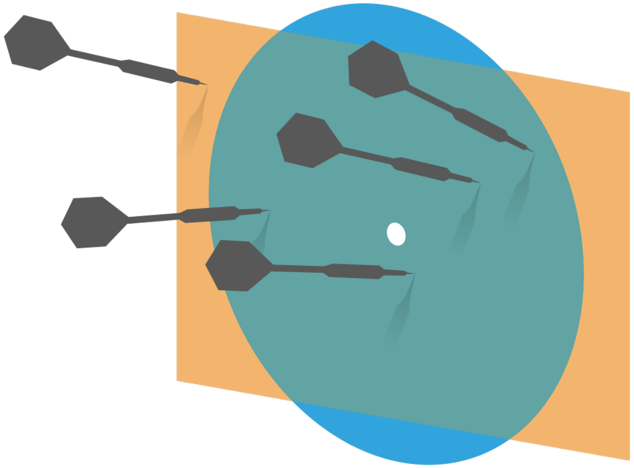
Probability and Statistics for Computer Science



Credit: wikipedia

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

Hongye Liu, Teaching Assistant Prof, CS361, UIUC, 11.03.2021

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?

  $\frac{1}{5} = 20\%$

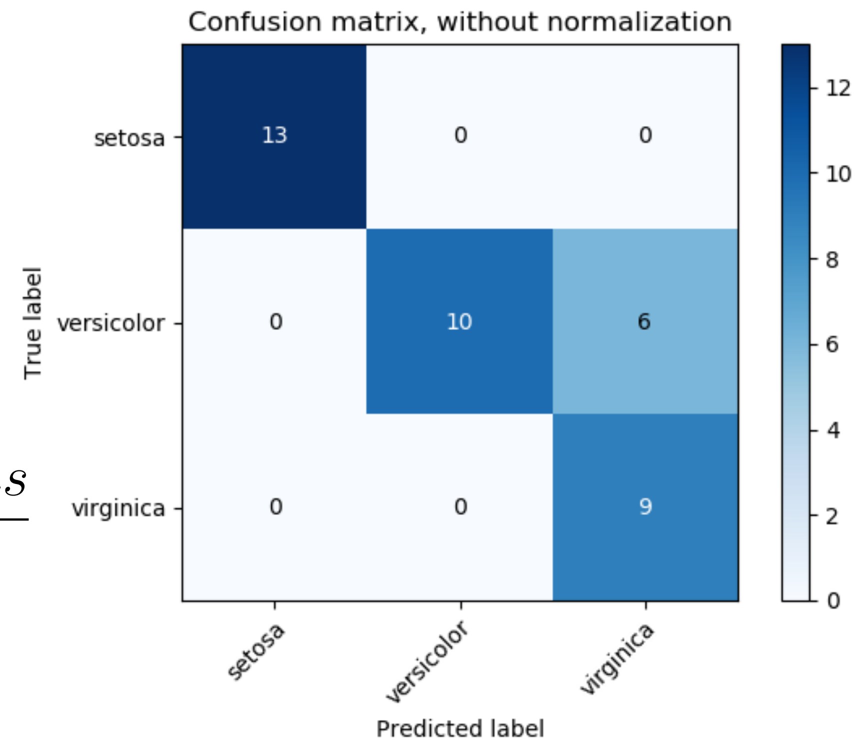
- What's validation and cross-validation in classification?

Performance of a multiclass classifier

- Assuming there are **c** classes:
- The class confusion matrix is c × 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

