Decision Trees

A naive example: cat v.s. non-cat

I want to build an APP that can distinguish cat and non-cat. The input feature from training images are:

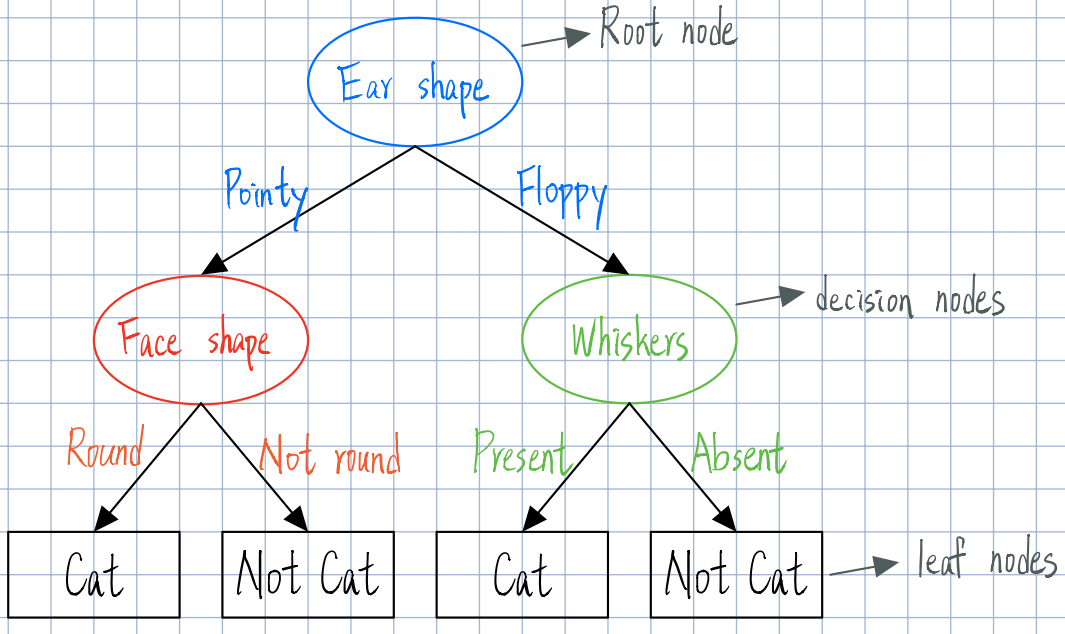
Ear shape: Pointy v.s. Floppy

Face shape: Round v.s. Not round

Whiskers: Present v.s. Absent

Notice that the features here are all discrete 1/0, but they don't have to be. The features in decision trees can also be continuous value.

These three features are then used to build a decision tree. E.g., here is one decision tree:



After a decision tree is found, it can be used to classify new images.

Cat classification example

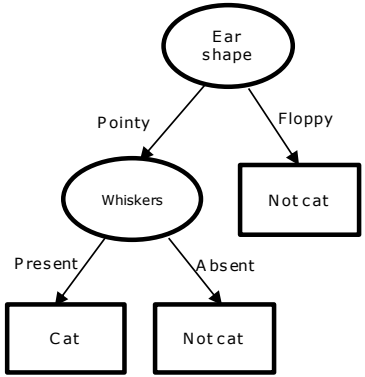
Ear shape (x_1)	Face shape (x_2)	Whiskers (x_3)	Cat
Pointy	Round	Present	1
Floppy	Not round	Present	1
Floppy	Round	Absent	0
Pointy	Not round	Present	0
Pointy	Round	Present	1
Pointy	Round	Absent	1
Floppy	Not round	Absent	0
Pointy	Round	Absent	1
Floppy	Round	Absent	0
Floppy	Round	Absent	0

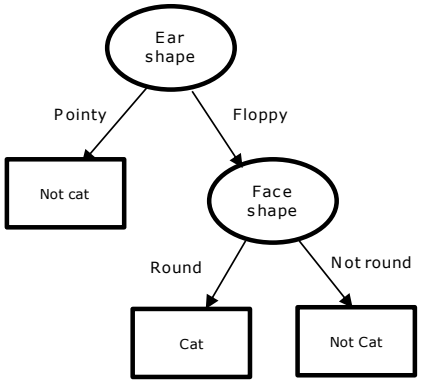
Categorical (discrete values)

