http://poloclub.gatech.edu/cse6242

CSE6242: Data & Visual Analytics

Classification Key Concepts

Duen Horng (Polo) Chau

Associate Professor, College of Computing

Associate Director, MS Analytics

Georgia Tech

Mahdi Roozbahani

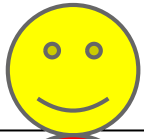
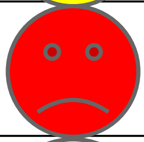
Lecturer, Computational Science & Engineering, Georgia Tech

Founder of Filio, a visual asset management platform

Partly based on materials by

Professors Guy Lebanon, Jeffrey Heer, John Stasko, Christos Faloutsos

How will I rate "Chopin's 5th Symphony"?

Songs	**Like?**
Some nights	
Skyfall	
Comfortably numb	
We are young	
...	...
...	...
Chopin's 5th	???

Classification

What tools do you need for classification?

1. **Data** $S = \{(x_i, y_i)\}_{i = 1,...,n}$
   - x_i : data example with d attributes
   - y_i : label of example (what **you** care about)

2. Classification **model** $f_{(a,b,c,....)}$ with some parameters $a, b, c, ...$
3. **Loss function** $L(y, f(x))$
   - how to penalize mistakes

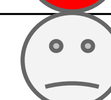
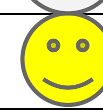
Terminology Explanation

data example = data instance
attribute = feature = dimension
label = target attribute

Data $S = \{(x_i, y_i)\}_{i = 1,\dots,n}$

- x_i : data example with d attributes
- y_i : label of example

$$x_i = (x_{i1}, \dots, x_{id})$$

Song name	Artist	Length	...	Like?
Some nights	Fun	4:23	...	
Skyfall	Adele	4:00	...	
Comf. numb	Pink Fl.	6:13	...	
We are young	Fun	3:50	...	
...	...	...	...	...
...	...	...	...	...
Chopin's 5th	Chopin	5:32	...	??

What is a "model"?

"a simplified representation of reality created to serve a purpose" *Data Science for Business*

Example: maps are abstract models of the physical world

There can be many models!!

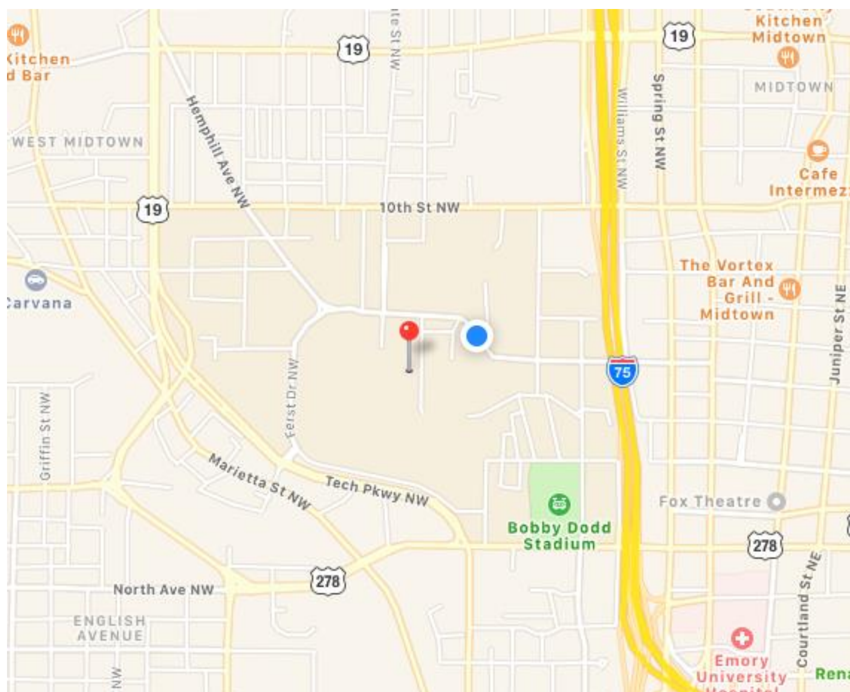
(Everyone sees the world differently, so each of us has a different model.)

In data science, a model is **formula to estimate what you care about**. The formula may be mathematical, a set of rules, a combination, etc.

Training a classifier = building the “model”

How do you learn appropriate values for parameters *a, b, c, ...* ?

Analogy: how do you know your map is a “good” map of the physical world?