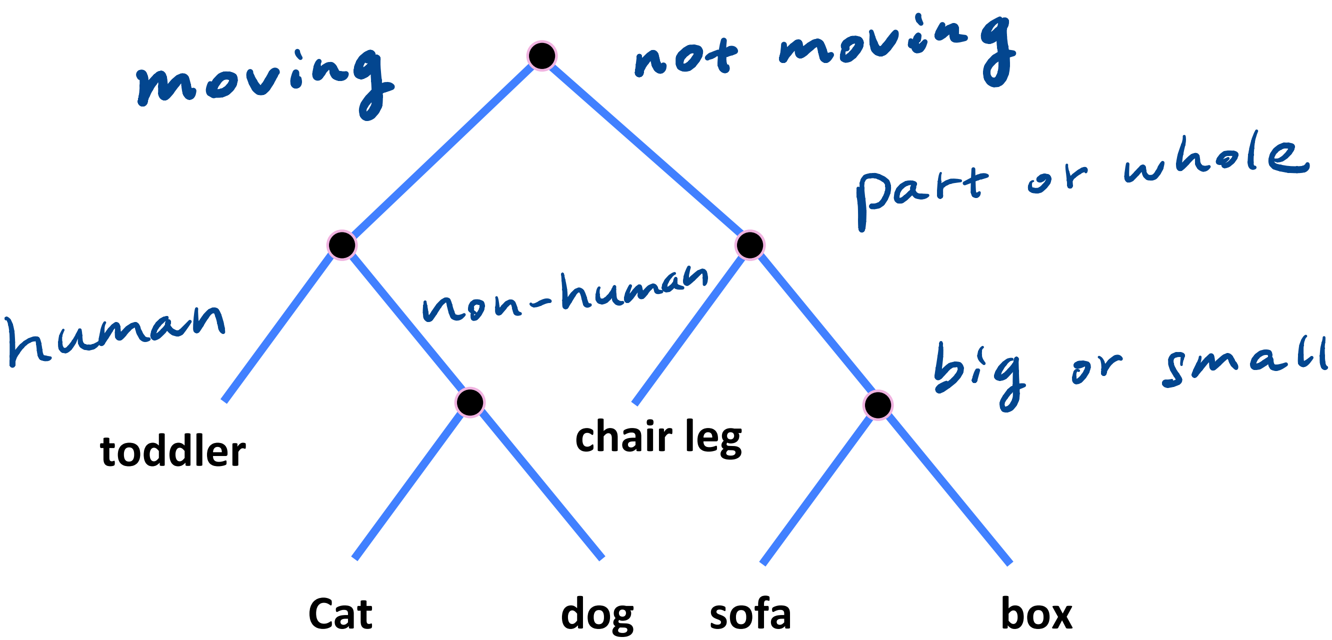
B. FALSE

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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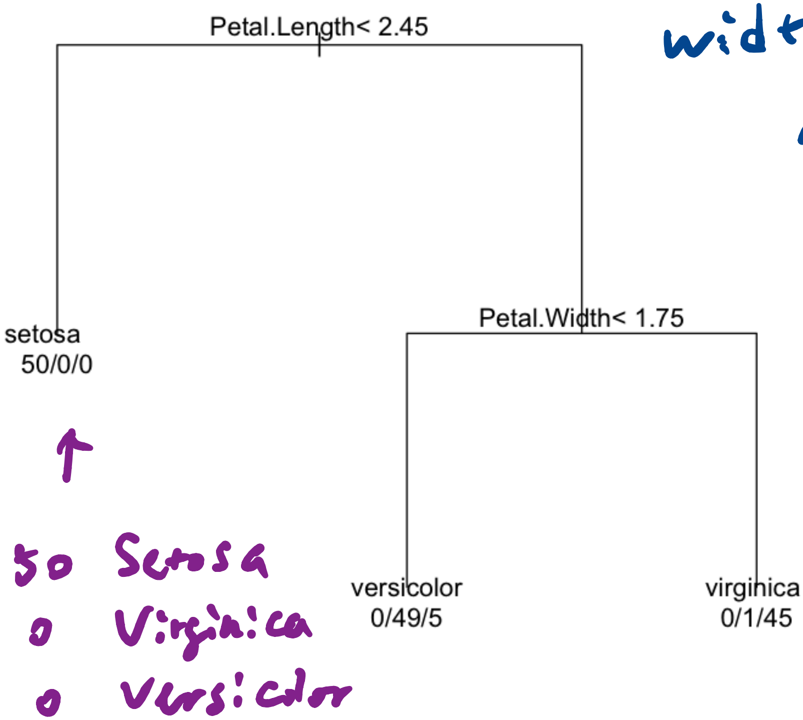
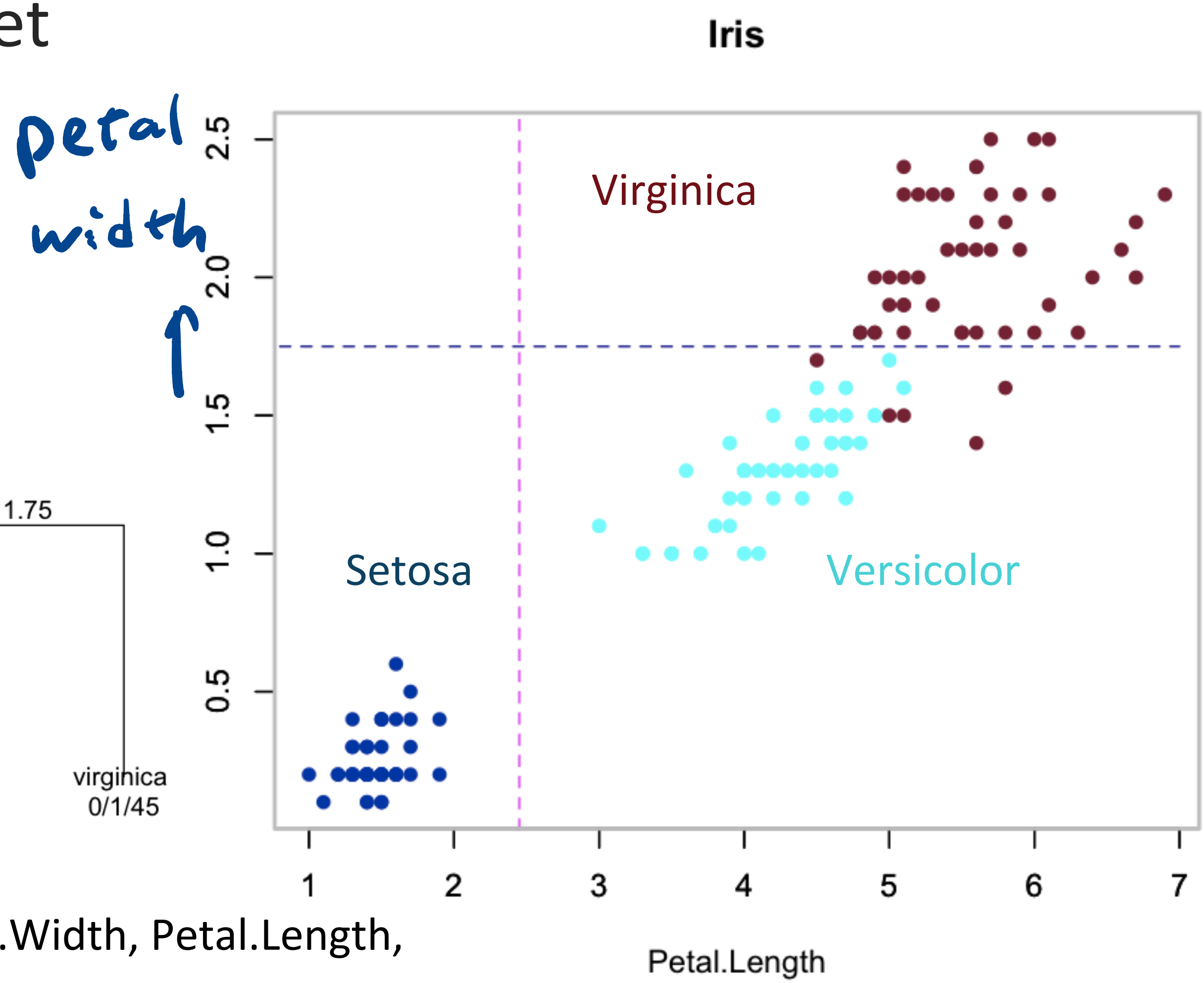
Training a decision tree: example

- The "Iris" data set





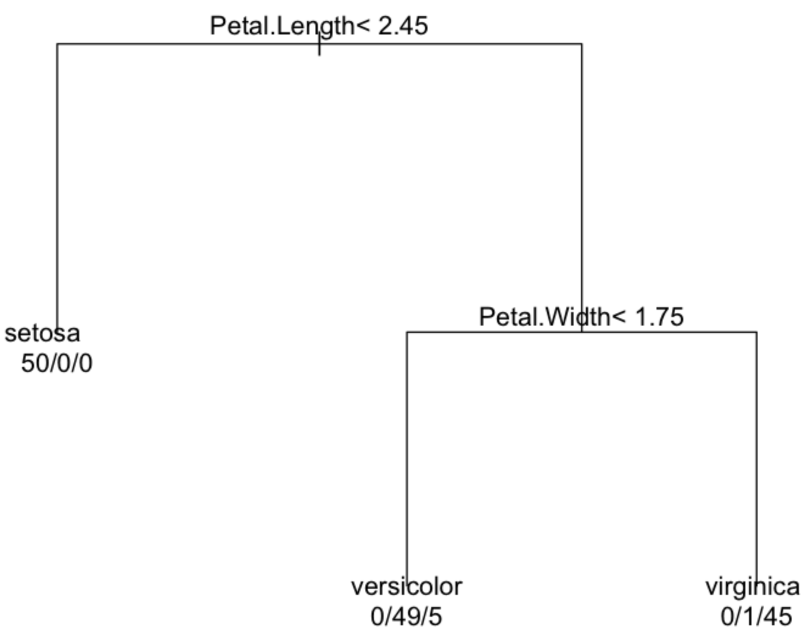
Features: Sepal.Length, Sepal.Width, Petal.Length, Petal.Width **Label**: Species

