### HOMEWORK 2: DECISION TREES

10-301/10-601 Introduction to Machine Learning (Spring 2023)

http://www.cs.cmu.edu/~mgormley/courses/10601/

OUT: Wednesday, September 6 DUE: Friday, September 15

TAs: Alisa, Annie, Bhargav, Erin, Sebastian, Neural the Narwhal

**Summary** It's time to build your first end-to-end learning system! In this assignment, you will build a Decision Tree classifier and apply it to several binary classification problems. This assignment consists of several parts: In the Written component, you will work through some Information Theory basics in order to "learn" a Decision Tree on paper, and also work through some pseudocode that will help you algorithmically think through the programming assignment. Then in the Programming component, you will implement Decision Tree learning, prediction, and evaluation. Using that implementation, you will answer the empirical questions found at the end of the Written component.

#### **START HERE: Instructions**

- Collaboration Policy: Please read the collaboration policy here: http://www.cs.cmu.edu/~mgormley/courses/10601/syllabus.html
- Late Submission Policy: See the late submission policy here: http://www.cs.cmu.edu/~mgormley/courses/10601/syllabus.html
- **Submitting your work:** You will use Gradescope to submit answers to all questions and code. Please follow instructions at the end of this PDF to correctly submit all your code to Gradescope.
  - Written: For written problems such as short answer, multiple choice, derivations, proofs, or plots, please use the provided template. Submissions can be handwritten onto the template, but should be labeled and clearly legible. If your writing is not legible, you will not be awarded marks. Alternatively, submissions can be written in LaTeX. Each derivation/proof should be completed in the boxes provided. You are responsible for ensuring that your submission contains exactly the same number of pages and the same alignment as our PDF template. If you do not follow the template, your assignment may not be graded correctly by our AI assisted grader and there will be a 2% penalty (e.g., if the homework is out of 100 points, 2 points will be deducted from your final score).
  - Programming: You will submit your code for programming questions on the homework to Gradescope. After uploading your code, our grading scripts will autograde your assignment by running your program on a virtual machine (VM). You are only permitted to use the Python Standard Library modules and numpy. Ensure that the version number of your programming language environment (i.e. Python 3.9.12) and versions of permitted libraries (i.e. numpy 1.23.0) match those used on Gradescope. You have 10 free Gradescope programming submissions, after which you will begin to lose points from your total programming score. We recommend debugging your implementation on your local machine (or the Linux servers) and making sure your code is running correctly first before submitting your code to Gradescope.

| • | <b>faterials:</b> The data and reference output that you will need in order to complete this assignment is osted along with the writeup and template on the course website. |  |  |  |  |
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# **Instructions for Specific Problem Types**

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| For "Select One" questions, please fill in the appropriate bubble completely:  |
| Select One: Who taught this course?  |
| Matt Gormley   |
| 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 th given space. You may cross out answers or parts of answers, but the final answer must still be within th given space. |
| Fill in the blank: What is the course number?  |
| 10-601 10-6301   |

## Written Questions (31 points)

### 1 LATEX Bonus Point and Template Alignment (1 points)

- 1. (1 point) **Select one:** Did you use LATEX for the entire written portion of this homework?
  - Yes
  - O No
- 2. (0 points) **Select one:** I have ensured that my final submission is aligned with the original template given to me in the handout file and that I haven't deleted or resized any items or made any other modifications which will result in a misaligned template. I understand that incorrectly responding yes to this question will result in a penalty equivalent to 2% of the points on this assignment.

Note: Failing to answer this question will not exempt you from the 2% misalignment penalty.

○ Yes

### 2 Warm-Up (11 points)

First, let's think a little bit about decision trees. The following dataset D consists of 8 examples, each with 3 attributes, (A, B, C), and a label, Y.

| A | B | C | Y |
|---|---|---|---|
| 1 | 2 | 0 | 1 |
| 0 | 1 | 0 | 0 |
| 0 | 0 | 1 | 0 |
| 0 | 2 | 0 | 1 |
| 1 | 1 | 0 | 1 |
| 1 | 0 | 1 | 0 |
| 1 | 2 | 1 | 0 |
| 1 | 1 | 0 | 1 |

Use the data above to answer the following questions.