Classification loss function

Most common loss: **0-1 loss function**

$$L_{0-1}(y, f(x)) = \mathbb{I}(y \neq f(x))$$

More general loss functions are defined by a *m x m* cost matrix *C* such that

$$L(y, f(x)) = C_{ab}$$

where *y* = *a* and *f(x)* = *b*

Class	P0	P1
T0	0	C_{10}
T1	C_{01}	0

T0 (true class 0), **T1** (true class 1)

P0 (predicted class 0), **P1** (predicted class 1)

An ideal model should correctly estimate:

- known or seen data examples' labels
- unknown or unseen data examples' labels

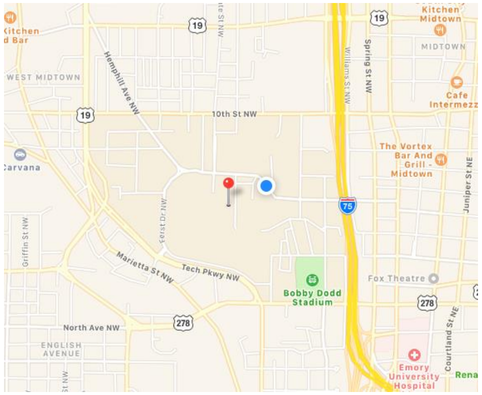
Song name	**Artist**	**Length**	**...**	**Like?**
Some nights	Fun	4:23	...	
Skyfall	Adele	4:00	...	
Comf. numb	Pink Fl.	6:13	...	
We are young	Fun	3:50	...	
...	...	...	...	...
...	...	...	...	...
Chopin's 5th	Chopin	5:32	...	??

Training a classifier = building the "model"

Q: How do you learn appropriate values for parameters *a, b, c, ...* ?
(Analogy: how do you know your map is a "good" map?)

- $y_i = f_{(a,b,c,....)}(x_i),\ i = 1, ..., n$
  - Low/no error on training data ("seen" or "known")
- $y = f_{(a,b,c,....)}(x)$, for any new x
  - Low/no error on test data ("unseen" or "unknown")

It is very easy to achieve perfect classification on training/seen/known data. Why?



If your model works really well for *training* data, but poorly for *test* data, your model is “overfitting”.

How to avoid overfitting?

Example: one run of *5-fold* cross validation

You should do a **few runs** and **compute the average**
(e.g., error rates if that's your evaluation metrics)

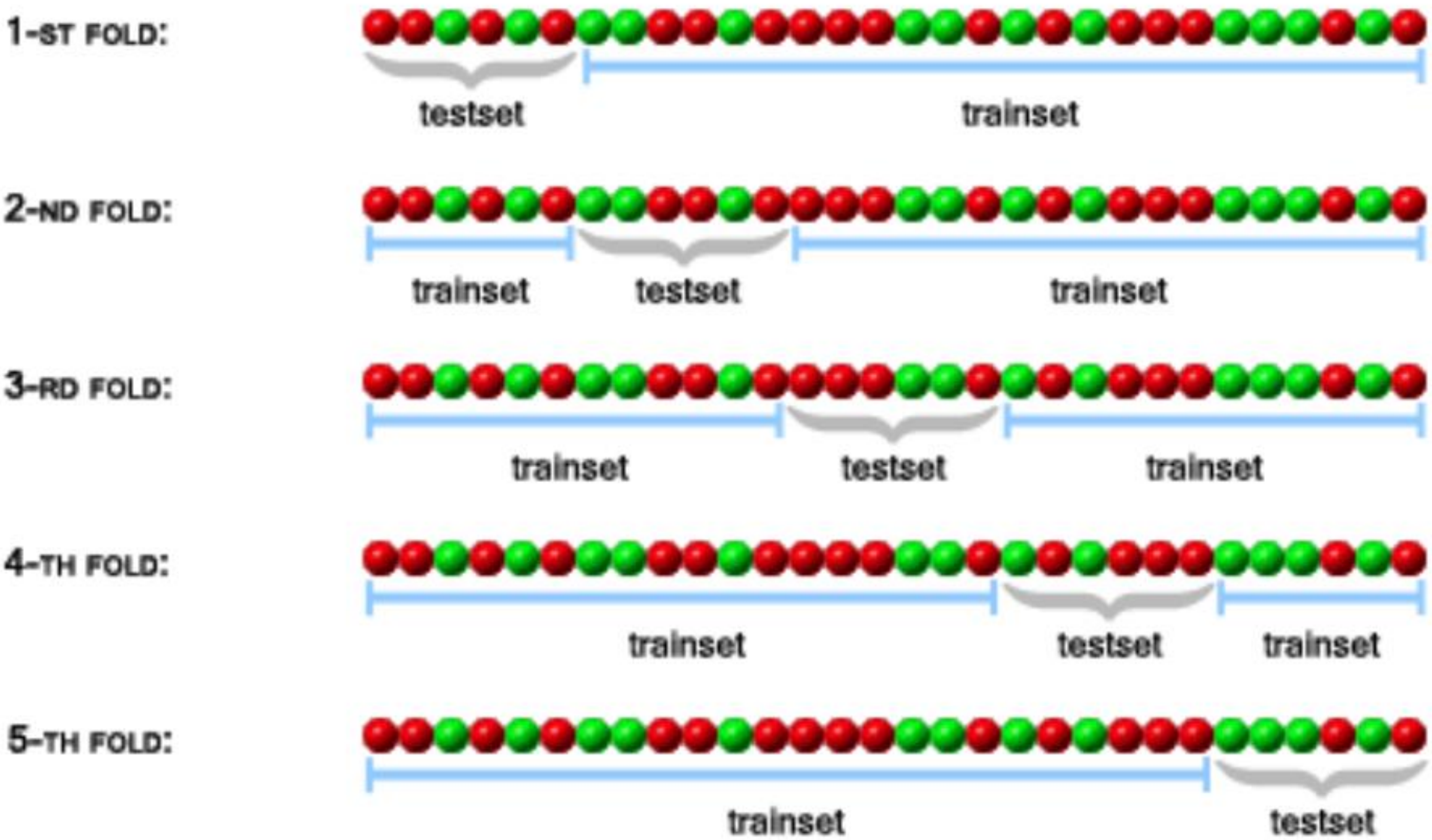
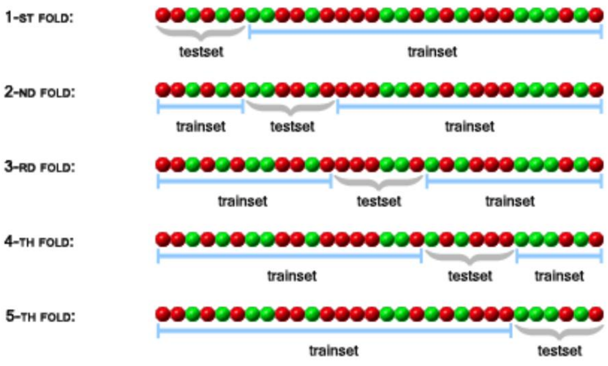


