Machine Learning 11

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TheMAD

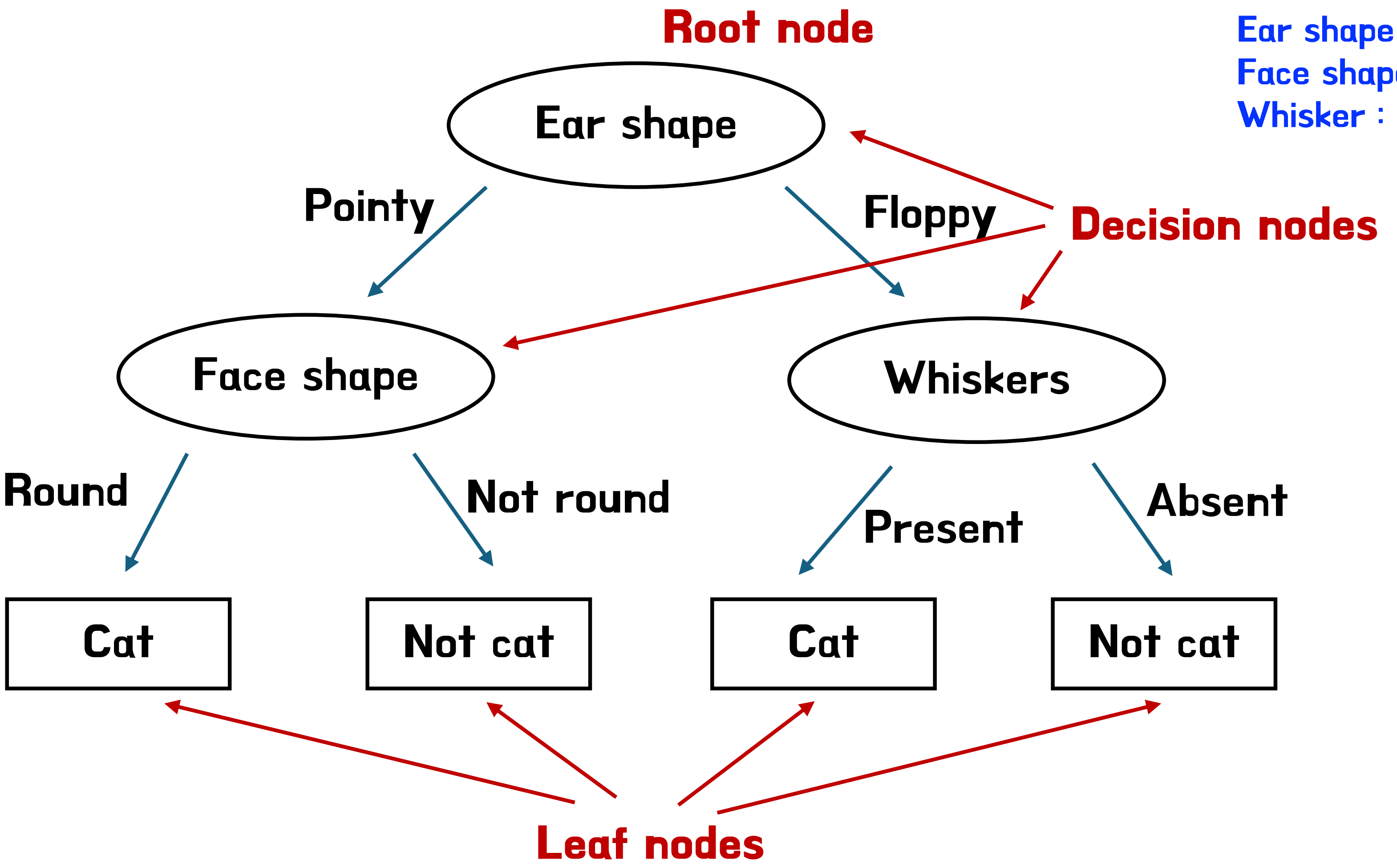
Decision tree

Cat classification example

	Ear shape (x_1)	Face shape (x_2)	Whiskers (x_3)	Cat (y)
	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

