CS167: Machine Learning

Decision Tree

Thursday, February 29th, 2024



Announcements

- Heads up: Quiz #1
 - due tonight by 11:59pm
- <u>Notebook #3: Cross Validation</u>
 - due tonight by 11:59pm
 - to submit, download the ipynb file from Colab

Review

- Evaluation Metrics
 - Classification metrics
 - Regression metrics

Review: classification metrics (accuracy)

- Accuracy: The fraction of test examples your model predicted correctly
 - *Example*: 17 out of 20 = 0.85 accuracy
- Issues with accuracy: suppose that a blood test for cancer has 99% accuracy
 - *can we safely assume this is a really good test?*
 - If the dataset is *unbalanced*, accuracy is not a reliable metric for the real performance of a classifier because it will yield misleading results
 - **Example**: Most people don't have cancer
 - Beware of what your metrics don't tell you

Review: classification metrics (confusion matrix)

- **Confusion matrix:** A specific table layout that allows the visualization of the performance of an algorithm.
- Each row represents instances in an actual class
- While each column represents the instances in a predicted class
 - It makes it easy to see where your model is confusing the predicted and actual results. For a binary classification problem:

		Predicted	condition		
	Total population = P + N	Positive (PP)	Negative (PN)		
ondition	Positive (P)	True positive (TP)	False negative (FN)		
Actual c	Negative (N)	False positive (FP)	True negative (TN)		

Review: example (confusion matrix)

 Confusion matrix: A specific table layout that allows the visualization of the performance of an algorithm

Individual Number	1	2	3	4	5	6	7	8	9	10	11	12
Actual Classification	1	1	1	1	1	1	1	1	0	0	0	0
Predicted Classification	0	0	1	1	1	1	1	1	1	0	0	0
Result	FN	FN	TP	TP	TP	TP	TP	TP	FP	TN	TN	TN

6

3

1

2

- Given the following confusion matrix:
 - how many true positive?
 - how many true negatives?
 - how many false positive?
 - how many false negatives?



Review: regression metrics (MAE vs. MSE)

• Mean Absolute Error (MAE): the average difference (absolute difference ie, always a positive value) between the actual and predicted target values

$$\frac{\sum_{\text{test example } x_i} |actual(x_i) - predicted(x_i)|}{\text{number of test examples}}$$

• **Mean Squared Error (MSE):** the average squared difference between the actual and predicted targets

$$\frac{\sum_{\text{test example } x_i} (actual(x_i) - predicted(x_i))^2}{\text{number of test examples}}$$

Today's Agenda

• Decision Tree

• Entropy

Decision: Are these comic book characters good or evil?



Problem: Is your date good or bad?

	mask	саре	tie	ears	smokes	height	class	
Batman	у	У	n	у	n	180	good	_
Robin	у	У	n	n	n	176	good	Training
Alfred	n	n	у	n	n	185	good	data
Penguin	n	n	у	n	у	140	evil	-
Catwoman	У	n	n	у	n	170	evil	-
Joker	n	n	n	n	n	179	evil	-
Batgirl	у	у	n	у	n	165	?	Test
Riddler	у	n	n	n	n	182	?	Data
Your Date	n	у	у	у	у	181	?	

Dataset and example from Dr. Kilian Weinberger @Cornell

	mask	cape	tie	ears	smokes	height	class
Batman	у	У	n	у	n	180	good
Robin	у	У	n	n	n	176	good
Alfred	n	n	у	n	n	185	good
Penguin	n	n	У	n	У	140	evil
Catwoman	У	n	n	У	n	170	evil
Joker	n	n	n	n	n	179	evil
Batgirl	У	У	n	У	n	165	?
Riddler	У	n	n	n	n	182	?
Your Date	n	у	у	у	у	181	?



Question: Is this a good tree?

Is this tree **<u>consistent</u>**: would it classify everyone correctly?





evil

yes

good

good

Question: Is this a good tree?

no

evil

Is this tree consistent: would it classify everyone correctly?