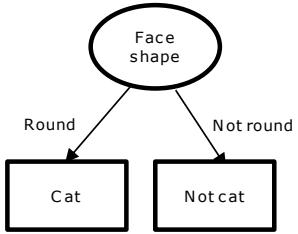
X

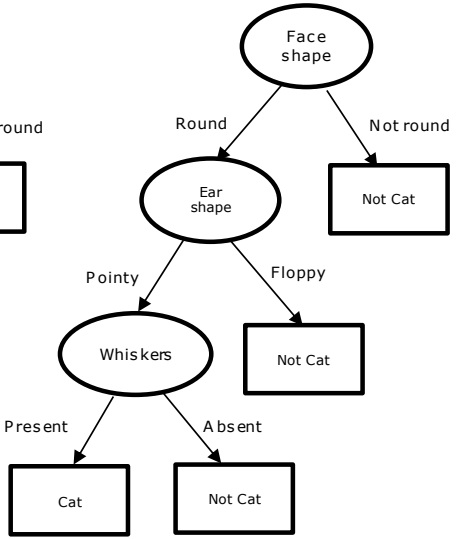
y

Decision Tree

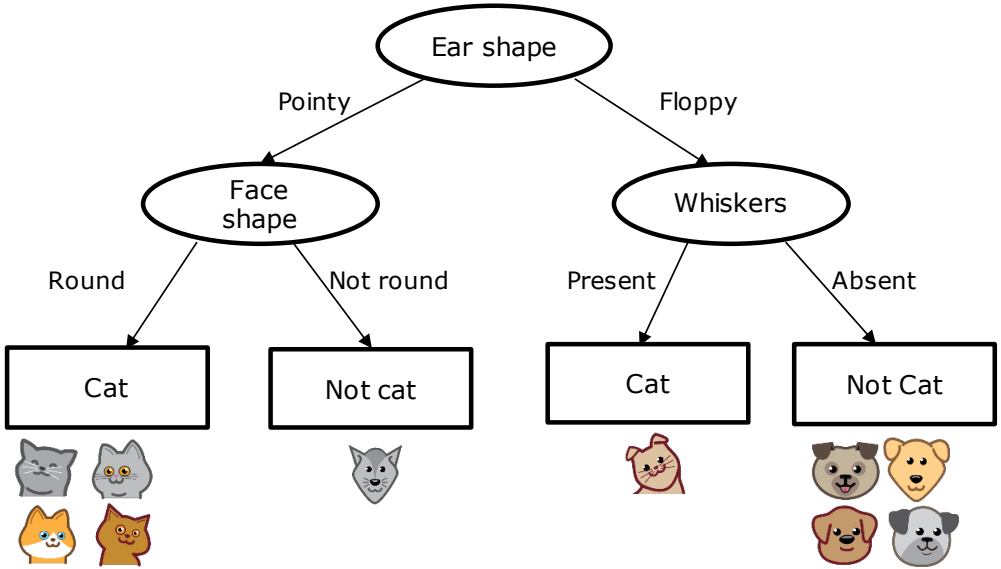








Decision Tree Learning

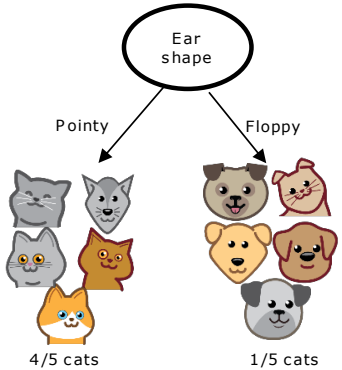


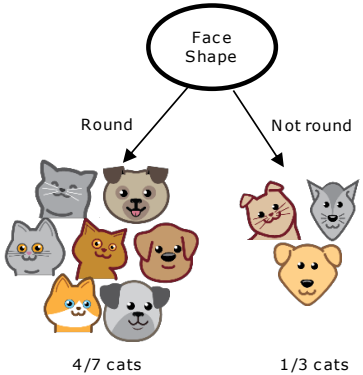
Decision Tree Learning

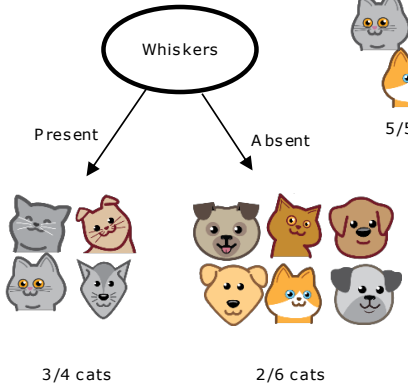
Decision 1: How to choose what feature to split on at each node?

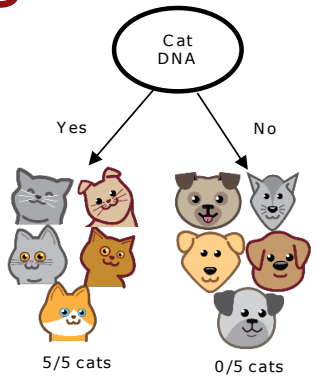
purity: we want to get what subsets, which are as close as possible to all cats or all dogs.

Maximize purity (or minimize impurity)

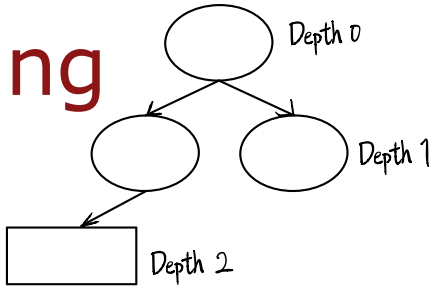








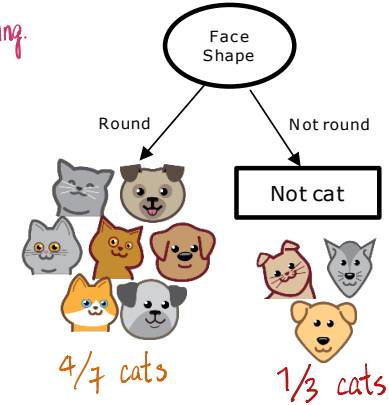
Decision Tree Learning



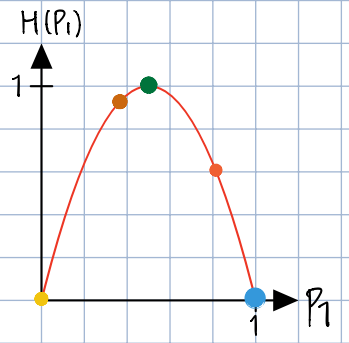
Decision 2: When do you stop splitting?

- When a node is 100% one class
- When splitting a node will result in the tree exceeding a maximum depth E.g. max depth = 2 Keep trees small can prevent overfitting.
- When improvements in purity score are below a threshold
- When number of examples in a node is below a threshold

E.g., there is only 1 cat in three samples. We don't want to split further. We can just put a leaf node.



Measuring Purity



Entropy is a measure of impurity of data.

Define P_1 = fraction of examples that are cats.

$H(P_1)$: Entropy function measures impurity.

$P_1 = 0/6$ $H(P_1) = 0$

$P_1 = 2/6$ $H(P_1) = 0.92$

$P_1 = 3/6$ $H(P_1) = 1$

$P_1 = 5/6$ $H(P_1) = 0.65$

$P_1 = 6/6$ $H(P_1) = 0$

The higher entropy means it's more impure.

The entropy equation: Define P_0 as fraction of examples that are not cats.

$$P_0 = 1 - P_1$$

$$H(P_1) = -P_1 \log_2(P_1) - P_0 \log_2(P_0)$$

$$= -P_1 \log_2(P_1) - (1-P_1) \log_2(1-P_1)$$

note: "$0 \log_2(0) = 0$"

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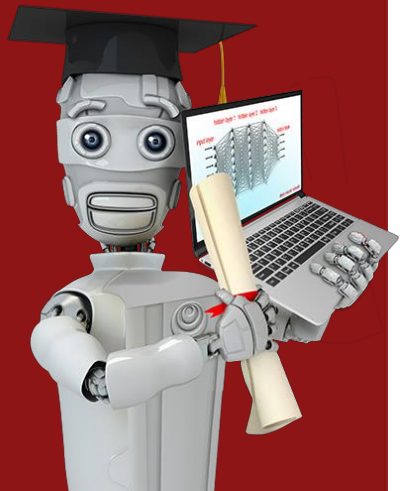


Decision Tree Learning

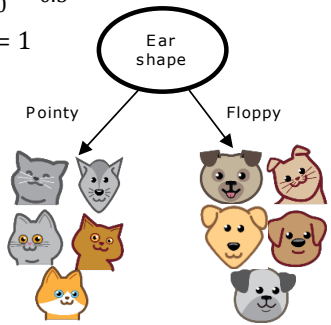
Choosing a split: Information Gain

Given 5 cats and 5 dogs, which feature should be used to split them? Before splitting, the entropy $H(P_1)$ is 1.