Image credit: http://stats.stackexchange.com/questions/1826/cross-validation-in-plain-english

Cross validation



1. Divide your data into n parts
2. Hold 1 part as “test set” or “hold out set”
3. Train classifier on remaining n-1 parts “training set”
4. Compute test error on test set
5. Repeat above steps n times, once for each n-th part
6. Compute the average test error over all n folds (i.e., cross-validation test error)

Cross-validation variations

K-fold cross-validation

- Test sets of size *(n / K)*
- K = 10 is most common (i.e., 10-fold CV)

Leave-one-out cross-validation (LOO-CV)

- test sets of size 1

Example:
k-Nearest-Neighbor classifier

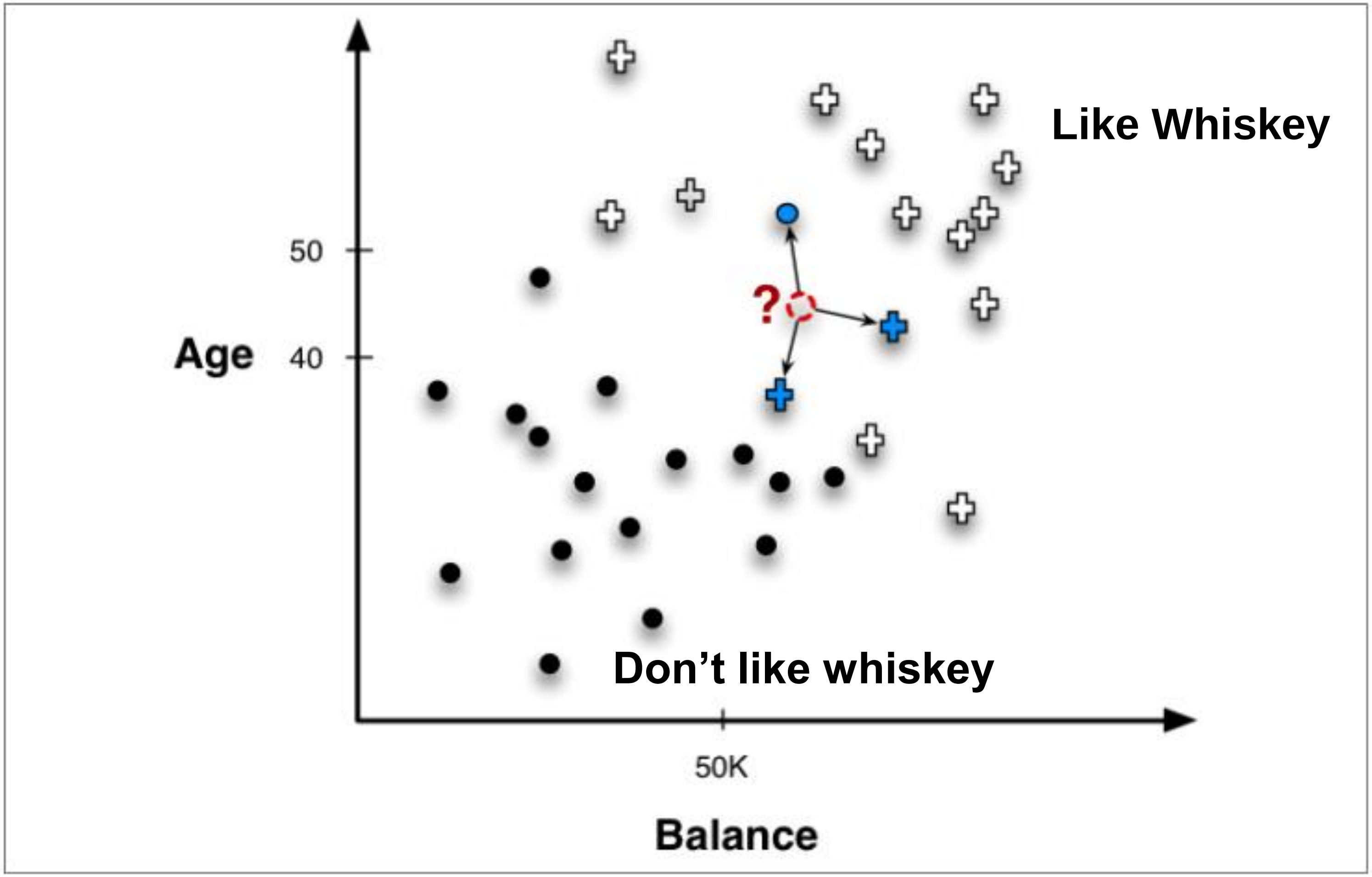


Figure 6-2. Nearest neighbor classification. The point to be classified, labeled with a question mark, would be classified + because the majority of its nearest (three) neighbors are +.

Image credit: Data Science for Business

But k-NN is so simple!