Let's classify the characters based on the value of attribute 'Smokes'

	mask	cape	tie	ears	smokes	height	class	Example Tree: Smokes ?
Batman	у	у	n	у	n	180	good	yes J
Robin	У	У	n	n	n	176	good	Mask?
Alfred	n	n	у	n	n	185	good	no yes no yes
Penguin	n	n	у	n	у	140	evil	evil no Height > evil good
Catwoman	у	n	n	у	n	170	evil	yes
Joker	n	n	n	n	n	179	evil	evil good
Batgirl	у	У	n	у	n	165	?	Question: Is this a good tree?
Riddler	у	n	n	n	n	182	?	Is this tree consistent: would it
Your Date	n	у	у	у	у	181	?	classify everyone correctly?

Let's classify the characters based on the value of attribute 'Ears'

	mask	cape	tie	ears	smokes	height	class	Example Tree: Smokes ?
Batman	у	У	n	у	n	180	good	yes
Robin	у	У	n	n	n	176	good	Mask? Ears?
Alfred	n	n	у	n	n	185	good	no yes no yes
Penguin	n	n	у	n	У	140	evil	Height > 175 evil good
Catwoman	у	n	n	у	n	170	evil	yes
Joker	n	n	n	n	n	179	evil	evil good
Batgirl	у	У	n	у	n	165	?	Question: Is this a good tree?
Riddler	У	n	n	n	n	182	?	Is this tree consistent: would it
Your Date	n	у	у	у	у	181	?	classify everyone correctly?

Let's classify the characters based on the value of attribute 'Mask'

	mask	cape	tie	ears	smokes	height	class	Example Tree: Smokes ?		
Batman	у	у	n	У	n	180	good	no yes		
Robin	у	у	n	n	n	176	good	Mask?		
Alfred	n	n	у	n	n	185	good	no ves		
Penguin	n	n	у	n	У	140	evil	Height > 175 evil good		
Catwoman	у	n	n	у	n	170	evil	yes		
Joker	n	n	n	n	n	179	evil	evil good		
Batgirl	У	У	n	У	n	165	?	Question: Is this a good tree?		
Riddler	У	n	n	n	n	182	?	Is this tree consistent: would it		
Your Date	n	у	у	у	у	181	?	classify everyone correctly?		

Let's classify the characters based on the value of attribute 'Height'

	mask	cape	tie	ears	smokes	height	class	Example Tree: Smokes ?		
Batman	у	У	n	у	n	180	good	no yes		
Robin	у	У	n	n	n	176	good	Mask? Ears?		
Alfred	n	n	у	n	n	185	good	no yes no yes		
Penguin	n	n	у	n	у	140	evil	Height > 175 evil good		
Catwoman	у	n	n	у	n	170	evil	yes		
Joker	n	n	n	n	n	179	evil	evi 🔨		
Batgirl	У	У	n	У	n	165	?			
Riddler	у	n	n	n	n	182	?	Answer: - No, it is not consistent. It		
Your Date	n	у	у	у	у	181	?	misclassified Alfred as evil		

	mask	cape	tie	ears	smokes	height	class	Example Tree: Smokes ?
Batman	у	у	n	у	n	180	good	no yes
Robin	у	у	n	n	n	176	good	Mask? Ears?
Alfred	n	n	у	n	n	185	good	no yes no yes
Penguin	n	n	у	n	у	140	evil	Height > 175 evil good
Catwoman	у	n	n	у	n	170	evil	yes yes
Joker	n	n	n	n	n	179	evil	evil good
Batgirl	у	у	n	у	n	165	?	
Riddler	у	n	n	n	n	182	?	
Your Date	n	у	у	у	у	181	?	this tree consistent?

	mask	cape	tie	ears	smokes	height	class	Example Tree: Smokes ?
Batman	у	У	n	у	n	180	good	no yes
Robin	у	У	n	n	n	176	good	Mask? Ears?
Alfred	n	n	У	n	n	185	good	no yes no yes
Penguin	n	n	у	n	У	140	evil	Height > 175 evil good
Catwoman	у	n	n	у	n	170	evil	Tie? yes yes yes
Joker	n	n	n	n	n	179	evil	
Batgirl	у	У	n	У	n	165	?	evil
Riddler	У	n	n	n	n	182	?	
Your Date	n	У	У	У	У	181	?	One Possibility: Add tie as an attribute