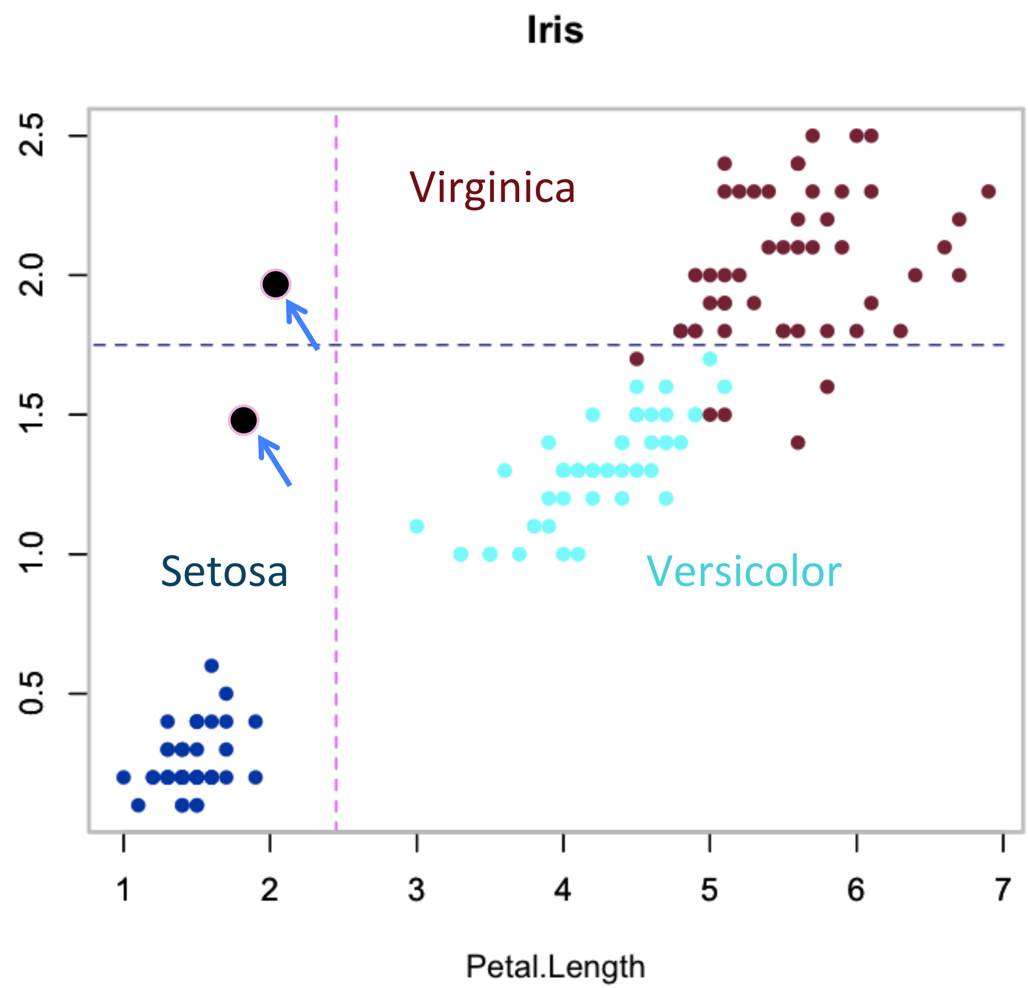
Training a decision tree

- 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





Q: What is accuracy of this decision tree given the confusion matrix ?