A few important notes:

- All calculations should be done without rounding! After you have finished all of your calculations, write your rounded solutions in the boxes below.
- Unless otherwise noted, numeric solutions should include 4 digits of precision (e.g. 0.1234).
- Note that, throughout this homework, we will use the convention that the leaves of the trees do not count as nodes, and as such are not included in calculations of depth and number of splits. (For example, a tree which classifies the data based on the value of a single attribute will have depth 1, and contain 1 split.)
- Note that the dataset contains duplicate rows; treat each of these as their own example, do not remove duplicate rows.

*Note*: Showing your work in these questions is optional, but it is recommended to help us understand where any misconceptions may occur. Only your numerical answer in the left box will be graded.

1. (1 point) What is the entropy of Y in bits, H(Y)? In this and subsequent questions, when we request the units in *bits*, this simply means that you need to use log base 2 in your calculations. (Please include one number rounded to the fourth decimal place, e.g. 0.1234)



2. (1 point) What is the mutual information of Y and A in bits, I(Y;A)? (Please include one number rounded to the fourth decimal place, e.g. 0.1234)



3. (1 point) What is the mutual information of Y and B in bits, I(Y;B)? (Please include one number rounded to the fourth decimal place, e.g. 0.1234)



<sup>&</sup>lt;sup>1</sup>If instead you used log base e, the units would be *nats*; log base 10 gives *bats*.

| 4. | (1 point) What is the mutual information of $Y$ and $C$ in bits, $I(Y;C)$ ? (Please include one number rounded to the fourth decimal place, e.g. $0.1234$ )  |
|----|--|
|    | I(Y;C) Work  |
| 5. | (1 point) <b>Select one:</b> Consider the dataset given above. Which attribute $(A, B, \text{ or } C)$ would a decision tree algorithm pick first to branch on, if its splitting criterion is mutual information?  |
|    | $\bigcirc$ A   |
|    | $\bigcirc$ B   |
|    | $\bigcirc$ $C$   |
| 6. | (1 point) <b>Select one:</b> Consider the dataset given above. After making the first split, which attribute would the algorithm pick to branch on next, if the splitting criterion is mutual information? ( <i>Hint:</i> Notice that this question correctly presupposes that there is <i>exactly one</i> second attribute.) $\bigcirc A$ |
|    | $\bigcirc B$   |
|    | $\bigcirc$ $C$   |
| 7. | (1 point) If the same algorithm continues until the tree perfectly classifies the data, what would the depth of the tree be?   |
|    | Depth  |

| 8. | (4 points) Draw your completed Decision Tree. Label the non-leaf nodes with which attribute the tree will split on (e.g. $B$ ), the edges with the value of the attribute (e.g. 1 or 0), and the leaf nodes with the classification decision (e.g. $Y=0$ ). You should include an image file below using the provided, commented out code in LATEX, switching out $DecTree.png$ to your file name as needed. The image may |
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|    | be hand-drawn.   |
|    | Decision Tree  |
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### 3 Pseudocode (6 points)

1. In the programming assignment, you will need to implement three main tasks: training a decision tree on an arbitrary training set, predicting new values with a trained tree given an arbitrary input dataset, and evaluating your predictions against an arbitrary dataset's true labels. For this problem, we will focus on thinking through the algorithm for the *second* task.

Below, you will write pseudocode for the function predict (node, example), which predicts the label of an example given a node of type Node representing the root of a *trained* tree. You must approach this problem recursively and use the Node class we have given to you.

```
class Node:
   def __init__(self, attr, v):
        self.attribute = attr
        self.left = None
        self.right = None
        self.vote = v
 (a) the left and right children of a node are denoted as
      node.left and node.right respectively, each is of type Node
  (b) the attribute for a node is denoted as node.attribute and has
     type str
 (c) if the node is a leaf, then node.vote of type str holds the
     prediction from the majority vote; if node is an internal
      node, then node.vote has value None
 (d) assume all attributes have values 0 and 1 only; further
     assume that the left child corresponds to an attribute value
     of 1, and the right child to a value of 0
def predict (node, example):
   # example is a dictionary which holds the attributes and the
    # values of the attribute (ex. example['X'] = 0)
        Part (a) :
        return Part (b)
   else:
           Part (c)
```

