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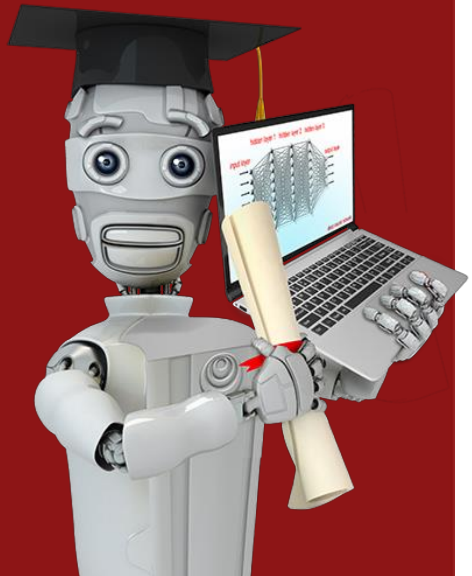


## Decision Trees

# Decision Tree Model

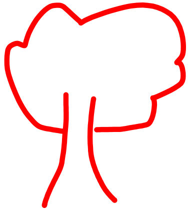
# Cat classification example

| 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 |

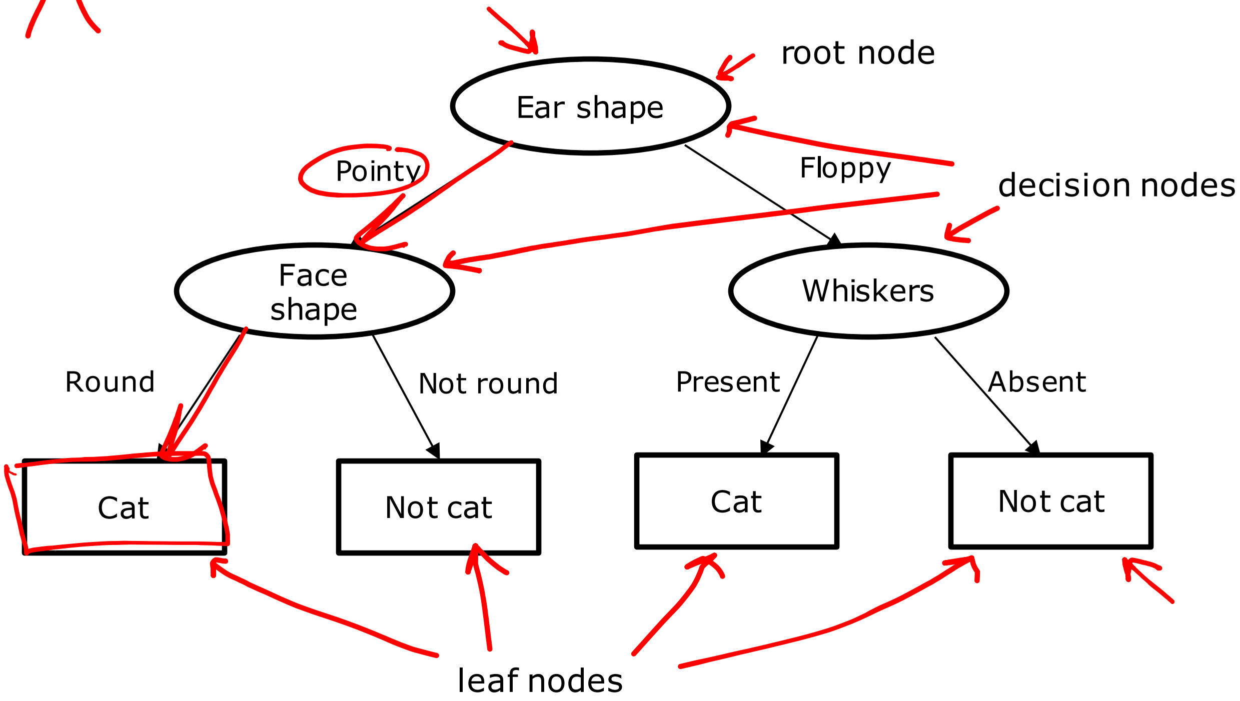
Categorical (discrete values)

X

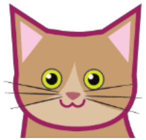
y



# Decision Tree

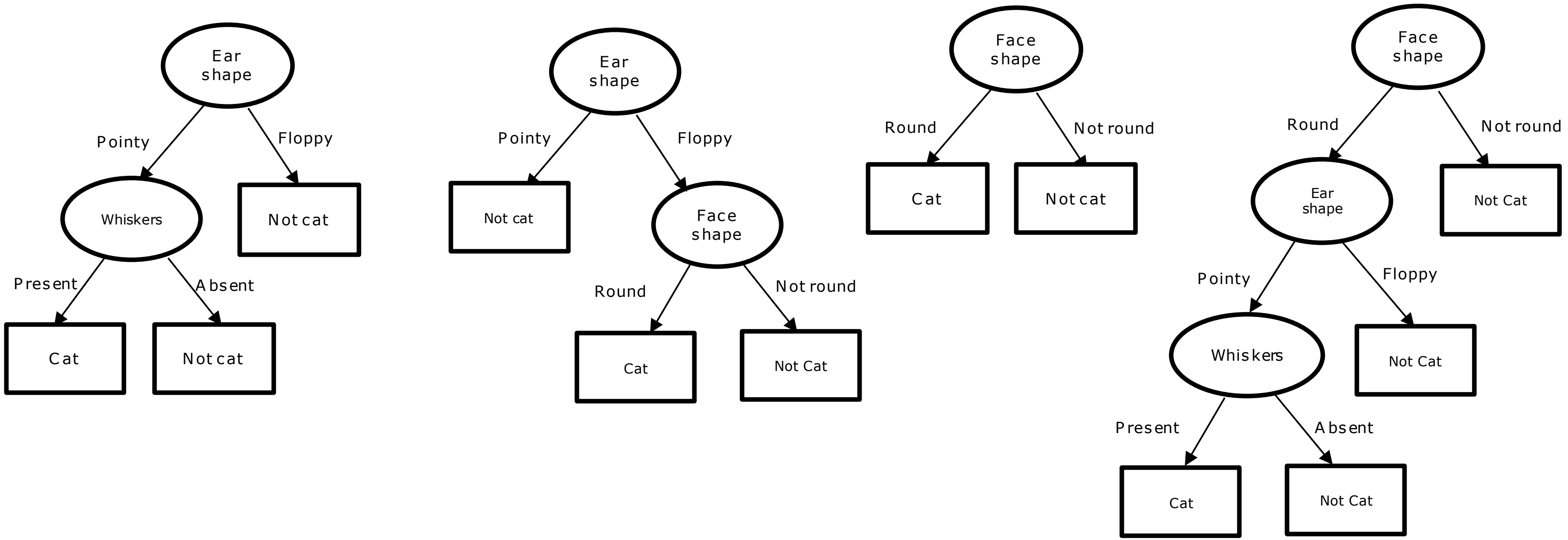



New test example



Ear shape: Pointy
Face shape: Round
Whiskers: Present

# Decision Tree



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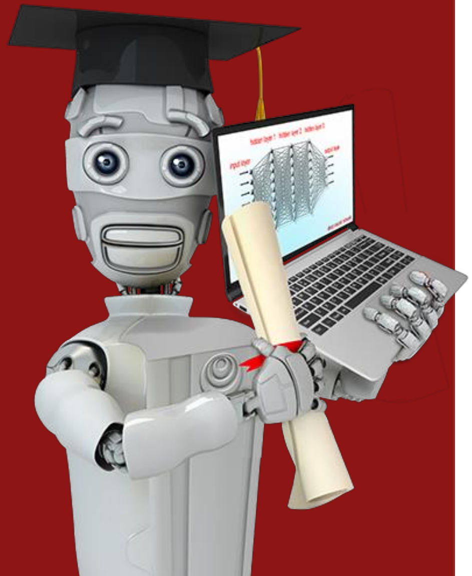