$$\begin{bmatrix} 50 & 0 & 0 \\ 0 & 49 & 5 \\ 0 & 1 & 45 \end{bmatrix}$$

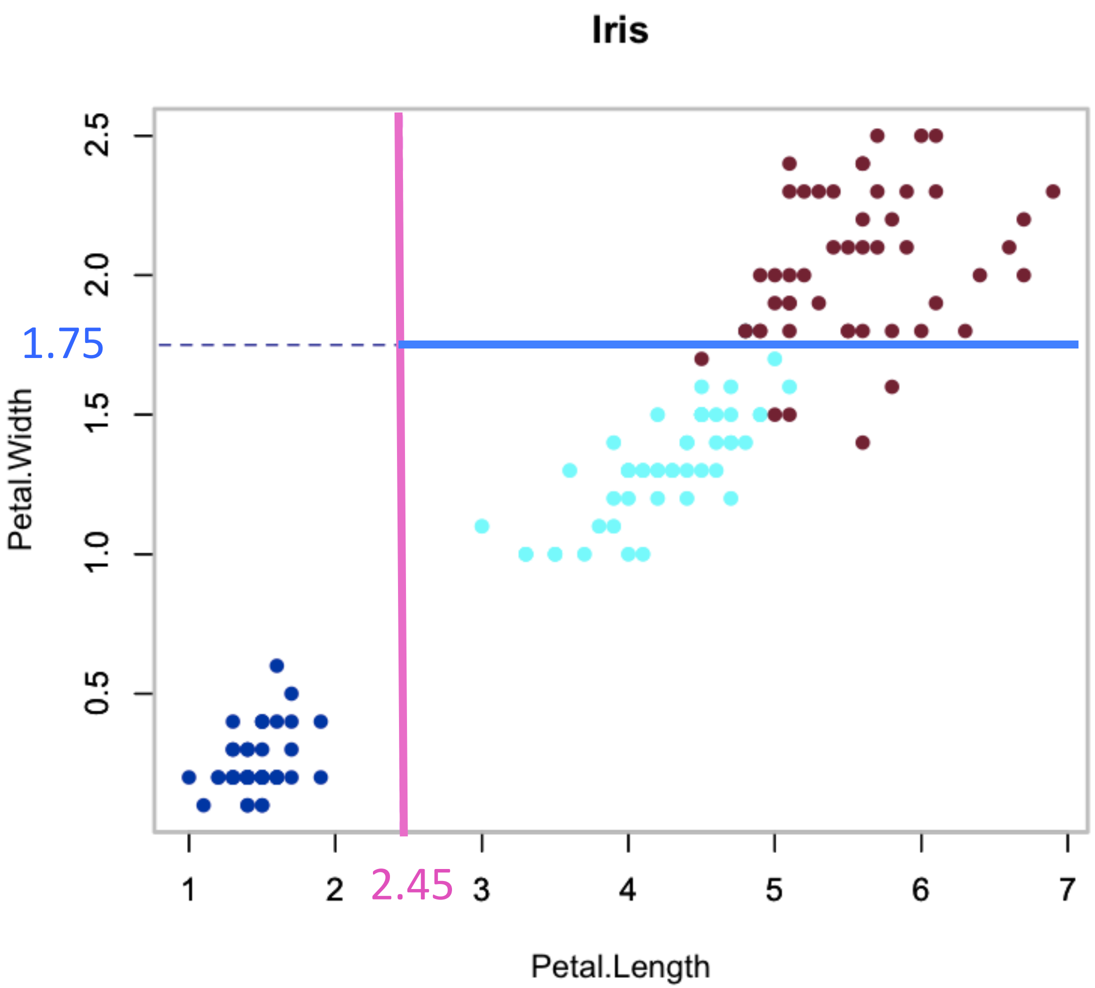
A. 6/150

B. $\boxed{\text{B.}}$ 144/150

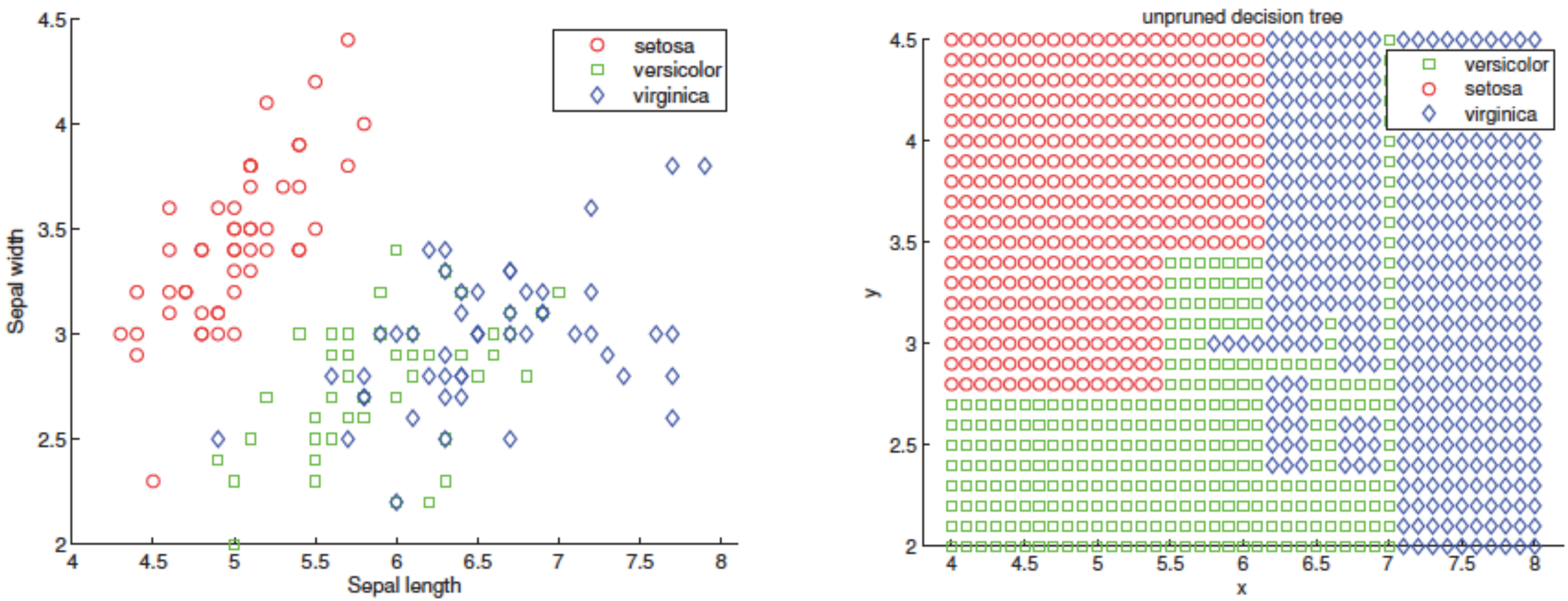
C. 145/150

$$\frac{150-6}{150}$$

Decision Boundary



Another Decision Boundary

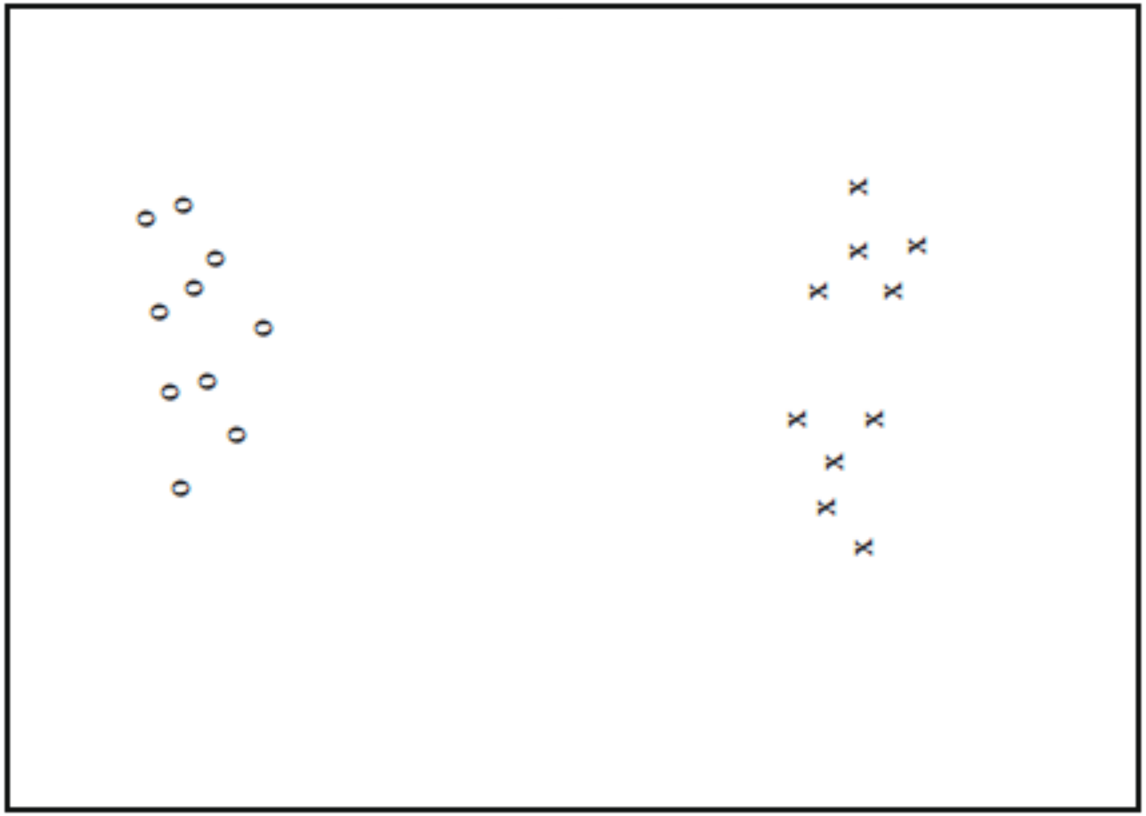


(a) (b)