(a) (2 points) Write the conditional statement of the base case of predict (node, example).

| Your Answer |  |  |
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| (b) | ) (1 point) Write the return statement of the base case of predict (node, example). |        |                 |  |           |                      |                  |
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| (c) | lines.  |        | cursive step of |  | example). | Limit your answer to | <del>-</del> ე 1 |
|     | Your A  | answer |                 |  |           |                      |                  |
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### 4 Empirical Questions (13 points)

The following questions should be completed as you work through the programming portion of this assignment.

1. (4 points) Train and test your decision tree on the heart dataset and the education dataset with four different values of max-depth, {0, 1, 2, 4}. Report your findings in the HW2 solutions template provided. A Decision Tree with max-depth 0 is simply a *majority vote classifier*; a Decision Tree with max-depth 1 is called a *decision stump*. (Please round each number to the fourth decimal place, e.g. 0.1234)

| Dataset   | Max-Depth | Train Error | Test Error |
|-----------|-----------|-------------|------------|
| heart     | 0         |             |            |
| heart     | 1         |             |            |
| heart     | 2         |             |            |
| heart     | 4         |             |            |
| education | 0         |             |            |
| education | 1         |             |            |
| education | 2         |             |            |
| education | 4         |             |            |

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2. (3 points) For the heart disease (heart) dataset, create a computer-generated plot showing error on

| 3. | (2 points) <b>Select one:</b> Suppose your research advisor asks you to run some model selection experiments and then report your results. You select the Decision Tree model's max-depth to be the one with lowes test error in metrics.txt and then report that model's test error as the performance of our classifier or held out test data. Is this a good experimental setup?   |
|----|---|
|    | Yes, because we are using the test set in order to choose the best model.   |
|    | O No, because we should be using the <i>training</i> set to optimize the max-depth, not the test set.   |
|    | Yes, because we are not using the training set to tune hyperparameters.   |
|    | O No, because we should be using a <i>validation</i> set to optimize the max-depth, not the test set.   |
| 4. | (2 points) <b>Select one:</b> In this assignment, we used max-depth as our stopping criterion, and as a mechanism to prevent overfitting. Alternatively, we could stop splitting a node whenever the mutual information for the best attribute is lower than a threshold value. This threshold would be another hyperparameter. Theoretically, how would increasing this threshold value affect the number of nodes and depth of the learned trees? |
|    | The higher this threshold value is, the <i>smaller</i> depth and the <i>fewer</i> nodes the decision tree contains.   |
|    | The higher this threshold value is, the smaller depth and the more nodes the decision tree contains.  |
|    | The higher this threshold value is, the higher depth and the fewer nodes the decision tree contains.  |
|    | The higher this threshold value is, the higher depth and the more nodes the decision tree contains.   |
|    | The depth and number of nodes in the decision tree will not vary as the threshold value increases.  |
|    |   |

5. (2 points) Print (do not handwrite!) the decision tree which is produced by your algorithm for the heart dataset with max depth 3. Instructions on how to print the tree could be found in section 6.3.5.

| Output  |
|---|
| <pre>% YOUR ANSWER % Text here will be compiled verbatim. % So do not add unnecessary indents</pre> |
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### **5** Collaboration Questions

After you have completed all other components of this assignment, report your answers to these questions regarding the collaboration policy. Details of the policy can be found here.

- 1. Did you receive any help whatsoever from anyone in solving this assignment? If so, include full details.
- 2. Did you give any help whatsoever to anyone in solving this assignment? If so, include full details.
- 3. Did you find or come across code that implements any part of this assignment? If so, include full details.

| Your Answer |  |
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### 6 Programming (70 points)

Your goal in this assignment is to implement a binary classifier, entirely from scratch—specifically a Decision Tree learner. In addition, we will ask you to run some end-to-end experiments on two tasks (predicting whether or not a patient has heart disease / predicting the final grade for high school students) and report your results. You will write two programs: inspection.py (Section 6.2) and decision\_tree.py (Section 6.3). The programs you write will be automatically graded using Gradescope.

