INTRODUCTION TO MACHINE LEARNING

Decision tree learning

Task of classification

- Automatically assign **class** to observations with **features**
- Observation: **vector** of **features**, with a **class**
- Automatically assign **class** to new observation with **features**, using previous observations
- **Binary** classification: two **classes**
- **Multiclass** classification: more than two **classes**

Example

- A dataset consisting of **persons**
- **Features**: age, weight and income
- **Class**:
  - **binary**: happy or not happy
  - **multiclass**: happy, satisfied or not happy

Examples of features

- Features can be **numerical**
  - age: 23, 25, 75, ...
  - height: 175.3, 179.5, ...
- Features can be **categorical**
  - travel_class: first class, business class, coach class
  - smokes?: yes, no

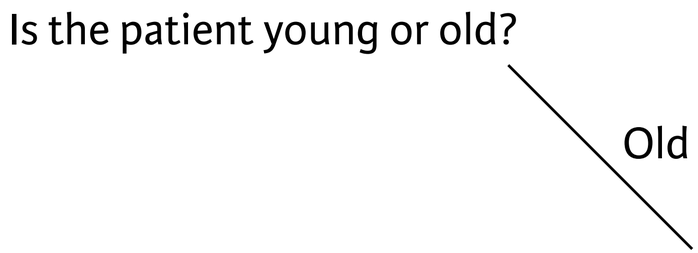
The decision tree

- Suppose you're classifying patients as **sick** or **not sick**
- Intuitive way of classifying: ask questions

Is the patient young or old?

The decision tree

- Suppose you're classifying patients as **sick** or **not sick**
- Intuitive way of classifying: ask questions



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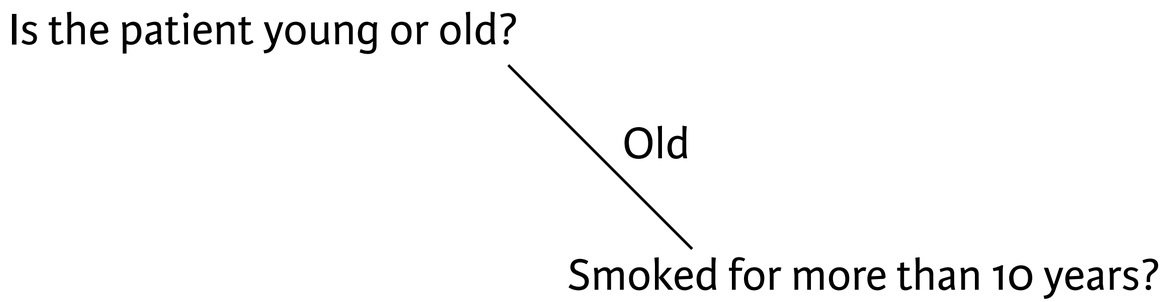

The decision tree

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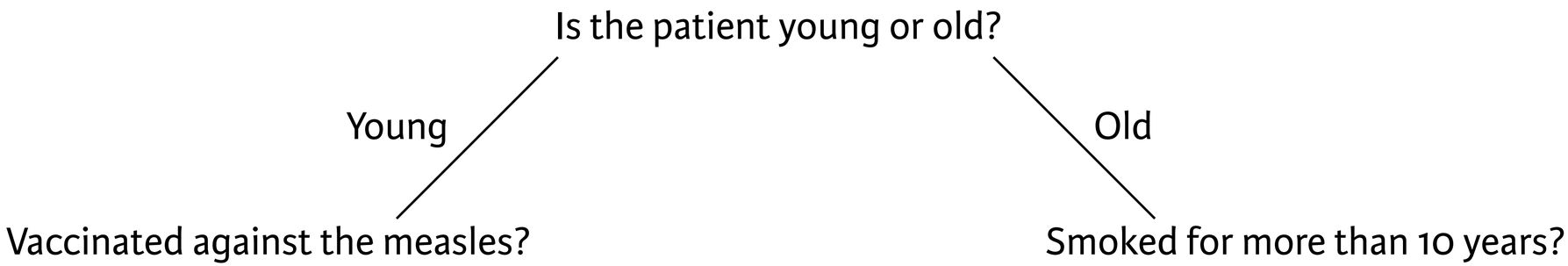

