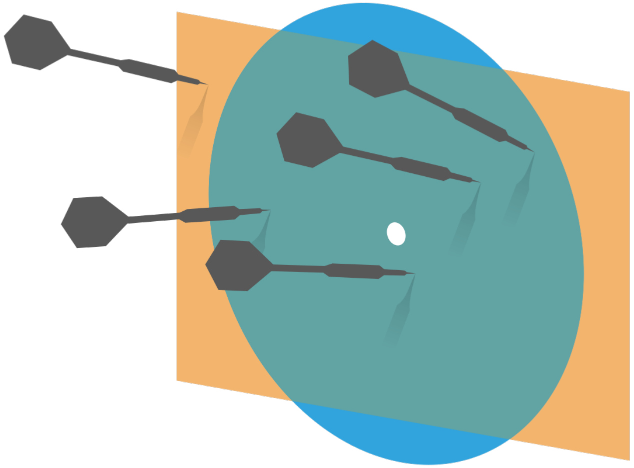
# Probability and Statistics for Computer Science



Credit: wikipedia

"…many problems are naturally classification problems"---Prof. Forsyth

Hongye Liu, Teaching Assistant Prof, CS361, UIUC, 04.06.2021

# Last time

- Demo of Principal Component Analysis
- Introduction to classification

# Classifiers

- Why do we need classifiers?
- What do we use to quantify the performance of a classifier?
- What is the baseline accuracy of a 5-class classifier using 0-1 loss function?  $\frac{1}{5} = 20\%$
- What's validation and cross-validation in classification?

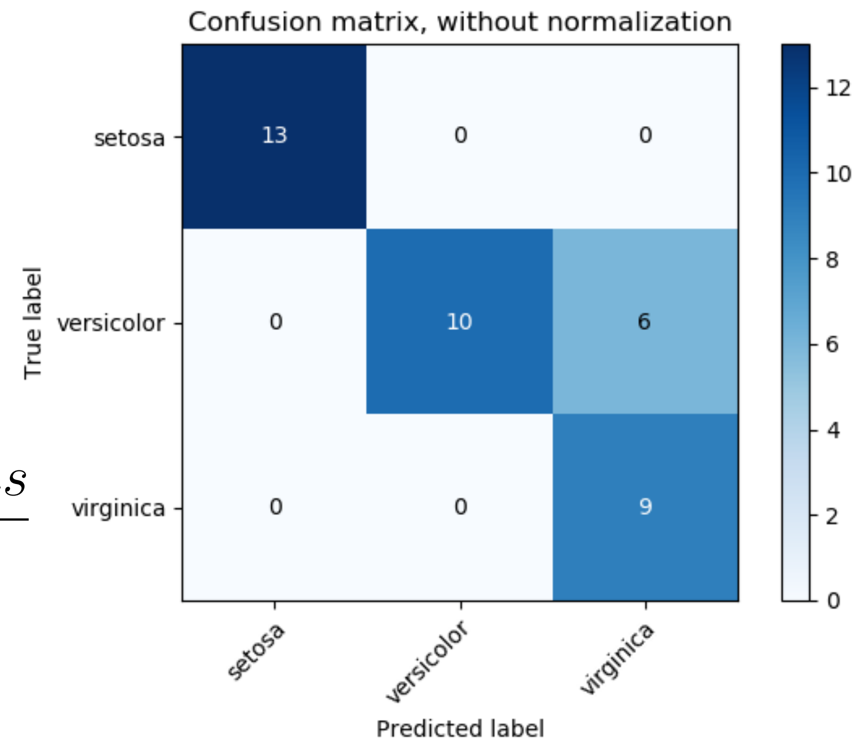
| | |
|---|---|
| TP | FT |
| FN | TN |

# Performance of a multiclass classifier

- Assuming there are **c** classes:
- The class confusion matrix is $c \times c$
- Under the 0-1 loss function

  accuracy= $\dfrac{sum\ of\ diagonal\ terms}{sum\ of\ all\ terms}$

  ie. in the right example, accuracy = 32/38=84%
- The baseline accuracy is 1/c.




Source: scikit-learn

# Cross-validation

- If we don't want to "waste" labeled data on validation, we can use **cross-validation** to see if our training method is sound.

- Split the labeled data into training and validation sets in multiple ways

- For each split (called a **fold**)
  - Train a classifier on the training set
  - Evaluate its accuracy on the validation set

- Average the accuracy to evaluate the training methodology

# Q1. Cross-validation

**Cross-validation** is a method used to prevent overfitting in classification.

A. TRUE

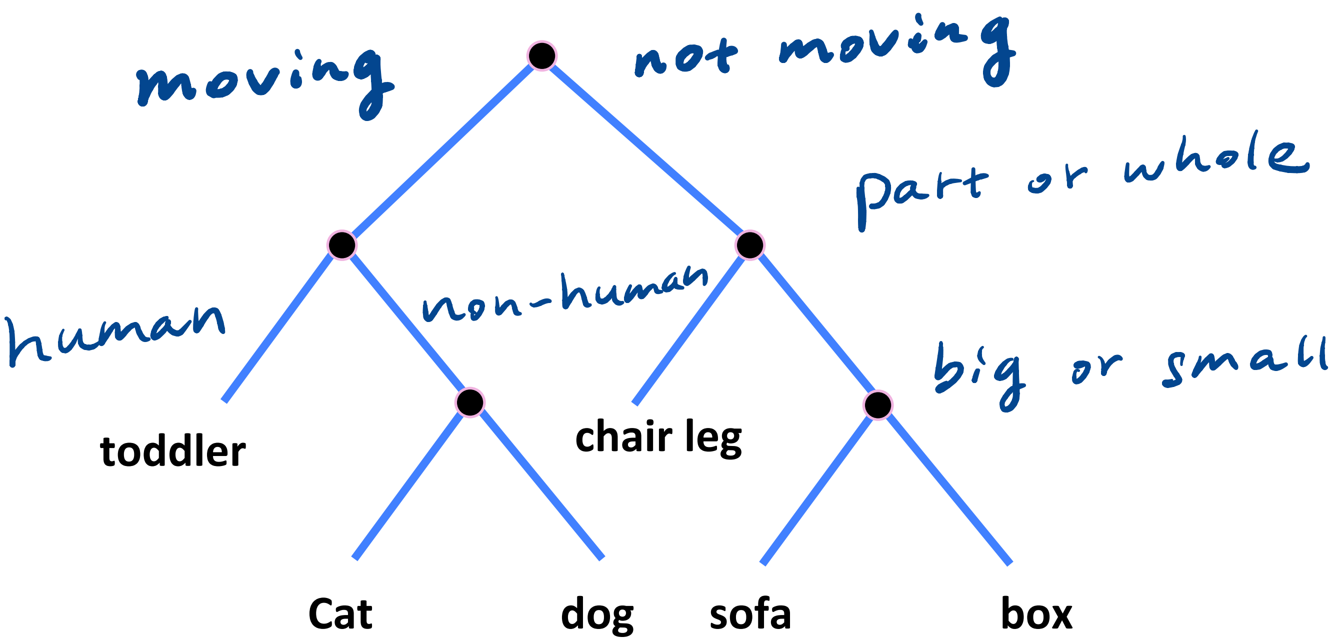
B. FALSE

# Objectives

- Decision tree (II)
- Random forest
- Support Vector Machine (I)

# Decision tree: object classification

- The object classification **decision tree** can classify objects into multiple classes using sequence of simple tests. It will naturally grow into a tree.