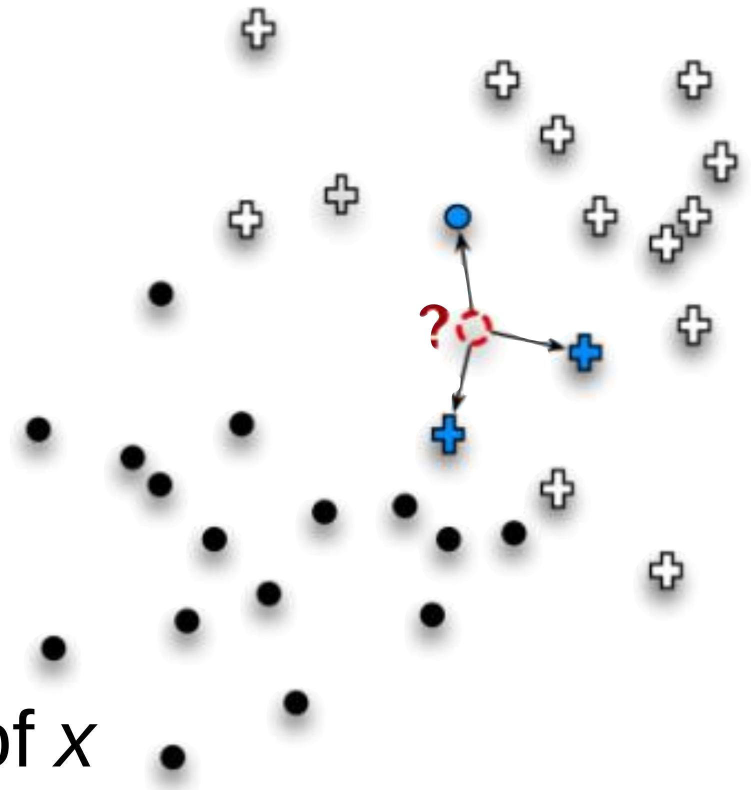
It can work really well! **Pandora** (acquired by SiriusXM) uses it or has used it: https://goo.gl/foLfMP
(from the book “Data Mining for Business Intelligence”)

Image credit: https://www.fool.com/investing/general/2015/03/16/will-the-music-industry-end-pandoras-business-mode.aspx

What are good models?

Simple (few parameters)	Effective	
Complex (more parameters)	Effective (if significantly more so than simple methods)	
Complex (many parameters)	Not-so-effective	😱

k-Nearest-Neighbor Classifier



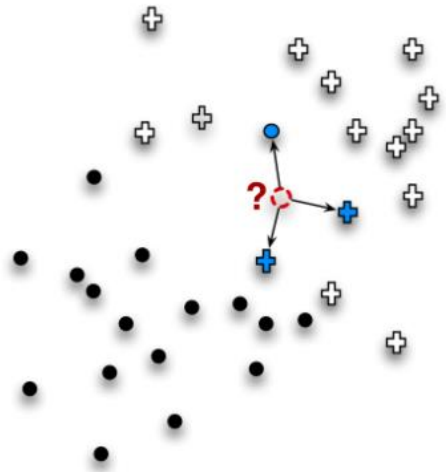
The classifier:

f(*x*) = majority label of the *k* nearest neighbors (NN) of *x*

Model parameters:

- Number of neighbors *k*
- Distance/similarity function *d(.,.)*

k-Nearest-Neighbor Classifier



If *k* and *d(.,.)* are fixed

Things to learn: ?

How to learn them: ?

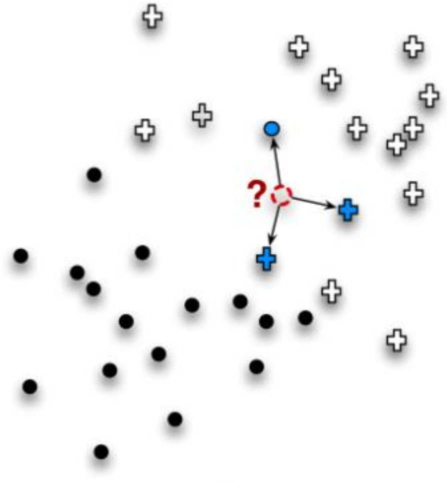
If *d(.,.)* is fixed, but you can change *k*

Things to learn: ?