Currently, Features are binary

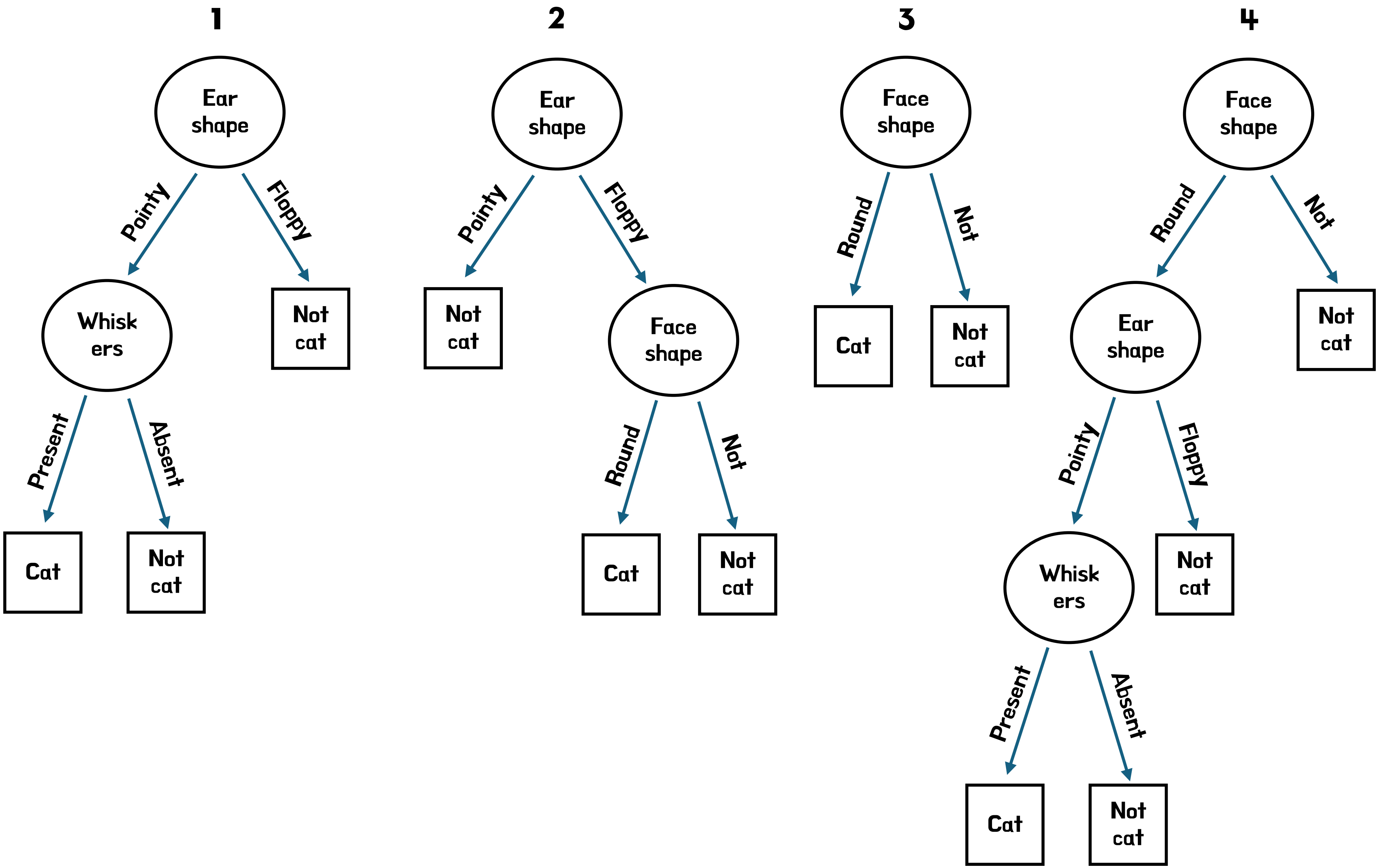
Decision tree



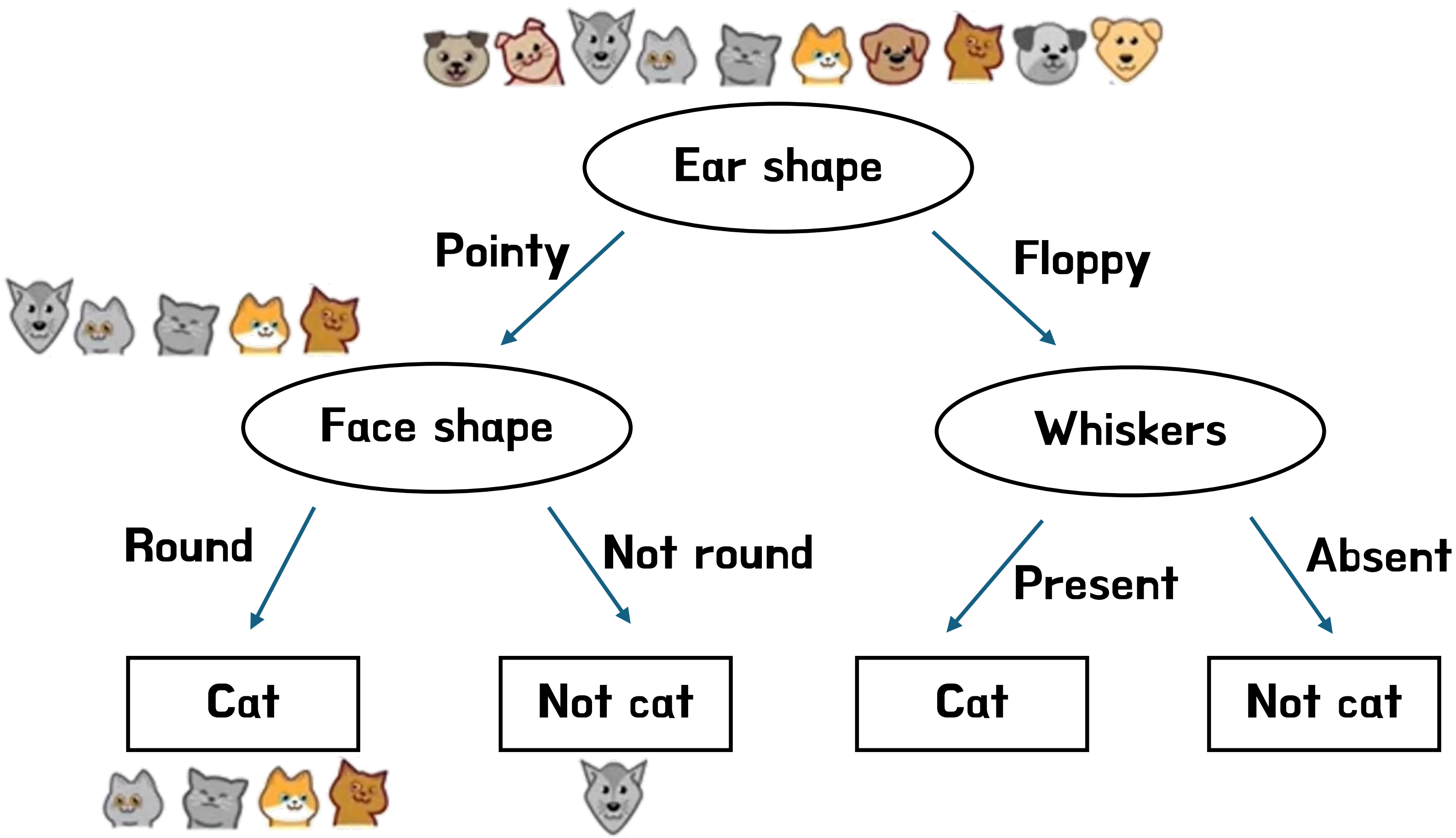
New test examples

Ear shape : Pointy
Face shape : Round
Whisker : Present

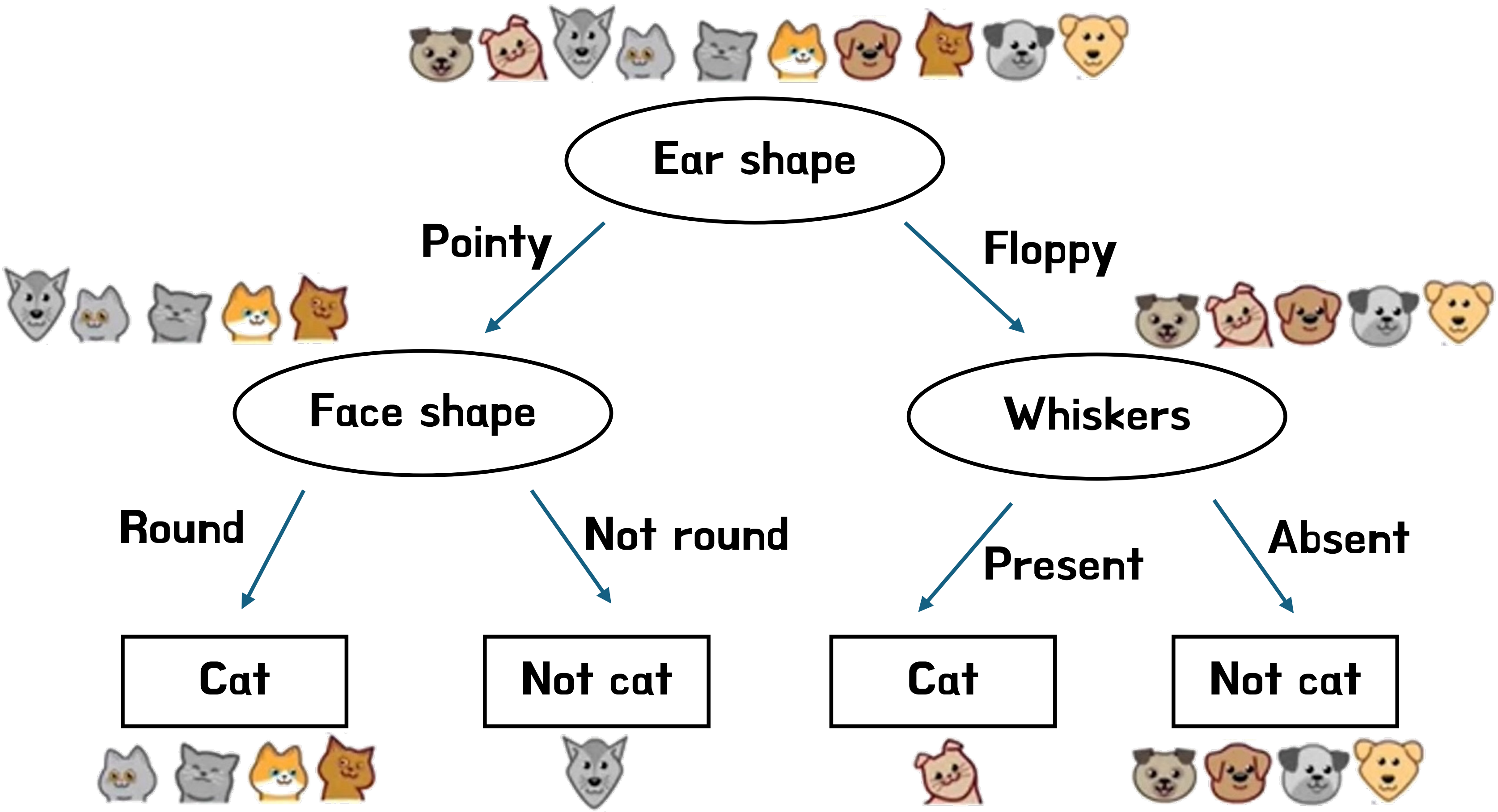
Decision tree



Decision tree learning



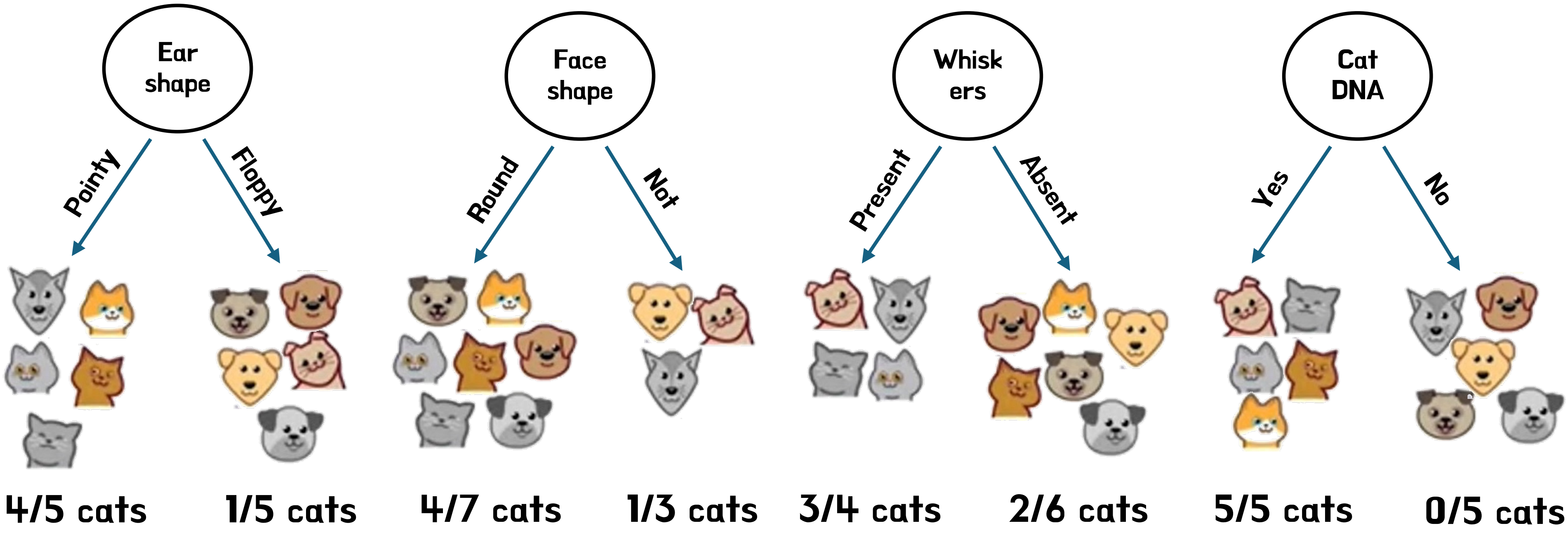
Decision tree learning



Decision tree learning