# Iris example · which type is this?

Irises

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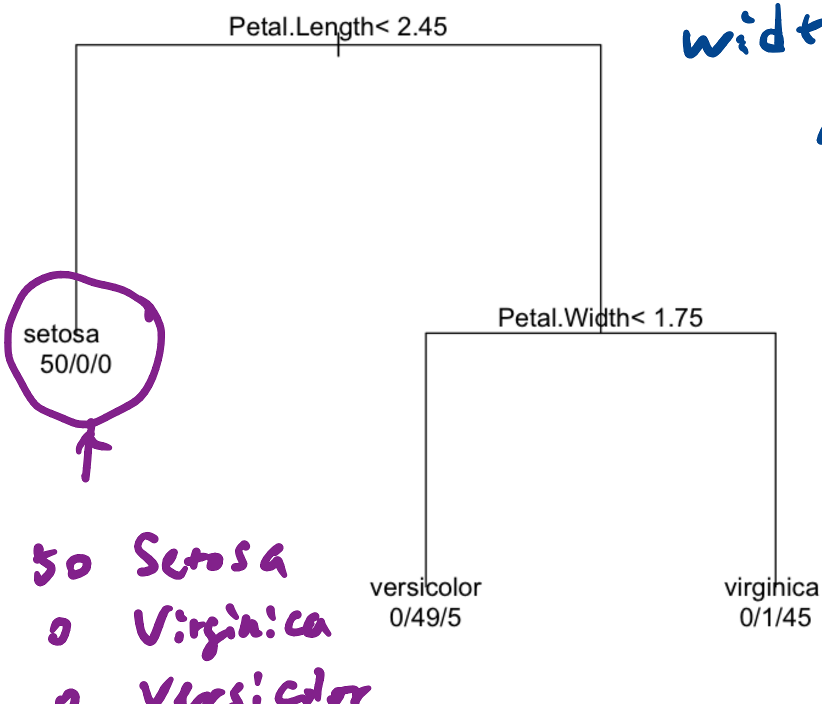
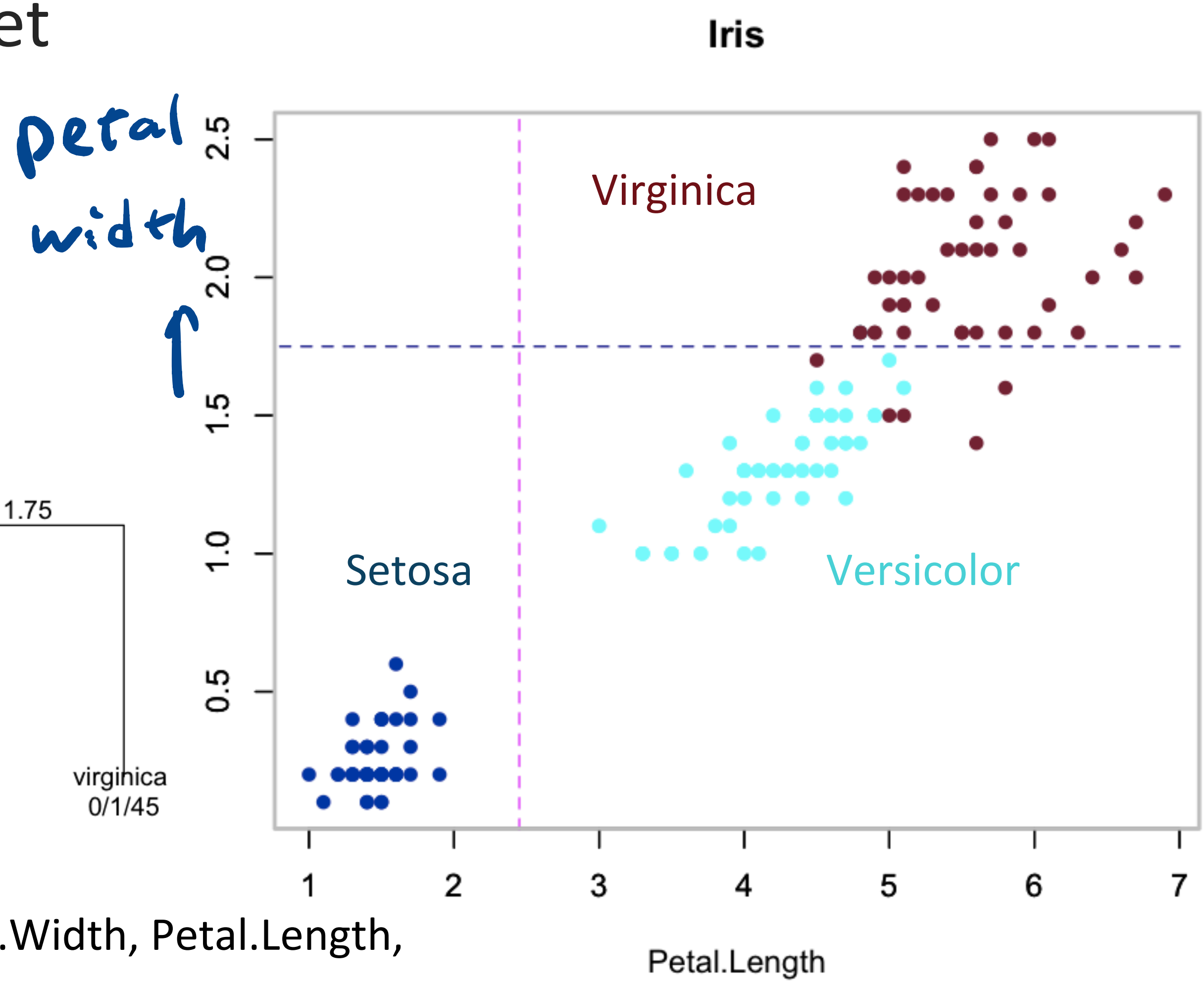
# Training a decision tree: example