Choosing a split

$p_1 = {}^5/_{10} = 0.5$

$H(0.5) = 1$



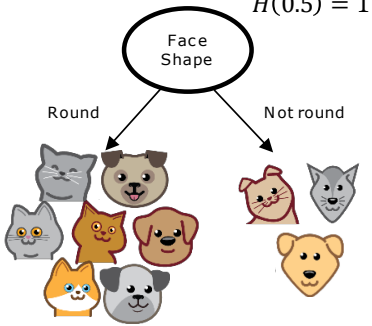
$p_1 = {}^4/_5 = 0.8 \quad p_1 = {}^1/_5 = 0.2$

$H(0.8) = 0.72 \quad H(0.2) = 0.72$

$$H(0.5) - \left(\frac{5}{10}H(0.8) + \frac{5}{10}H(0.2)\right)$$

$= 0.28$ Choose this feature to split on because 0.28 is the largest.

$H(0.5) = 1$



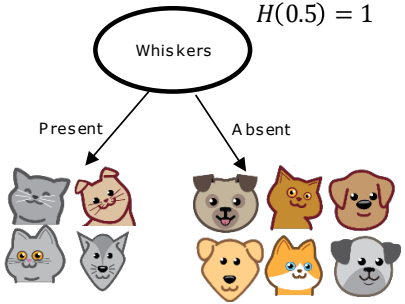
$p_1 = {}^4/_7 = 0.57 \quad p_1 = {}^1/_3 = 0.33$

$H(0.57) = 0.99 \quad H(0.33) = 0.92$

$$H(0.5) - \left(\frac{7}{10}H(0.57) + \frac{3}{10}H(0.33)\right)$$

$= 0.03$

$H(0.5) = 1$



$p_1 = {}^3/_4 = 0.75 \quad p_1 = {}^2/_6 = 0.33$

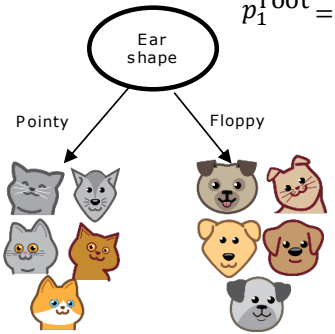
$H(0.75) = 0.81 \quad H(0.33) = 0.92$

$$H(0.5) - \left(\frac{4}{10}H(0.75) + \frac{6}{10}H(0.33)\right)$$

$= 0.12$

Information Gain

$p_1^{\text{root}} = 5/10 = 0.5$



$p_1^{\text{left}} = 4/5$

$w^{\text{left}} = 5/10$

$p_1^{\text{right}} = 1/5$

$w^{\text{right}} = 5/10$

weight

We need to fuse multiple factors into a single value so we can make a decision.

Information gain

$$= \text{H}(p_1^{\text{root}}) - \left(w^{\text{left}} H\left(p_1^{\text{left}}\right) + w^{\text{right}} H\left(p_1^{\text{right}}\right) \right)$$

The higher the information gain, the better.

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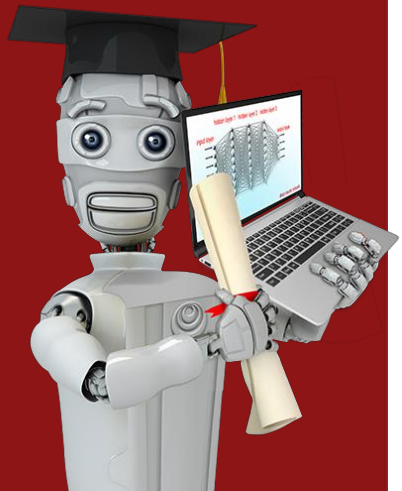


Decision Tree Learning

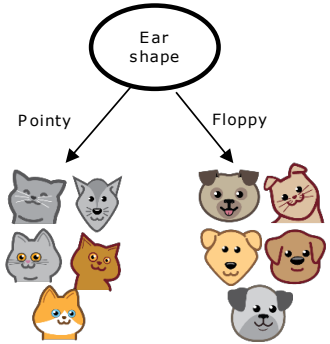
Putting it together

Decision Tree Learning

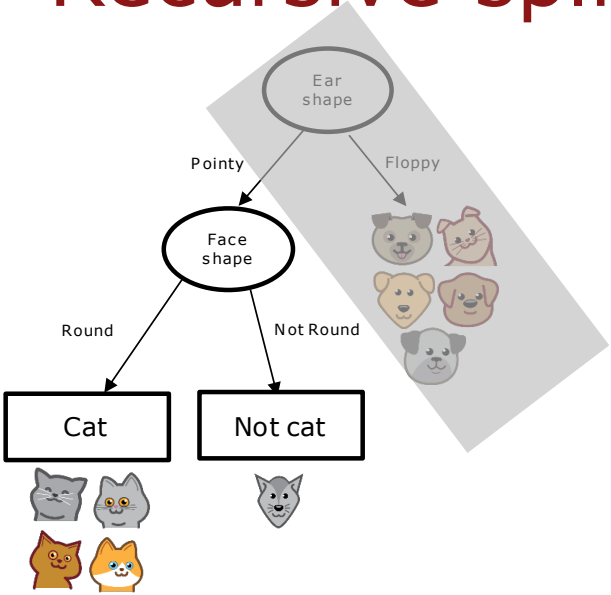
- Start with all examples at the root node
- Calculate information gain for all possible features, and pick the one with the highest information gain
- Split dataset according to selected feature, and create left and right branches of the tree
- Keep repeating splitting process until stopping criteria is met:
  - When a node is 100% one class
  - When splitting a node will result in the tree exceeding a maximum depth
  - Information gain from additional splits is less than threshold
  - When number of examples in a node is below a threshold