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

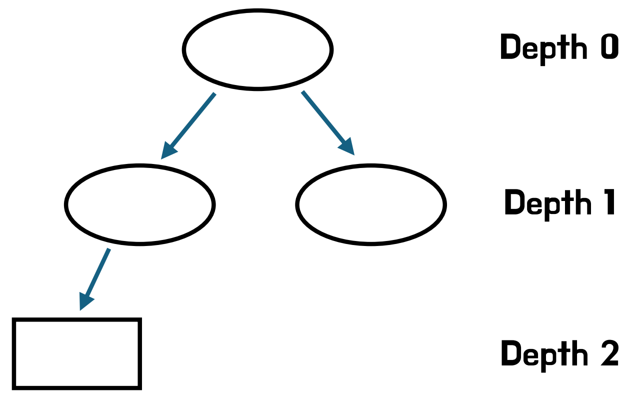
- Maximize purity (or minimize impurity)

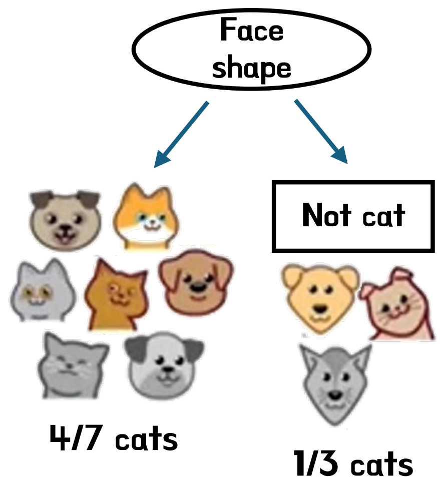


Decision tree learning

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
- When improvements in purity score are below a threshold
- When number of examples in a node is below a threshold