How to learn them: ?

$x_i = (x_{i1}, \ldots, x_{id}); y_i = \{1, \ldots, m\}$

k-Nearest-Neighbor Classifier



If *k* and *d(.,.)* are fixed

Things to learn: Nothing

How to learn them: N/A

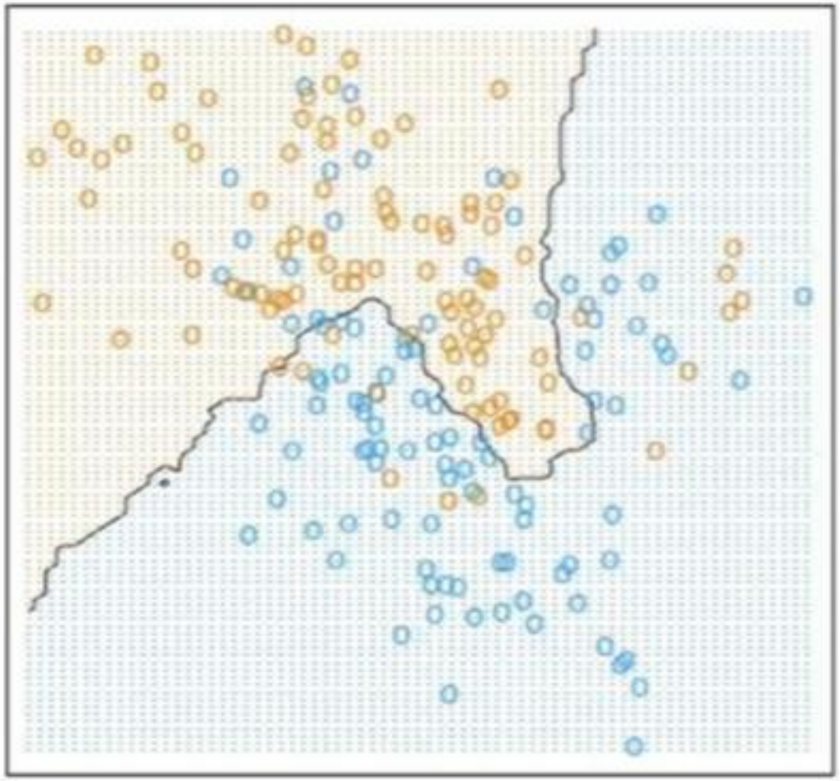
If *d(.,.)* is fixed, but you can change *k*

Selecting *k*: How?

How to find best k in k-NN?

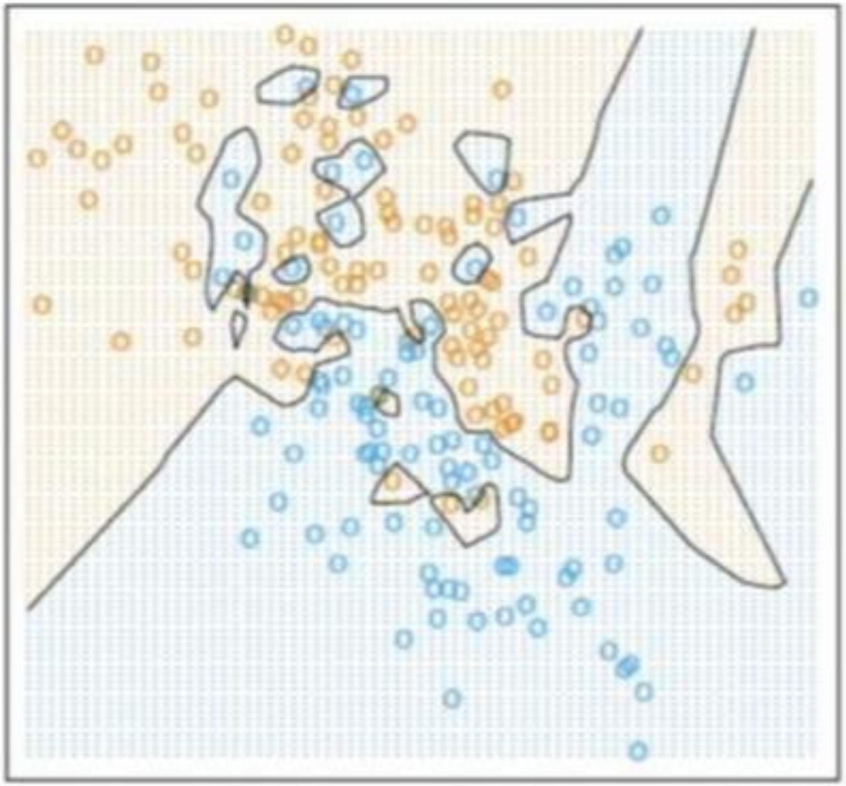
Use **cross validation (CV)**.