Recursive splitting

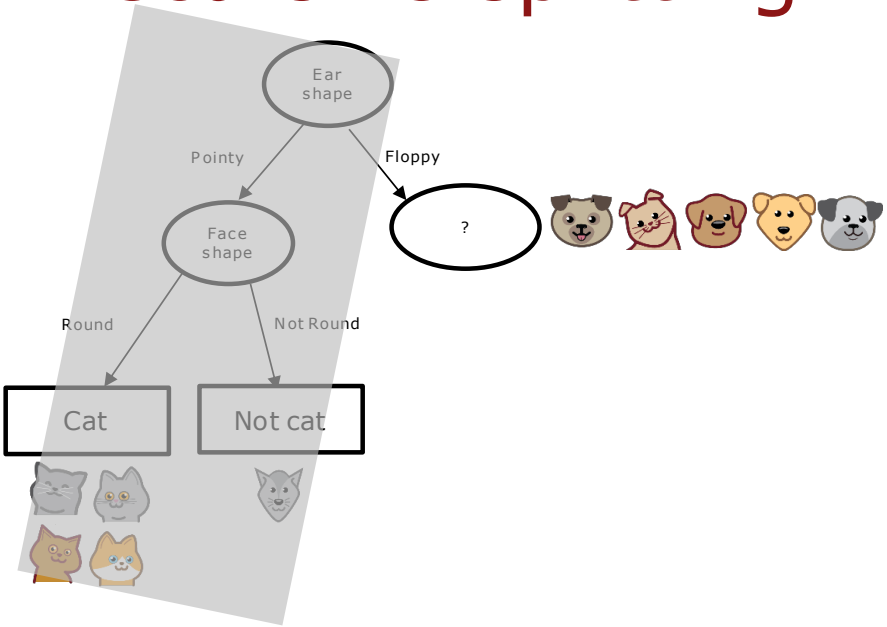
Recursive splitting



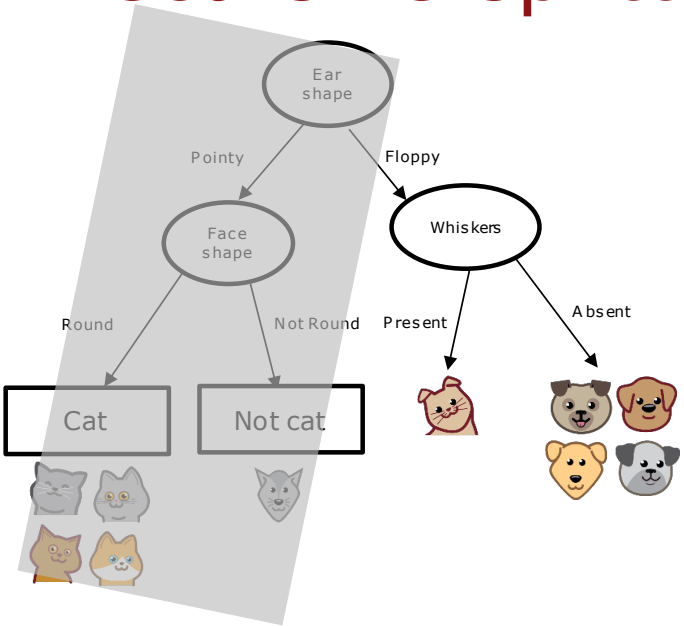
Recursive splitting



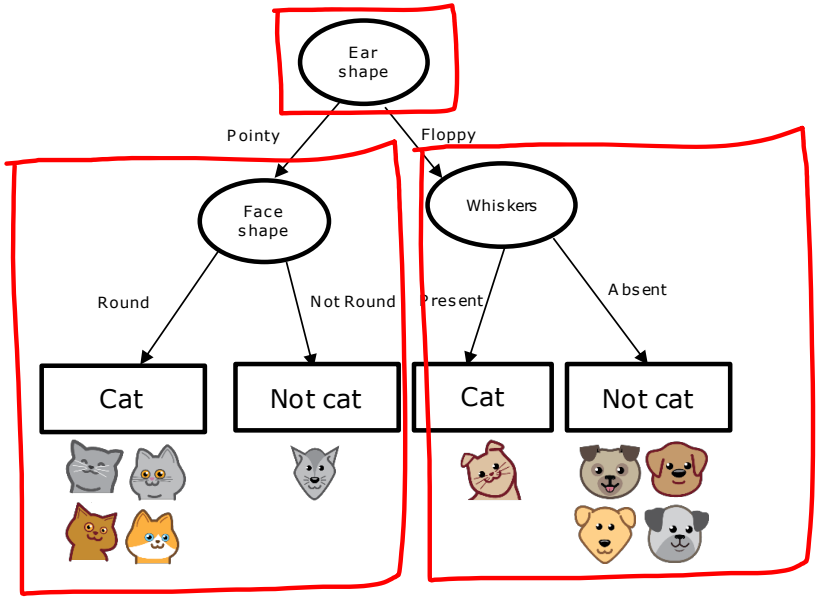
Recursive splitting



Recursive splitting



Recursive splitting



Recursive algorithm

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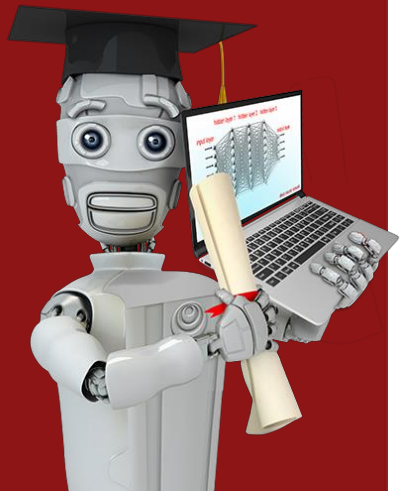


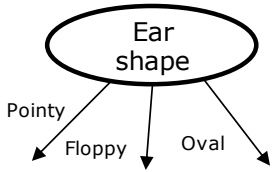
Decision Tree Learning

Using one-hot encoding of categorical features

Features with three possible values

	Ear shape (x_1)	Face shape (x_2)	Whiskers (x_3)	Cat (y)
	Pointy	Round	Present	1
	Oval	Not round	Present	1
	Oval	Round	Absent	0
	Pointy	Not round	Present	0
	Oval	Round	Present	1
	Pointy	Round	Absent	1
	Floppy	Not round	Absent	0
	Oval	Round	Absent	1
	Floppy	Round	Absent	0
	Floppy	Round	Absent	0

3 possible values



One hot encoding

If a categorical feature can take on k values, create k binary features (0 or 1 valued).