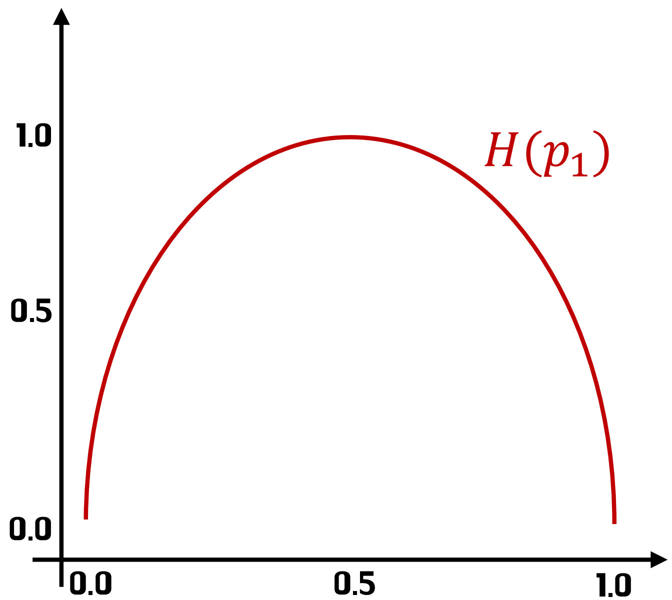
We can chose the depth

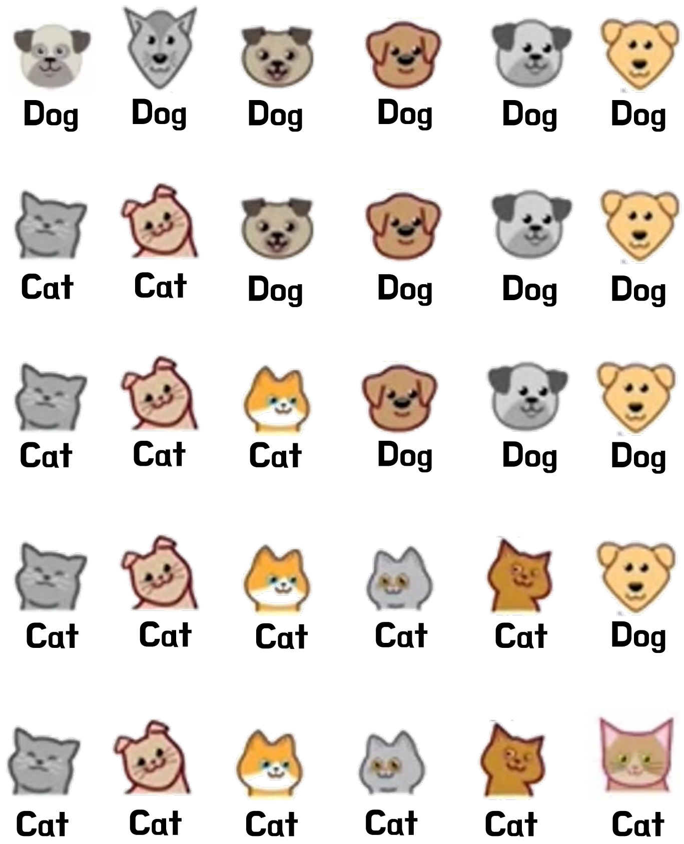
- Too deep: overfitting
- When do we have to stop ?

Decision tree Learning

Entropy as a measure of impurity

p_1 = fraction of examples that are cats





$p_1 = 0 \quad H(p_1) = 0$

$p_1 = 2/6 \quad H(p_1) = 0.92$

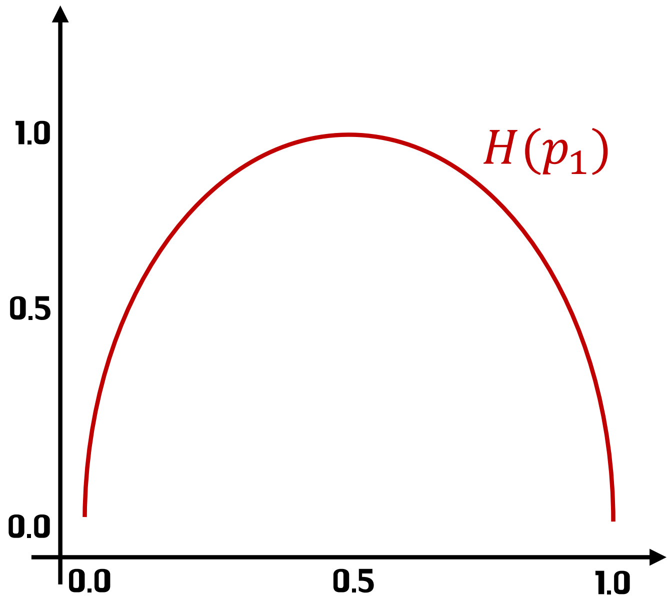
$p_1 = 3/6 \quad H(p_1) = 1$

$p_1 = 5/6 \quad H(p_1) = 0.65$

$p_1 = 6/6 \quad H(p_1) = 0$

Entropy as a measure of impurity

p_1 = fraction of examples that are cats



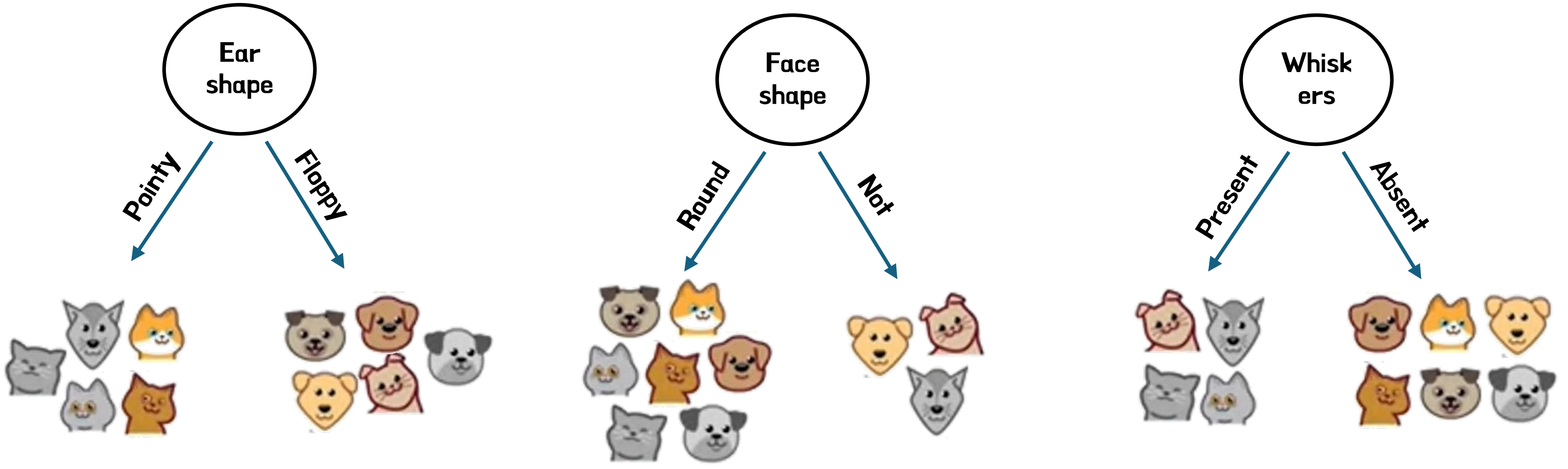
$p_0 = 1 - p_1$
(fraction of example that are not cats)

$$H(p_1) = -p_1 \log_2(p_1) - p_0 \log_2(p_0)$$
$$= -p_1 \log_2(p_1) - (1 - p_1) \log_2(1 - p_1)$$

***Note**: $0 \log_2(0) = 0$

Choosing a split

Root node: $p_1 = \frac{5}{10} = 0.5 \quad H(0.5) = 1$



$p_1 = 4/5 = 0.8$ | $p_1 = 1/5 = 0.2$ | $p_1 = 4/7 = 0.57$ | $p_1 = 1/3 = 0.33$ | $p_1 = 3/4 = 0.75$ | $p_1 = 2/6 = 0.33$