- The “Iris” data set



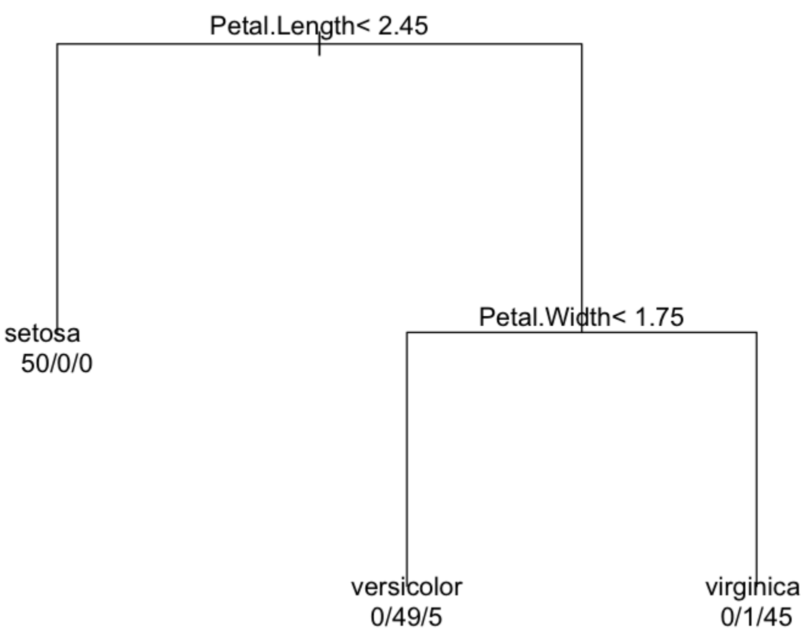

**Features**: Sepal.Length, Sepal.Width, Petal.Length, Petal.Width **Label**: Species

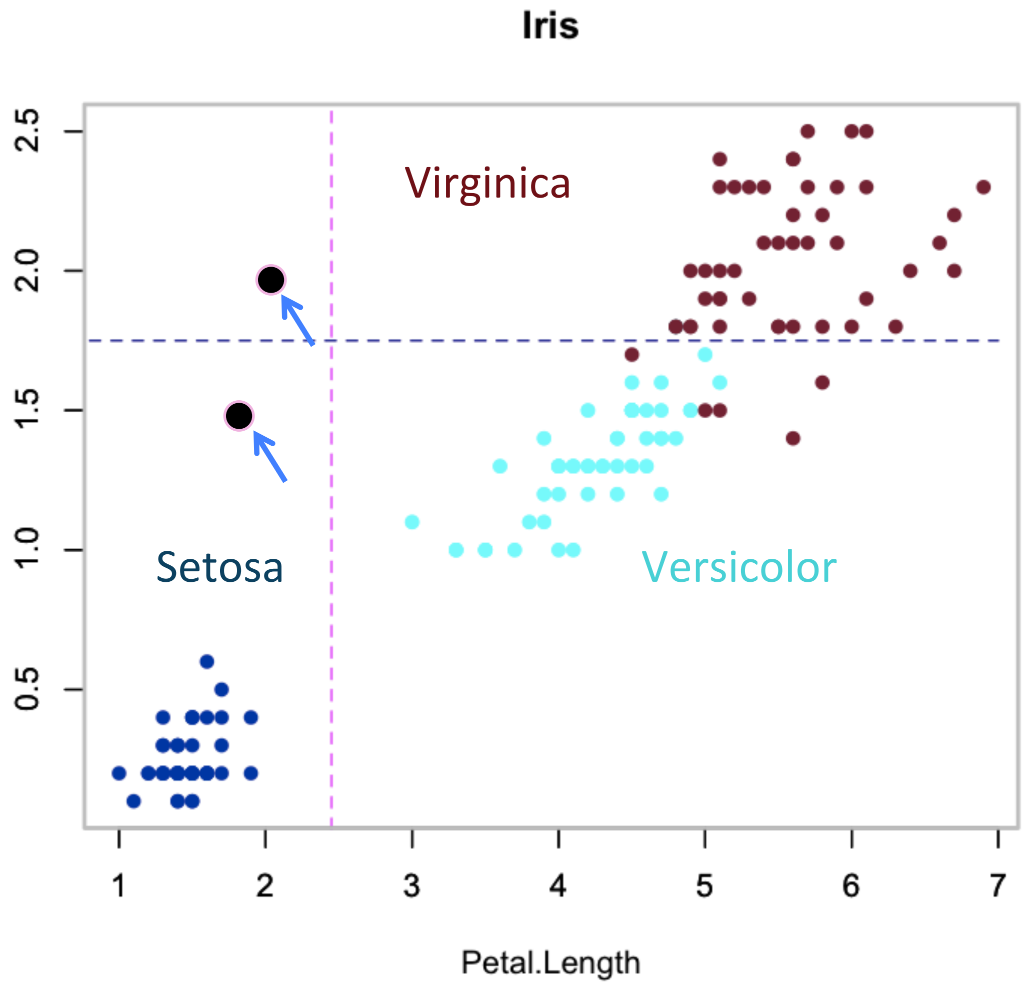
# Training a decision tree

- Choose a dimension/feature and a split
- Split the training Data into left- and right-child subsets $D_l$ and $D_r$
- Repeat the two steps above recursively on each child
- Stop the recursion based on some conditions
- Label the leaves with class labels

# Classifying with a decision tree: example

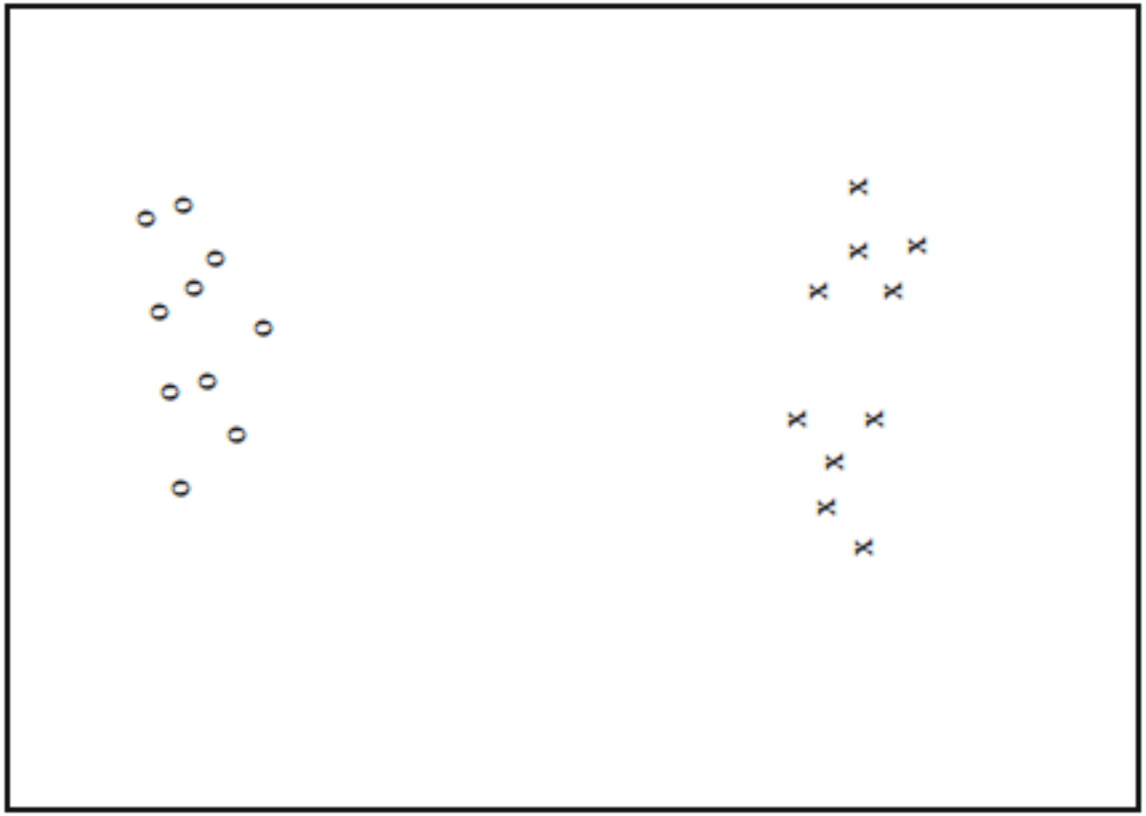
- The "Iris" data set



# Choosing a split

- An informative split makes the subsets more concentrated and reduces uncertainty about class labels