Activity: What is the smallest consistent tree?

	mask	cape	tie	ears	smokes	height	class	Example Tree: Smokes ?
Batman	у	у	n	у	n	180	good	no yes
Robin	у	у	n	n	n	176	good	Mask? Ears?
Alfred	n	n	у	n	n	185	good	no yes no yes
Penguin	n	n	у	n	у	140	evil	Height > 175 evil good
Catwoman	У	n	n	у	n	170	evil	yes
Joker	n	n	n	n	n	179	evil	evil good
Batgirl	У	У	n	У	n	165	?	
Riddler	у	n	n	n	n	182	?	
Your Date	n	у	у	у	у	181	?	



	mask	cape	tie	ears	smokes	height	class	Example Tree: Cape?
Batman	у	у	n	у	n	180	good	no yes
Robin	У	У	n	n	n	176	good	Height > good
Alfred	n	n	у	n	n	185	good	no
Penguin	n	n	у	n	У	140	evil	evil good
Catwoman	у	n	n	у	n	170	evil	
Joker	n	n	n	n	n	179	evil	
Batgirl	У	У	n	У	n	165	?	
Riddler	у	n	n	n	n	182	?	
Your Date	n	у	у	у	у	181	?	

	mask	cape	tie	ears	smokes	height	class	Example Tree: Cape?
Batman	у	у	n	У	n	180	good	no yes
Robin	у	у	n	n	n	176	good	Height > good
Alfred	n	n	у	n	n	185	good	no
Penguin	n	n	у	n	У	140	evil	evil good
Catwoman	у	n	n	у	n	170	evil	
Joker	n	n	n	n	n	179	evil	
Batgirl	у	У	n	У	n	165	?	
Riddler	у	n	n	n	n	182	?	
Your Date	n	у	у	у	у	181	?	

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Tree Data Structure

• **Tree:** a common data structure that simulates a hierarchical tree structure, with a root value and subtrees of children with a parent node, represented as a set of liked nodes.





Today's Agenda

• Decision Tree

• Entropy

Features or Attributes:

Target feature is whether or not a person will stay at a restaurant (T, F) with the following predictor features:

- 1. **Alternate:** whether there is a suitable alternative restaurant nearby.
- 2. Bar: whether the restaurant has a comfortable bar area to wait in.
- 3. Fri/Sat: true on Fridays and Saturdays.
- 4. Hungry: whether we are hungry.
- 5. **Patrons:** how many people are in the restaurant (values are None, Some, and Full).
- 6. **Price:** the restaurant's price range (one, two, or three \$'s)
- 7. **Raining:** whether it is raining outside.
- 8. **Reservation:** whether we made a reservation.
- 9. **Type:** the kind of restaurant (French, Italian, Thai, or burger).
- 10. **Est:** the wait estimated by the host (0–10 minutes, 10–30, 30–60, or >60).

Restaurant dataset

	Predictor feature											
Ex	Alt	Bar	Fri	Hun	Pat	Price	Rain	Res	Туре	Est	Wait	
X ₁	Т	F	F	Т	Some	\$\$\$	F	Т	French	0–10	Т	
X ₂	Т	F	F	Т	Full	\$	F	F	Thai	30–60	F	
X ₃	F	T	F	F	Some	\$	F	F	Burger	0–10	Т	
X4	Т	F	Т	Т	Full	\$	F	F	Thai	10–30	Т	
X5	Т	F	Т	F	Full	\$\$\$	F	Т	French	>60	F	
X ₆	F	Т	F	Т	Some	\$\$	Т	Т	Italian	0–10	Т	
X7	F	Т	F	F	None	\$	Т	F	Burger	0–10	F	
X ₈	F	F	F	Т	Some	\$\$	Т	Т	Thai	0–10	Т	
X9	F	Т	Т	F	Full	\$	Т	F	Burger	>60	F	
X ₁₀	Т	Т	Т	Т	Full	\$\$\$	F	Т	Italian	10–30	F	
X ₁₁	F	F	F	F	None	\$	F	F	Thai	0–10	F	
X ₁₂	Т	Т	T	Т	Full	\$	F	F	Burger	30–60	Т	

Target feature

Example Tree



Example Tree



- Target feature

Consistent and **Generalize**

- Is this tree consistent with the training examples?
 - do all of the training examples get categorized appropriately?