The decision tree

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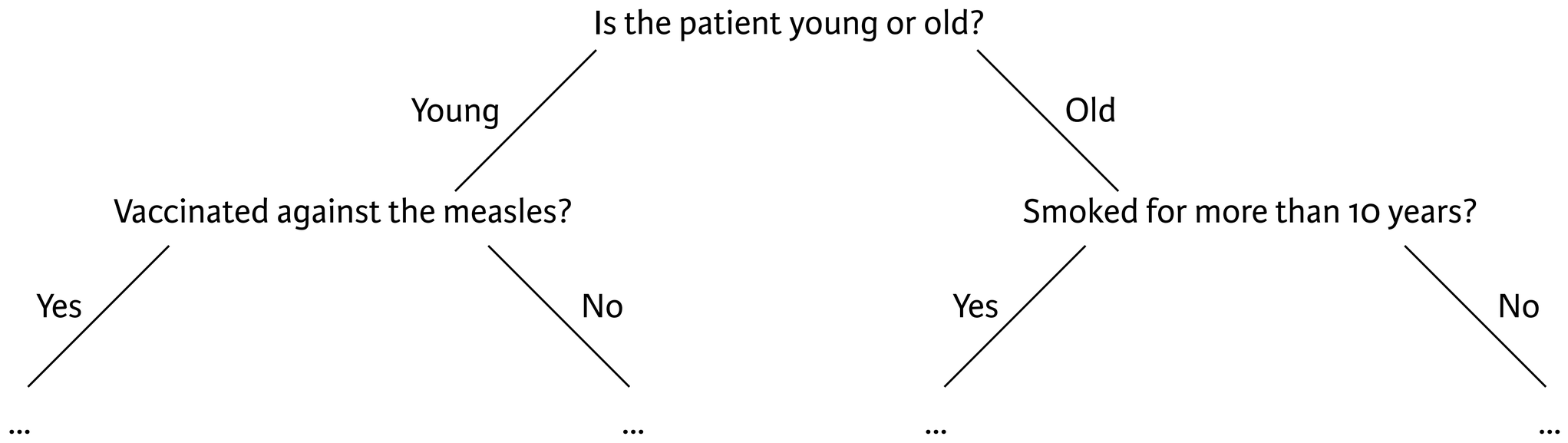
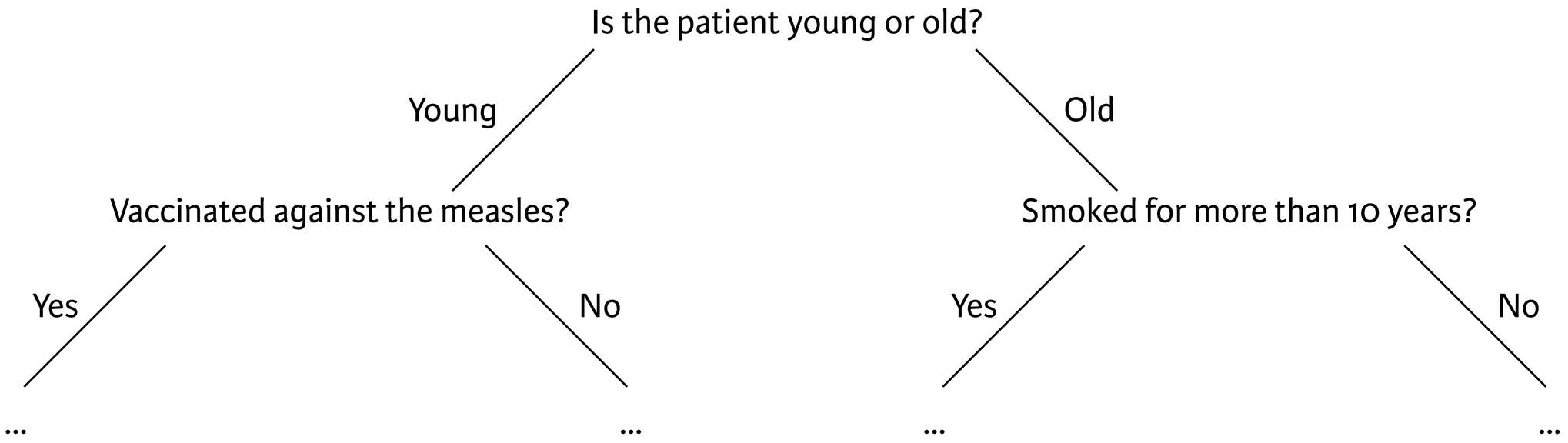


