that the VC-dimension equals $2d$.

3. In the lectures, we considered the VC dimensions of infinite concept classes. However, the same argument can be applied to finite concept classes too. In this question, we will explore this setting.

   (a) [10 points] Show that for a finite hypothesis class $\mathcal{C}$, its VC dimension can be at most $\log_2(|\mathcal{C}|)$. (Hint: You can use contradiction for this proof. But not necessarily!)

   Response: Suppose the finite concept class C has a VC-dimension d larger than $lg(|C|)$, then $d > lg(|C|)$. However, $2^d > |C|$ implies that are more unique labelings than C contains as a finite concept class. Therefore, the VC-dimensions of a finite hypothesis class can be at most $lg(|C|)$.

   (b) [5 points] Find an example of a class $\mathcal{C}$ of functions over the real interval $X = [0, 1]$ such that $\mathcal{C}$ is an **infinite** set, while its VC dimension is exactly one.

   Response: The concept class under consideration involves half intervals. As demonstrated in the lecture, the hypothesis class consists of intervals on the real axis: $[a, b]$ where a and b are real numbers and $b > a$. In this specific instance, $a = 0$ and $b = 1$. It has been established that while there exists a dataset of size 1 that can be shattered, no dataset of size 2 can be fully classified.

   (c) [5 points] Give an example of a **finite** class $\mathcal{C}$ of functions over the same domain $X = [0, 1]$ whose VC dimension is exactly $\log_2(|\mathcal{C}|)$.

   Response: The collection of disjoint sub-intervals is a finite class within the interval [0, 1]. It partitions the interval into discrete, equal segments, rendering it finite. By assigning a value of +1 to points residing within the intervals of this partition and -1 to those outside of it, complete classification can be achieved.

   It can be readily proven that the VC dimension is $lg(|C|)$. This is because we can easily shatter two points if they fall within one of these intervals. Moreover, all possible labelings can be attained by executing the various combinations of $|C|$ labelings.

4 Extra Credit - Decision Lists [25 points]

In this problem, we are going to learn the class of k-decision lists. A decision list is an ordered sequence of if-then-else statements. The sequence of if-then-else conditions are tested in order, and the answer associated to the first satisfied condition is output. See Figure 1 for an example of a 2-decision list.

A *k-decision list* over the variables $x_1, \ldots, x_n$ is an ordered sequence $L = (c_1, b_1), \ldots, (c_l, b_l)$ and a bit b, in which each c_i is a conjunction of at most k literals over $x_1, \ldots, x_n$. The bit b is called the *default* value, and b_i is referred to as the bit *associated* with condition c_i. For any

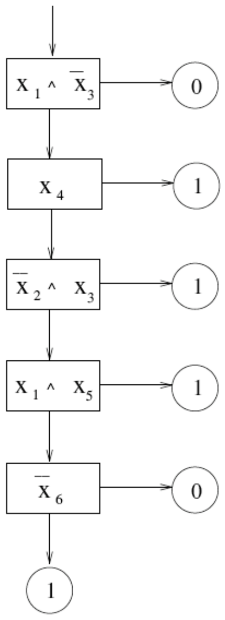


Figure 1: A 2-decision list.

input $x \in \{0,1\}^n$, $L(x)$ is defined to be the bit b_j, where j is the smallest index satisfying $c_j(x) = 1$; if no such index exists, then $L(x) = b$.

We denote by *k-DL* the class of concepts that can be represented by a k-decision list.

1. [8 points] Show that if a concept c can be represented as a k-decision list so can its complement, $\neg c$. You can show this by providing a k-decision list that represents $\neg c$, given $c = \{(c_1, b_1), \ldots, (c_l, b_l), b)$.

   Response: By leveraging *a priori* from Ron Rivest in *Learning Decision Lists*, we come to find that the solution is trivial and involves a minute manipulation of the decision list (DL). The complement $\neg c$ can be derived by negating all the leaves of the DL due to k-DL trees being closed under complementation. So,

$$\neg c = \{(c_1, \neg b_1), \ldots, (c_l, \neg b_l), \neg b)$$

2. [9 points] Use Occam's Razor to show:
   For any constant $k \geq 1$, the class of k-decision lists is PAC-learnable.

   Response: We know that k-DL is polynomial-sized, that is, $|k\text{-DL(n)}| = O(3^{|C_k^n|}(|C_k^n|)!)$, where C_k^n is the set of all conjuctions of size at most k with literals drawn from L_n. Furthermore, each term can either be paired with 1 or 0 or missing in arbitrary order. Taking the 2-base lg:

$$lg|k\text{-DL(n)}| = lg(O(3^{|C_k^n|}(|C_k^n|)!))$$

Thus, for some constant t,

$$lg|k\text{-DL(n)}| = O(n^t)$$

Finally, we have shown that k-DL is PAC learnable in polynomial time for $k \geq 1$

3. [8 points] Show that 1-decision lists are a linearly separable functions. (Hint: Find a weight vector that will make the same predictions a given 1-decision list.)

   Response: For instance, suppose we have a conjunctive clause $c = x_1^{\neg}x_2$. Now, let's consider a weight vector w such that $w^T x$ yields the decision d. We can set w to be the same as the conjunction c itself, treating the literals as weights. Specifically, if the literal appears positively in c, we assign $w_i = 1$; if it appears negatively, we assign $w_i = -1$. So w = [1, -1] for c.

$$d = w^T x = x_1 - \neg x_2$$