- Will this tree generalize well to new examples?
 - how well will new examples (test set) perform?

Growing or Building a Decision Tree

- Great, now how do I build (grow) a tree?
 - One algorithm that builds a decision tree is called:
 - ID3 Decision Tree Learning Algorithm

ID3 Decision Tree Learning (Main Loop)

- 1. A ← select the "best" decision feature for next node
- 2. Assign A as decision feature for node
- 3. For each possible attribute of A, create new descendant of node
- 4. Sort training examples to leaf nodes
- 5. If training examples perfectly classified, Then STOP, Else iterate over new leaf nodes

But... what does 'best' mean?

How would we go about deciding which node is the 'best?

Choosing a feature

Which of these features do you think is a better choice for putting at the root of the decision tree?

					♦				↓		
					Predict	tor feat	ure				
E×	Alt	Bar	Fri	Hun	Pat	Price	Rain	Res	Type	Est	Wait
X_1	Т	F	F	Т	Some	\$\$\$	F	Т	French	0-10	Т
X_2	Т	F	F	Т	Full	\$	F	F	Thai	30-60	F
X_3	F	Т	F	F	Some	\$	F	F	Burger	0-10	Т
X_4	Т	F	Т	Т	Full	\$	F	F	Thai	10-30	Т
X_5	Т	F	Т	F	Full	\$\$\$	F	Т	French	>60	F
X_6	F	Т	F	Т	Some	\$\$	Т	Т	Italian	0-10	Т
X_7	F	Т	F	F	None	\$	Т	F	Burger	0-10	F
X_8	F	F	F	Т	Some	\$\$	Т	Т	Thai	0-10	Т
X_9	F	т	Т	F	Full	\$	Т	F	Burger	>60	F
X10	Т	Т	Т	Т	Full	\$\$\$	F	Т	Italian	10-30	F
X11	F	F	F	F	None	\$	F	F	Thai	0-10	F
X_{12}	Т	Т	Т	Т	Full	\$	F	F	Burger	30-60	Т

Target feature

Choosing a feature

Which of these features do you think is a better choice for putting at the root of the decision tree?



- Wait column is the target value

Decision Tree: Choosing a feature

Idea: a good feature splits the examples into subsets that are as pure as possible (ideally) "all positive" or "all negative"

- Patrons is a better choice--it gives more information about the classification

Red = false target value, Green = true target value



Wait column is the target value

Decision Tree: Entropy

Entropy is a measure of impurity/randomness

- High entropy: more evenly split classes highly unpredictable
- Low entropy: mostly one class highly predictable



Decision Tree: Calculating Entropy Prior

Prior Probability: aka the 'prior'

- the split of the examples
- Out of 14 examples, if I have 9 positive examples and 5 negative examples my prior is:

<<u>9</u>/14, <u>5</u>/14> ≈ <<u>0.64</u>, <u>0.36</u>>

Calculating the entropy when prior is $\langle P_1, ..., P_c \rangle$ is:

$$Entropy(\langle P_1,\ldots,P_c\rangle) = \sum_{i=1}^{c} -P_i \log_2 P_i$$

Decision Tree: Calculating Entropy Prior

Calculating the entropy when prior is $\langle P_1, ..., P_c \rangle$ is:

$$Entropy(\langle P_1,\ldots,P_c\rangle) = \sum_{i=1}^c -P_i \log_2 P_i$$

- entropy of prior $\langle 0.5, 0.5 \rangle$
 - $-0.5 \log_2 (0.5) 0.5 \log_2 (0.5) = 1$
- entropy of prior $\langle 0.9, 0.1 \rangle$
 - $-0.9 \log_2 (0.9) 0.1 \log_2 (0.1) \approx 0.47$
- entropy of prior (0.64, 0.36)
 - -0.64 log₂ (0.64) 0.36 log₂ (0.36) ≈ 0.94
- entropy of prior $\langle 0.25,\, 0.25,\, 0.5\rangle$
 - $-0.25 \log_2 (0.25) 0.25 \log_2 (0.25) 0.5 \log_2 (0.5) = 1.5$