# Decision Trees

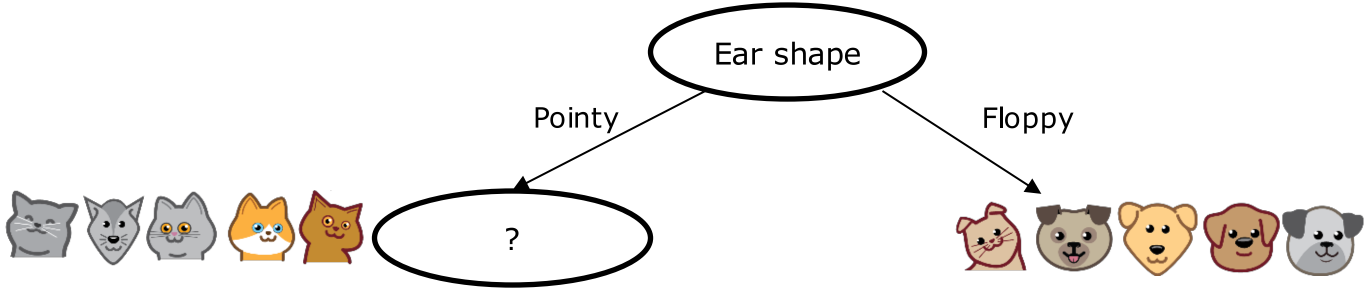
# Learning Process

# Decision Tree Learning

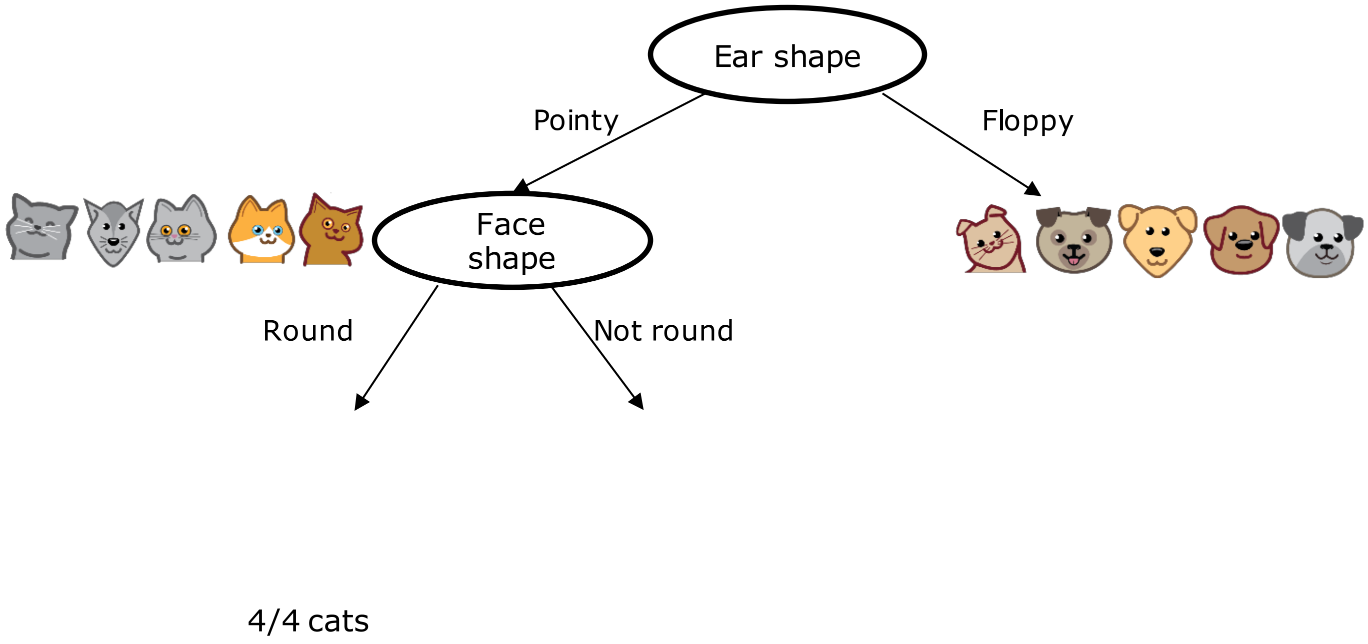
# Decision Tree Learning

# Decision Tree Learning

# Decision Tree Learning



# Decision Tree Learning



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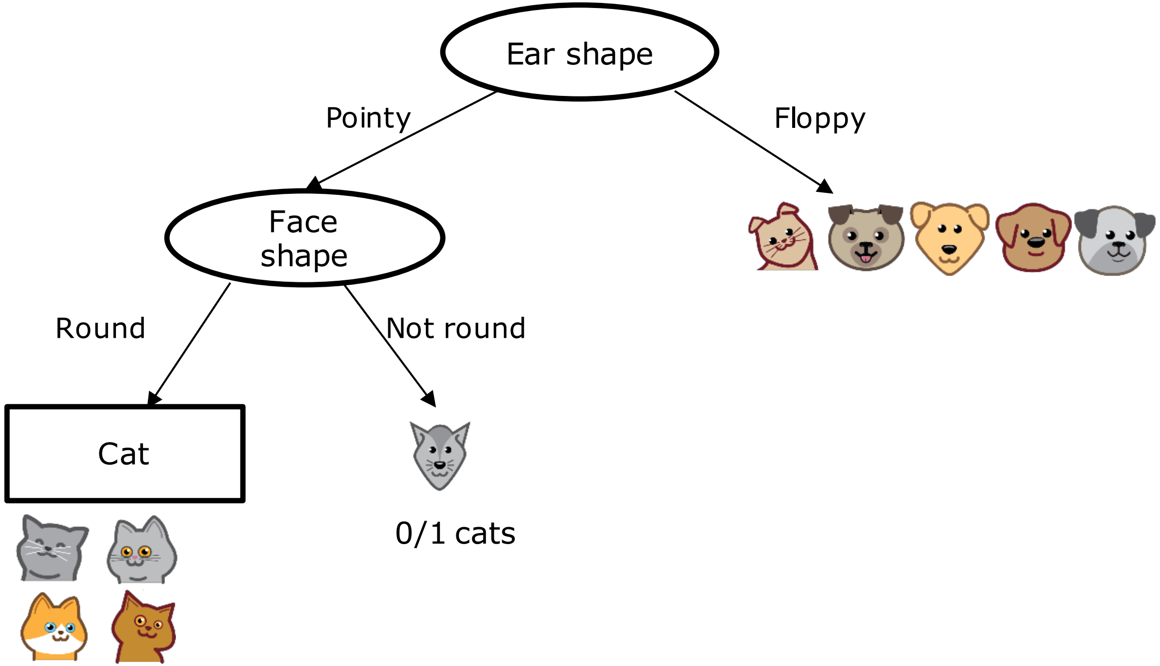

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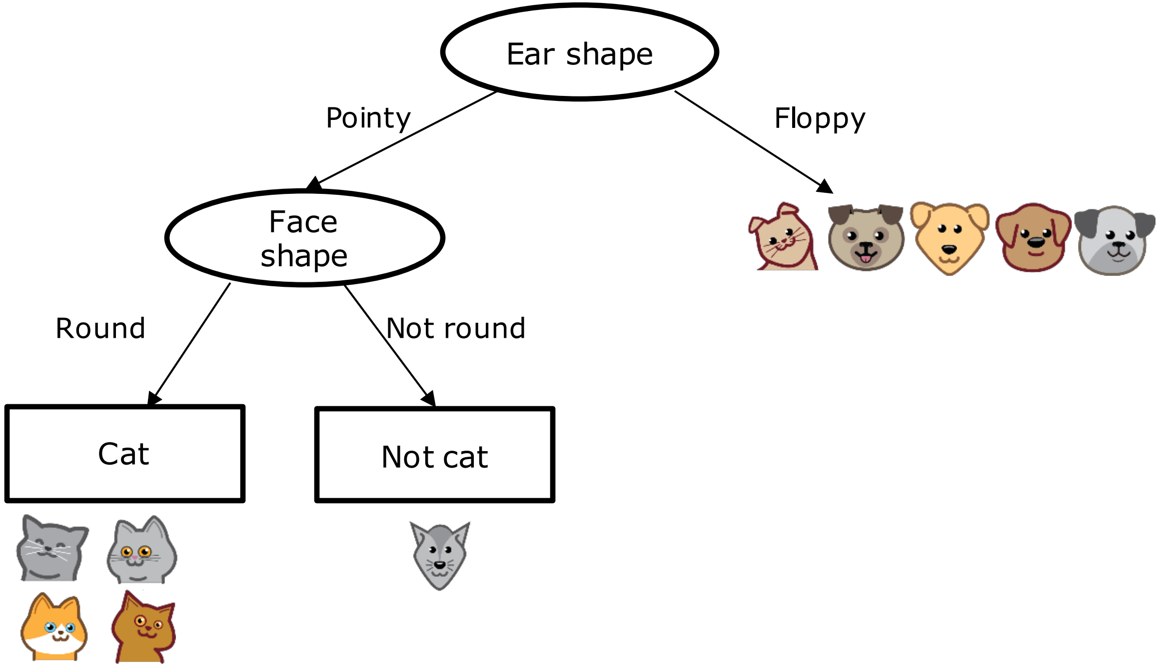

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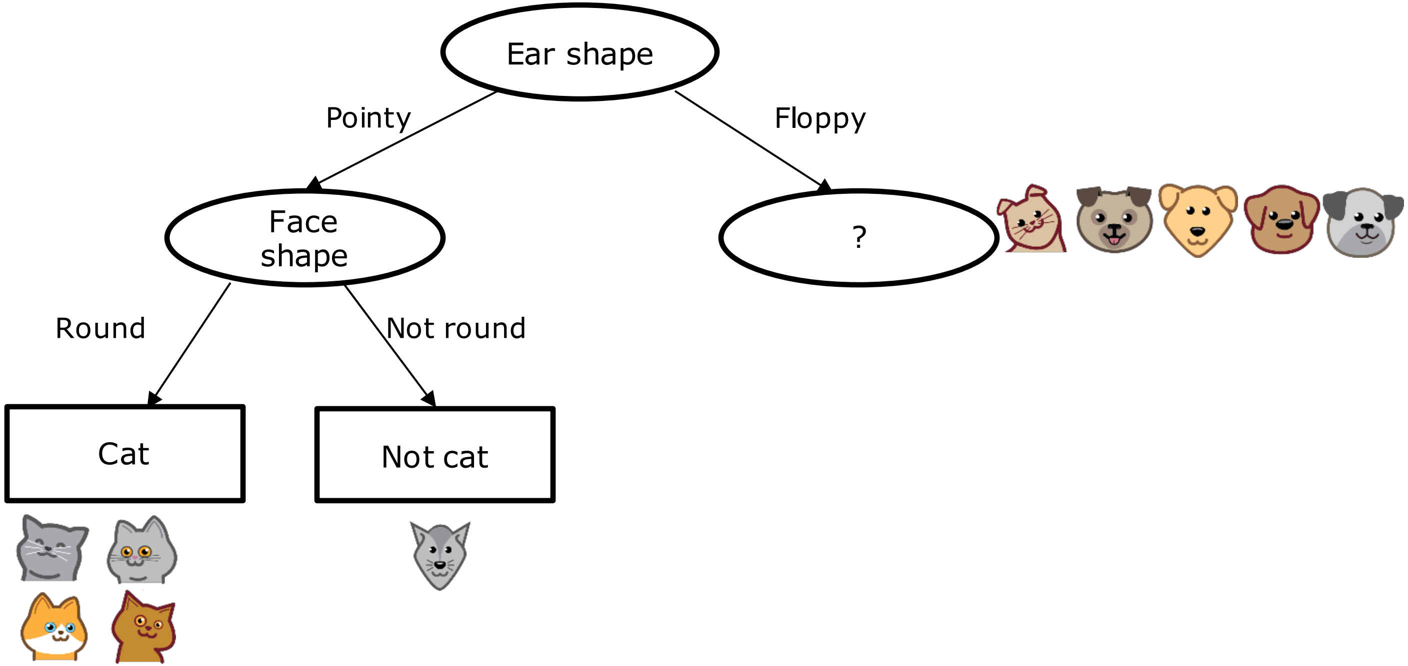
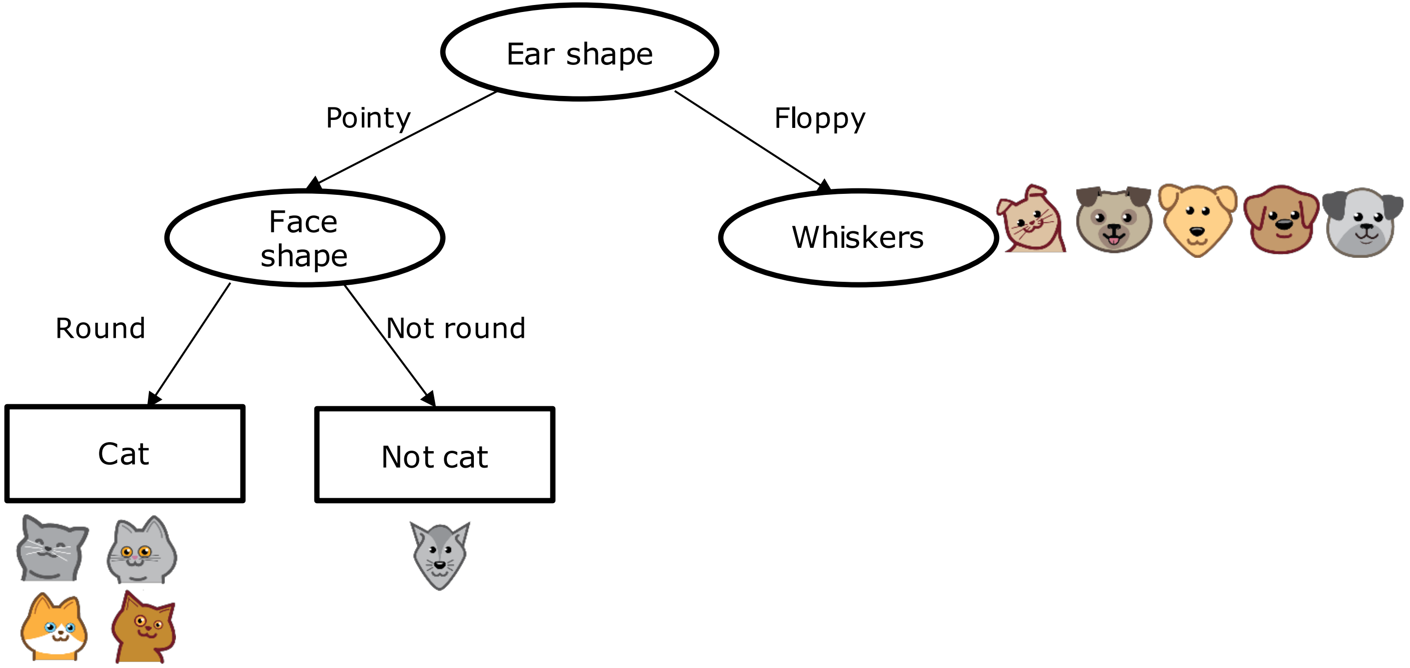