$H(0.8) = 0.72$ | $H(0.2) = 0.72$ | $H(0.57) = 0.99$ | $H(0.33) = 0.92$ | $H(0.75) = 0.81$ | $H(0.33) = 0.92$

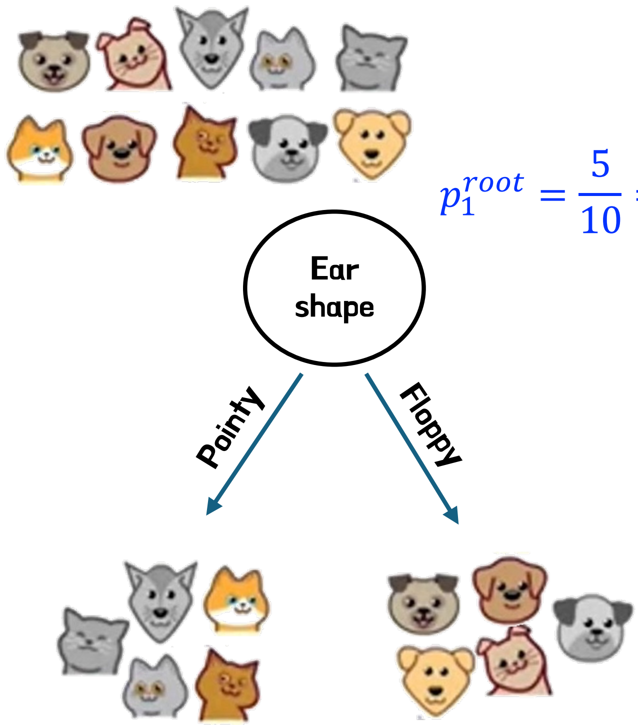
$$H(0.5) - (\frac{5}{10}H(0.8) + \frac{5}{10}H(0.2)) = 0.28$$

$$H(0.5) - (\frac{7}{10}H(0.57) + \frac{3}{10}H(0.33)) = 0.03$$

$$H(0.5) - (\frac{4}{10}H(0.75) + \frac{6}{10}H(0.33)) = 0.12$$

Entropy reduction (weighted average) = Information gain

Information gain



$p_1^{root} = \frac{5}{10} = 0.5$

$p_1^{left} = 4/5$

$w^{left} = 5/10$

$p_1^{right} = 1/5$

$w^{left} = 5/10$

Information gain

(or entropy reduction)

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

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

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

Features are not binary (three possible values)

One hot encoding

	~~Ear shape (x_1)~~	Pointy ears	Floppy ears	Oval ears	Face shape (x_2)	Whiskers (x_3)	Cat (y)
	~~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

Features are not binary (three 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 and neural networks

	~~Ear shape (x_1)~~	Pointy ears	Floppy ears	Oval ears	Face shape (x_2)	Whiskers (x_3)	Cat (y)
	~~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

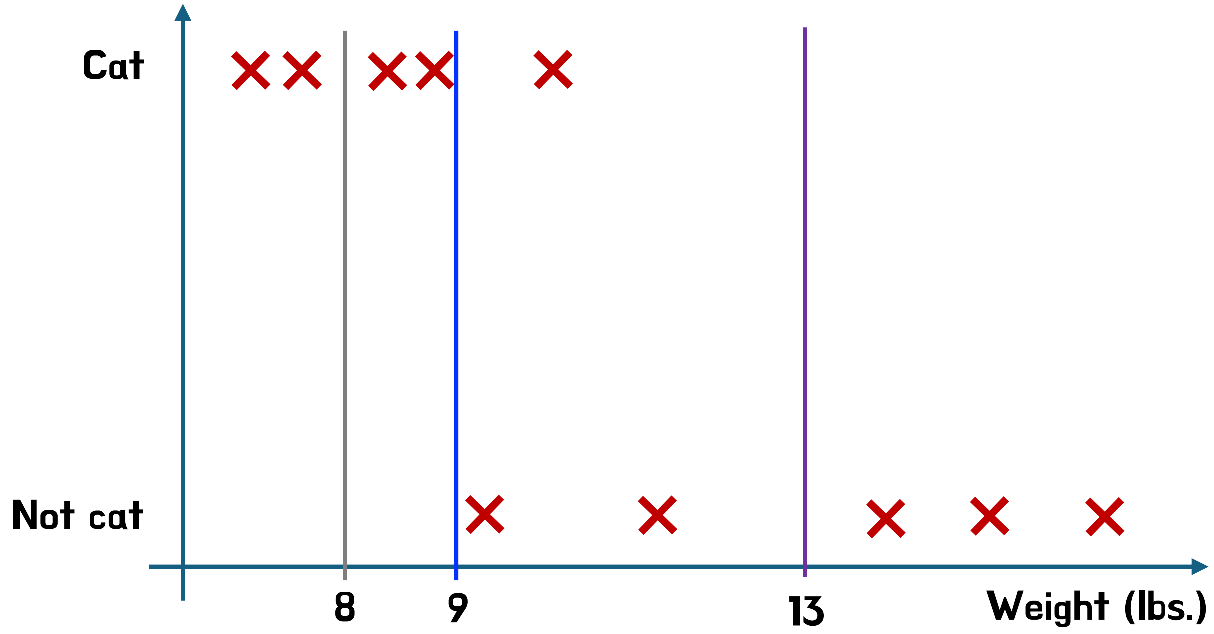
One hot encoding and neural networks

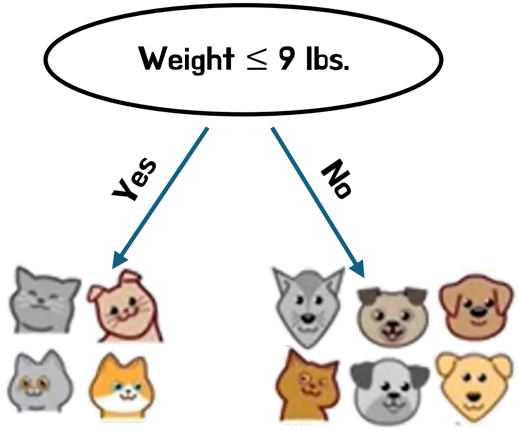
	Pointy ears	Floppy ears	Oval ears	Face shape (x_2)	Whiskers (x_3)	Cat (y)
	1	0	0	1	1	1
	0	0	1	0	1	1
	0	0	1	1	0	0
	1	0	0	0	1	0
	0	0	1	1	1	1
	1	0	0	1	0	1
	0	1	0	0	0	0
	0	0	1	1	0	1
	0	1	0	1	0	0
	0	1	0	1	0	0

Continuous features

	Ear shape (x_1)	Face shape (x_2)	Whiskers (x_3)	Weight (lbs.)	Cat (y)
	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