Credit: Kelvin Murphy, "Machine Learning: A Probabilistic Perspective", 2012

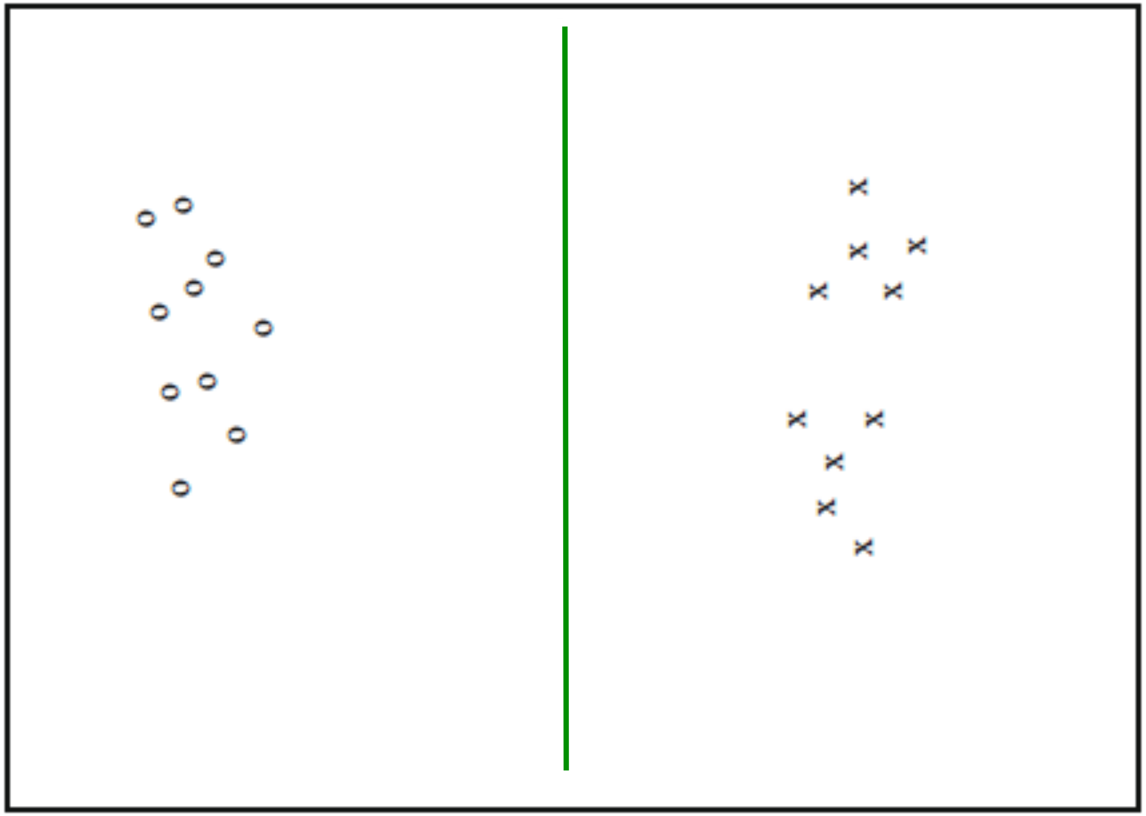
Choosing a split

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



Choosing a split

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



Choosing a split

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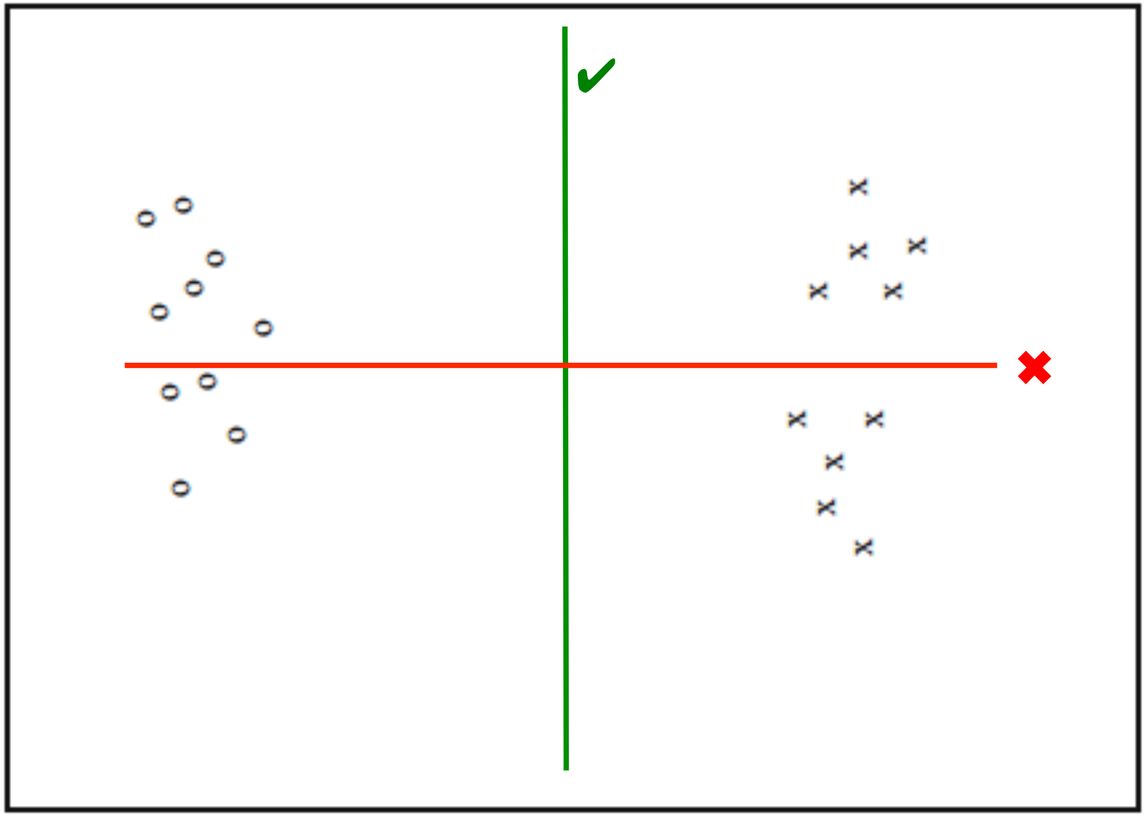
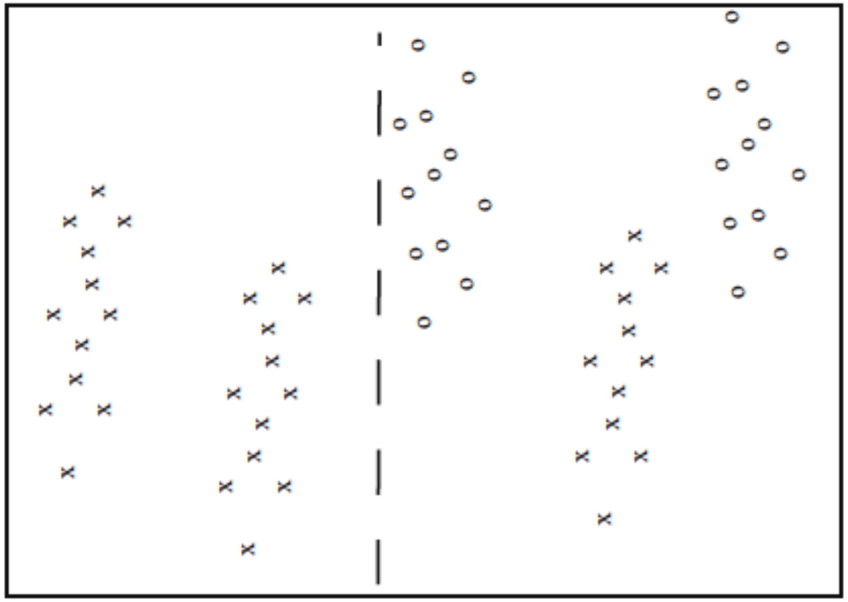
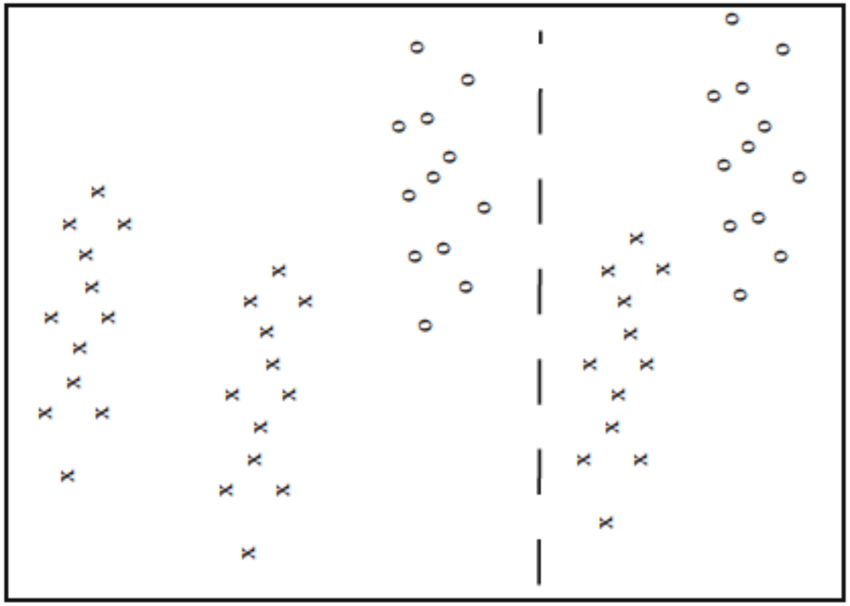


Which is more informative?

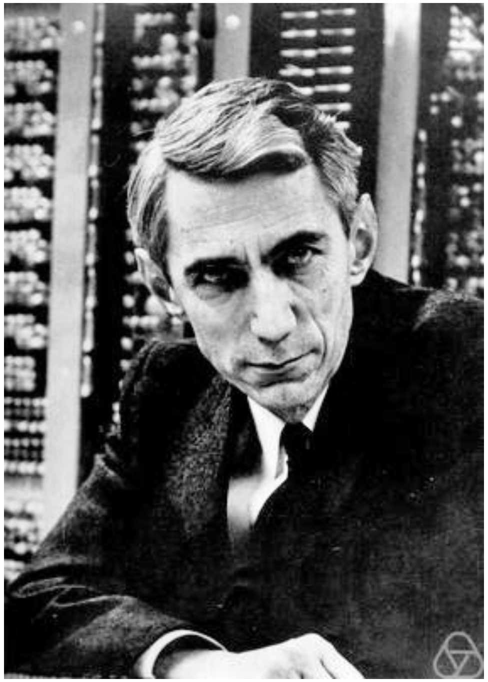




Quantifying uncertainty using entropy

- 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 $Log_2\ 2 = 1$ bit to distinguish 2 equal classes
  - We need $Log_2\ 4 = 2$ bit to distinguish 4 equal classes

0 0
0 1
1 0
1 1



Claude Shannon (1916-2001)