# Decision Tree Learning



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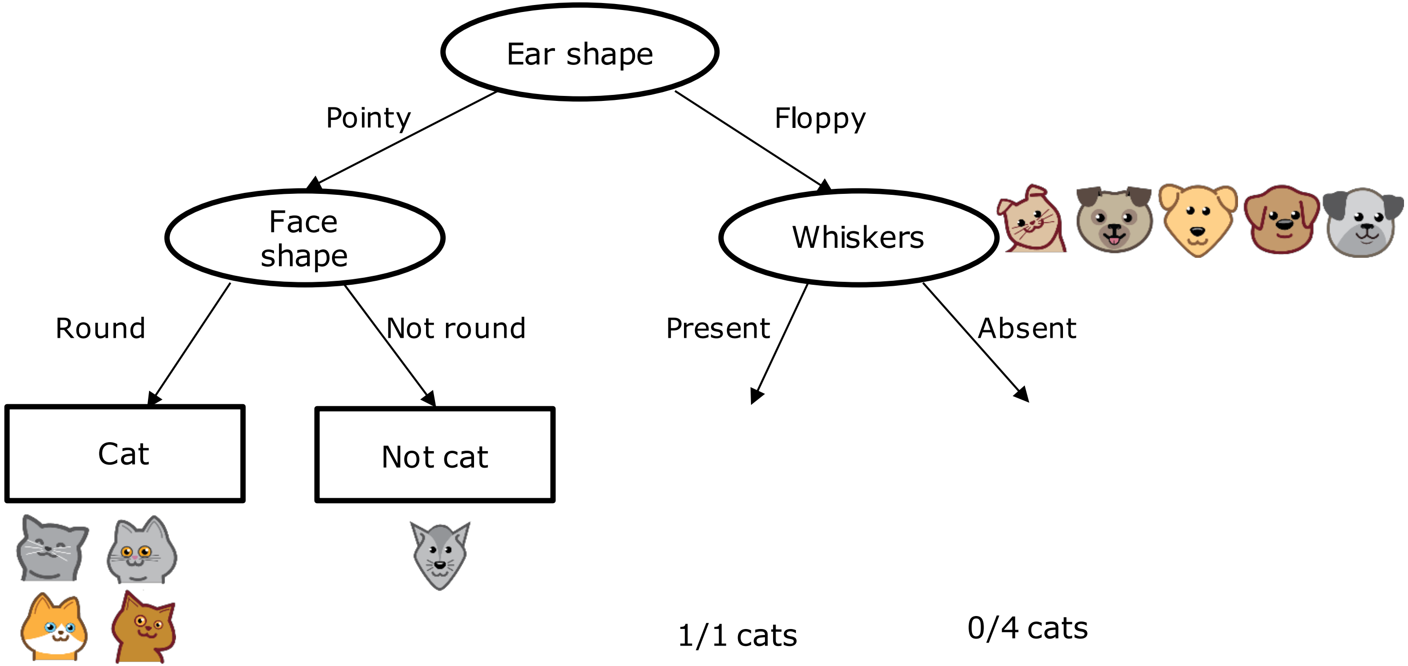
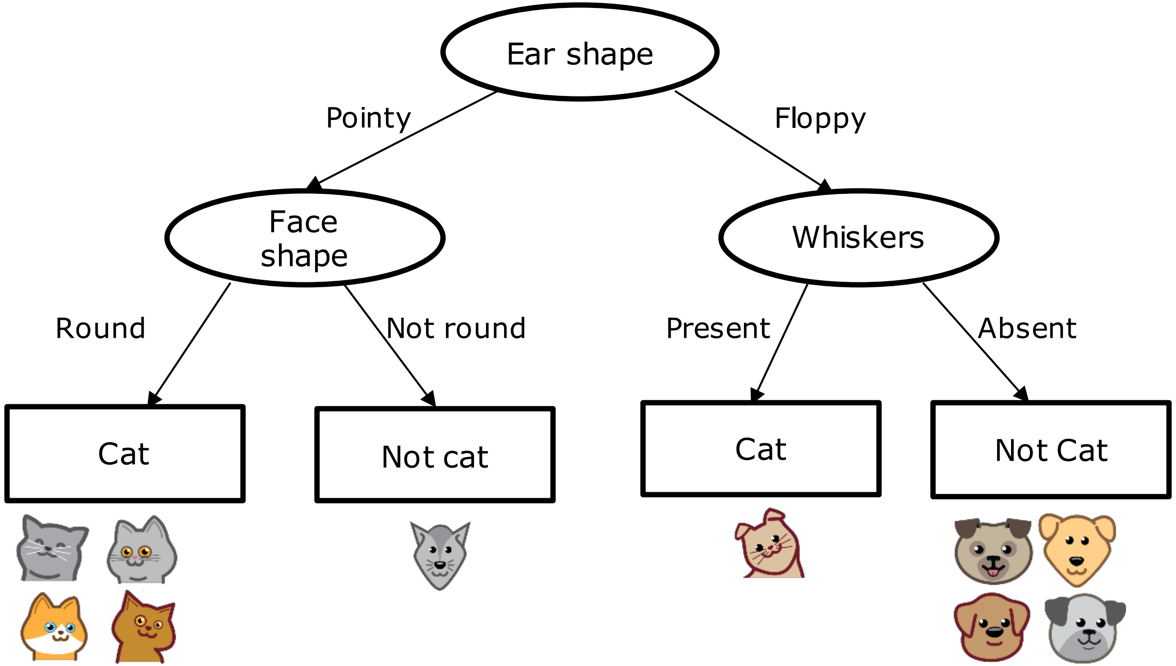


# Decision Tree Learning



# Decision Tree Learning

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

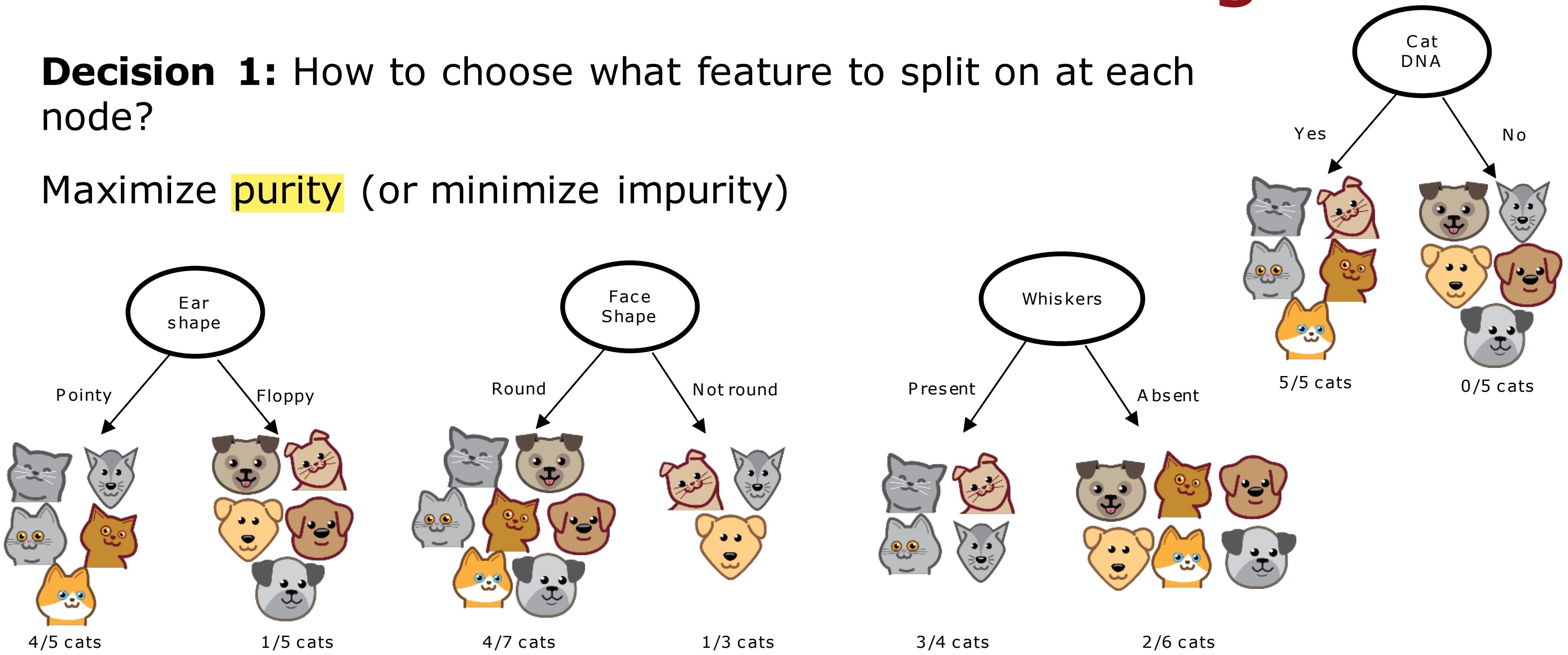
?

Maximize purity (or minimize impurity)

# Decision Tree Learning

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

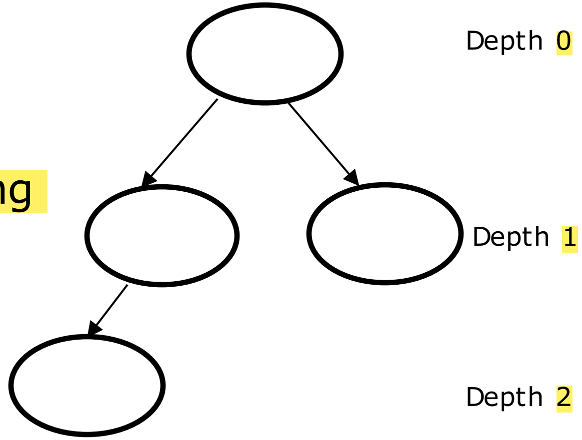
Maximize purity (or minimize impurity)



# 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



# Decision Tree Learning

**Decision 2:** When do you stop splitting?

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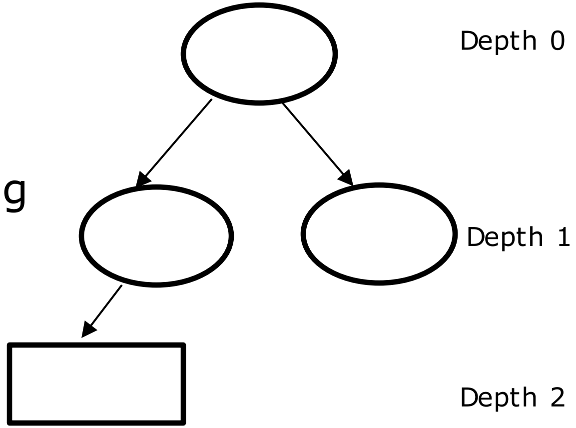
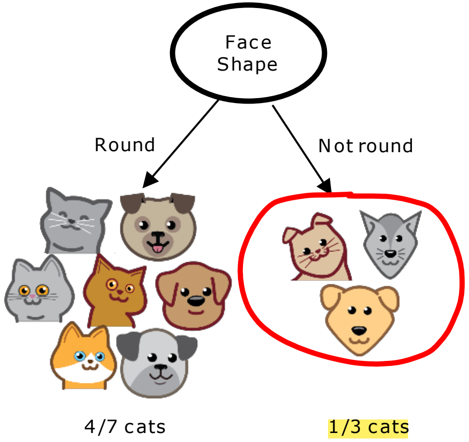


# Decision Tree Learning

**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



# Decision Tree Learning

**Decision 2:** When do you stop splitting?

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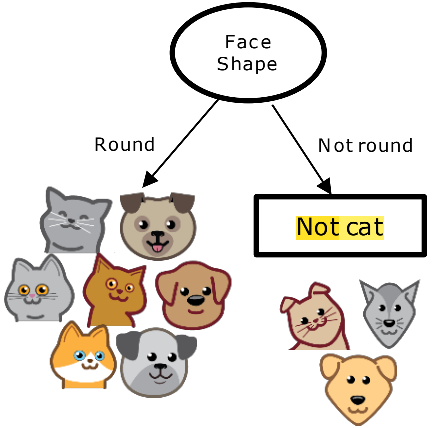

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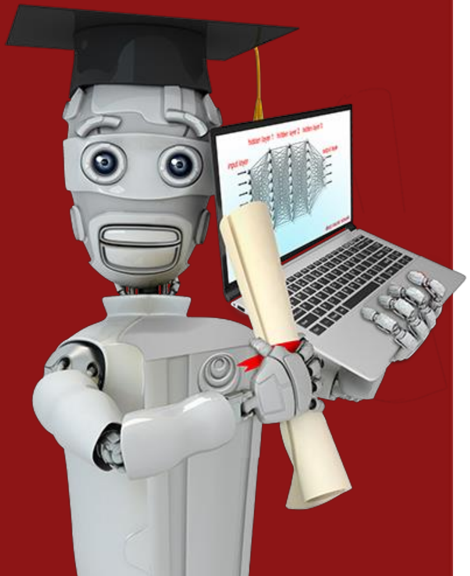
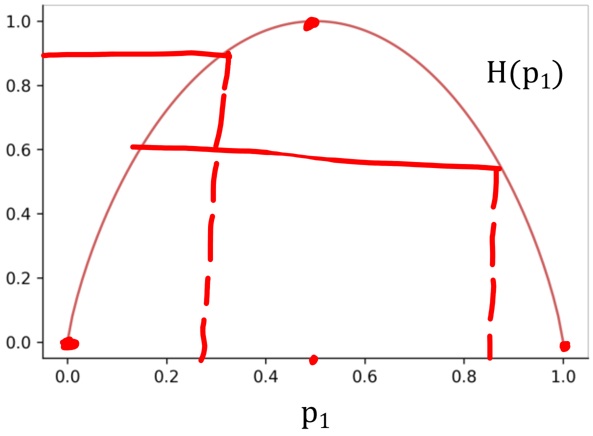