#### 6.1 The Tasks and Datasets

**Materials** Download the zip file from the course website. The zip file will have a handout folder that contains all the data that you will need in order to complete this assignment.

**Starter Code** The handout will contain a preexisting decision\_tree.py file that itself contains some starter code for the assignment. While we do not require that you use the starter code in your final submission, we *heavily* recommend building upon the structure laid out in the starter code.

**Datasets** The handout contains three datasets. Each one contains attributes and labels and is already split into training and testing data. The first line of each .tsv file contains the name of each attribute, and *the class label is always the last column*.

- 1. **heart:** The first task is to predict whether a patient has been (or will be) diagnosed with heart disease, based on available patient information. The attributes (aka. features) are:
  - (a) sex: The sex of the patient—1 if the patient is male, and 0 if the patient is female.
  - (b) chest pain: 1 if the patient has chest pain, and 0 otherwise.
  - (c) high\_blood\_sugar: 1 if the patient has high blood sugar (>120 mg/dl fasting), or 0 otherwise.
  - (d) abnormal\_ecg: 1 if exercise induced angina in the patient, and 0 otherwise. Angina is a type of severe chest pain.
  - (e) flat\_ST: 1 if the patient's ST segment (a section of an ECG) was flat during exercise, or 0 if it had some slope.
  - (f) fluoroscopy: 1 if a physician used fluoroscopy, and 0 otherwise. Fluoroscopy is an imaging technique used to see the flow of blood through the heart.
  - (g) thalassemia: 1 if the patient is known to have thalassemia, and 0 otherwise. Thalassemia is a blood disorder that may impair the oxygen-carrying capacity of the patient's red blood cells.
  - (h) heart\_disease: 1 if the patient was diagnosed with heart disease, and 0 otherwise. This is the class label you should predict.

The training data is in heart\_train.tsv, and the test data in heart\_test.tsv.

- 2. **education:** The second task is to predict the final grade for high school students. The attributes (covariates, predictors) are student grades on 5 multiple choice assignments *M1* through *M5*, 4 programming assignments *P1* through *P4*, and the final exam *F*. Values of 1 indicate that a student received an A, and 0 indicates that the student did not receive an A. The training data is in education train.tsv, and the test data in education test.tsv.
- 3. **small:** We also include small\_train.tsv and small\_test.tsv—a small, purely for demonstration version of the **heart** dataset, with *only* attributes chest\_pain and thalassemia. For this small dataset, the handout folder also contains the predictions from a reference implementation of

a Decision Tree with max-depth 3 (see small\_3\_train.labels, small\_3\_test.labels, small\_3\_metrics.txt). You can check your own output against these to see if your implementation is correct.

**Note:** For simplicity, all attributes are discretized into just two categories (i.e. each node will have at most two descendents). This applies to all the datasets in the handout, as well as the additional datasets on which we will evaluate your Decision Tree.

#### 6.2 Program #1: Inspecting the Data (5 points)

Create and write a program inspection.py to calculate the label entropy at the root (i.e. the entropy of the labels before any splits) and the error rate (the percent of incorrectly classified instances) of classifying using a majority vote (picking the label with the most examples). You do not need to look at the values of any of the attributes to do these calculations; knowing the labels of each example is sufficient. **Entropy should be calculated in bits using log base 2.** 

**Command Line Arguments** The autograder runs and evaluates the output from the files generated, using the following command:

```
$ python inspection.py <input> <output>
```

Your program should accept two command line arguments: an input file and an output file. It should read the .tsv input file (of the format described in Section 6.1), compute the quantities above, and write them to the output file so that it contains:

```
entropy: <entropy value>
error: <error value>
```

**Example** For example, suppose you wanted to inspect the file small\_train.tsv and write out the results to small\_inspect.txt. You would run the following command:

```
$ python inspection.py small_train.tsv small_inspect.txt
```

Afterwards, your output file small\_inspect.txt should contain the following:

```
entropy: 1.000000
error: 0.500000
```

Our autograder will run your program on several input datasets to check that it correctly computes entropy and error, and will take minor differences due to rounding into account. You do not need to round your reported numbers! The autograder will automatically incorporate the right tolerance for float comparisons.