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

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

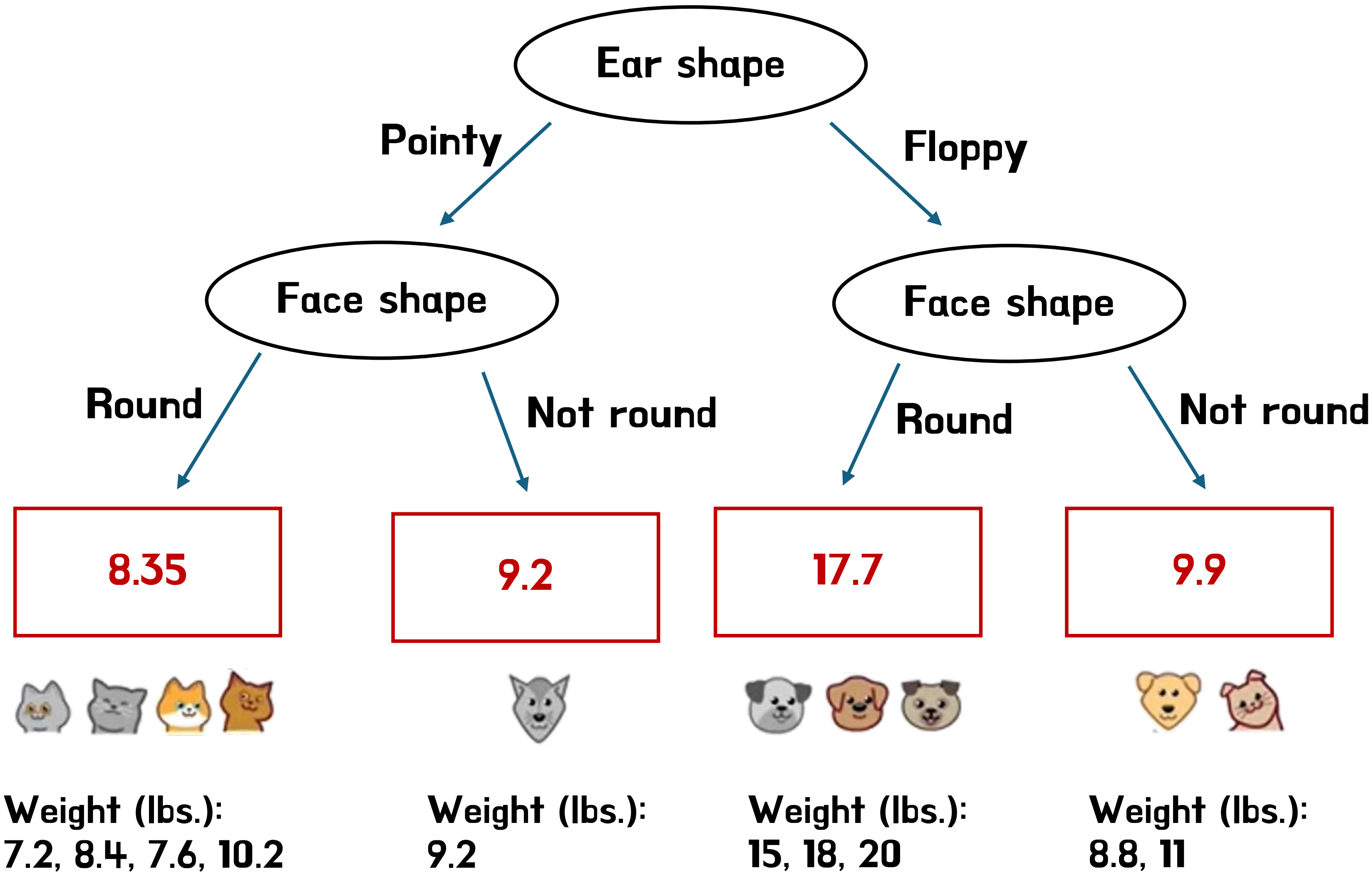
$$H(0.5) - \left(\frac{7}{10}H\left(\frac{5}{7}\right) + \frac{3}{10}H\left(\frac{0}{3}\right)\right) = 0.40$$

Regression with decision trees

	Ear shape (x_1)	Face shape (x_2)	Whiskers (x_3)	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

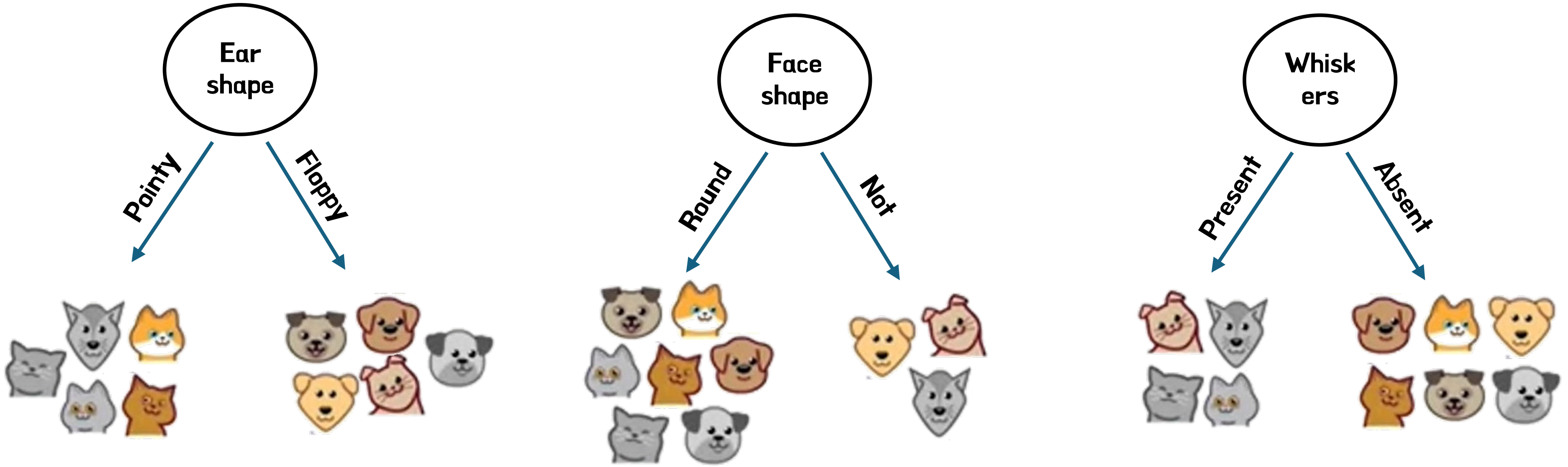
x y

Regression with decision trees



Choosing a split

Variance at root node: 20.51



Ear shape: Pointy	Ear shape: Floppy	Face shape: Round	Face shape: Not	Whiskers: Present	Whiskers: Absent
Weights: 7.2, 9.2, 8.4, 7.6, 10.2	Weights: 8.8, 15, 11, 18, 20	Weights: 7.2, 15, 8.4, 7.6, 10.2, 18, 20	Weights: 8.8, 9.2, 11	Weights: 7.2, 8.8, 9.2, 8.4	Weights: 15, 7.6, 11, 10.2, 18, 20
Variance: 1.47	Variance: 21.87	Variance: 27.80	Variance: 1.37	Variance: 0.75	Variance: 23.32
$w^{left} = 5/10$	$w^{right} = 5/10$	$w^{left} = 7/10$	$w^{right} = 3/10$	$w^{left} = 4/10$	$w^{right} = 6/10$