## Decision Tree Learning

# Measuring purity

# Entropy as a measure of impurity

$p_1 =$ fraction of examples that are cats





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

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

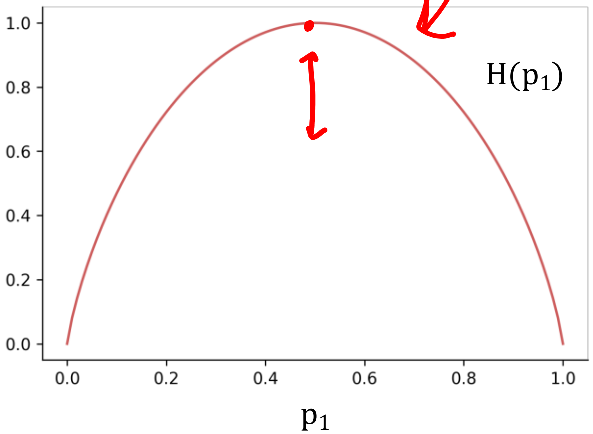
$p_1 = 3/6 \quad H(p_1) = 1$

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

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

# Entropy as a measure of impurity

$p_1 =$ fraction of examples that are cats




$$p_0 = 1 - p_1$$

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

Note: "$0 \log(0)$" $= 0$

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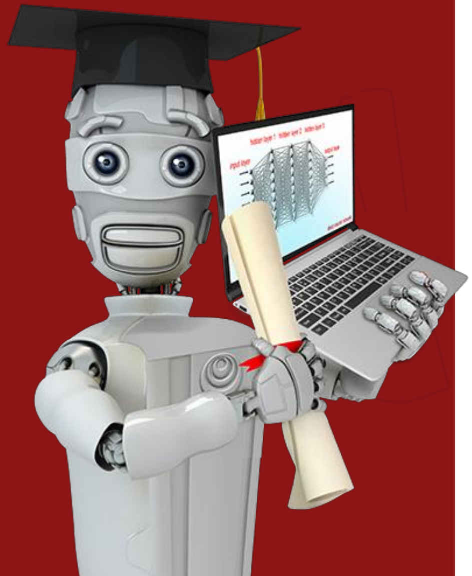


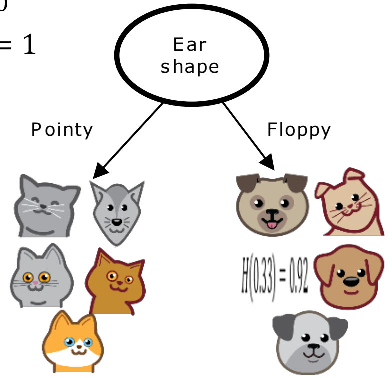
# Decision Tree Learning

## Choosing a split: Information Gain

# Choosing a split

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

$H(0.5) = 1$



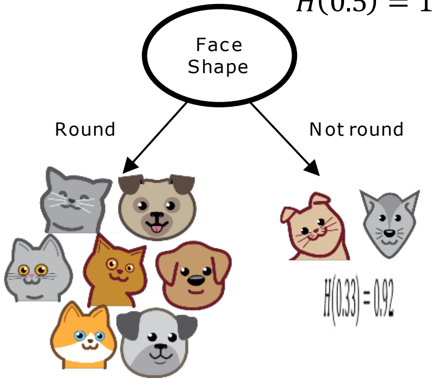

$p_1 = {}^{4}/_{5} = 0.8$ $\quad p_1 = {}^{1}/_{5} = 0.2$

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

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

$= 0.28$

$H(0.5) = 1$



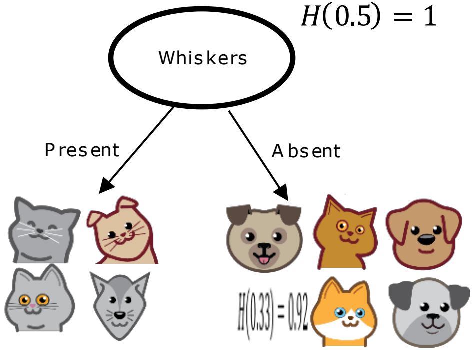

$p_1 = {}^{4}/_{7} = 0.57$ $\quad p_1 = {}^{1}/_{3} = 0.33$

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

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

$= 0.03$

$H(0.5) = 1$




$p_1 = {}^{3}/_{4} = 0.75$ $\quad p_1 = {}^{2}/_{6} = 0.33$

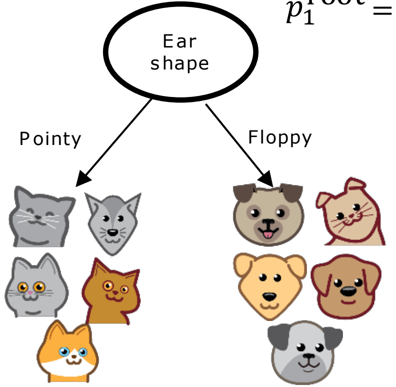
$H(0.75) = 0.81$ $\quad H(0.33) = 0.92$

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

$= 0.12$

# Information Gain

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

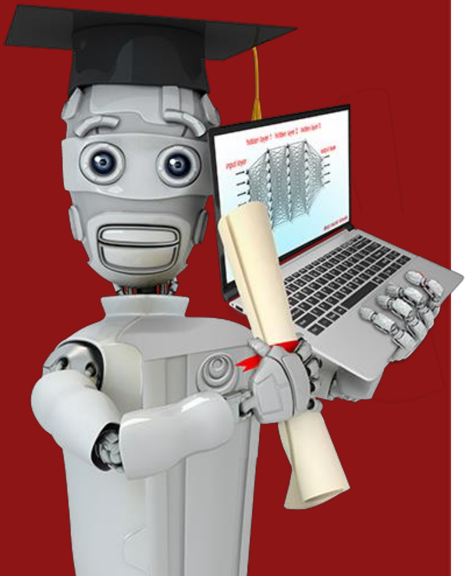



$p_1^{\text{left}} = 4/5$ $\qquad$ $p_1^{\text{right}} = 1/5$

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

## Information gain

$$= \mathrm{H}(\mathrm{p}_1^{\text{root}}) - \left(w^{\text{left}} H\left(p_1^{\text{left}}\right) + w^{\text{right}} H\left(p_1^{\text{right}}\right)\right)$$



# 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

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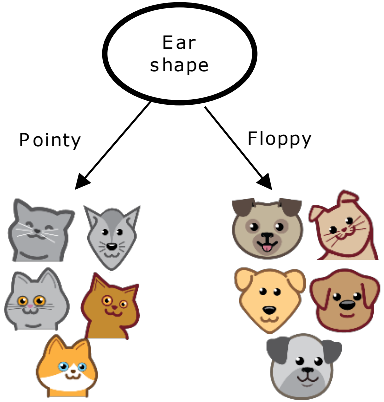
# Recursive splitting



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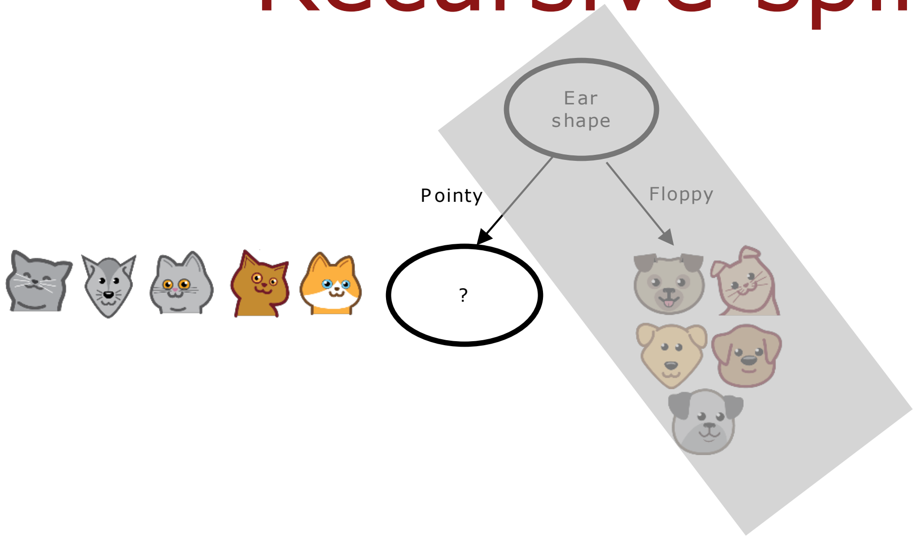

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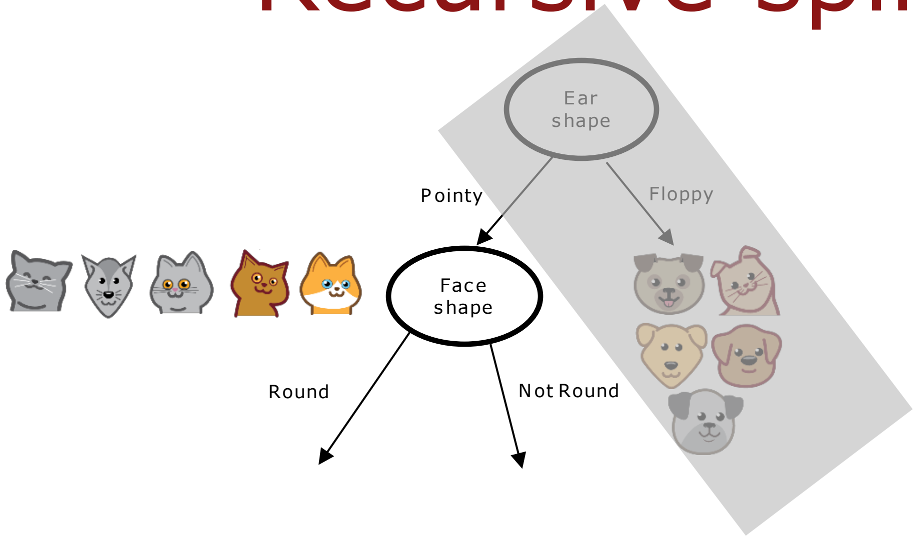
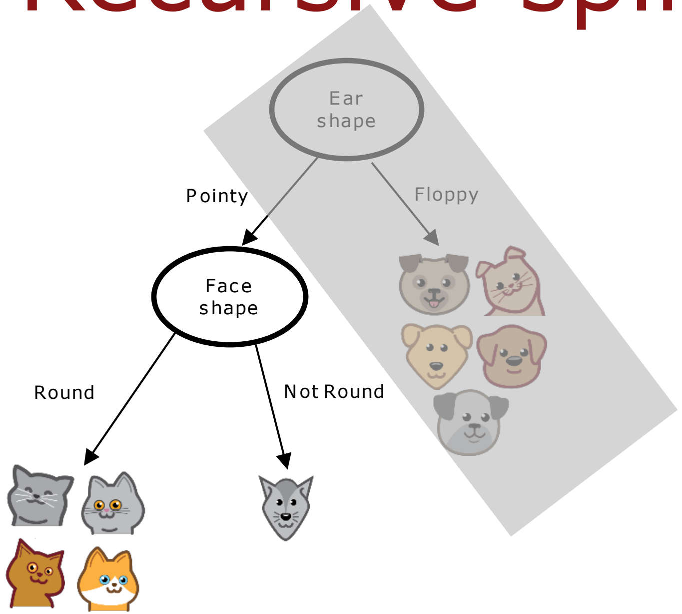


# Recursive splitting



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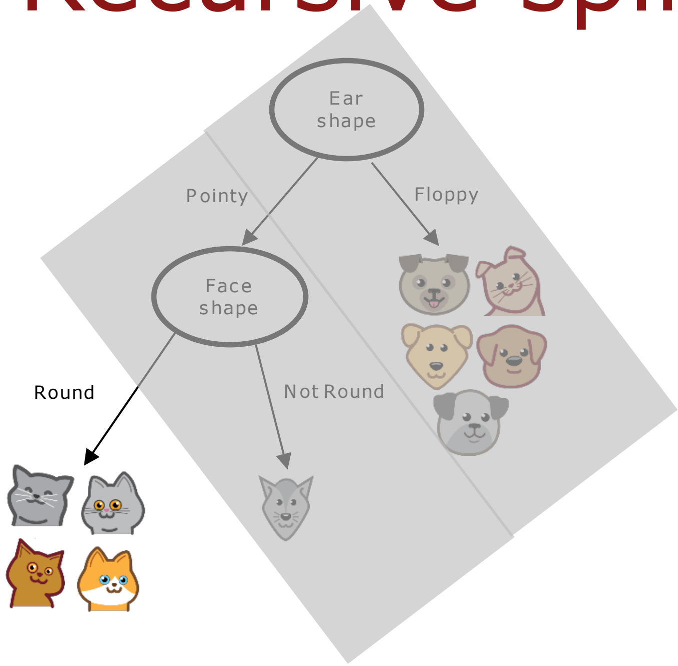