For your own records, run your program on each of the datasets provided in the handout—this error rate for a *majority vote* classifier is a baseline over which we would (ideally) like to improve.

#### 6.3 Program #2: Decision Tree Learner (65 points)

In decision\_tree.py, implement a Decision Tree learner. This file should learn a decision tree with a specified maximum depth, print the decision tree in a specified format, predict the labels of the training and testing examples, and calculate training and testing errors.

#### Your implementation must satisfy the following requirements:

- Use mutual information to determine which attribute to split on.
- Be sure you're correctly weighting your calculation of mutual information. For a split on attribute X, I(Y;X) = H(Y) H(Y|X) = H(Y) P(X=0)H(Y|X=0) P(X=1)H(Y|X=1).
- As a stopping rule, only split on an attribute if the mutual information is > 0.
- Do not grow the tree beyond a max-depth specified on the command line. For example, for a maximum depth of 3, split a node only if the mutual information is > 0 and the current level of the node is < 3.
- Use a majority vote of the labels at each leaf to make classification decisions. If the vote is tied, choose the label that is higher (i.e. 1 should be chosen before 0)
- It is possible for different columns to have equal values for mutual information. In this case, you should split on the *first column to break ties* (e.g. if column 0 and column 4 have the same mutual information, use column 0).
- Do not hard-code any aspects of the datasets into your code. We may autograde your programs on hidden datasets that include different attributes and output labels.

#### **6.3.1** Getting Started

Careful planning will help you to correctly and concisely implement your Decision Tree learner. Here are a few *hints* to get you started:

- Write helper functions to calculate entropy and mutual information.
- It is best to think of a Decision Tree as a collection of nodes, where nodes are either leaf nodes (where final decisions are made) or interior nodes (where we split on attributes). It is helpful to design a function to train a single node (i.e. a depth-0 tree), and then recursively call that function to create sub-trees.
- In the recursion, keep track of the depth of the current tree so you can stop growing the tree beyond the max-depth.
- Implement a function that takes a learned decision tree and data as inputs, and generates predicted labels. You can write a separate function to calculate the error of the predicted labels with respect to the given (ground-truth) labels.
- Be sure to correctly handle the case where the specified maximum depth is greater than the total number of attributes.
- Be sure to handle the case where max-depth is zero (i.e. a majority vote classifier).
- Look under the FAQ post on Piazza for more useful clarifications about the assignment.

Look out for the HW2 debugging checklist on Piazza!

#### **6.3.2** Command Line Arguments

The autograder runs and evaluates the output from the files generated, using the following command:

```
$ python decision_tree.py [args...]
```

Where above [args...] is a placeholder for six command-line arguments: <train input> <test input> <max depth> <train out> <test out> <metrics out>. These arguments are described in detail below:

- 1. <train input>: path to the training input .tsv file (see Section 6.1)
- 2. <test input>: path to the test input .tsv file (see Section 6.1)
- 3. <max depth>: maximum depth to which the tree should be built
- 4. <train out>: path of output .txt file to which the predictions on the *training* data should be written (see Section 6.3.3)
- 5. <test out>: path of output .txt file to which the predictions on the *test* data should be written (see Section 6.3.3)
- 6. <metrics out>: path of the output .txt file to which metrics such as train and test error should be written (see Section 6.3.4)

As an example, the following command line would run your program on the heart dataset and learn a tree with a max-depth of 2. The train predictions would be written to heart\_2\_train.txt, the test predictions to heart\_2\_test.txt, and the metrics to heart\_2\_metrics.txt.

```
$ python decision_tree.py heart_train.tsv heart_test.tsv 2 \
    heart_2_train.txt heart_2_test.txt heart_2_metrics.txt
```

The following example would run the same learning setup except with a max-depth of 3, and conveniently writing to analogously named output files, so you can can compare the two runs.

```
$ python decision_tree.py heart_train.tsv heart_test.tsv 3 \
    heart_3_train.txt heart_3_test.txt heart_3_metrics.txt
```

#### **6.3.3** Output: Labels Files

Your program should write two output .txt files containing the predictions of your model on training data (<train out>) and test data (<test out>). Each should contain the predicted labels for each example printed on a new line. Use '\n' to create a new line.