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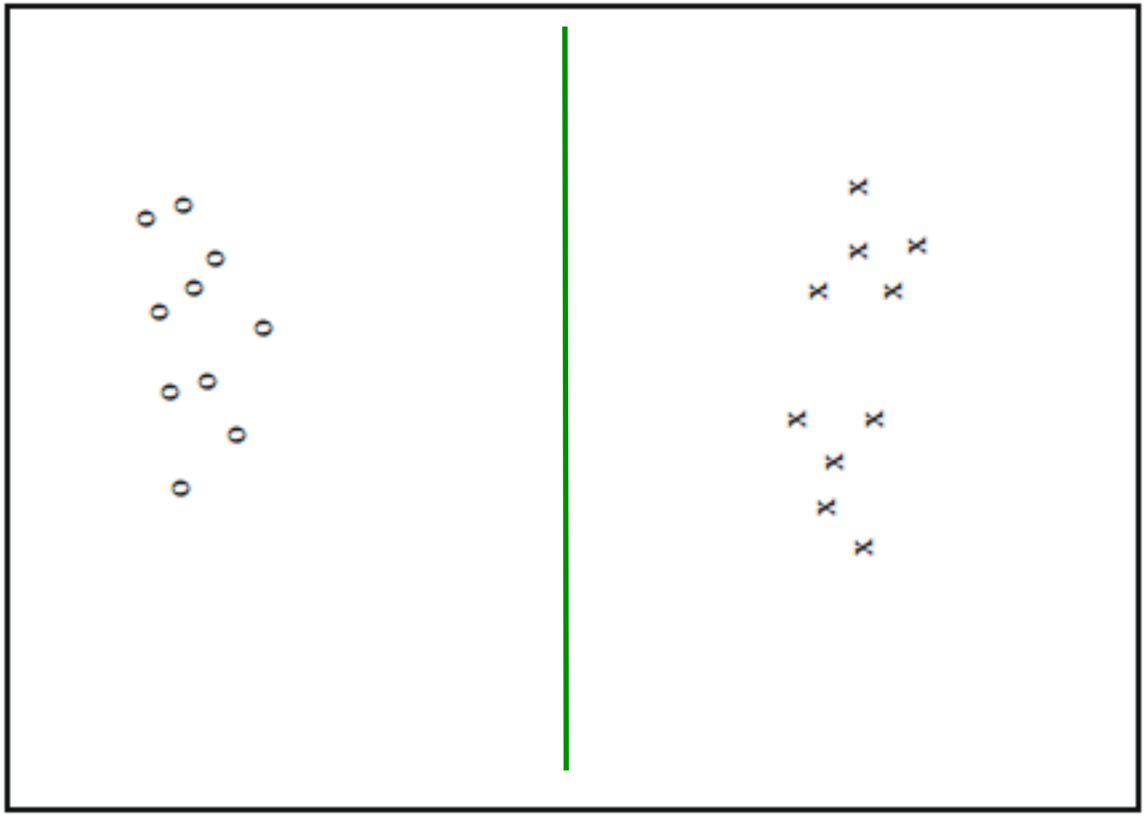
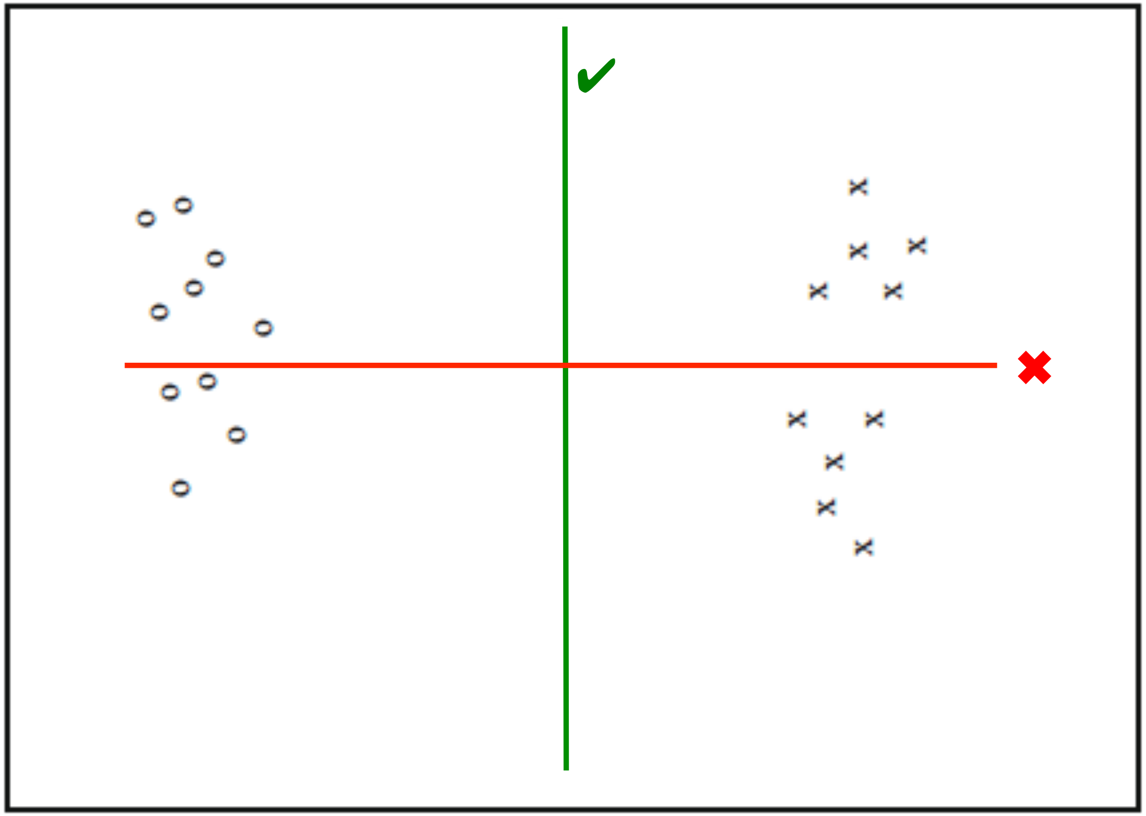
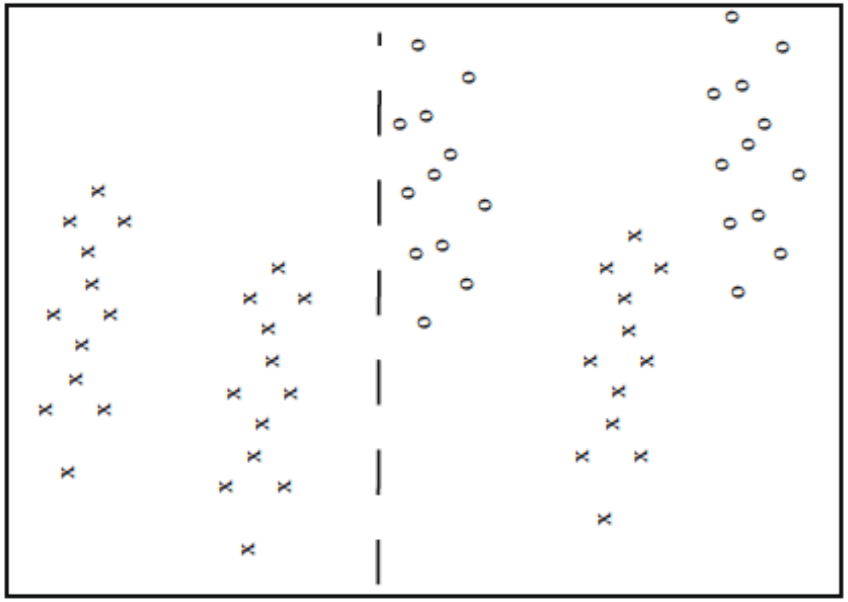


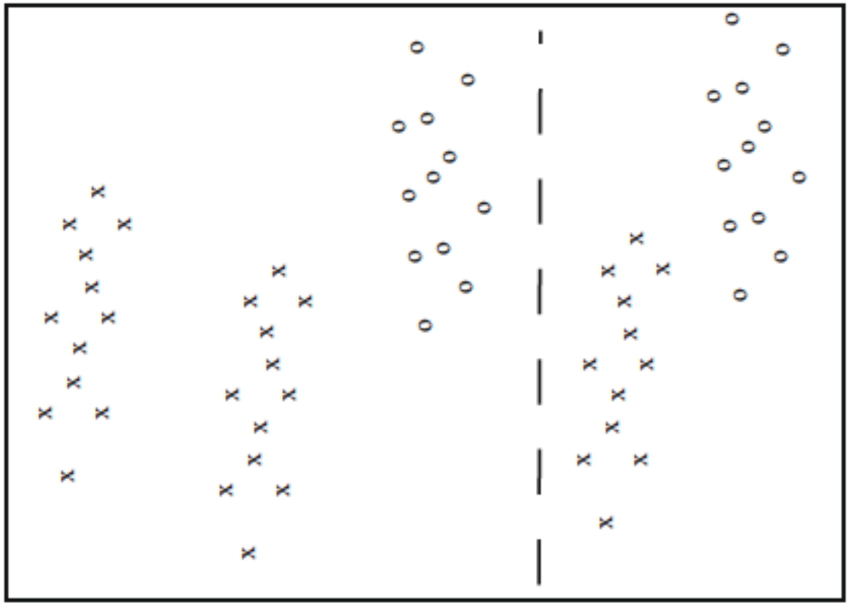
# Choosing a split

- An informative split makes the subsets more concentrated and reduces uncertainty about class labels