One hot encoding

	~~Ear shape~~	Pointy ears	Floppy ears	Oval ears	Face shape	Whiskers	Cat
	~~Pointy~~	1	0	0	Round	Present	1
	~~Oval~~	0	0	1	Not round	Present	1
	~~Oval~~	0	0	1	Round	Absent	0
	~~Pointy~~	1	0	0	Not round	Present	0
	~~Oval~~	0	0	1	Round	Present	1
	~~Pointy~~	1	0	0	Round	Absent	1
	~~Floppy~~	0	1	0	Not round	Absent	0
	~~Oval~~	0	0	1	Round	Absent	1
	~~Floppy~~	0	1	0	Round	Absent	0
	~~Floppy~~	0	1	0	Round	Absent	0

Only 1 feature of ears can be True.

One hot encoding and neural networks

	Pointy ears	Floppy ears	Round ears	Face shape	Whiskers	Cat
	1	0	0	~~Round~~ 1	~~Present~~ 1	1
	0	0	1	~~Not round~~ 0	~~Present~~ 1	1
	0	0	1	~~Round~~ 1	~~Absent~~ 0	0
	1	0	0	~~Not round~~ 0	~~Present~~ 1	0
	0	0	1	~~Round~~ 1	~~Present~~ 1	1
	1	0	0	~~Round~~ 1	~~Absent~~ 0	1
	0	1	0	~~Not round~~ 0	~~Absent~~ 0	1
	0	0	1	~~Round~~ 1	~~Absent~~ 0	1
	0	1	0	~~Round~~ 1	~~Absent~~ 0	1
	0	1	0	~~Round~~ 1	~~Absent~~ 0	1

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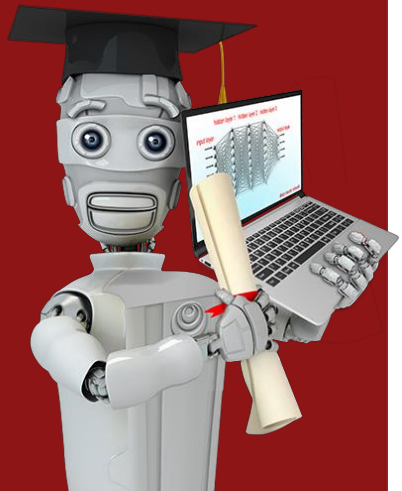


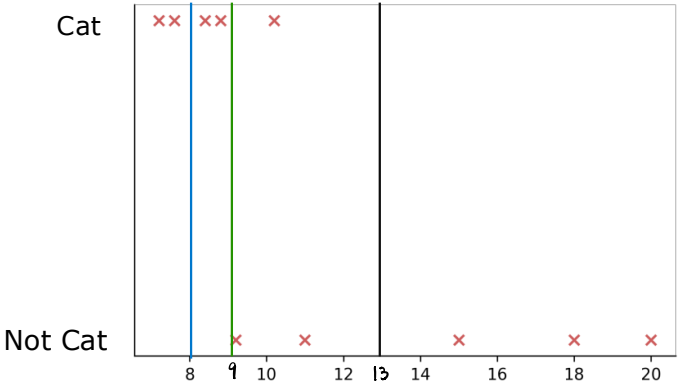
Decision Tree Learning

Continuous valued features

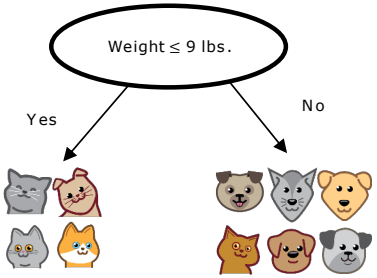
Continuous features

	Ear shape	Face shape	Whiskers	Weight (lbs.)	Cat
	Pointy	Round	Present	7.2	1
	Floppy	Not round	Present	8.8	1
	Floppy	Round	Absent	15	0
	Pointy	Not round	Present	9.2	0
	Pointy	Round	Present	8.4	1
	Pointy	Round	Absent	7.6	1
	Floppy	Not round	Absent	11	0
	Pointy	Round	Absent	10.2	1
	Floppy	Round	Absent	18	0
	Floppy	Round	Absent	20	0

Splitting on a continuous variable



We can choose 9 mid-points between the 10 examples as possible splits, and find the split that gives the highest information gain.



$$H(0.5) - \left(\frac{2}{10}H\left(\frac{2}{2}\right) + \frac{8}{10}H\left(\frac{3}{8}\right)\right) = 0.24$$ threshold = 8

$$H(0.5) - \left(\frac{4}{10}H\left(\frac{4}{4}\right) + \frac{6}{10}H\left(\frac{1}{6}\right)\right) = 0.61$$ threshold = 9

$$H(0.5) - \left(\frac{7}{10}H\left(\frac{5}{7}\right) + \frac{3}{10}H\left(\frac{0}{3}\right)\right) = 0.40$$ threshold = 13

Given 5 cats and 5 dogs, what threshold of weights should be used to split them?

Before splitting, the entropy $H(P_1)$ is $H(\frac{5}{10}) = 1$

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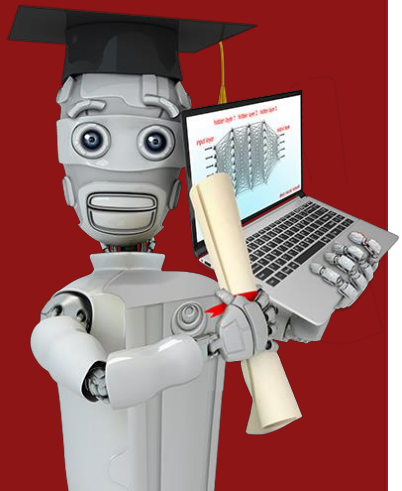


So far, Andrew has been talking about decision trees as classification algorithm. Now, he will generalize decision trees to be regression algorithms so that algorithms can predict a number.