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

$$= 8.84$$

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

$$= 0.64$$

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

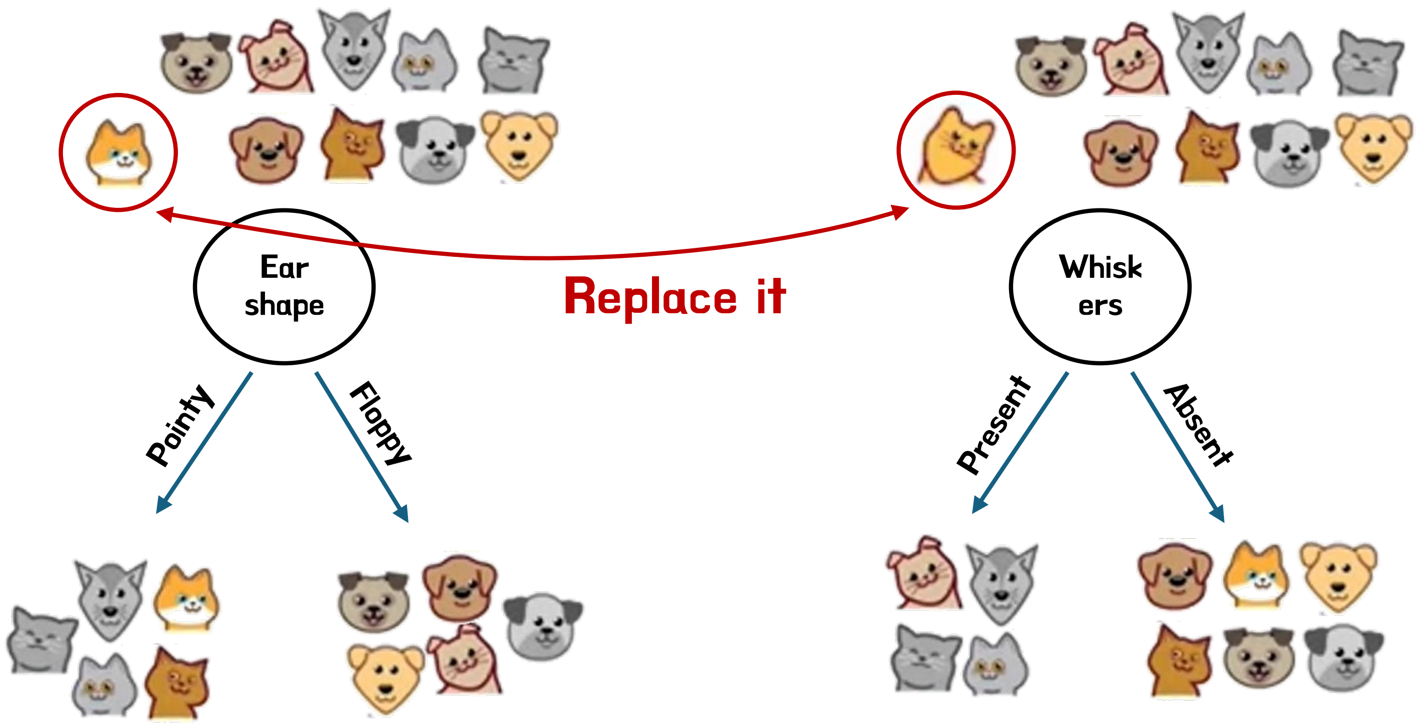
$$= 6.22$$

Variance reduction = Information gain

Tree ensembles

Tree ensemble

Highly sensitive to small changes of the data

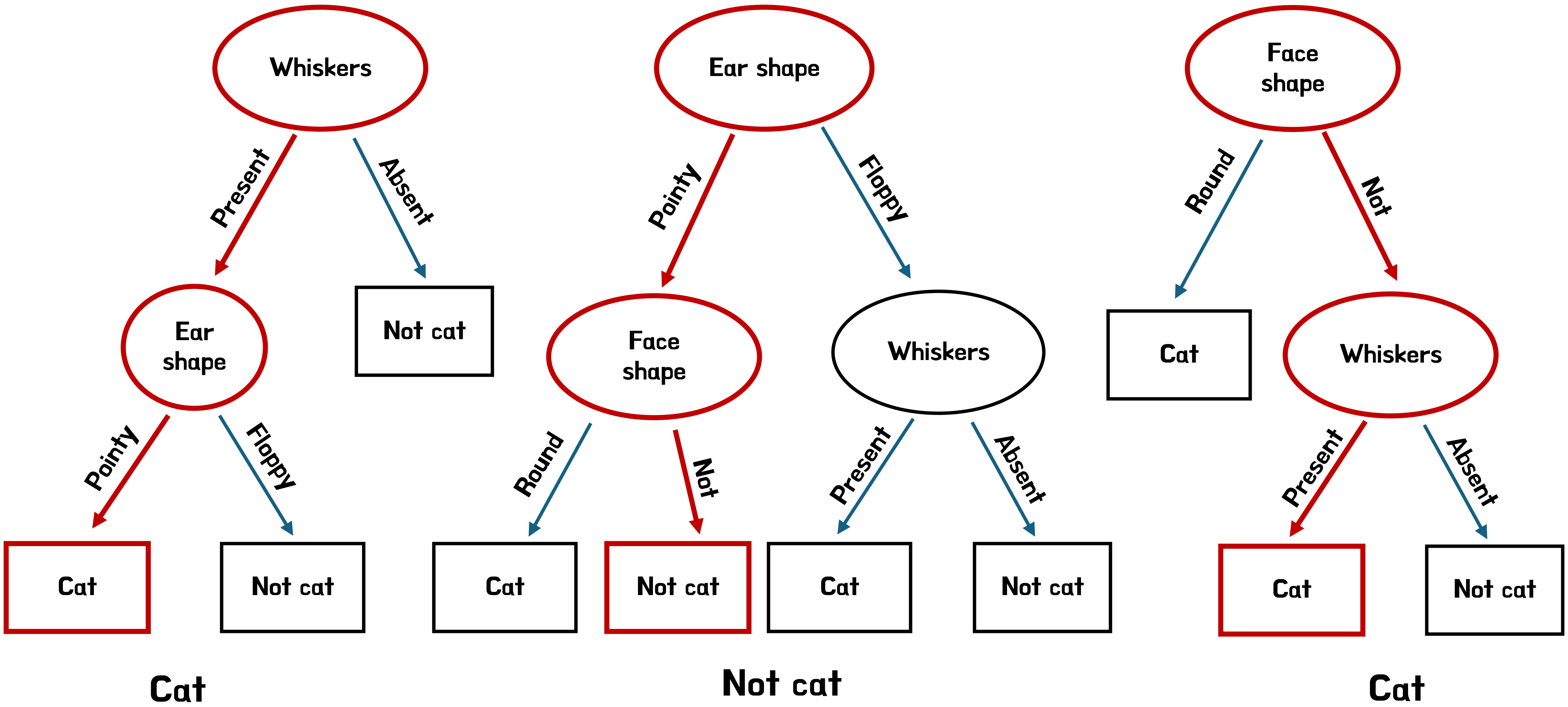


Single data change → change of optimal tree

Using collections of tree will be better

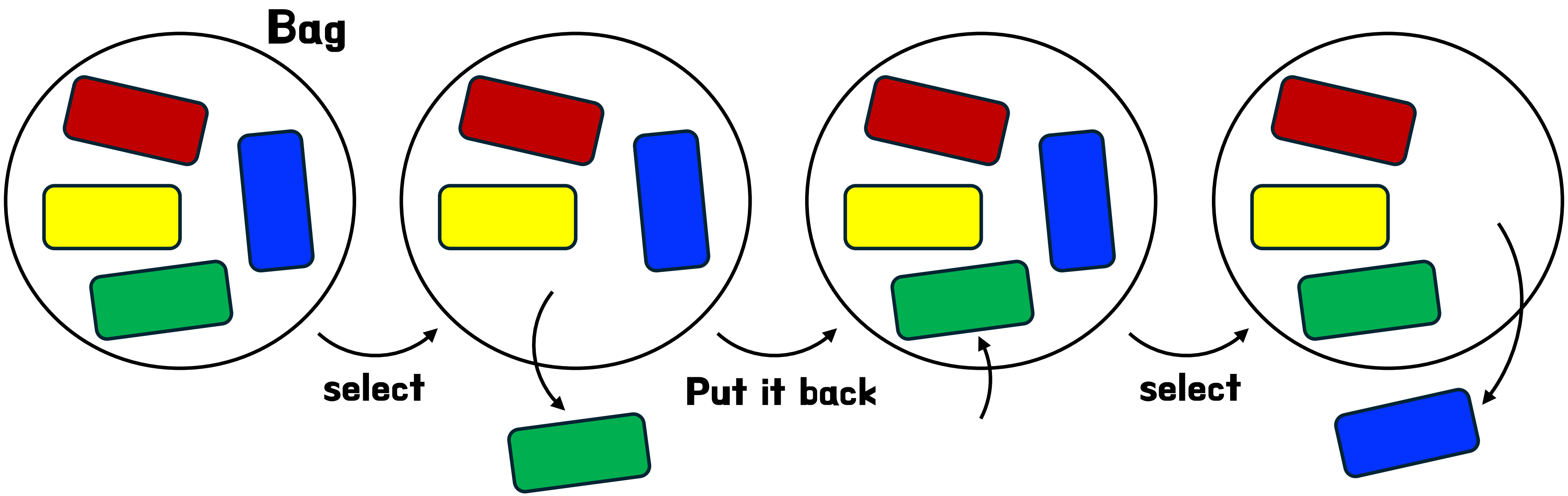
Tree ensemble

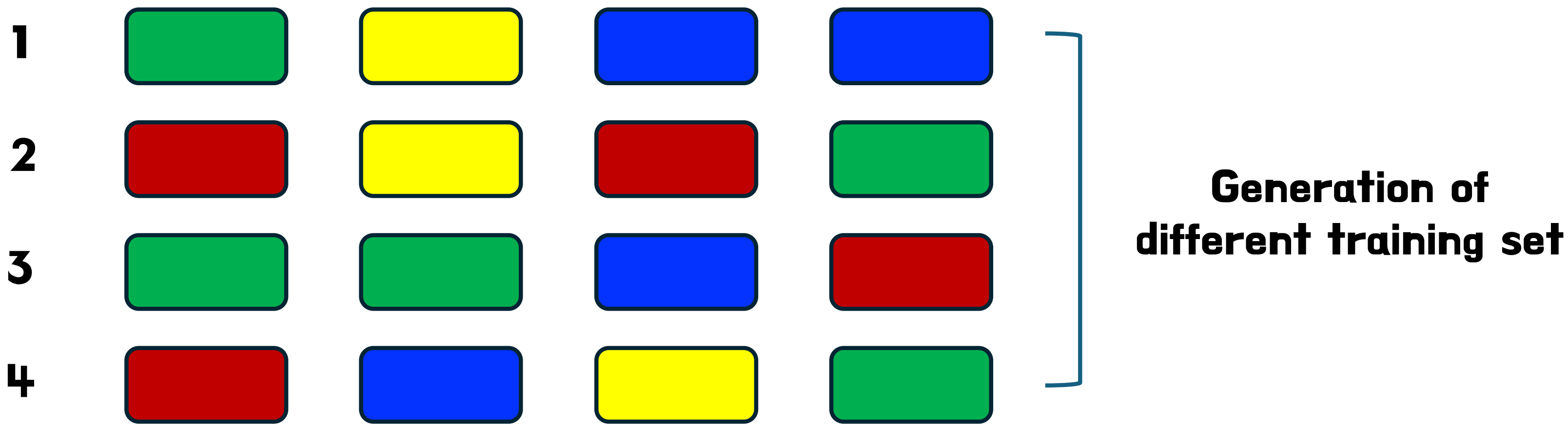
New test example
Ear shape: Pointy
Face shape : not round
Whisker : present



Prediction based on voting

Sampling with replacement





Sampling with replacement

Bag

	Ear shape (x_1)	Face shape (x_2)	Whiskers (x_3)	Cat (y)
	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

Random forest: generating a tree sample

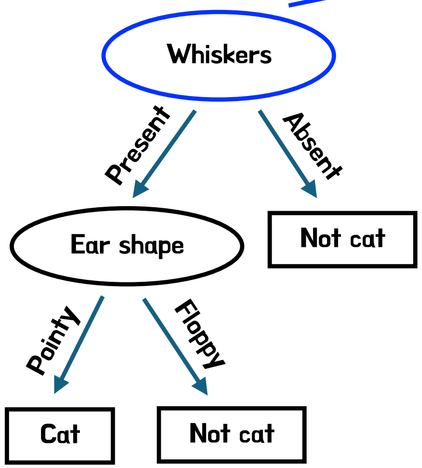
Given training set of size m

For $b = 1$ to B (*usually* 100)

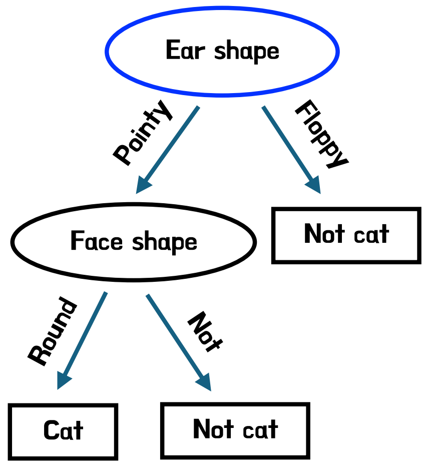
- **Use sampling with replacement to create a new training set of size m**
- **Train a decision tree on the new dataset**

Usually, root node is identical