15-NN



Pretty good!

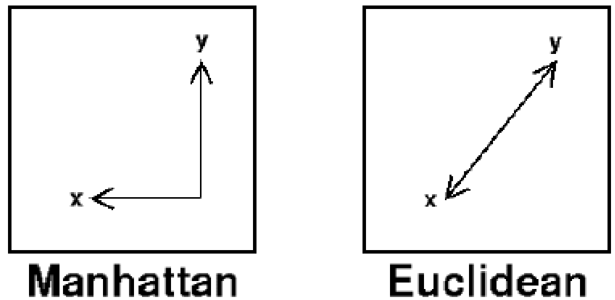
1-NN



Overfitted

k-Nearest-Neighbor Classifier

If *k* is fixed, but you can change *d(.,.)*



Possible distance functions:

- Euclidean distance: $\|x_i - x_j\|_2 = \sqrt{(x_i - x_j)^\top (x_i - x_j)}$
- Manhattan distance: $\|x_i - x_j\|_1 = \sum_{l=1}^{d} |x_{il} - x_{jl}|$
- …

$x_i = (x_{i1}, \ldots, x_{id}); y_i = \{1, \ldots, m\}$

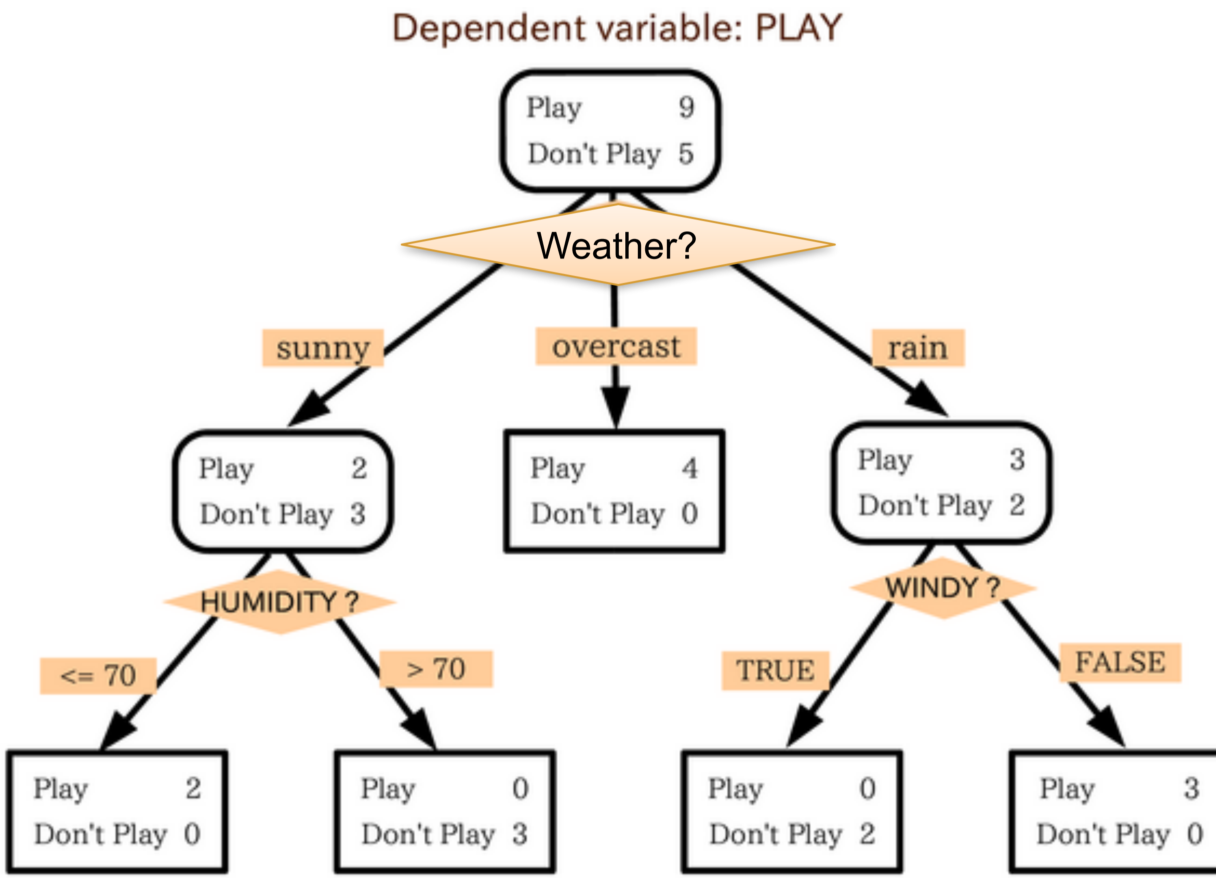
Summary on k-NN classifier

- Advantages
  - Little learning (unless you are learning the distance functions)
  - Quite powerful in practice (and has theoretical guarantees)
- Caveats
  - Computationally expensive at test time

Reading material:

- The Elements of Statistical Learning (ESL) book, Chapter 13.3
  https://web.stanford.edu/~hastie/ElemStatLearn/

Decision trees (DT)



The classifier:

$f_T(x)$: majority class in the leaf in the tree T containing x

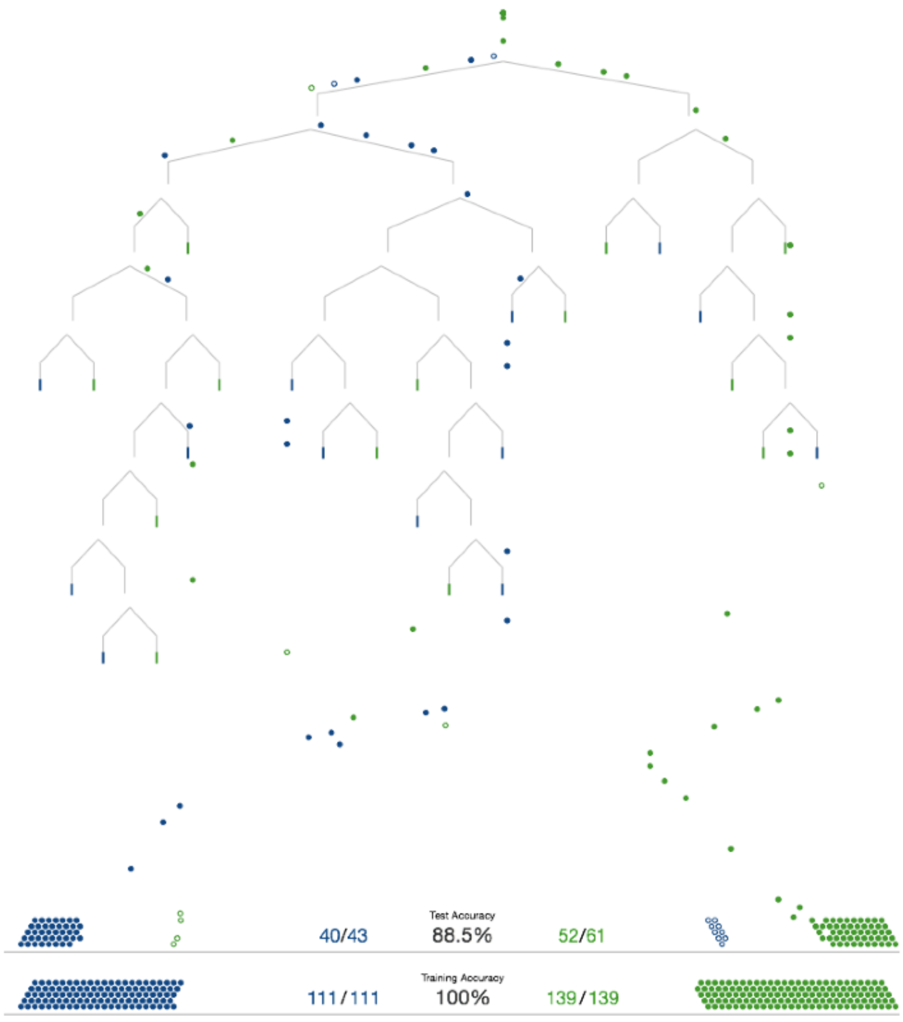
Model parameters: The tree structure and size

Highly recommended!

Visual Introduction to Decision Tree

Building a tree to distinguish homes in New York from homes in San Francisco

http://www.r2d3.us/visual-intro-to-machine-learning-part-1/

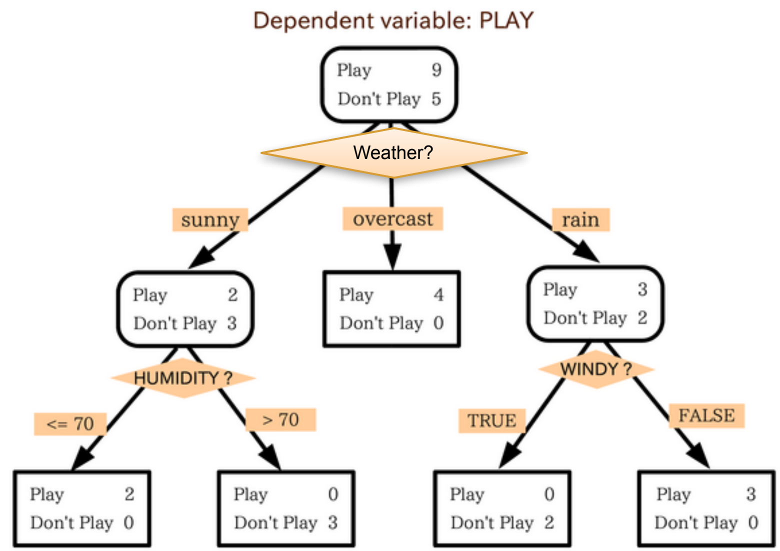


Decision trees

Things to learn: ?

How to learn them: ?

Cross-validation: ?