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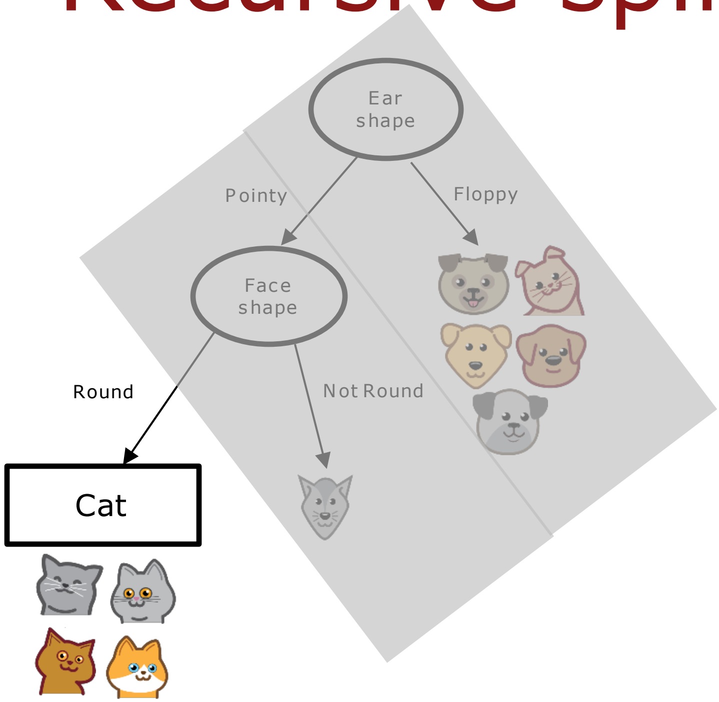

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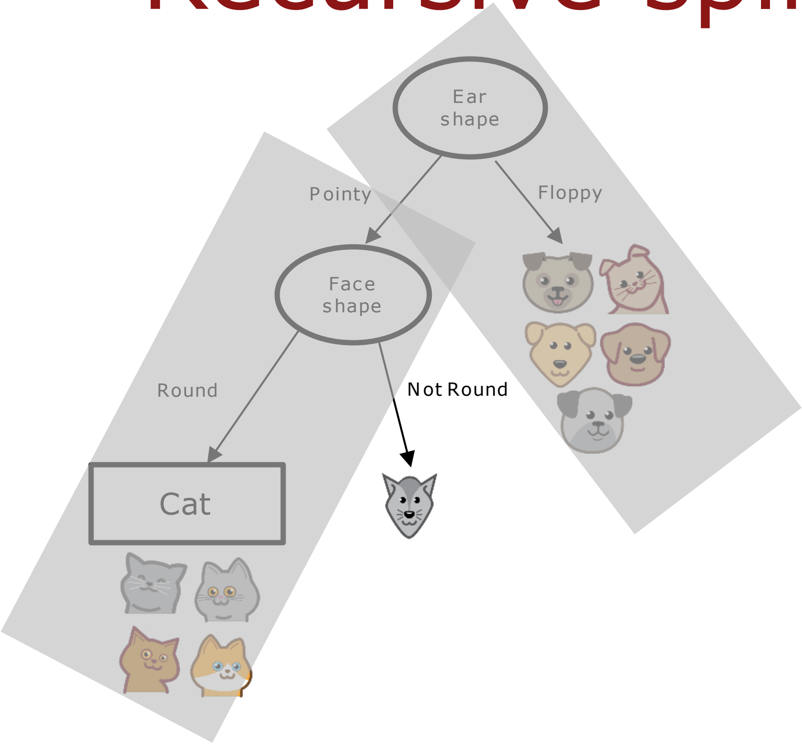

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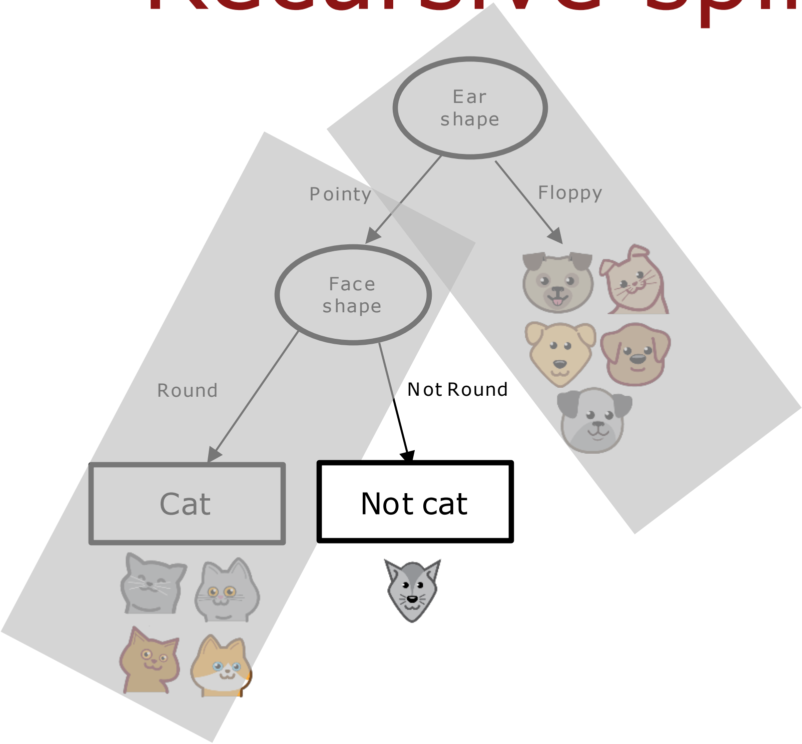

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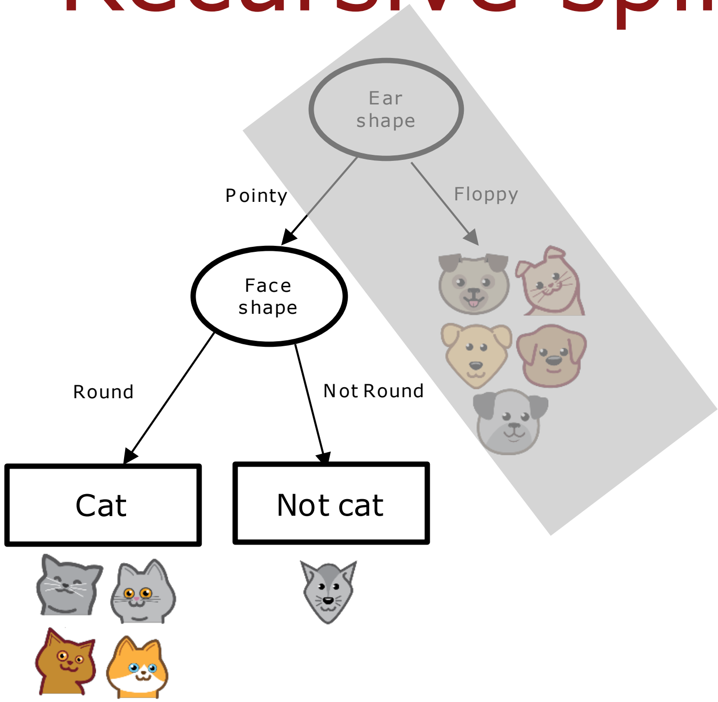

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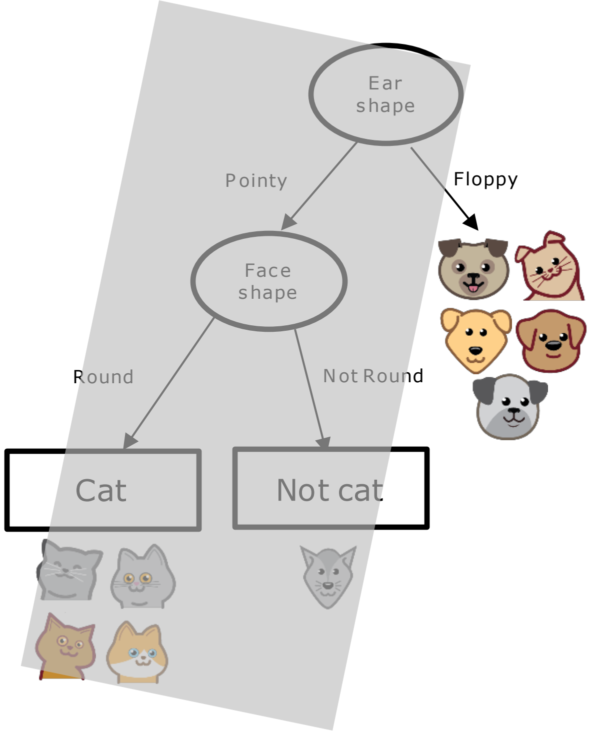

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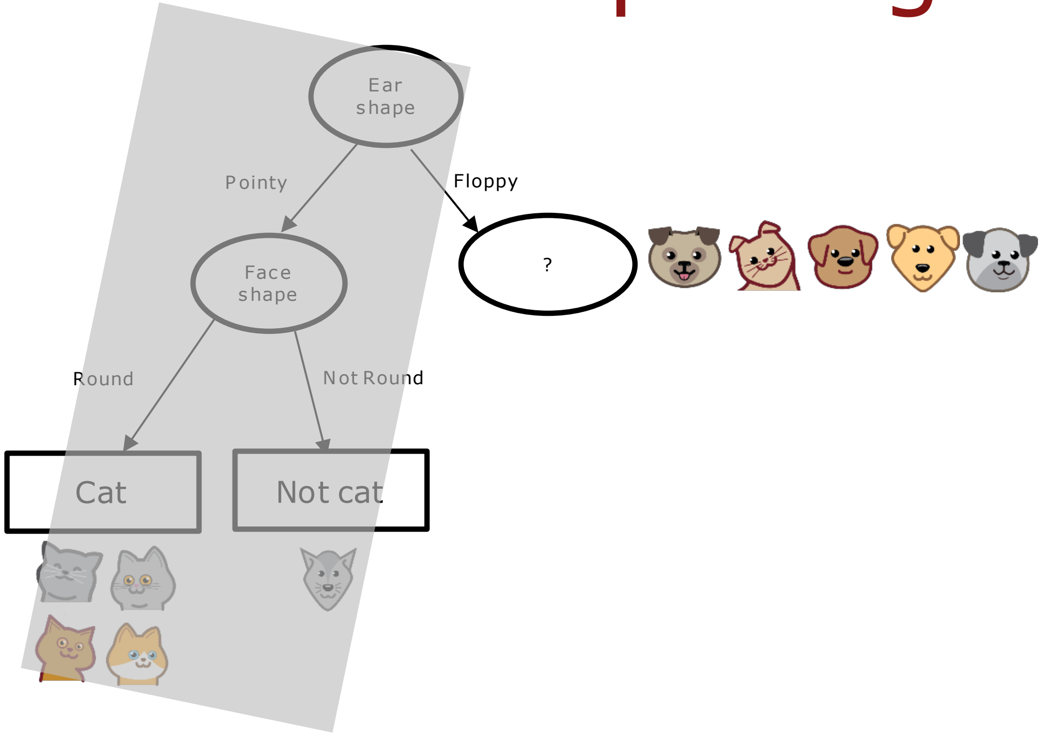

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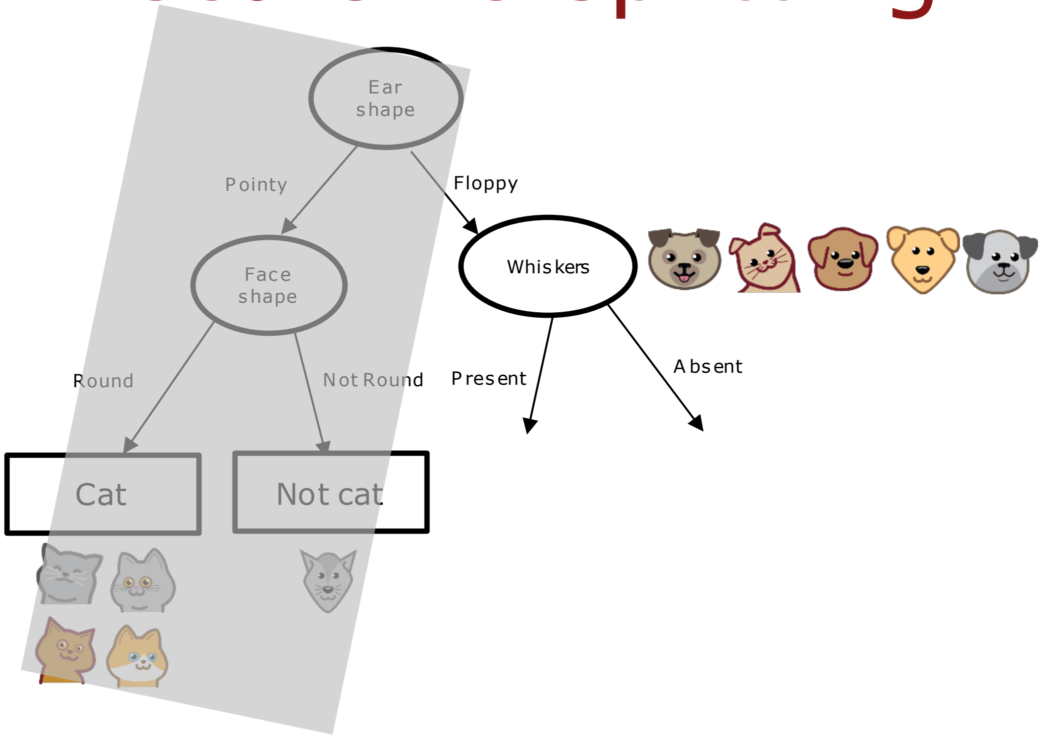