Decision Tree Learning

Regression Trees (optional)

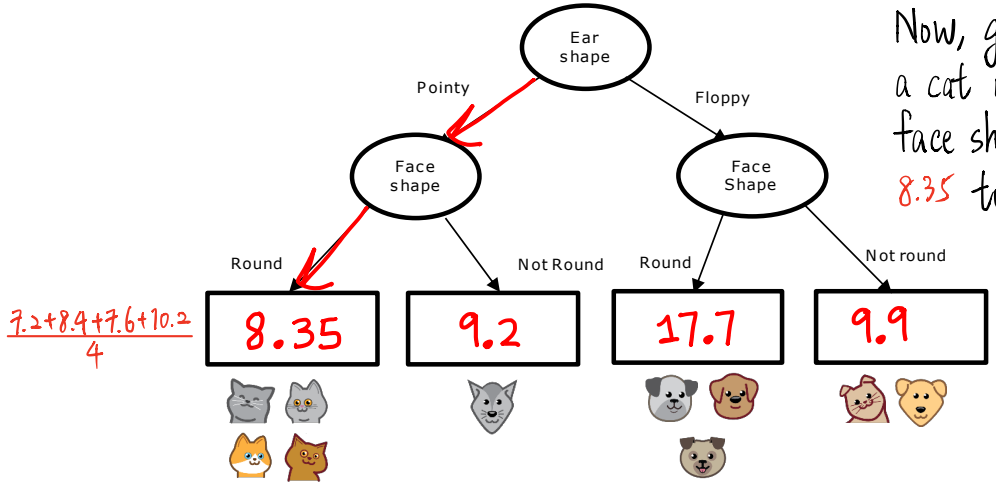
Regression with Decision Trees: Predicting a number

Ear shape	Face shape	Whiskers	Weight (lbs.)
Pointy	Round	Present	7.2
Floppy	Not round	Present	8.8
Floppy	Round	Absent	15
Pointy	Not round	Present	9.2
Pointy	Round	Present	8.4
Pointy	Round	Absent	7.6
Floppy	Not round	Absent	11
Pointy	Round	Absent	10.2
Floppy	Round	Absent	18
Floppy	Round	Absent	20

Input features X

y Target output

Regression with Decision Trees

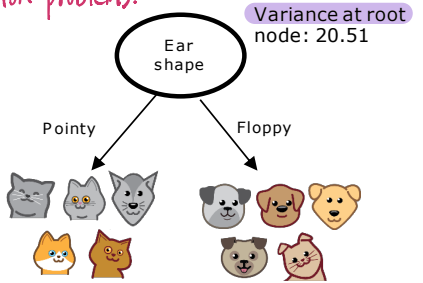


Now, given a new testing example, a cat with pointy ear and a round face shape, we can just assign 8.35 to it.

Unlike reducing entropy in classification algorithms, we want to reduce variance in regression problems.

Now, let's train a regression tree.

Choosing a split



Variance at root node: 20.51

Weights: 7.2, 9.2, 8.4,7.6, 10.2

Variance: 1.47

Weights: 8.8, 15, 11, 18, 20

Variance: 21.87

$w^{\text{left}} = 5/10$

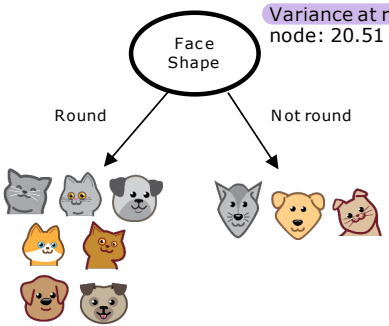
$w^{\text{right}} = 5/10$

$$20.51 - \left(\frac{5}{10} * 1.47 + \frac{5}{10} * 21.87\right)$$

$$= 8.84$$

information gain

Choose this feature to split on because 8.84 is the largest.



Variance at root node: 20.51

Weights: 7.2, 15, 8.4, 7.6,10.2, 18, 20

Variance: 27.80

Weights: 8.8,9.2,11

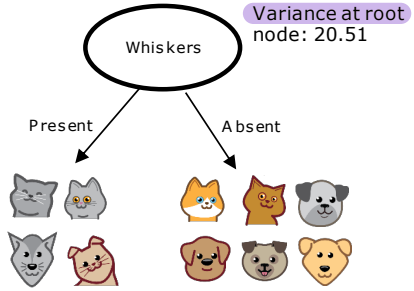
Variance: 1.37

$w^{\text{left}} = 7/10$

$w^{\text{right}} = 3/10$

$$20.51 - \left(\frac{7}{10} * 27.80 + \frac{3}{10} * 1.37\right)$$

$$= 0.64$$



Variance at root node: 20.51

Weights: 7.2, 8.8, 9.2, 8.4

Variance: 0.75

Weights: 15, 7.6, 11, 10.2, 18, 20

Variance: 23.32

$w^{\text{left}} = 4/10$

$w^{\text{right}} = 6/10$

$$20.51 - \left(\frac{4}{10} * 0.75 + \frac{6}{10} * 23.32\right)$$

$$= 6.22$$

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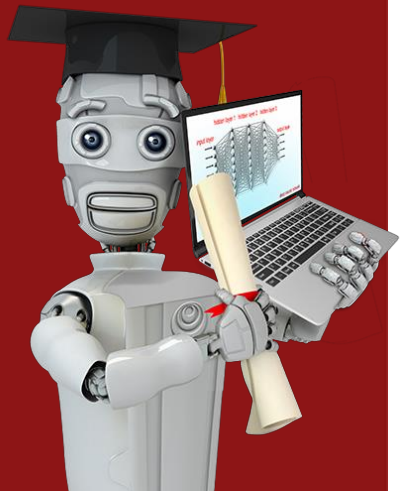
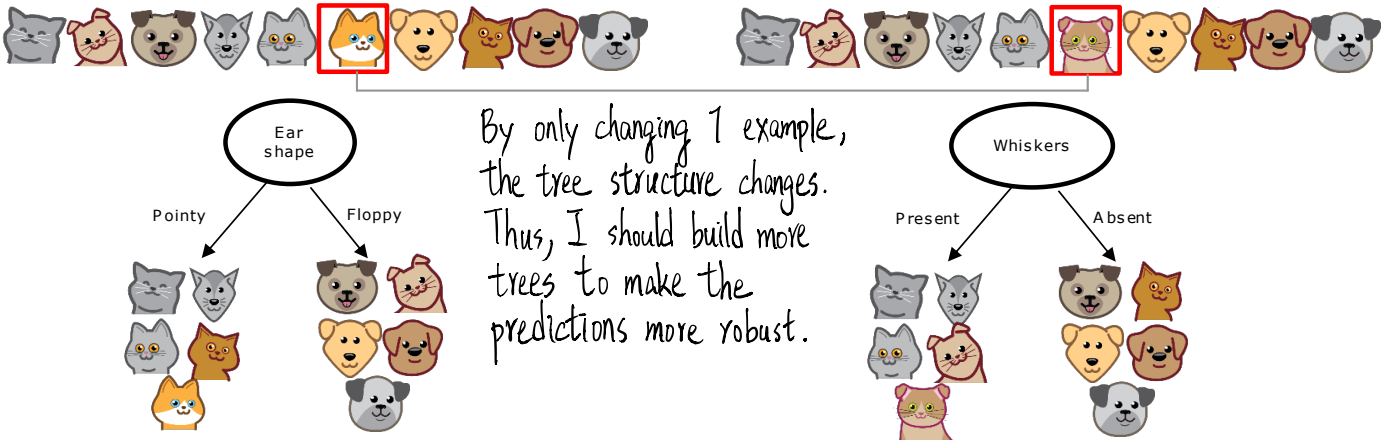