# Which is more informative?

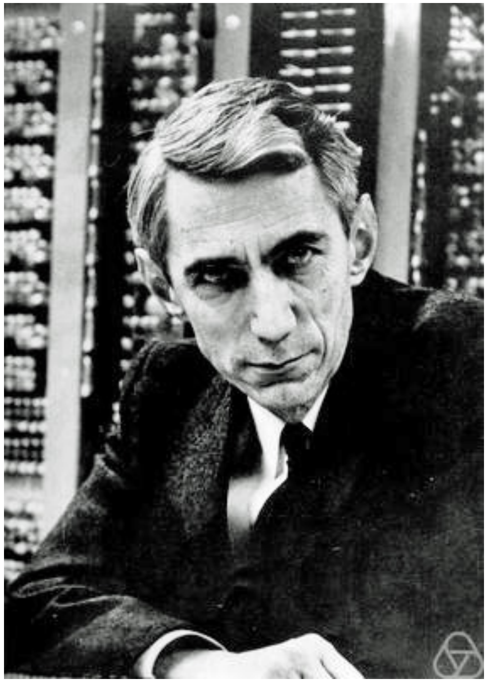




# Quantifying uncertainty using entropy

- We can measure uncertainty as the number of bits of information needed to distinguish between classes in a dataset (first introduced by Claude Shannon)
  - We need $\text{Log}_2\ 2 = 1$ bit to distinguish 2 equal classes
  - We need $\text{Log}_2\ 4 = 2$ bit to distinguish 4 equal classes

00
01
10
11



Claude Shannon (1916-2001)

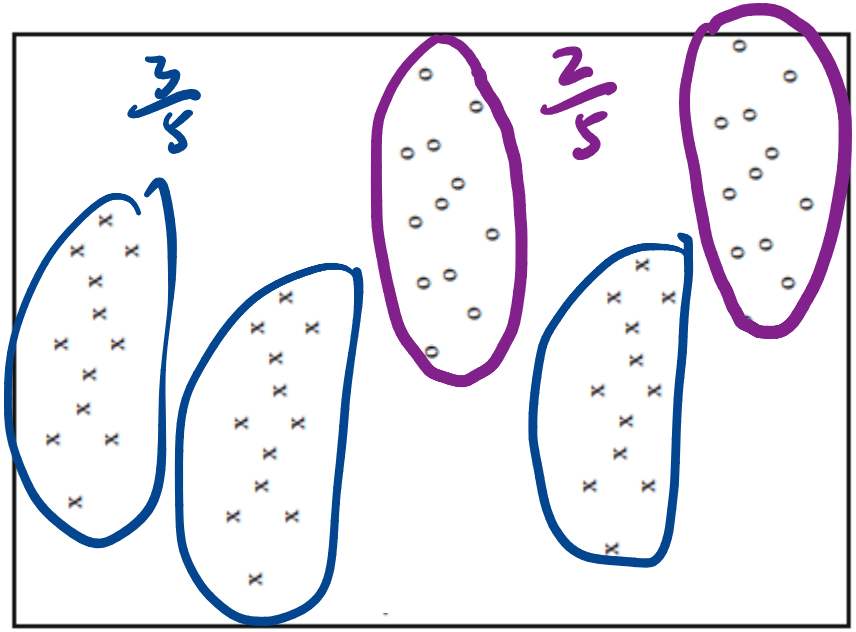
# Quantifying uncertainty using entropy

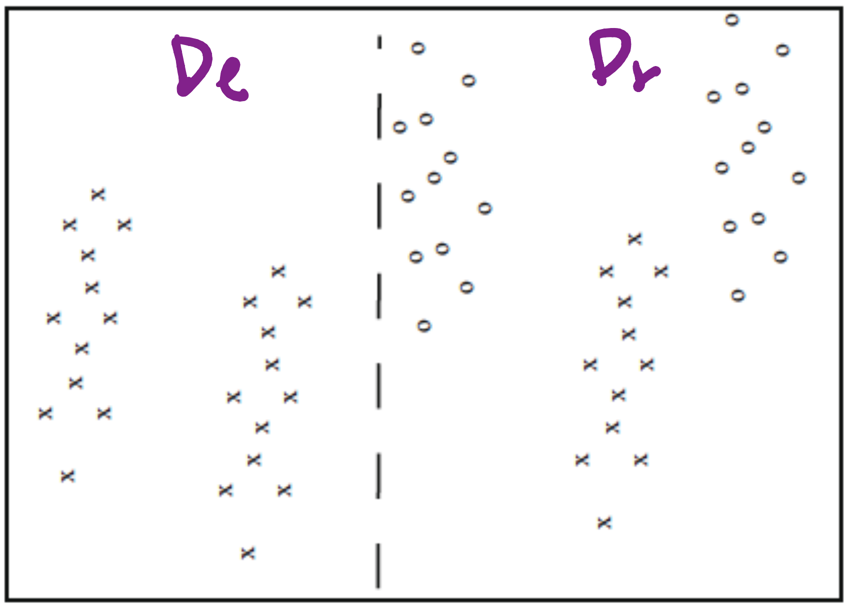
- **Entropy** (Shannon entropy) is the measure of uncertainty for a general distribution
  - If class $\boldsymbol{i}$ contains a fraction $\boldsymbol{P}(\boldsymbol{i})$ of the data, we need $log_2 \dfrac{1}{P(i)}$ bits for that class
  - The entropy H(D) of a dataset is defined as the **weighted mean** of entropy for every class:

$$H(D) = \sum_{i=1}^{c} P(i) log_2 \frac{1}{P(i)}$$

$$= \sum_{i=1}^{c} -P(i) \log P(i)$$

# Entropy: before the split

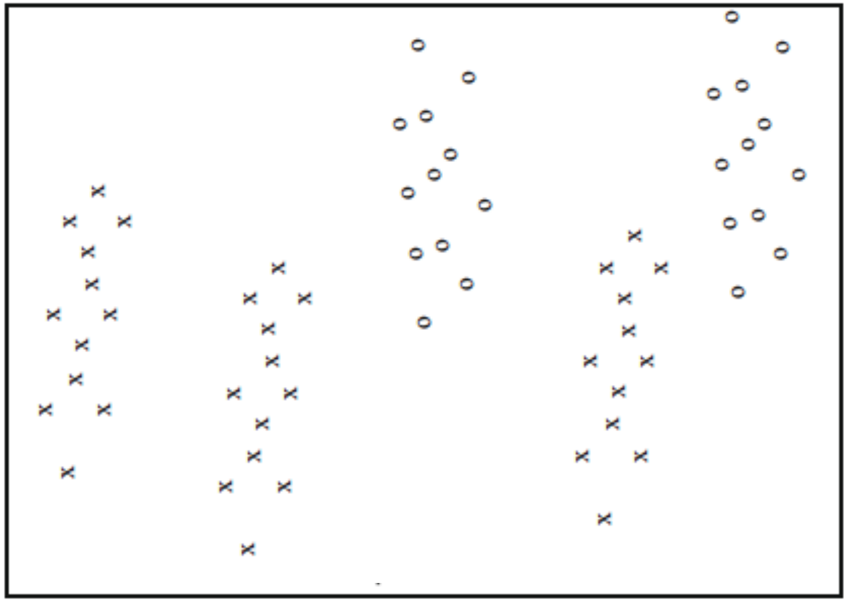


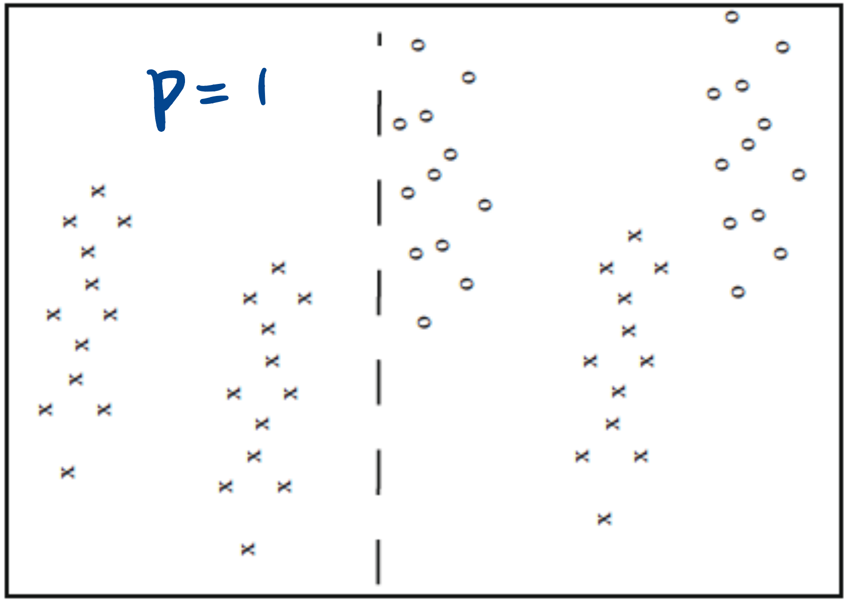




$$H(D) = -\frac{3}{5}log_2\frac{3}{5} - \frac{2}{5}log_2\frac{2}{5}$$

$$= 0.971\ bits$$

# Entropy: examples





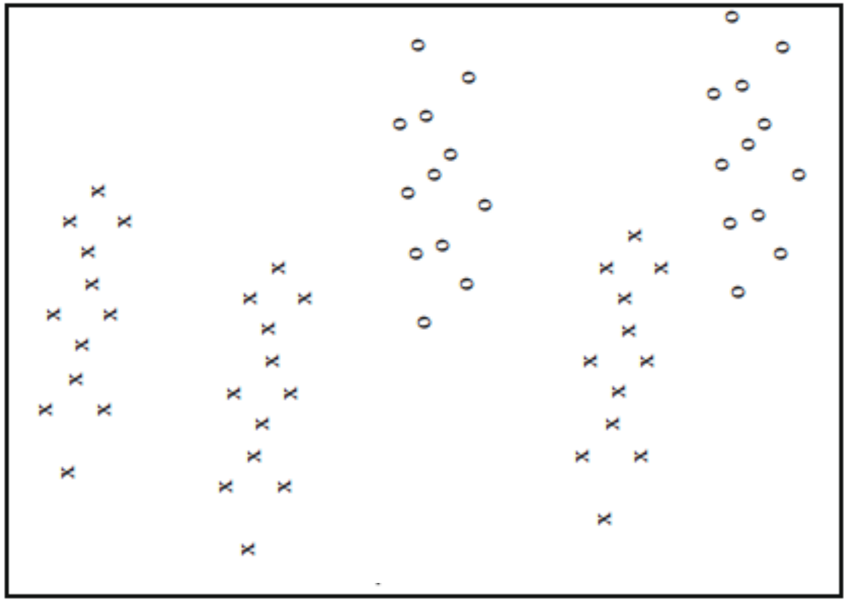

$$H(D) = -\frac{3}{5} log_2 \frac{3}{5} - \frac{2}{5} log_2 \frac{2}{5}$$

$$= 0.971 \ bits$$

$$H(D_l) = -1 \ log_2 1 = \underline{0} \ bits$$

$$H(D_r) = ?$$

# Entropy: examples



$$H(D) = -\frac{3}{5}log_2\frac{3}{5} - \frac{2}{5}log_2\frac{2}{5}$$

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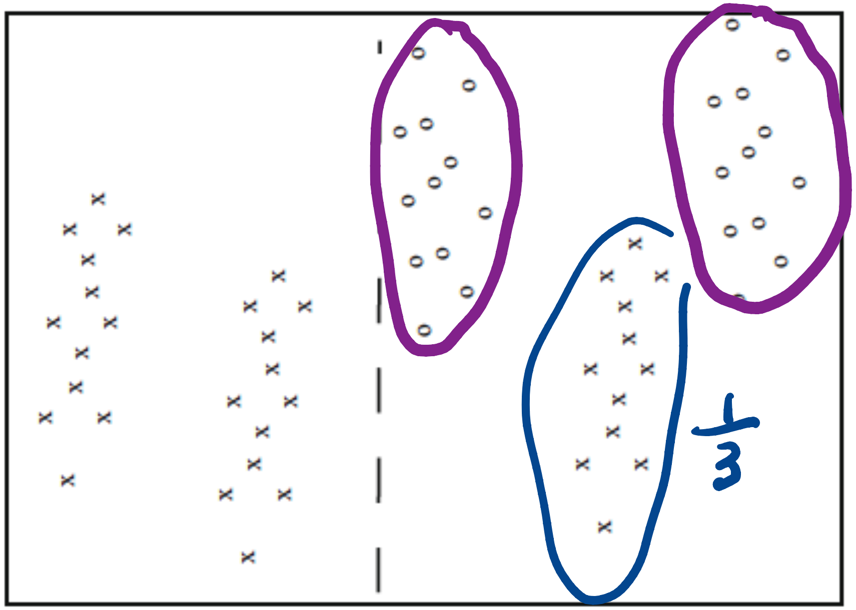