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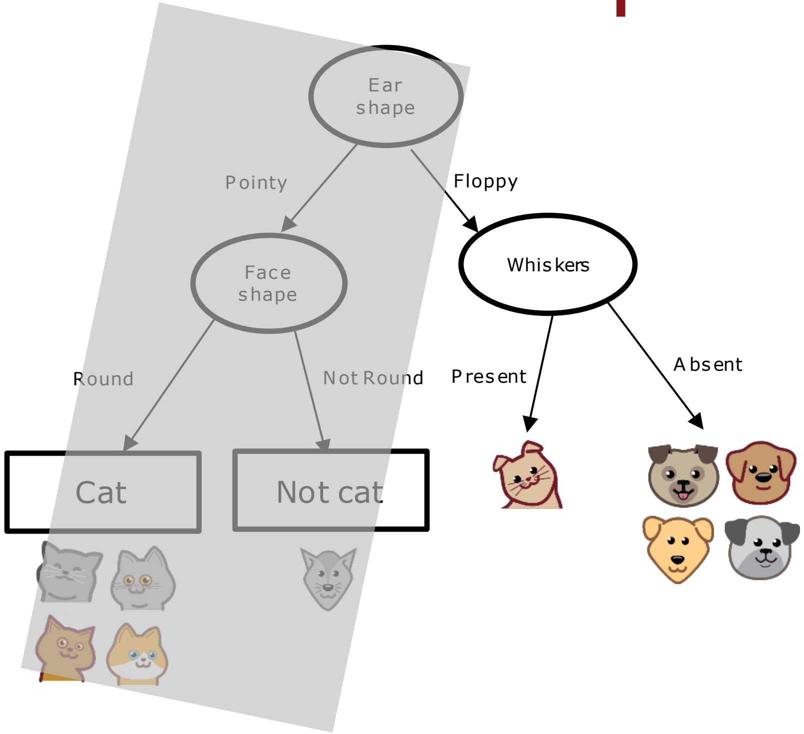

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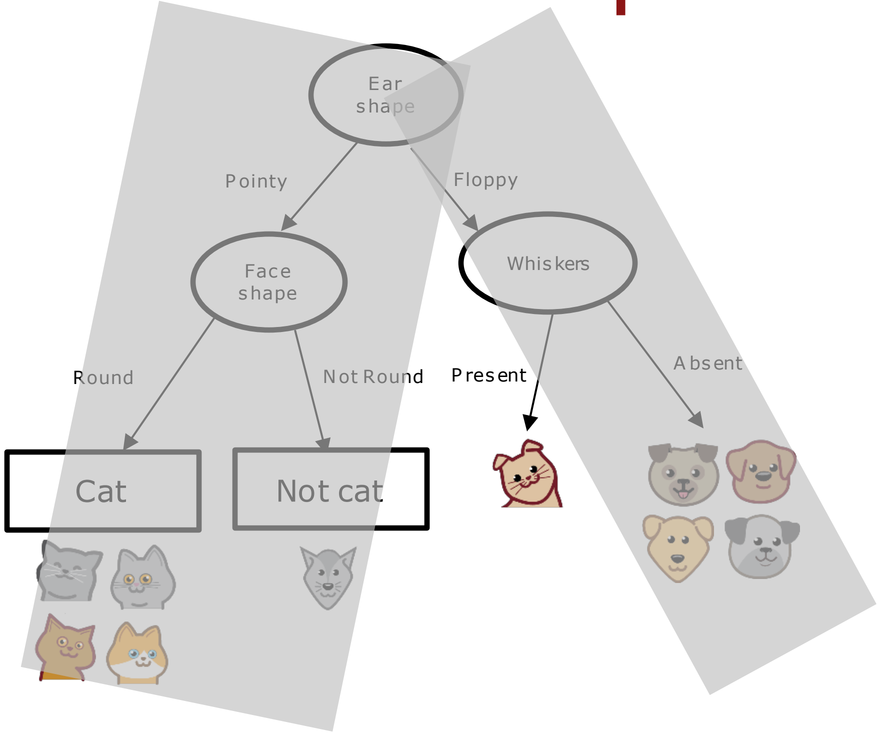

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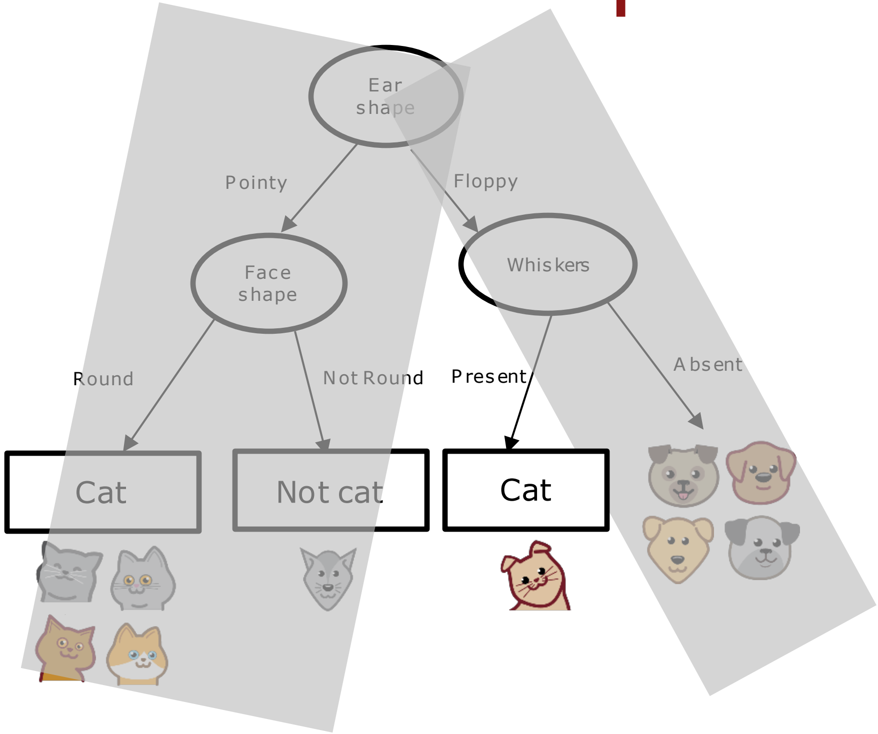

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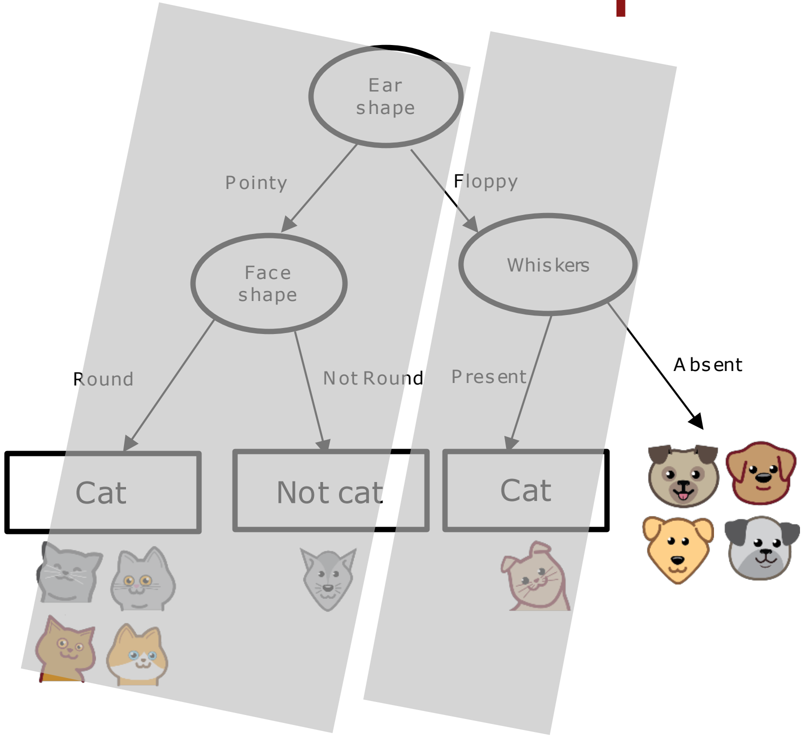

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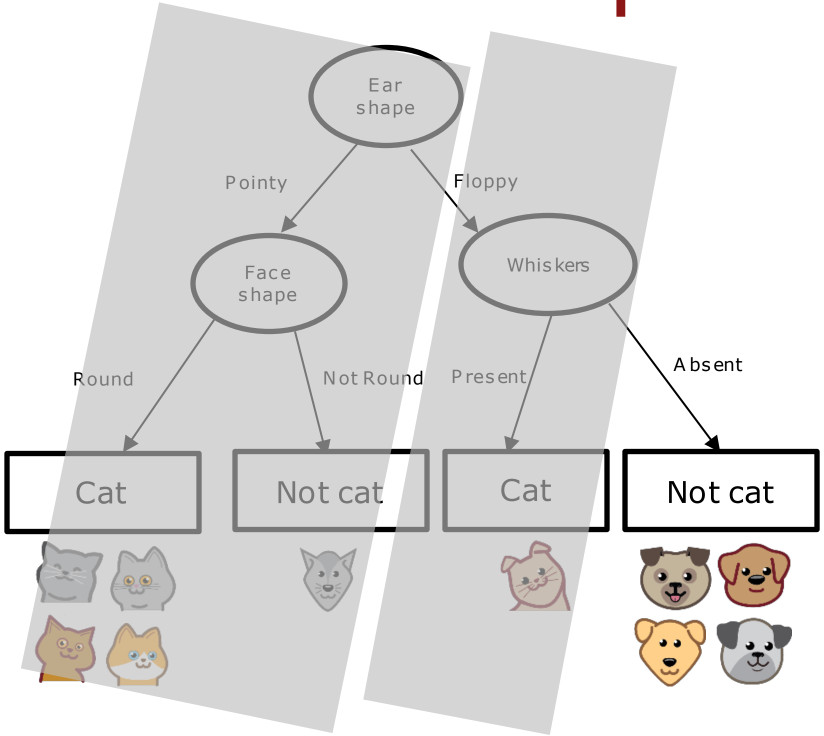

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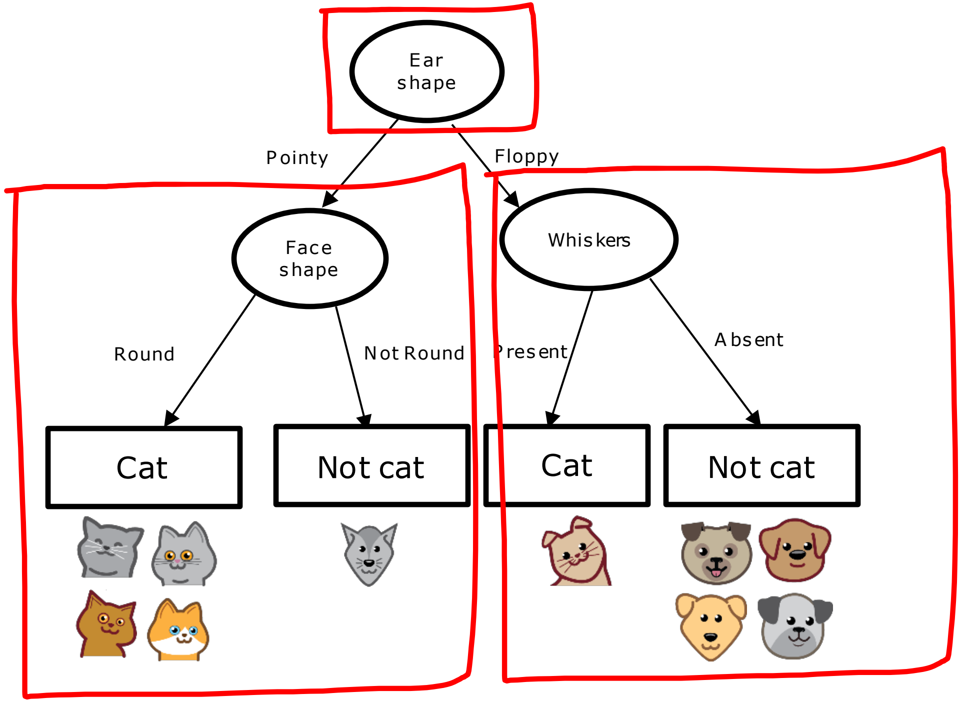


