Homework 3: Decision trees

Unless otherwise stated,

1. All problems below are binary classification and the two classes are $+1$ and -1.
2. When comparing a feature value F against a threshold T, the case $F == T$ goes with the "less than" case. Thus, the two branches of a node on the decision tree are: $F \leq T$ and $F > T$.
3. On a decision tree, let the condition at each node always be the "greater than" case. For the two branches of a node, the left branch is always the True case ("greater than") and the right branch is the False ("less than or equal to") case.

How to view this in nice PDF

```
pandoc -s hw3.md -o hw3.pdf
```

A precompiled PDF is here

Hand computation [4pts]

You may develop a program to do the computation for you here.

1. [1pt] Given the dataset (where each sample has 3 feature values: a, b, and c) below, compute the gini impurity for the condition $S1 : a > 10$. Please show the estimations of $Pr(class = +1|a > 10)$ and $Pr(class = -1|a > 10)$. If you do not show these two but a final result, you will get no point.

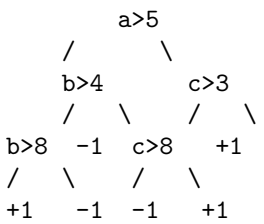
Sample Number	feature a	feature b	feature c	class
1	12	3	5	+1
2	4	7	6	+1
3	5	4	8	+1
4	6	6	7	+1
5	7	5	1	-1
6	8	2	2	-1
7	9	6	3	-1
8	11	8	1	-1

2. [1pt] Do the same for a condition $S2 : a \leq 5$. Again, intermediate steps need to be shown.

3. [1pt] Based on the results from the two problems above, compute the expectation for gini impurity for the feature a and the threshold 5. Please show the estimatons of the probabilities of both conditions, i.e., $P(a > 5)$

and $P(a \leq 5)$. If you just show a final result, no point.

4. [1pt] Using the decision tree below, decide the classification outcomes for all samples in Problem 1. Left branch is True and right branch is False. Present your result as a two-column table.



Programming [6pts]

Now, let's try to implement node split using grid search and compare the result with scikit-learn's implementation. Please work from a provided file `hw3.py` and just upload this file.

5. [2pt] **Estimating Gini impurity**

   Turn the computational steps you did for Problems 1 and 2 into a function `estimate_gini_impurity` that computes the Gini impurity given

   a. values of a feature on a set of samples,
   b. a threshold,
   c. labels corresponding to the samples,
   d. and, the polarity of comparison.

   The variable `polarity` takes value from `operator.lt` and `operator.ge` in Python standard module `operator`. They are functions applied to two operands, e.g.,

```
>>> import operator
>>> operator.lt(5,4)
False
>>> operator.lt(4,5)
True
>>> operator.ge(4,5)
False
>>> operator.ge(5,4)
True
>>> operator.ge(5,5)
True
```

   Note that there may be no sample satisfying a comparison expression at all. In such cases, when computing $Pr(class = s|S)$, it will result devision by zero. To avoid that, please set $Pr(class = s|S)$ to a very small number

`numpy.finfo(float).eps` when it is zero. AND, in such a case, the gini impurity should be 1 because $Pr(class = c|S)$ is zero for either class.

6. [2pt] **The expectation of Gini impurity.** Turn the computational steps you did in Problem 3 into the function `estimate_gini_impurity_expectation` that computes the expectation of Gini impurity given

   - values of a feature on a set of samples,
   - a threshold,
   - and, labels corresponding to the samples.

7. [2pt] **The split of a node** Each node of a decision tree is a comparison on a feature against a threshold. To determine the feature and the threshold, a common practice is a grid search. Search over every feature, against a set of thresholds. In the end, pick the combination of feature and threshold that minimize the expectation of Gini impurity.

   There are many ways to establish the thresholds. Here we use a common practice that for each feature, the thresholds are the means of all pairs of its two consecutive values on all samples. For example, if the values on a feature is `[5,4,2,1,3]`, then the thresholds are `[1.5, 2.5, 3.5, 4.5]`. Note that because values on features differ (e.g., in feature 1, `[1,2,3,4,5]` and in feature 2, `[0.1, 0.2, 0.9, 0.1, -0.8]`]), thresholds for features differ. To help you start, the thresholds for each feature are constructed the function `grid_search_split_midpoint` in `hw3` already. So you can directly make use of the variable `thresholds`, each column of which corresponds to a feature dimension.

   The function shall return 3 variables:

   a. `grid`: 2D numpy array, the expectations of Gini impurity. Each column corresponds to one feature and each row orresponds to a threshold.
   b. `best_feature`: int, the index of the column containing the minimal value in `grid`.
   c. `best_threshold`: float, the threshold of the `best_feature` that minimizes the value in `grid`.

How to test your submission

Test cases for all functions are provided in `doctest`. You can visually compare the outputs of your functions. Or you can run the `hw3.py` script as `python3 hw3.py`. If you see no error, then all your functions are correct.

In addition to the doctest cases, an additional function `you_rock` is provided. It generates many random datasets and compares the results computed by your functions against those by scikit-learn's `tree` module. Because of the slight implementation difference, your `best_feature` and `best_threshold` may not

be always the same as scikit-learns'. But you should see they are the same for 70% of the cases or more, when calling it as `you_rock(1000, 100, 3)` (1000 samples, feature values ranging from 1 to 100, 3 features).

Hints for programming:

1. Instead of for-loops, take advantage of numpy's array-wise operations. For example,

   ```
   numpy.array([1,2,3,4]) > 3
   ```

   returns an array containing the comparison result between every element of the array against the threshold 3: `array([False, False, False, True])`

2. You can `logical_and` two arrays to find elements satisfying both conditions (instead of using for-loops to check both conditions over elements):

   ```
   numpy.logical_and(
       numpy.array([1,2,3,4]) > 2,
       numpy.array([+1,-1,+1,-1]) == +1
       )
   ```

   shall return `array([False, False, True, False])`

   There are many other logic operations in Numpy. Click here to see.

3. You can sum over a Boolean array to count how many elemens are True or False.

   ```
   sum(numpy.array([True, False, True]))
   ```

   shall return `2`.

How to submit

For hand computation part, upload one PDF file. For programming part, upload your edited `hw3.py`. Do NOT delete contents in the template for programming.