Tree ensembles

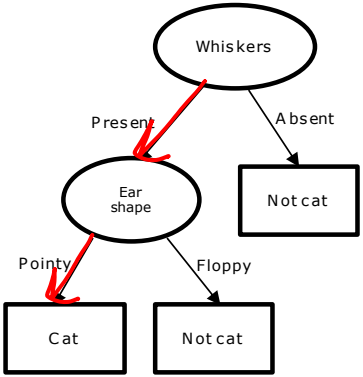
Using multiple decision trees

Trees are highly sensitive to small changes of the data

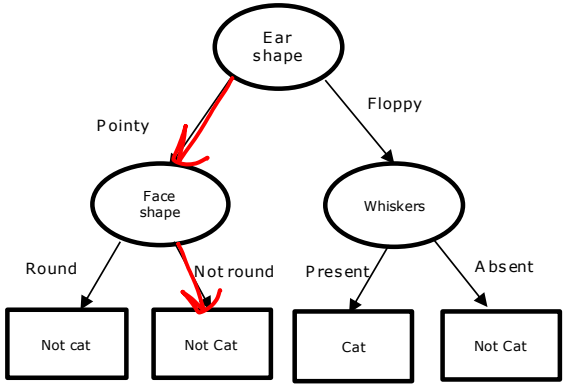


It makes predictions more robust.

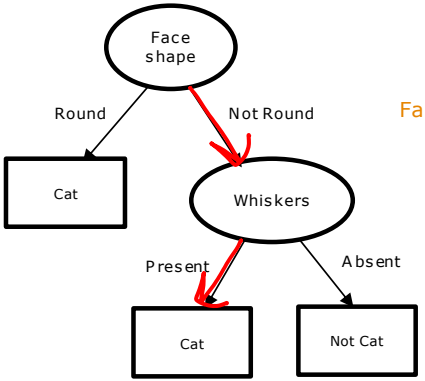
Tree ensemble



Prediction: Cat



Prediction: Not cat



Prediction: Cat

New test example

Ear shape: Pointy
Face shape: Not Round
Whiskers: Present

Voting Majority wins

Final prediction: Cat

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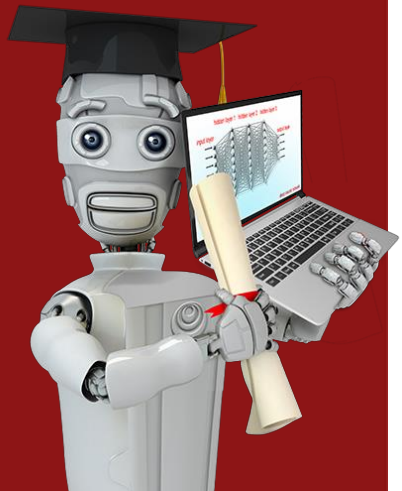


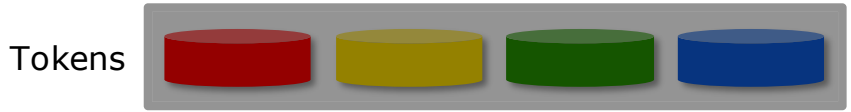
We know that tree ensembles is more robust than a single decision tree. But how to build tree ensembles?

Sampling with Replacement

Tree ensembles

Sampling with replacement

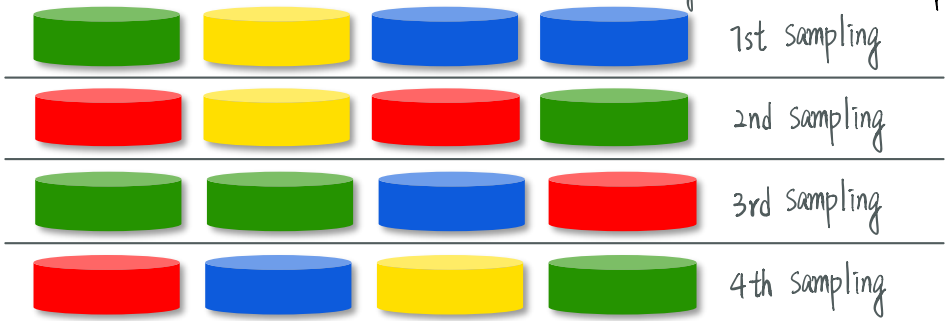
Sampling with replacement



A token is drawn out of the black bag and put back at a time. Thus, a repeated token is possible.

Sampling with replacement:

In each sampling, I can draw 4 times from the black bag.



Sampling with replacement

A bag with 10 examples

Ear shape	Face shape	Whiskers	Cat
Pointy	Round	Present	1
Floppy	Not round	Absent	0
Pointy	Round	Absent	1
Pointy	Not round	Present	0
Floppy	Not round	Absent	0
Pointy	Round	Absent	1
Pointy	Round	Present	1
Floppy	Not round	Present	1
Floppy	Round	Absent	0
Pointy	Round	Absent	1

After 1 sampling process (drawing 10 samples from the bag), now we have a new training set (with repeated data) which is slightly different than the original set.