$$H(D_l) = -1\ log_2 1 = 0\ bits$$

$$H(D_r) = -\frac{1}{3}log_2\frac{1}{3} - \frac{2}{3}log_2\frac{2}{3}$$

$$= 0.918\ bits$$

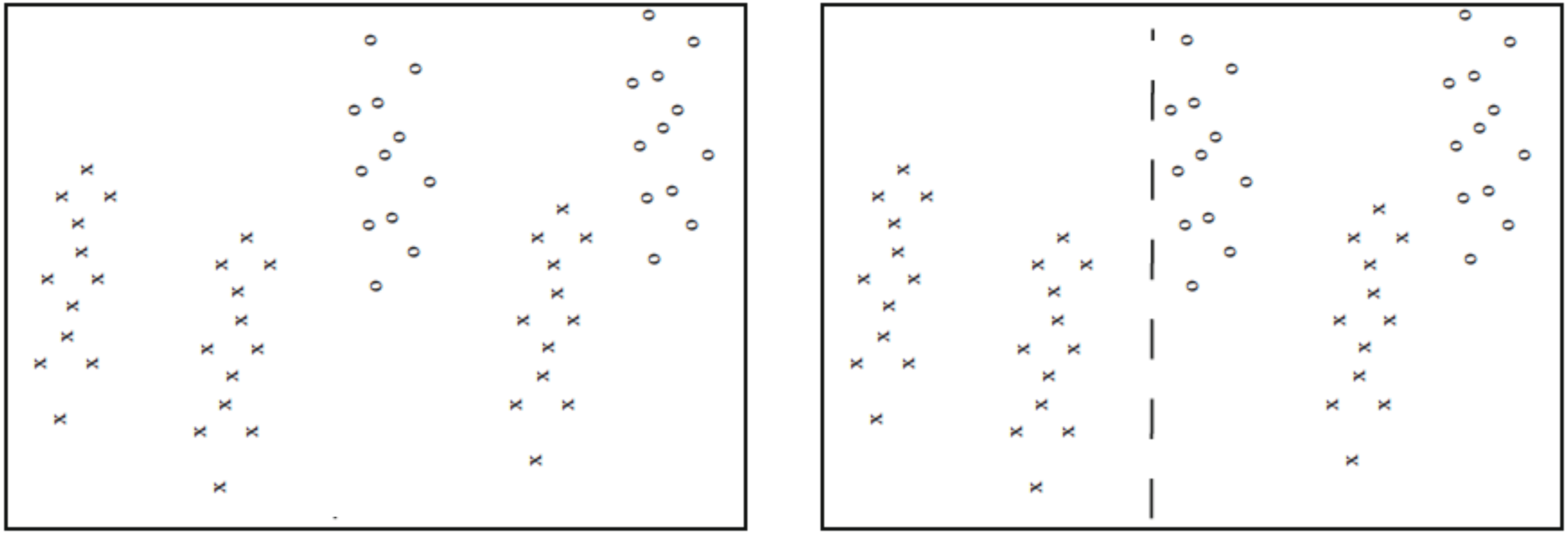
# Information gain of a split

- The information gain of a split is the amount of entropy that was reduced on average after the split

$$I = H(D) - (\frac{N_{Dl}}{N_D} H(D_l) + \frac{N_{Dr}}{N_D} H(D_r))$$

- where
  - $N_D$ is the number of items in the dataset $D$
  - $N_{Dl}$ is the number of items in the left-child dataset $D_l$
  - $N_{Dr}$ is the number of items in the left-child dataset $D_r$

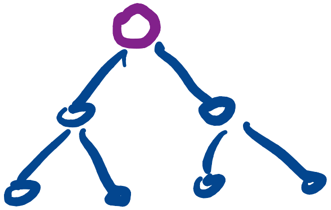
# Information gain: examples



$$I = H(D) - (\frac{N_{Dl}}{N_D} H(D_l) + \frac{N_{Dr}}{N_D} H(D_r))$$
$$= 0.971 - (\frac{24}{60} \times 0 + \frac{36}{60} \times 0.918)$$
$$= 0.420 \ bits$$

# Q. Is the splitting method global optimum?

local optimum



A. Yes
B. No

# How to choose a dimension and split

- If there are **d** dimensions, choose approximately $\sqrt{d}$ of them as candidates at random
- For each candidate, find the split that maximizes the information gain
- Choose the best overall dimension and split
- Note that splitting can be generalized to categorical features for which there is no natural ordering of the data

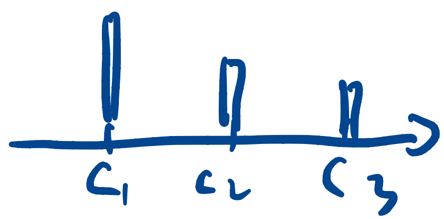
# When to stop growing the decision tree?

- Growing the tree too deep can lead to overfitting to the training data

- Stop recursion on a data subset if any of the following occurs:
  - All items in the data subset are in the same class
  - The data subset becomes smaller than a predetermined size
  - A predetermined maximum tree depth has been reached.

# How to label the leaves of a decision tree

- A leaf will usually have a data subset containing many class labels
- Choose the class that has the most items in the subset
- Alternatively, label the leaf with the number it contains in each class for a probabilistic "soft" classification.



# Pros and Cons of a decision tree

- Pros:

  Quick.

  Interpretable

  Decision boundary is clear

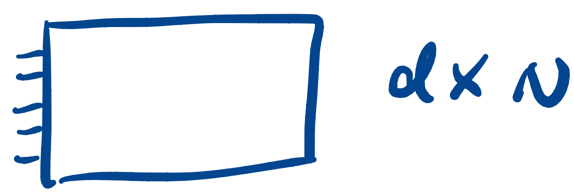
- Cons:

  overfitting

  Accuracy is low

# Random Forest – forest of decision trees

- Build the random forest by training each decision tree on a random subset with replacement from the training data and subset of features are also randomly selected--- "Bagging"
- Evaluate the random forest by testing on its out-of-bag items
- Classify by merging the classifications of individual decision trees
  - By simple vote
  - Or by adding soft classifications together and then take a vote



# An example of bagging

Drawing random samples from our training set with replacement. E.g., if our training set consists of 7 training samples, our bootstrap samples (here: n=7) can look as follows, where $C_1$, $C_2$, … $C_m$ shall symbolize the decision tree classifiers.

| Sample indices | Bagging Round 1 | Bagging Round 2 | … | Bagging Round M |
|---|---|---|---|---|
| 1 | 2 | 7 | | |
| 2 | 2 | 3 | | |
| 3 | 1 | 2 | | |
| 4 | 3 | 1 | | |
| 5 | 4 | 1 | | |
| 6 | 7 | 7 | | |
| 7 | 2 | 1 | | |

$C_1$ — one tree

$C_2$

… $C_M$

$d = 9$

$d_* = 3$ → 5, 6 (for $C_1$); 5, 6 (for $C_2$); $\binom{9}{3}$

# Pros and Cons of Random forest

- Pros: Less prone to overfitting
  better accuracy

- Cons: longer time; bigger complexity
  not intuitive as to
  decision boundary

# Q2. Do you think random forest will always outperform simple decision tree?

A. Yes
B. No

# Considerations in choosing a classifier

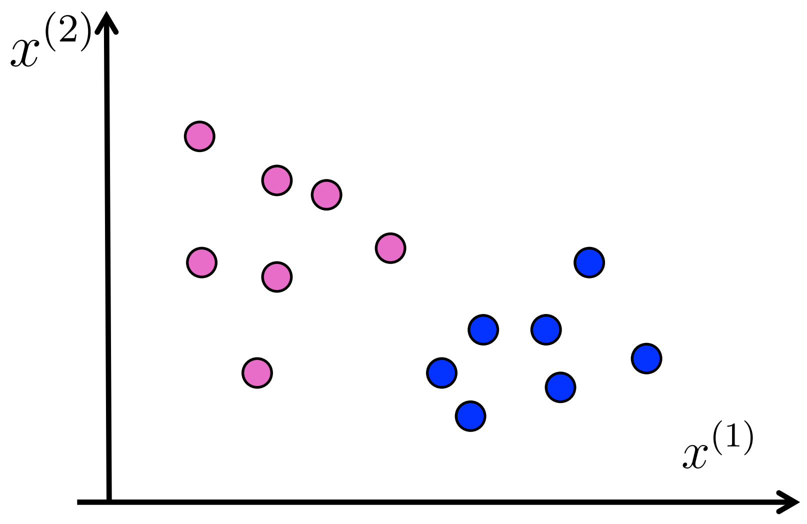
- When solving a classification problem, it is good to try several techniques.
- Criteria to consider in choosing the classifier include
  - * Accuracy
  - * Speed ( testing, and classification)
  - * flexibility (variety of data, small or big)
  - * Intepretation ( decision boundary)
  - * scaling effect

# Support Vector Machine (SVM) overview

- The Decision boundary and function of a Support Vector Machine
- Loss function (cost function in the book)
- Training
- Validation
- Extension to multiclass classification