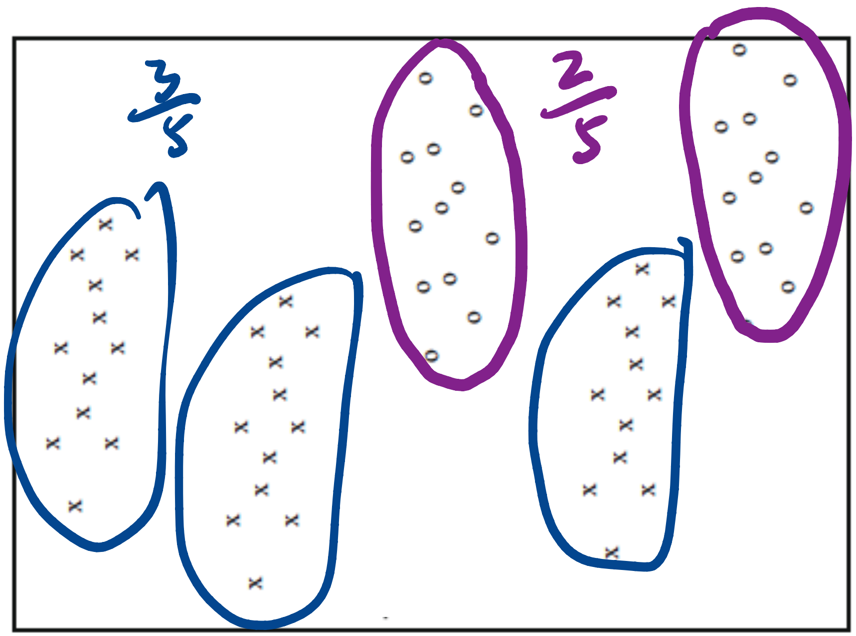
Quantifying uncertainty using entropy

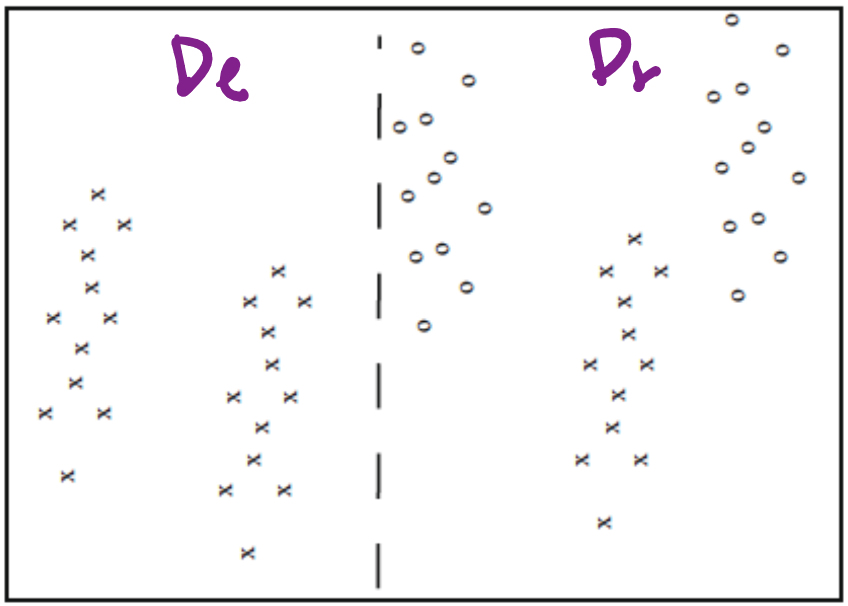
- **Entropy** (Shannon entropy) is the measure of uncertainty for a general distribution
  - If class $\boldsymbol{i}$ contains a fraction $\boldsymbol{P}(\boldsymbol{i})$ of the data, we need $log_2 \dfrac{1}{P(i)}$ bits for that class
  - The entropy H(D) of a dataset is defined as the **weighted mean**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



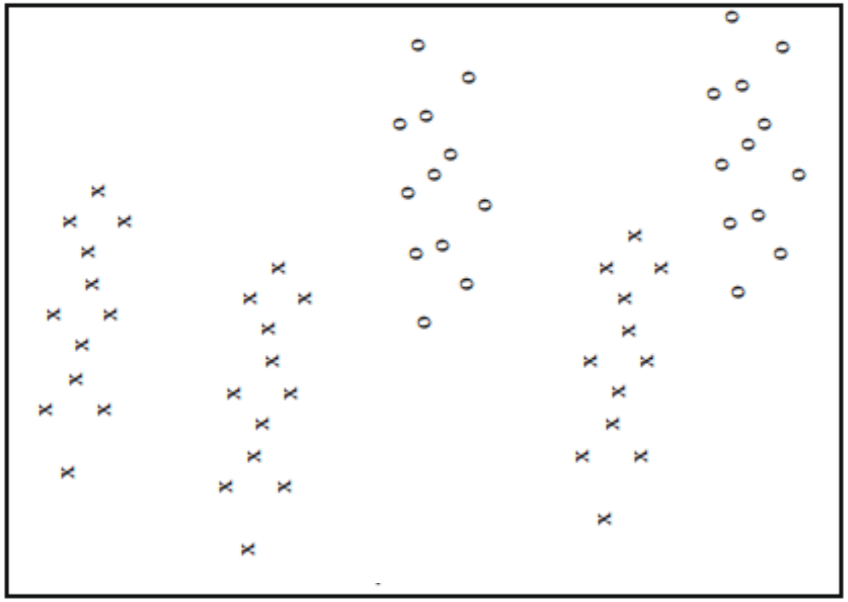


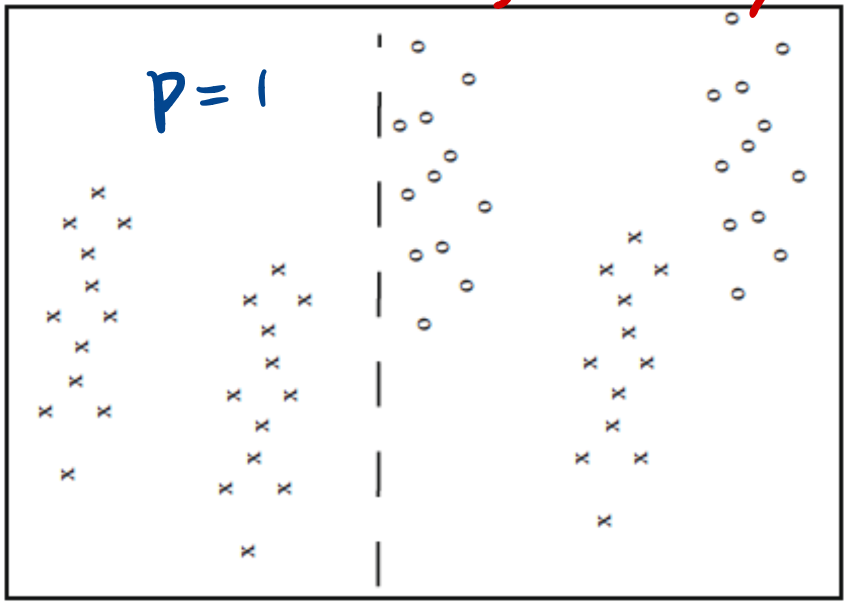
$$H(D) = -\frac{3}{5}log_2\frac{3}{5} - \frac{2}{5}log_2\frac{2}{5}$$

$$= 0.971\ bits$$

Entropy: examples

$\frac{2}{3}$ o $\frac{1}{3}$ x





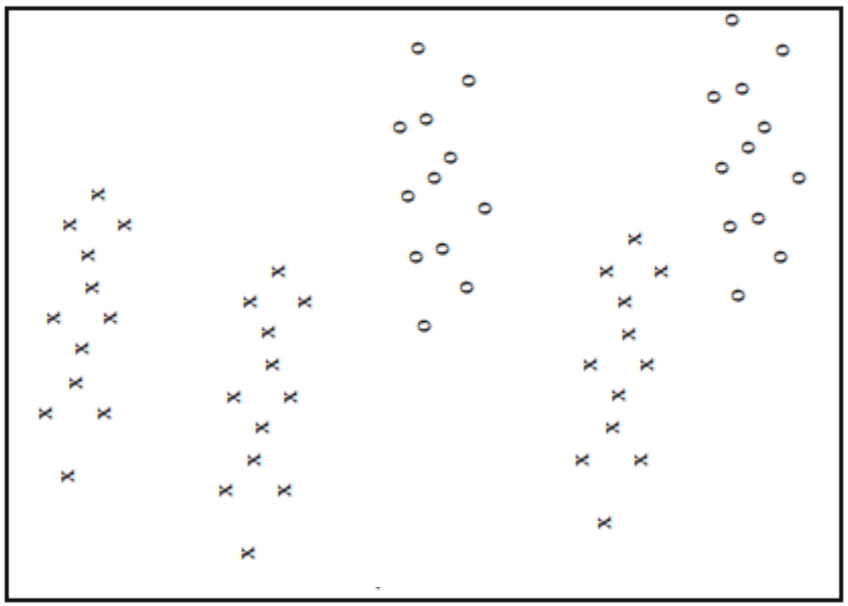
$$H(D) = -\frac{3}{5}log_2\frac{3}{5} - \frac{2}{5}log_2\frac{2}{5}$$