The maximum entropy is log₂(k) where k is the number of categories. It is not always bounded by 0 and 1

$$\log_2(3) = 1.584962501$$

Decision Tree: Entropy Calculation Example



So, the entropy for the three sets after sorting according to Patrons is

$$\begin{aligned} &-\frac{0}{2}\log_2\frac{0}{2} - \frac{2}{2}\log_2\frac{2}{2} = 0,\\ &-\frac{4}{4}\log_2\frac{4}{4} - \frac{0}{2}\log_2\frac{0}{2} = 0,\\ &\text{and} \ -\frac{2}{6}\log_2\frac{2}{6} - \frac{4}{6}\log_2\frac{4}{6} \approx 0.918 \end{aligned}$$

Decision Tree: Entropy Calculation Exercise

The <u>expected entropy</u> for a feature is defined as the weighted sum of entropies multiplied by the fraction of samples that belong to each set.



Then, the *expected entropy* remaining after testing the *Patrons* is

$$pprox rac{2}{12} \cdot 0 + rac{4}{12} \cdot 0 + rac{6}{12} \cdot 0.918 pprox 0.459$$

Decision Tree: Entropy Calculation Example

What is the expected entropy for Type?

Can you say without doing the math?



Decision Tree: Information Gain Example

• We need to calculate entropy for each feature (eg, *Patron, Type*) as a candidate



Decision Tree: Information Gain Example

• Calculate entropy for feature *Patron* as a candidate



Decision Tree: Information Gain Example

• The *difference* between the entropy before the test and the expected entropy after the test is the **information gain**

InformationGain() = Entropy (before) - Expected Entropy (after)

InformationGain(Patrons) = 1.0 - 0.459 = 0.541



- <u>Step 1:</u> Calculate the entropy of the distribution of the classes before the node you are testing.
 - this is the entropy_before



- entropy of prior $\langle 0.5, \, 0.5 \rangle$
 - -0.5 log₂ (0.5) 0.5 log₂ (0.5) = 1

So, Entropy_before = 1

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• <u>Step 1:</u> Calculate the entropy of the distribution of the classes before the node you are testing. This is the entropy before



Then, the *expected entropy* remaining after testing the *Patrons* is

$$\approx \frac{2}{12} \cdot 0 + \frac{4}{12} \cdot 0 + \frac{6}{12} \cdot 0.918 \approx 0.459$$

 Step 1: Calculate the entropy of the distribution of the classes before the node you are testing. This is the entropy before

- Step 2: Calculate the expected entropy
 - The weighted sum of the entropy of each split of the data

- Step 3: Find the difference between the entropy before and expected entropy
 - Information Gain(Patron) = Entropy_before(Patron) Expected_entropy(Patron)

```
= 1 - 0.459
= 0.541
```

Decision Tree: Entropy Calculation Example

• Calculate entropy for feature *Type* as a candidate





Decision Tree: Exercise Information Gain

• Calculate the Information Gain for *Hun*:



Ex	Alt	Bar	Fri	Hun	Pat	Price	Rain	Res	Туре	Est	Wait
X1	Т	F	F	Т	Some	\$\$\$	F	Т	French	0–10	Т
X_2	Т	F	F	T	Full	\$	F	F	Thai	30–60	F
X ₃	F	Т	F	F	Some	\$	F	F	Burger	0–10	Т
X_4	Т	F	Т	Т	Full	\$	F	F	Thai	10-30	Т
X_5	Т	F	Т	F	Full	\$\$\$	F	Т	French	>60	F
X_6	F	Т	F	T	Some	\$\$	Т	Т	Italian	0–10	Т
X7	F	Т	F	F	None	\$	Т	F	Burger	0–10	F
X ₈	F	F	F	T	Some	\$\$	Т	Т	Thai	0–10	Т
X_9	F	Т	Т	F	Full	\$	Т	F	Burger	>60	F
X10	Т	Т	Т	Т	Full	\$\$\$	F	Т	Italian	10-30	F
X11	F	F	F	F	None	\$	F	F	Thai	0–10	F
X ₁₂	Т	Т	Т	Т	Full	\$	F	F	Burger	30–60	Т

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Decision Tree: Exercise Information Gain

• Calculate the Information Gain for *Hun*:



Ex	Alt	Bar	Fri	Hun	Pat	Price	Rain	Res	Туре	Est	Wait
X1	Т	F	F	Т	Some	\$\$\$	F	Т	French	0–10	Т
X2	Т	F	F	Т	Full	\$	F	F	Thai	30–60	F
<i>X</i> ₃	F	Т	F	F	Some	\$	F	F	Burger	0–10	Т
X_4	Т	F	Т	Т	Full	\$	F	F	Thai	10-30	Т
X_5	Т	F	Т	F	Full	\$\$\$	F	Т	French	>60	F
X ₆	F	Т	F	Т	Some	\$\$	Т	Т	Italian	0–10	Т
X7	F	Т	F	F	None	\$	Т	F	Burger	0–10	F
X ₈	F	F	F	Т	Some	\$\$	Т	Т	Thai	0–10	Т
X_9	F	Т	Т	F	Full	\$	Т	F	Burger	>60	F
X10	Т	Т	Т	Т	Full	\$\$\$	F	Т	Italian	10-30	F
X11	F	F	F	F	None	\$	F	F	Thai	0–10	F
X ₁₂	Т	Т	Т	Т	Full	\$	F	F	Burger	30–60	Т

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Decision Tree: Exercise Information Gain

• Information Gain results

- Gain(Alt) = 1 1 = 0
- Gain (Bar) = 1 1 = 0
- Gain(Fri) = 1 0.979 = 0.021
- Gain(Hun) = 1 0.804 = 0.196
- Gain(Patrons) = 1 0.459 = 0.541
- Gain(Price) = 1 0.804 = 0.196
- Gain(Rain) = 1 1 = 0
- Gain(Res) = 1 0.979 = 0.021
- Gain(Type) = 1 1 = 0
- Gain(Est) = 1 0.792 = 0.208



Decision Tree: What to do with numeric features?

What do we do if we have numeric (even continuous-valued) features like age from the titanic dataset or petal length from the iris dataset?

Idea: Decision Tree thresholds: if age > 70

Unfortunate annoying thing: Even though decision tree algorithms work well with categorical data, the Python library we will work with still wants all predictor features converted to a number, so we will have to work with numbers no matter what.

Decision Tree Size Discussion

Decision tree learned from the 12 examples:



Decision Tree Size Discussion

Many different consistent trees possible:

What quality is preferably?

More nodes v fewer nodes?

What are the consequences of having a deep tree with many nodes?



Inductive Bias of ID3 Algorithm

Shorter trees are preferred in ID3, trees with high-information features closer to the root are preferred

Biases allow us to learn, but you should understand what your algorithm's bias is.

Overfitting

 Big idea: You <u>overfit</u> if you do well on the training set, but not so well on the testing set.



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Avoid Overfitting

- Make the tree smaller
- Some ideas on avoiding overly complex trees:
- Stop growing when data split is not statistically significant
- Grow full tree, then post-prune

Avoid Overfitting

- What are the benefits of decision trees compared to kNN
- Disadvantages?
- When would you use one over the other?
 - if one column highly predicts the target variable \rightarrow decision tree
 - If lots of predictors have similar weight in decision \rightarrow kNN
 - If you must be able to interpret the data clearly \rightarrow decision tree