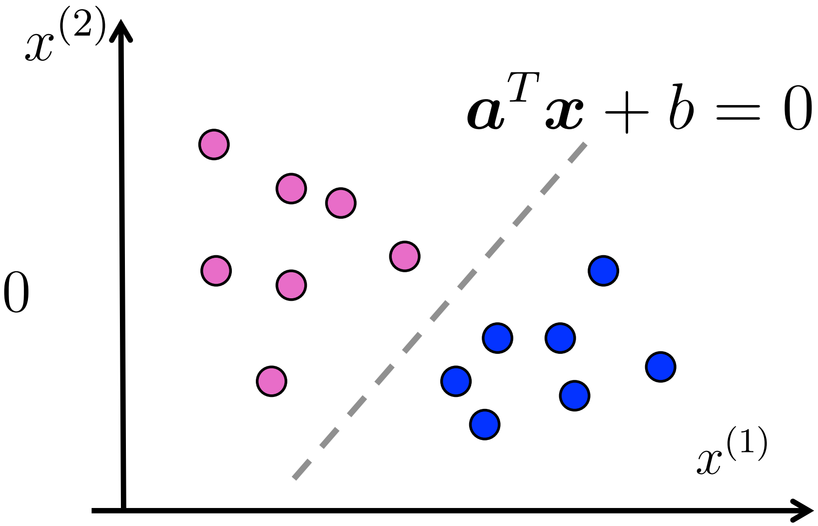
# SVM problem formulation

- At first we assume a binary classification problem
- The training set consists of N items
  - Feature vectors $x_i$ of dimension d
  - Corresponding class labels $y_i \in \{\pm 1\}$
- We can picture the training data as a d-dimensional scatter plot with colored labels



# Decision boundary of SVM

- SVM uses a hyperplane as its **decision boundary**




- The decision boundary is:

$$a_1 x^{(1)} + a_2 x^{(2)} + \ldots + a_d x^{(d)} + b = 0$$

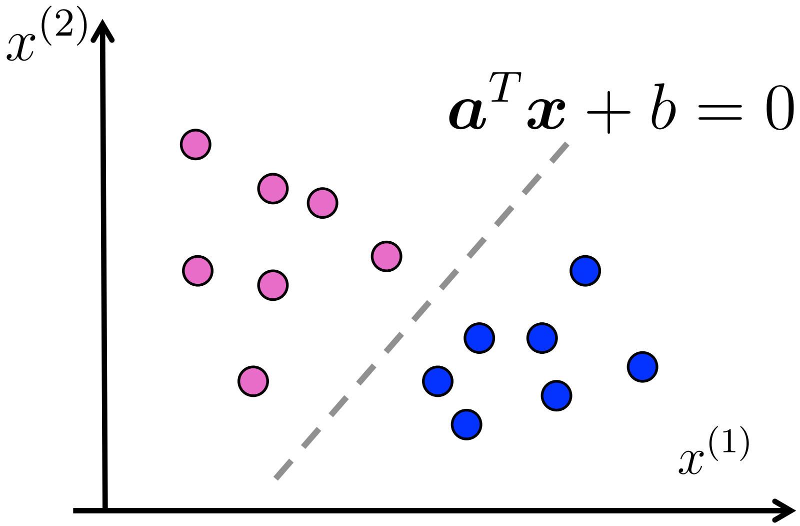
- In vector notation, the hyperplane can be written as:

$$\boldsymbol{a}^T\boldsymbol{x} + b = 0$$

$$\boldsymbol{a} = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_d \end{bmatrix} \quad \boldsymbol{x} = \begin{bmatrix} x^{(1)} \\ x^{(2)} \\ \vdots \\ x^{(d)} \end{bmatrix}$$

# Q3. How many solutions can we have for the decision boundary?

A. One
B. Several
C. Infinite

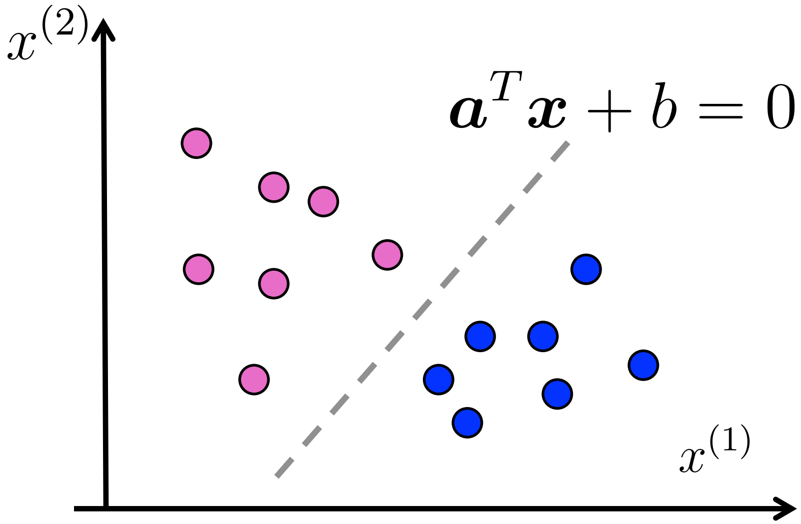


# Classification function of SVM

- SVM assigns a class label to a feature vector according to the following rule:

  +1 if $\boldsymbol{a}^T \boldsymbol{x}_i + b \geq 0$

  -1 if $\boldsymbol{a}^T \boldsymbol{x}_i + b < 0$

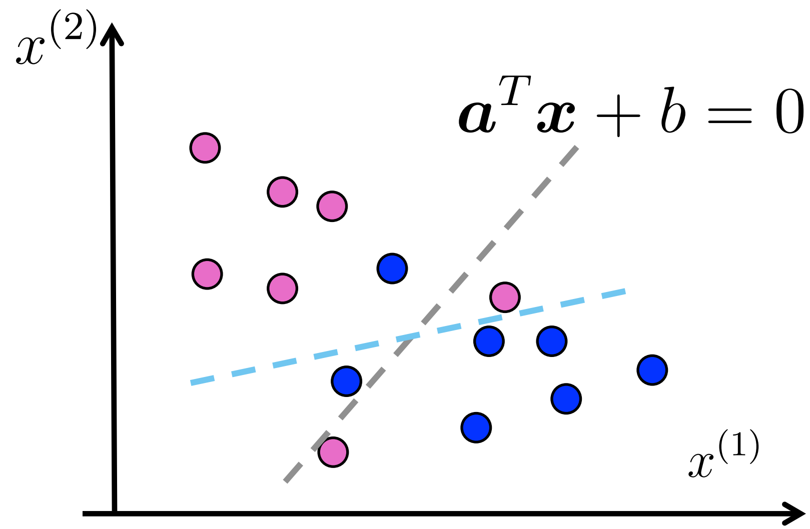



- In other words, the classification function is: $sign(\boldsymbol{a}^T \boldsymbol{x}_i + b)$

- Note that
  - If $|\boldsymbol{a}^T \boldsymbol{x}_i + b|$ is small, then $\boldsymbol{x}_i$ was close to the decision boundary
  - If $|\boldsymbol{a}^T \boldsymbol{x}_i + b|$ is large, then $\boldsymbol{x}_i$ was far from the decision boundary

# What if there is no clean cut boundary?

- Some boundaries are better than others for the training data
- Some boundaries are likely more robust for run-time data
- We need to a quantitative measure to decide about the boundary
- The **loss function** can help decide if one boundary is better than others



# Assignments

- Read Chapter 11 of the textbook
- Next time: SVM-regularization, Stochastic descent

# Additional References


- Robert V. Hogg, Elliot A. Tanis and Dale L. Zimmerman. "Probability and Statistical Inference"
- Morris H. Degroot and Mark J. Schervish "Probability and Statistics"
- Kelvin Murphy, "Machine learning, A Probabilistic perspective"

# See you next time

*See You!*