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



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



Random forest: random 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.

$$k = \sqrt{n}$$

Boosted trees intuition

Given training set of size m

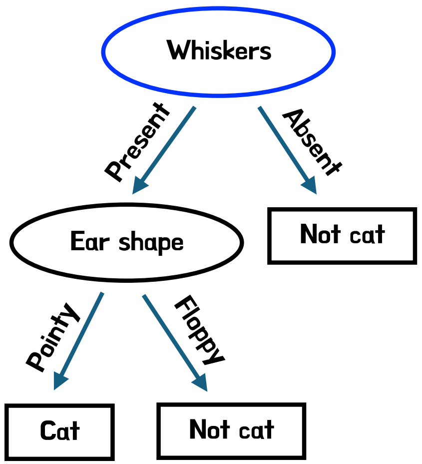
For $b = 1$ to B

- **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 misclassified examples from previous trained trees

- **Train a decision tree on the new dataset**

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



Ear shape (x_1)	Face shape (x_2)	Whiskers (x_3)	Prediction	
Pointy	Round	Present	Cat	O
Floppy	Not round	Absent	Cat	X
Pointy	Round	Absent	Not cat	O
Pointy	Not round	Present	Not cat	O
Floppy	Not round	Present	Cat	O
Pointy	Round	Absent	Cat	X
Pointy	Round	Present	Cat	O
Floppy	Not round	Absent	Cat	X
Floppy	Round	Absent	Not cat	O
Pointy	Round	Present	Cat	O

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 (e. g. Kaggle competitions)

Deep learning as well

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)

Simple to use

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 tress 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 multiple neural networks