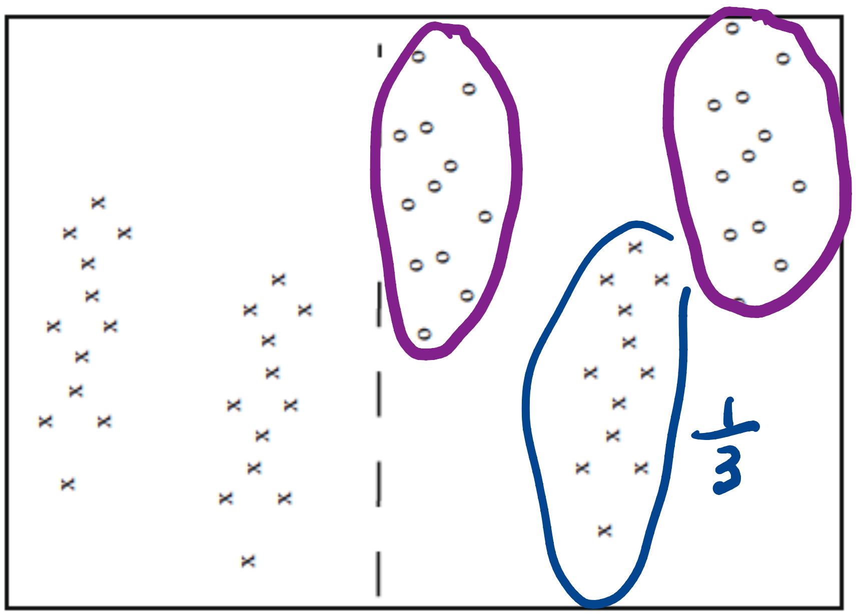
$$= 0.971\ bits$$

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

$H(D_r) = ?$

Entropy: examples





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

$$= 0.971\ bits$$

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

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

$$= 0.918\ bits$$

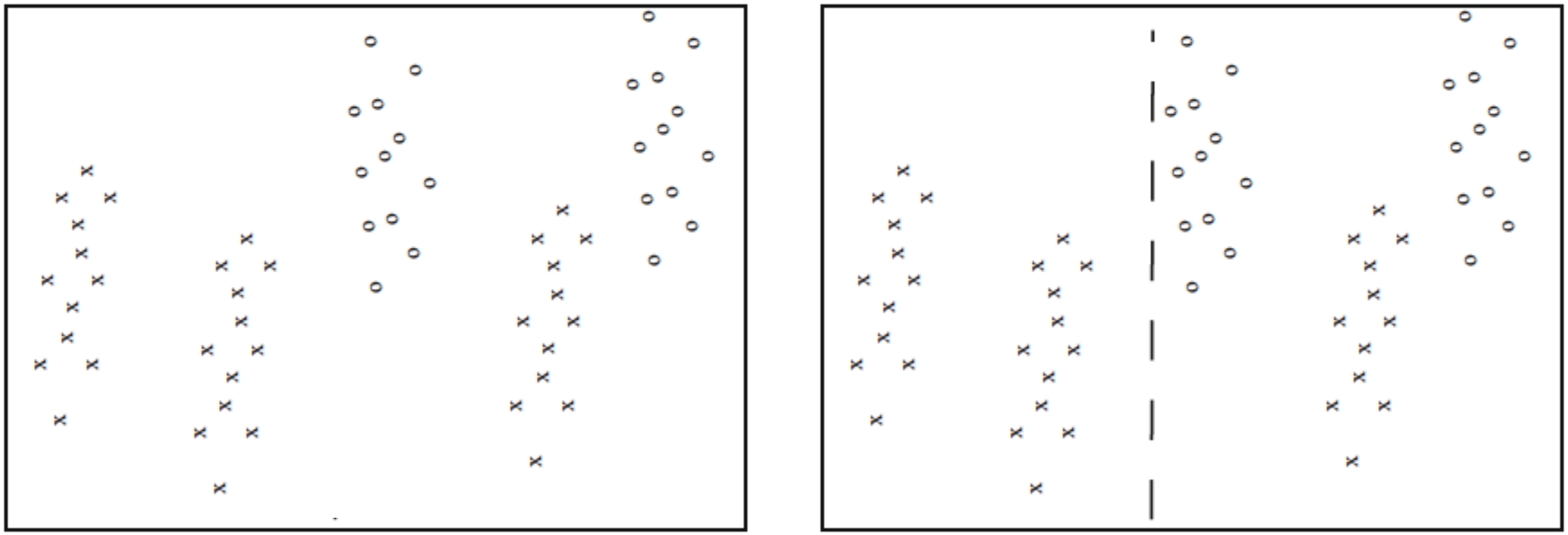
Information gain of a split

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

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

- 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

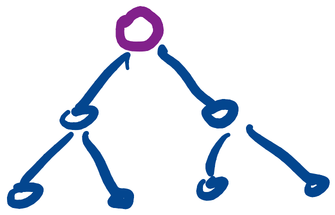


$$I = H(D) - (\frac{N_{Dl}}{N_D}H(D_l) + \frac{N_{Dr}}{N_D}H(D_r))$$
$$= 0.971 - (\frac{24}{60} \times 0 + \frac{36}{60} \times 0.918)$$
$$= 0.420\ bits$$

Q. Is the splitting method global optimum?

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

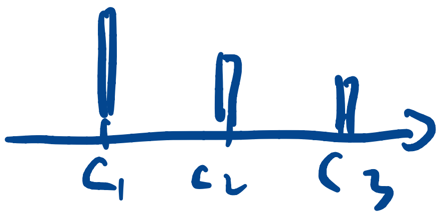
When to stop growing the decision tree?

- 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:

  Flexible (all data types)

  Interpretable

  clear decision boundary

  Quick

- Cons:

  overfit

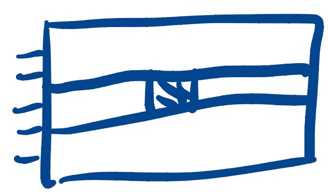
  Accuracy is low

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



$d \times N$

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 C_2 ... C_m

d^*

5
6

Pros and Cons of Random forest

- Pros: better accu.

  less prone to overfitting.

- Cons: longer

  complex

  no clear decision boundary

  Not interpretable

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

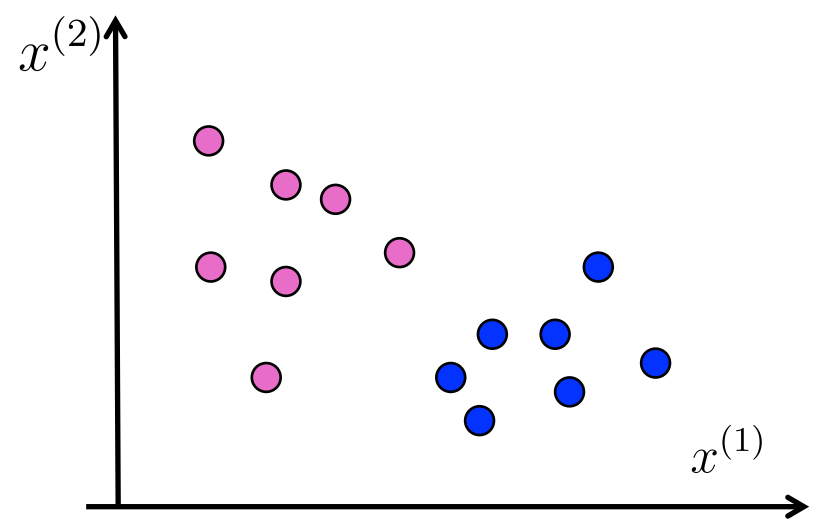
* Accuracy
* Speed (testing, and classification)
* flexibility (variety of data, small or big)
* Intepretation (decision boundary)
* scaling effect