Recursive algorithm

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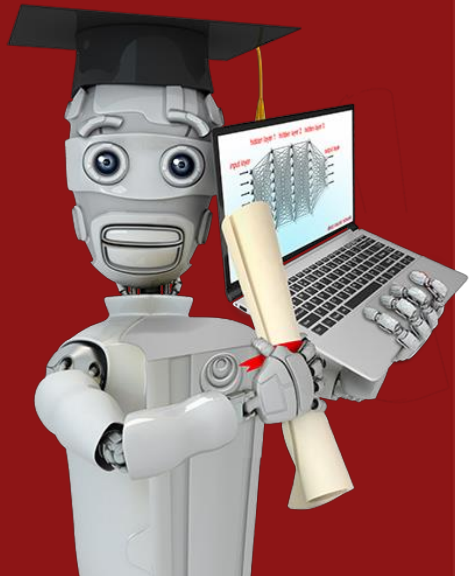
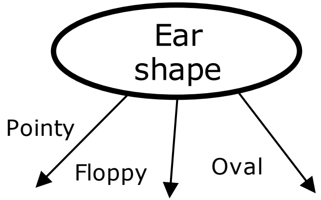


# Decision Tree Learning

## 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

| | ~~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 |

# 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 |

# 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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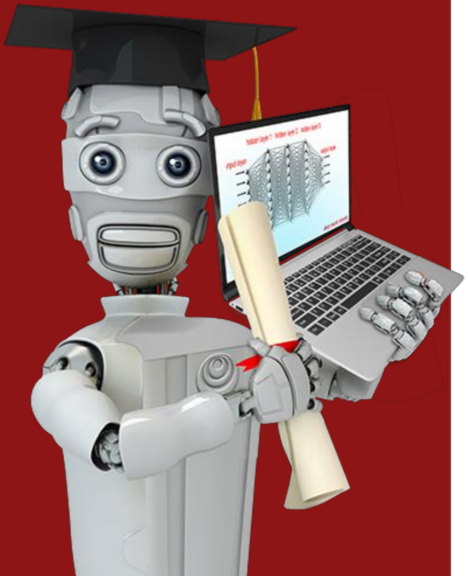


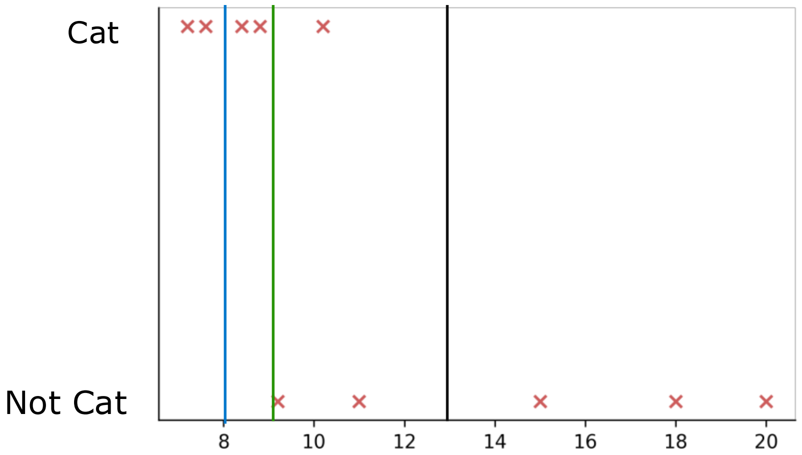
# Decision Tree Learning

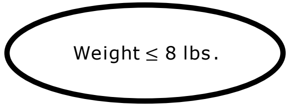
## Continuous valued features

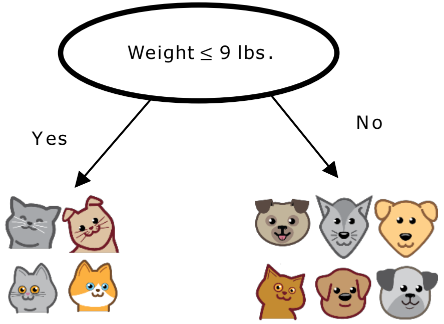
# Continuous features

| | 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




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

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

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

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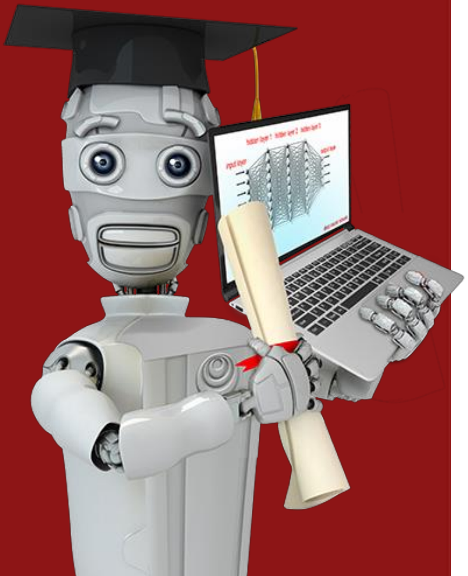


# Decision Tree Learning

## Regression Trees (optional)

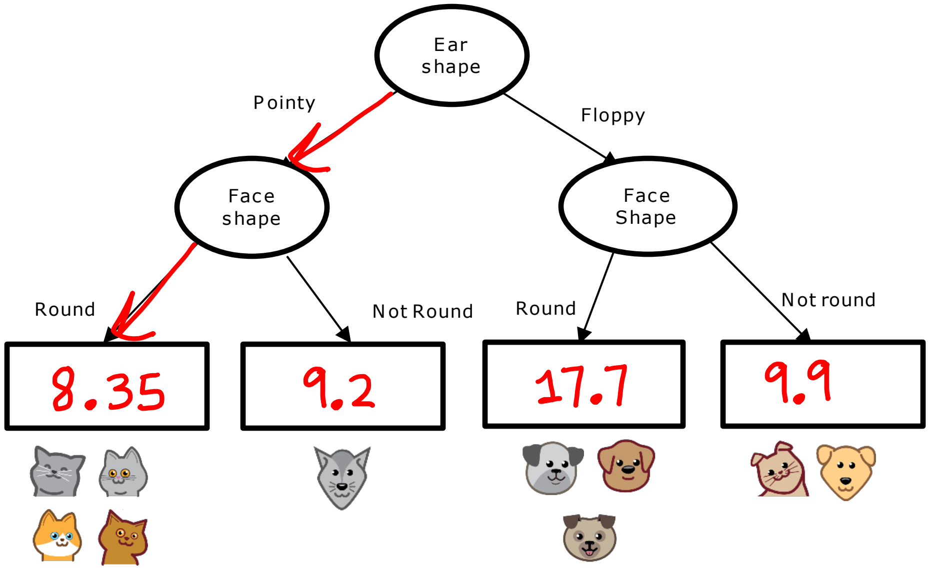
# Regression with Decision Trees: Predicting a number

| 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 |

X

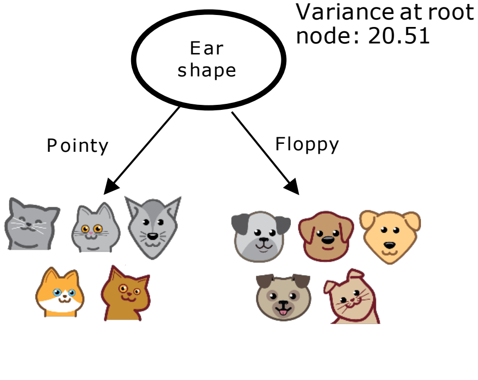
y

# Regression with Decision Trees




| **Weights(lbs.):** | **Weights(lbs.):** | **Weights (lbs.):** | **Weights(lbs.):** |
|---|---|---|---|
| 7.2, 8.4, 7.6, 10.2 | 9.2 | 15, 18, 20 | 8.8,11 |

# Choosing a split




Weights: 7.2, 9.2, 8.4,7.6, 10.2

Variance: 1.47

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

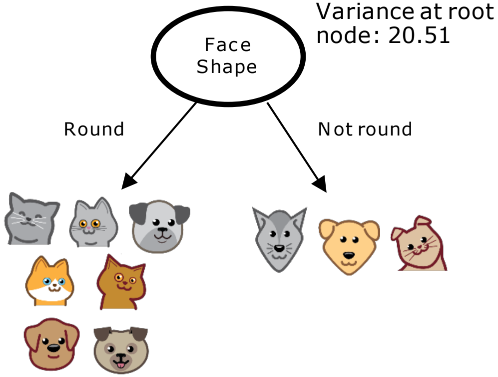
Weights: 8.8, 15, 11, 18, 20

Variance: 21.87

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

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

$= 8.84$




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

Variance: 27.80

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

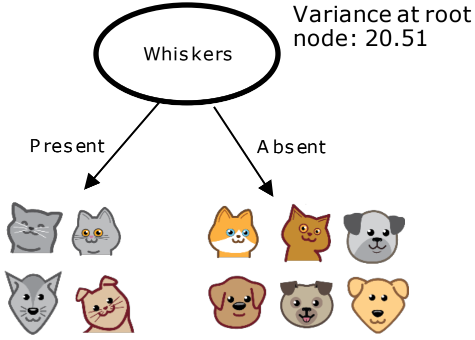
Weights: 8.8,9.2,11

Variance: 1.37

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

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

$= 0.64$




Weights: 7.2, 8.8, 9.2, 8.4

Variance: 0.75

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

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

Variance: 23.32

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

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

$= 6.22$

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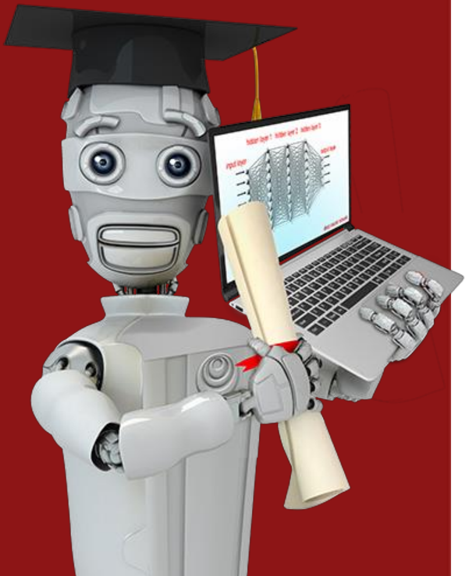
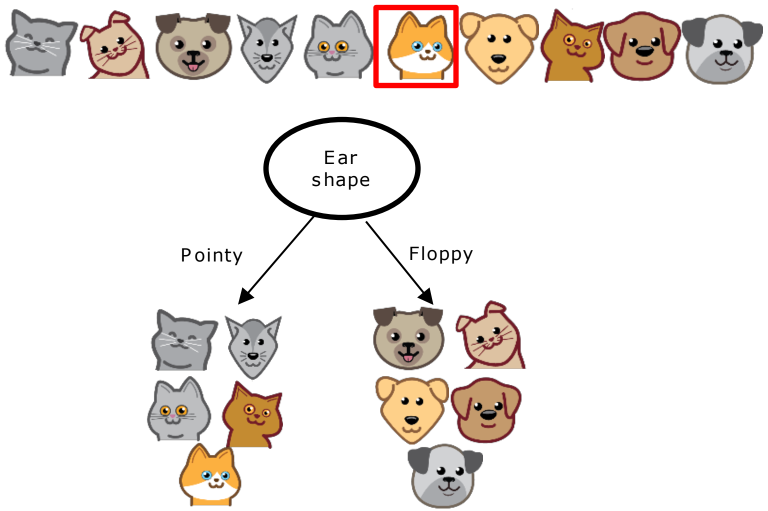
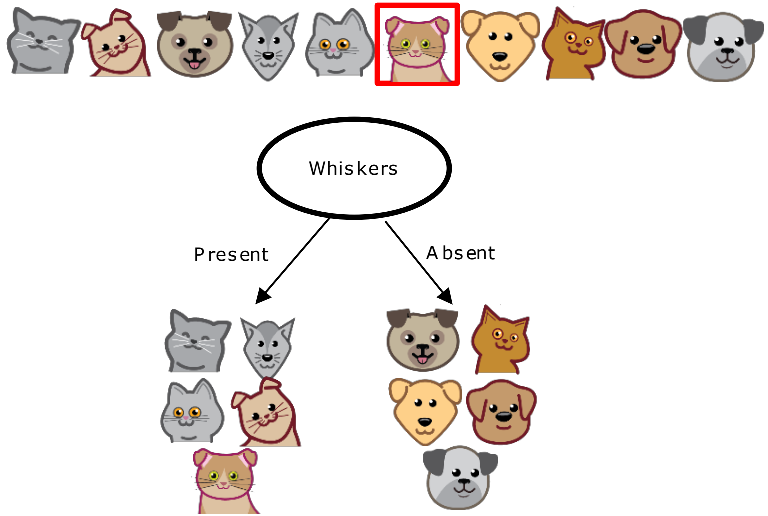