Learning the Tree Structure

Things to learn: the tree structure

How to learn them: (greedily) minimize the overall classification loss

Cross-validation: finding the best sized tree with K-fold cross-validation

Decision trees

Pieces:

1. Find the best attribute to split on
2. Find the best split on the chosen attribute
3. Decide on when to stop splitting
4. Cross-validation

Highly recommended lecture slides from CMU

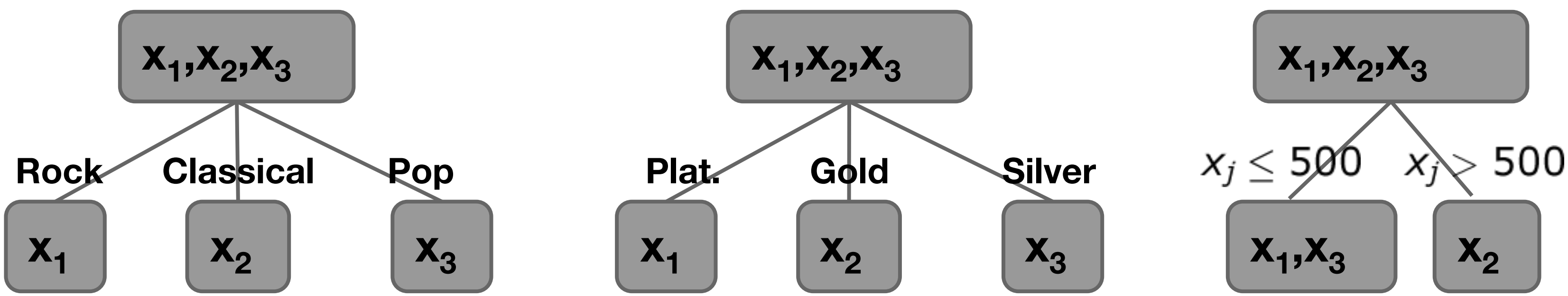
http://www.cs.cmu.edu/afs/cs.cmu.edu/academic/class/15381-s06/www/DTs.pdf

$$x_i = (x_{i1}, \ldots, x_{id}); y_i = \{1, \ldots, m\}$$

Choosing the split point

Split types for a selected attribute j:

1. Categorical attribute (e.g. "genre")
   x_{1j} = Rock, x_{2j} = Classical, x_{3j} = Pop
2. Ordinal attribute (e.g., "achievement")
   x_{1j}=Platinum, x_{2j}=Gold, x_{3j}=Silver
3. Continuous attribute (e.g., song duration)
   $x_{1j} = 235$, $x_{2j} = 543$, $x_{3j} = 378$



Split on genre Split on achievement Split on duration

$$x_i = (x_{i1}, \dots, x_{id}); y_i = \{1, \dots, m\}$$

Choosing the split point

At a node T for a given attribute d,

select a split s as following:

$$min_s \; loss(T_L) + loss(T_R)$$

where $loss(T)$ is the loss at node T

Common node loss functions:

- Misclassification rate
- Expected loss
- Normalized negative log-likelihood (= cross-entropy)

More details on loss functions, see Chapter 3.3:
http://www.stat.cmu.edu/~cshalizi/350/lectures/22/lecture-22.pdf

Choosing the attribute

Choice of attribute:

1. Attribute providing the maximum improvement in training loss
2. Attribute with highest information gain

   (mutual information)

Intuition: an attribute with highest information gain helps most rapidly describe an instance (i.e., most rapidly reduces "uncertainty")

Excellent refresher on **information gain**: using it pick **splitting attribute** and **split point** (for that attribute)

http://www.cs.cmu.edu/afs/cs.cmu.edu/academic/class/15381-s06/www/DTs.pdf

PDF page 7 to 21

When to stop splitting? Common strategies:

1. Pure and impure leave nodes
   - All points belong to the same class; OR
   - All points from one class completely overlap with points from another class (i.e., same attributes)
     - Output majority class as this leaf’s label

2. Node contains points fewer than some threshold
3. Node purity is higher than some threshold
4. Further splits provide no improvement in *training loss*
   ($loss(T) <= loss(T_L) + loss(T_R)$)

Graphics from: http://www.cs.cmu.edu/afs/cs.cmu.edu/academic/class/15381-s06/www/DTs.pdf

Parameters vs Hyper-parameters

Example **hyper-parameters** (need to experiment/try)

- k-NN: k, similarity function
- Decision tree: #node,
- Can be determined using **CV** and **optimization strategies**, e.g., “grid search” (fancy way to say “try all combinations”), random search, etc. (http://scikit-learn.org/stable/modules/grid_search.html)

Example **parameters**
(can be “learned” / “estimated” / “computed” directly from data)

- Decision tree (entropy-based):
  - which attribute to split
  - split point for an attribute

Summary on decision trees

Advantages

- Easy to implement
- Interpretable
- Very fast test time
- Can work seamlessly with mixed attributes
- Works quite well in practice

Caveats

- “Too basic” — but OK if it works!
- Training can be very expensive
- Cross-validation is hard (node-level CV)