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

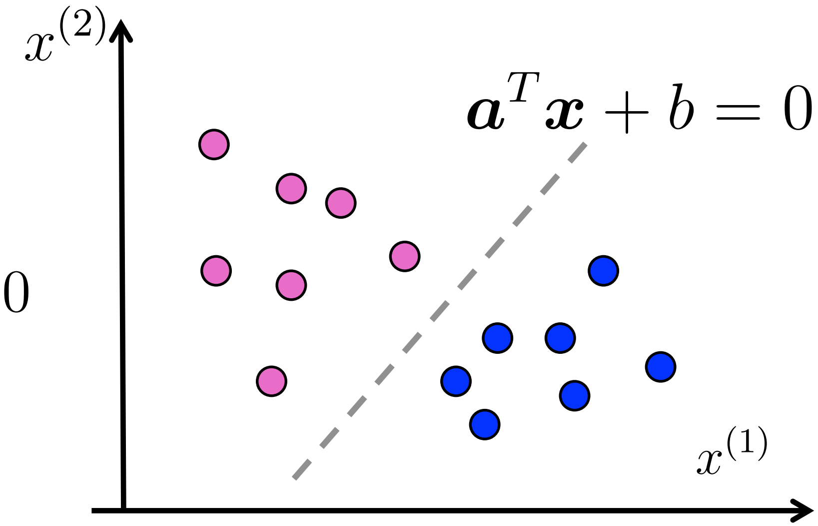
SVM problem formulation

- 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:

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

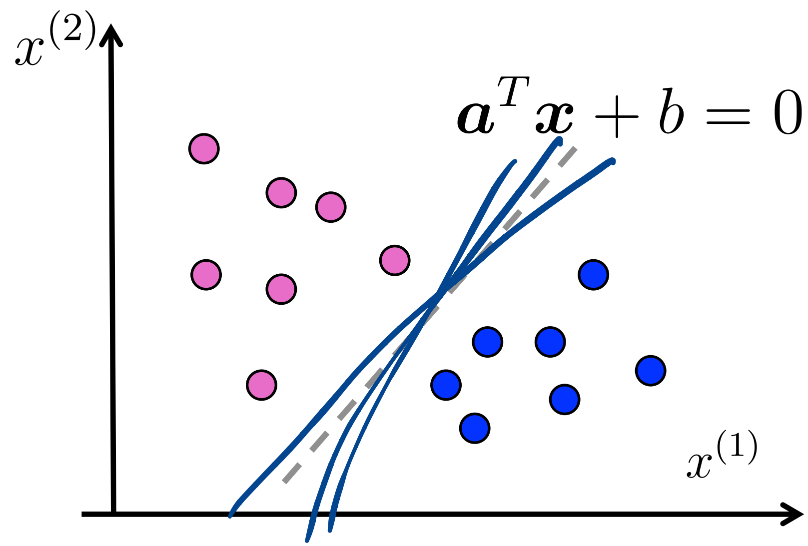
- In vector notation, the hyperplane can be written as:

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

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

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

A. One
B. Several
C. Infinite

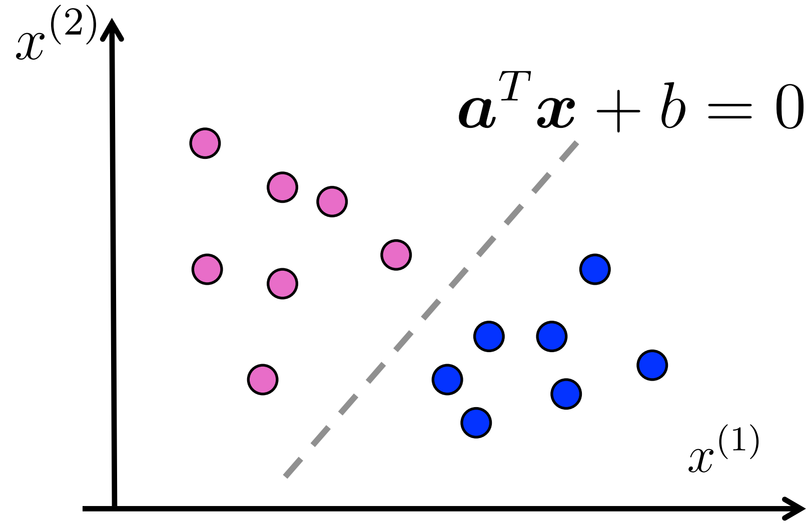


Classification function of SVM

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

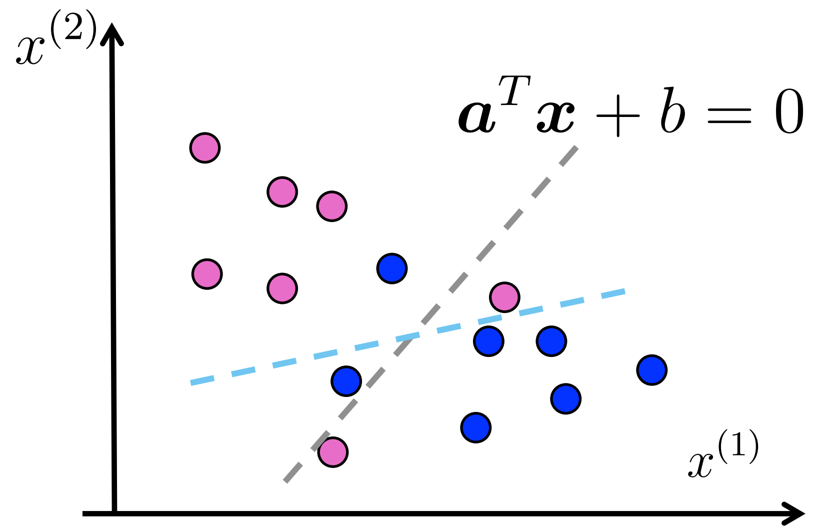
- In other words, the classification function is: $sign(\boldsymbol{a}^T\boldsymbol{x}_i + b)$



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

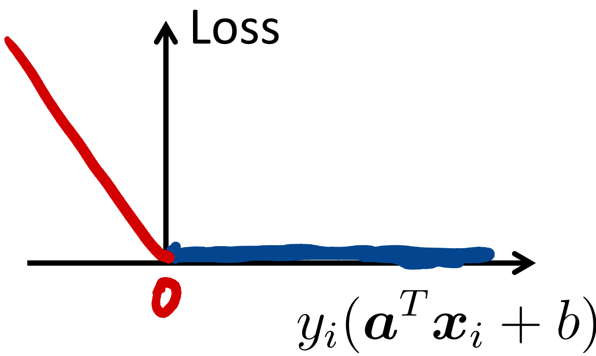


Loss function 1

- For any given feature vector $\boldsymbol{x}_i$ with class label $y_i \in \{\pm 1\}$, we want
  - Zero loss if $\boldsymbol{x}_i$ is classified correctly $sign(\boldsymbol{a}^T\boldsymbol{x}_i + b) = y_i$
  - Positive loss if $\boldsymbol{x}_i$ is misclassified $sign(\boldsymbol{a}^T\boldsymbol{x}_i + b) \neq y_i$
  - If $\boldsymbol{x}_i$ is misclassified, more loss is assigned if it's further away from the boundary

- This loss function 1 meets the criteria above:

$$max(0, -y_i(\boldsymbol{a}^T\boldsymbol{x}_i + b))$$



- Training error cost

$$S(\boldsymbol{a}, b) = \frac{1}{N}\sum_{i=1}^{N} max(0, -y_i(\boldsymbol{a}^T\boldsymbol{x}_i + b))$$

Q4. What's the value of this function ?

$$max(0, -y_i(\boldsymbol{a}^T\boldsymbol{x}_i + b)) \quad \text{if} \quad sign(\boldsymbol{a}^T\boldsymbol{x}_i + b) = y_i$$

A. 0.
B. others.

Q5. What's the value of this function ?

$$max(0, -y_i(\boldsymbol{a}^T\boldsymbol{x}_i + b)) \quad \text{if} \quad sign(\boldsymbol{a}^T\boldsymbol{x}_i + b) \neq y_i$$

A. 0.
B. A value greater than or equal to 0.

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!