# Tree ensembles

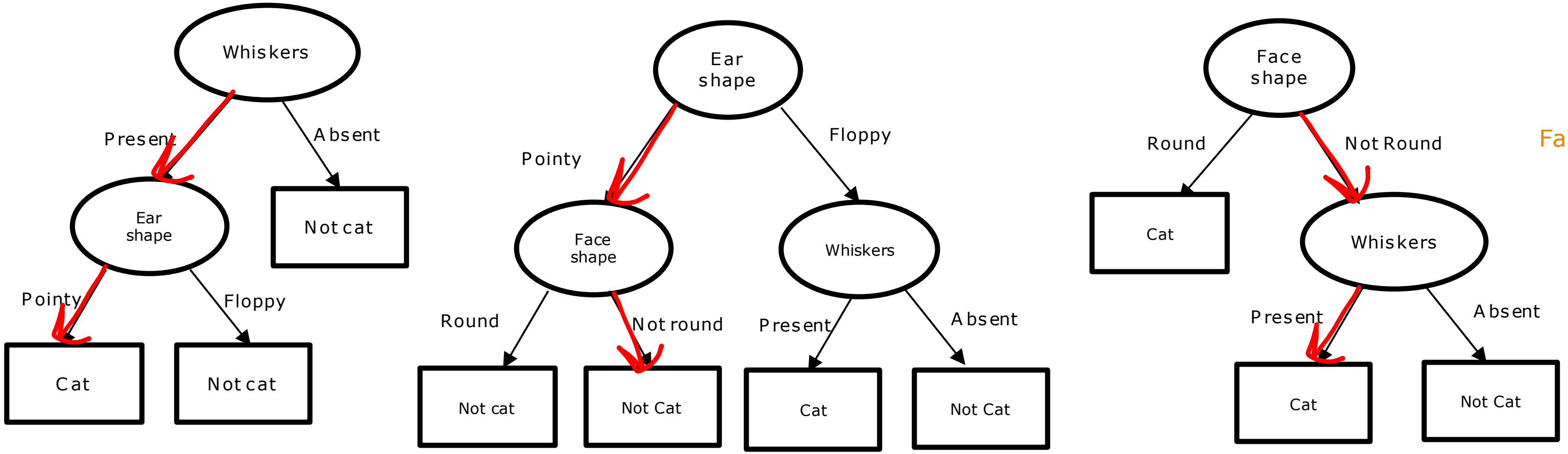
## Using multiple decision trees

# Trees are highly sensitive to small changes of the data



# Tree ensemble




New test example

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

Prediction: Cat

Prediction: Not cat

Prediction: Cat

Final prediction: Cat

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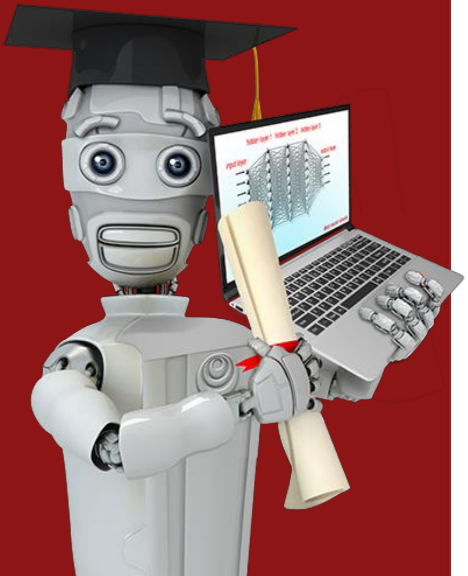
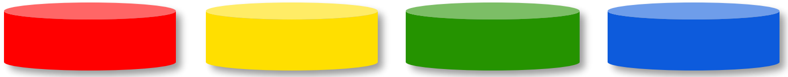


# Tree ensembles

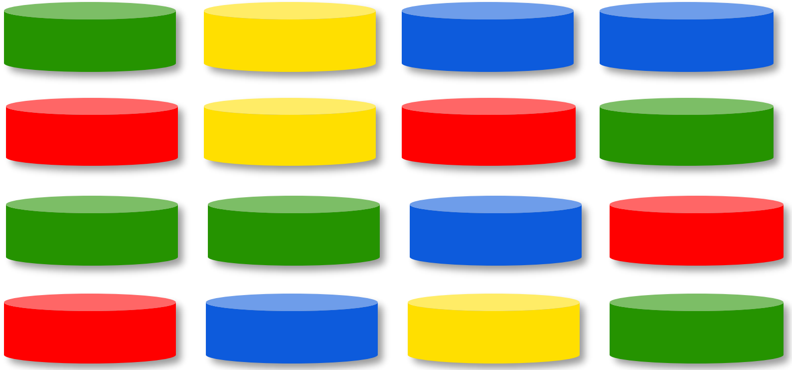
## Sampling with replacement

# Sampling with replacement

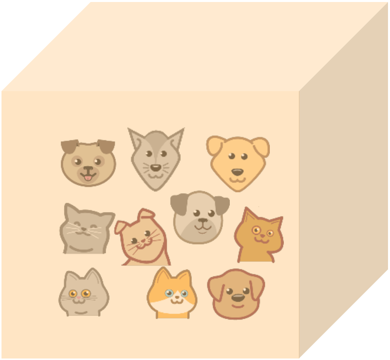
Tokens



Sampling with replacement:



# Sampling with replacement



| 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 |

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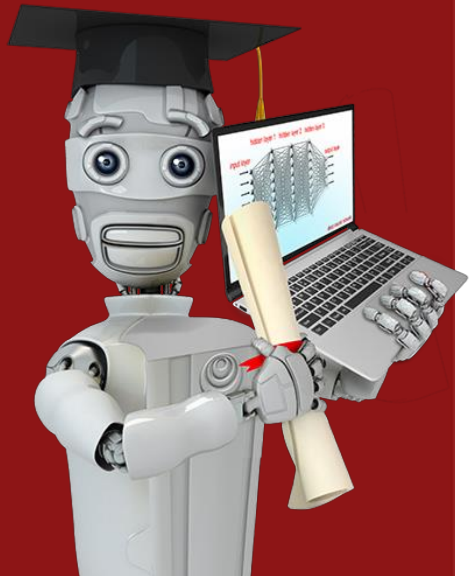


## Tree ensembles

# Random forest algorithm

# Generating a tree sample

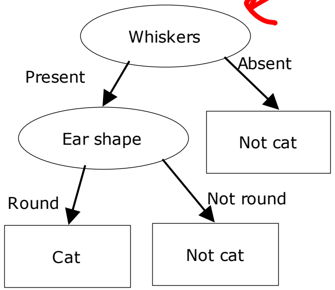
Given training set of size $m$

For $b = 1$ to $B$:

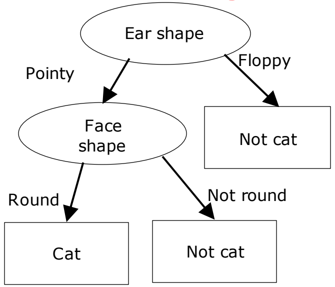
Use sampling with replacement to create a new training set of size $m$

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

# 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.

$$K = \sqrt{n}$$

Random forest algorithm

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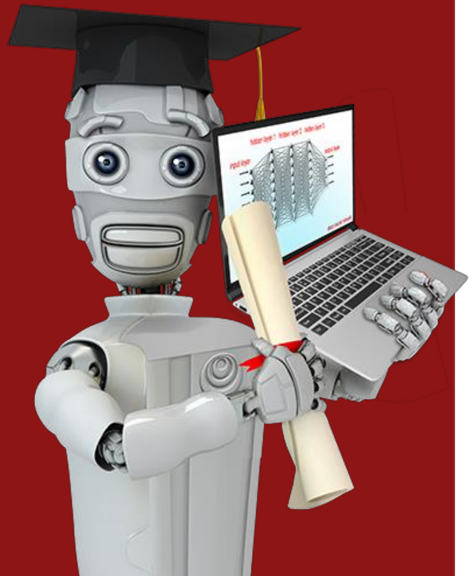


# Tree ensembles

# XGBoost

# Boosted trees intuition

Given training set of size $m$

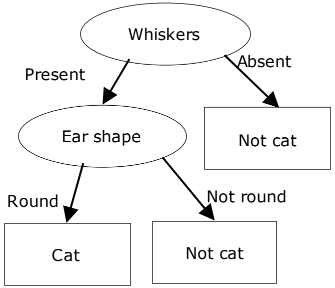
For $b = 1$ to $B$:

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 |




$\underbrace{1, 2, \ldots, b-1}$

$b$

| 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 | ✓ |

# 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)

# 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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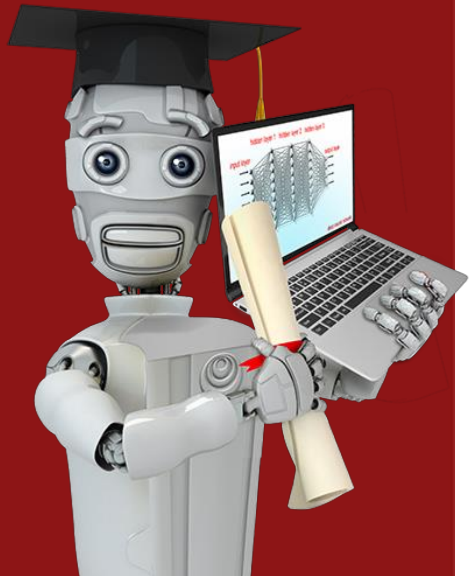


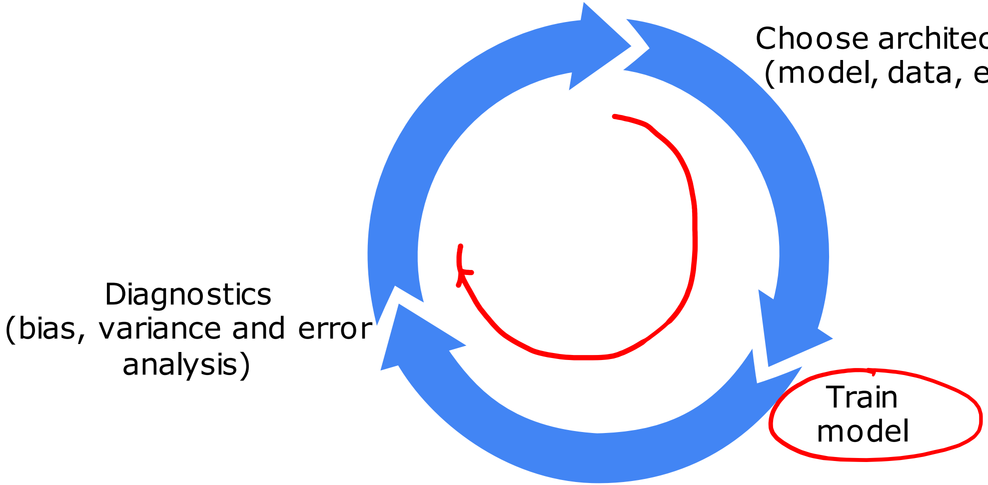
# Conclusion

## 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



# 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