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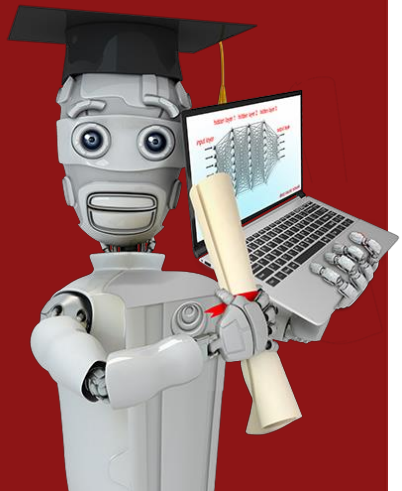


Tree ensembles

Random forest algorithm

Generating a tree sample

Given training set of size m

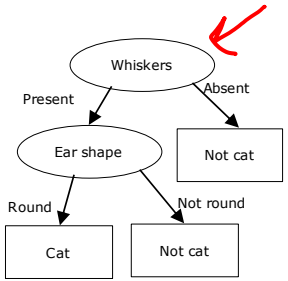
B: the number of times of sampling

For $b = 1$ to B:

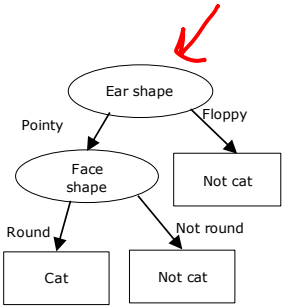
Use sampling with replacement to create a new training set of size m

Train a decision tree on the new dataset

Ear shape	Face shape	Whiskers	Cat
Pointy	Round	Present	Yes
Floppy	Round	Absent	No
Floppy	Round	Absent	No
Pointy	Round	Present	Yes
Pointy	Not Round	Present	Yes
Floppy	Round	Absent	No
Floppy	Round	Present	Yes
Pointy	Not Round	Absent	No
Pointy	Not Round	Absent	No
Pointy	Not Round	Present	Yes



Ear shape	Face shape	Whiskers	Cat
Pointy	Round	Present	Yes
Pointy	Round	Absent	Yes
Floppy	Not Round	Absent	No
Floppy	Not Round	Absent	No
Pointy	Round	Absent	Yes
Floppy	Round	Absent	No
Floppy	Round	Absent	No
Floppy	Round	Absent	No
Pointy	Not Round	Absent	No
Pointy	Round	Present	Yes



...

Bagged decision tree

The recommend value for B is 64 ~ 128. Choosing a bigger B like 1000 is usually meaningless because the performance isn't improved significantly and computation is slow down noticeably.

Randomizing the feature choice

At each node, when choosing a feature to use to split, if n features are available, pick a random subset of $k < n$ features and allow the algorithm to only choose from that subset of features.

When n is large, like $10^2 \sim 10^3$ or more, k could be $k = \sqrt{n}$

Random forest algorithm is usually more robust than Bagged decision tree.

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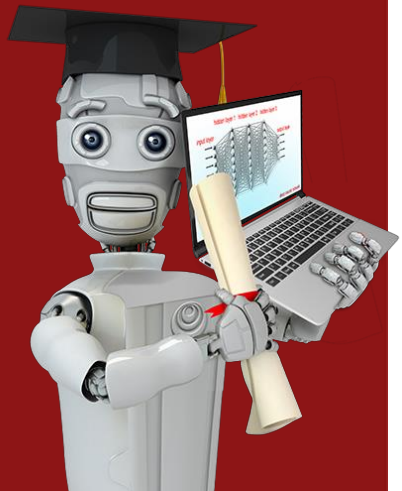


Tree ensembles

XGBoost

Boosted trees intuition

Given training set of size m

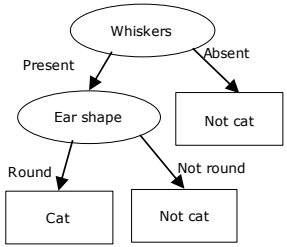
For b = 1 to B:

Use sampling with replacement to create a new training set of size m

But instead of picking from all examples with equal (1/m) probability, make it more likely to pick examples that the previously trained trees misclassify

Train a decision tree on the new dataset

Ear shape	Face shape	Whiskers	Cat
Pointy	Round	Present	Yes
Floppy	Round	Absent	No
Floppy	Round	Absent	No
Pointy	Round	Present	Yes
Pointy	Not Round	Present	Yes
Floppy	Round	Absent	No
Floppy	Round	Present	Yes
Pointy	Not Round	Absent	No
Pointy	Not Round	Absent	No
Pointy	Not Round	Present	Yes



Ear shape	Face shape	Whiskers	Prediction
Pointy	Round	Present	Cat ✓
Floppy	Not Round	Present	Not cat ✗
Floppy	Round	Absent	Not cat ✓
Pointy	Not Round	Present	Not cat ✓
Pointy	Round	Present	Cat ✓
Pointy	Round	Absent	Not cat ✗
Floppy	Not Round	Absent	Not cat ✓
Pointy	Round	Absent	Not cat ✗
Floppy	Round	Absent	Not cat ✓
Floppy	Round	Absent	Not cat ✓

$1, 2, \ldots, b-1$

b

XGBoost (eXtreme Gradient Boosting)

- Open source implementation of boosted trees
- Fast efficient implementation
- Good choice of default splitting criteria and criteria for when to stop splitting
- Built in regularization to prevent overfitting
- Highly competitive algorithm for machine learning competitions (eg: Kaggle competitions)

XGBoost is generally better than Random forest.

Using XGBoost

Classification

```
from xgboost import XGBClassifier

model = XGBClassifier()

model.fit(X_train, y_train)
y_pred = model.predict(X_test)
```

Regression

```
from xgboost import XGBRegressor

model = XGBRegressor()

model.fit(X_train, y_train)
y_pred = model.predict(X_test)
```

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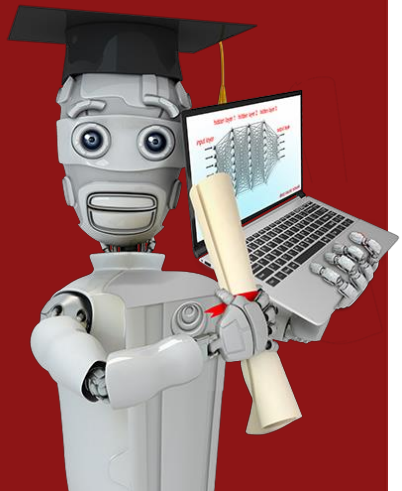

Conclusion

When to use decision trees

Decision Trees vs Neural Networks

Decision Trees and Tree ensembles

- Works well on tabular (structured) data
- Not recommended for unstructured data (images, audio, text)
- Fast
- Small decision trees may be human interpretable

Neural Networks

- Works well on all types of data, including tabular (structured) and unstructured data
- May be slower than a decision tree
- Works with transfer learning
- When building a system of multiple models working together, it might be easier to string together multiple neural networks