Your labels should exactly match those of a reference decision tree implementation—this will be checked by the autograder by running your program and evaluating your output file against the reference solution.

The first few lines of an example output file is given below for the small dataset:

#### 6.3.4 Output: Metrics File

Generate another file where you should report the training error and testing error. This file should be written to the path specified by the command line argument <metrics out>. Your reported numbers should be within 0.0001 of the reference solution. You do not need to round your reported numbers! The autograder will automatically incorporate the right tolerance for float comparisons. The file should be formatted as follows:

```
error(train): 0.214286
error(test): 0.285714
```

The values above correspond to the results from training a tree of depth 3 on small\_train.tsv and testing on small\_test.tsv. (Note that there is one space between the colon and value.)

#### 6.3.5 Output: Printing the Tree

Finally, you should write a function to pretty-print your learned decision tree. Your function should print your tree only after you are done generating the fully-trained tree. Each row should correspond to a node in the tree. They should be printed using a pre-order depth-first-search traversal (but you may print left-to-right or right-to-left, i.e. your answer does not need to have exactly the same order as the reference below). Print the attribute of the node's parent and the attribute value corresponding to the node. Also include the sufficient statistics (i.e. count of positive / negative examples) for the data passed to that node. The row for the root should include only those sufficient statistics. A node at depth d, should be prefixed by d copies of the string '| '.

Below, we have provided the recommended format for printing the tree. You can print it directly rather than to a file. **This functionality of your program will NOT be autograded**.

```
$ python decision_tree.py small_train.tsv small_test.tsv 2 \
small_2_train.txt small_2_test.txt small_2_metrics.txt

[14 0/14 1]
| chest_pain = 0: [4 0/12 1]
| | thalassemia = 0: [3 0/4 1]
| | thalassemia = 1: [1 0/8 1]
| chest_pain = 1: [10 0/2 1]
| | thalassemia = 0: [7 0/0 1]
| | thalassemia = 1: [3 0/2 1]
```

However, you should be careful that the tree might not be full. For example, with a different subset of the small dataset, there may be no nodes under chest\_pain = 0 if all labels are the same.

The following pretty-print shows the education dataset with max-depth 3. Use this example to check your code before submitting your pretty-print of the heart dataset (asked in question 5 of the Empirical questions).

```
$ python decision_tree.py education_train.tsv education_test.tsv 3 \
edu_3_train.txt edu_3_test.txt edu_3_metrics.txt
[65 0/135 1]
| F = 0: [42 0/16 1]
 | M2 = 0 : [27 0/3 1]
   | M4 = 0 : [22 0/0 1]
 | M4 = 1: [5 0/3 1]
  | M2 = 1: [15 0/13 1]
 | M4 = 0: [14 0/7 1]
 | M4 = 1: [1 0/6 1]
| F = 1: [23 \ 0/119 \ 1]
 | M4 = 0: [21 0/63 1]
   | M2 = 0: [18 0/26 1]
 | M2 = 1: [3 0/37 1]
  | M4 = 1: [2 0/56 1]
| | | P1 = 0: [2 0/15 1]
| | | P1 = 1: [0 0/41 1]
```

The numbers in brackets give the number of positive and negative labels from the training data in that part of the tree.

At this point, you should be able to go back and answer questions 1-5 in the "Empirical Questions" section of this handout. Write your solutions in the template provided.

#### **6.4 Submission Instructions**

**Programming** Please ensure you have completed the following files for submission.

```
inspection.py
decision_tree.py
```

When submitting your solution, make sure to select and upload both files. **Any other files will be deleted.** Ensure the files have the exact same spelling and letter casing as above. You can either directly zip the two files (by selecting the two files and compressing them – do not compress the folder containing the files) or directly drag them to Gradescope for submission.

**Written Questions** Make sure you have completed all questions from Written component (including the collaboration policy questions) in the template provided. When you have done so, please submit your document in **PDF format** to the corresponding assignment slot on Gradescope.