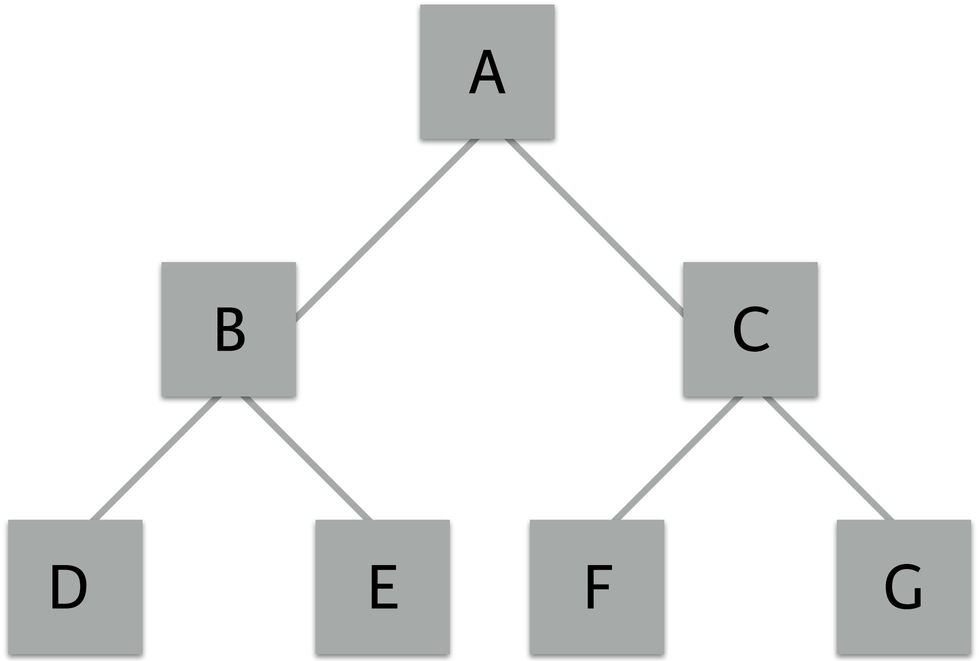
The decision tree

- Suppose you're classifying patients as **sick** or **not sick**
- Intuitive way of classifying: ask questions



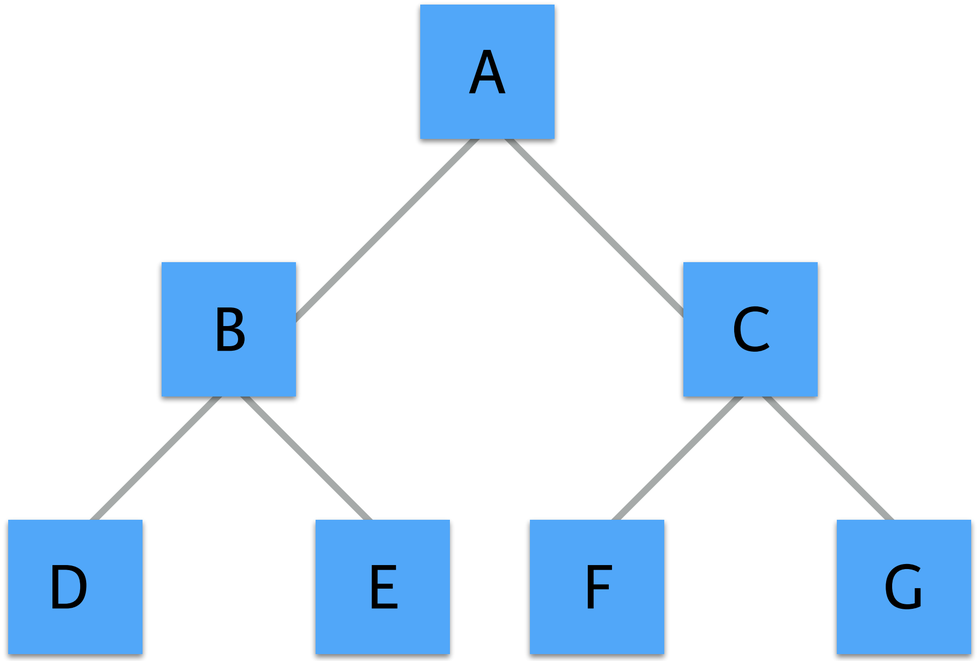
It's a decision tree!!!

Define the tree



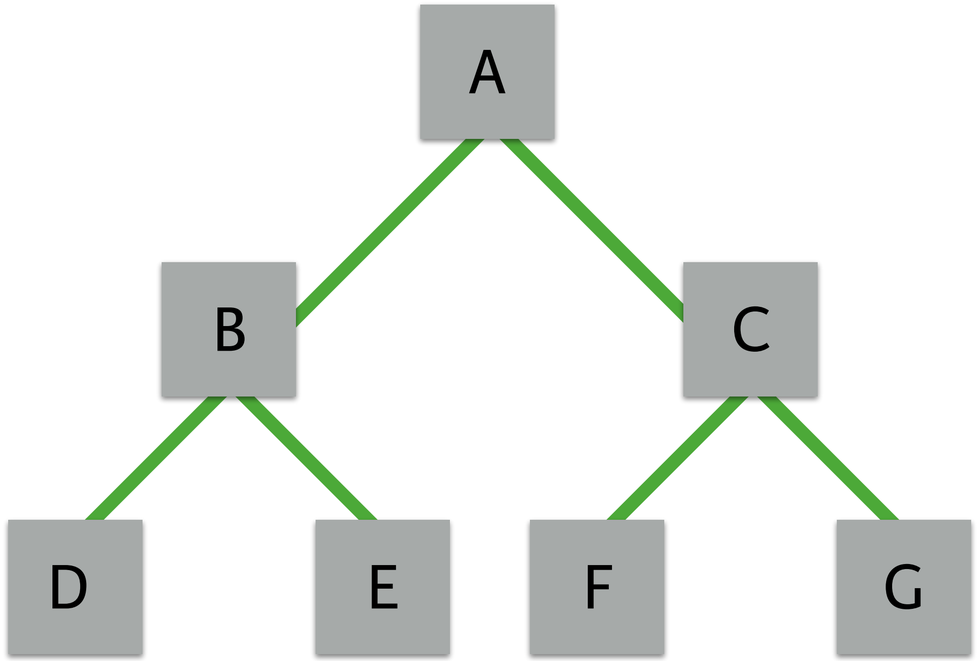
Define the tree

Nodes

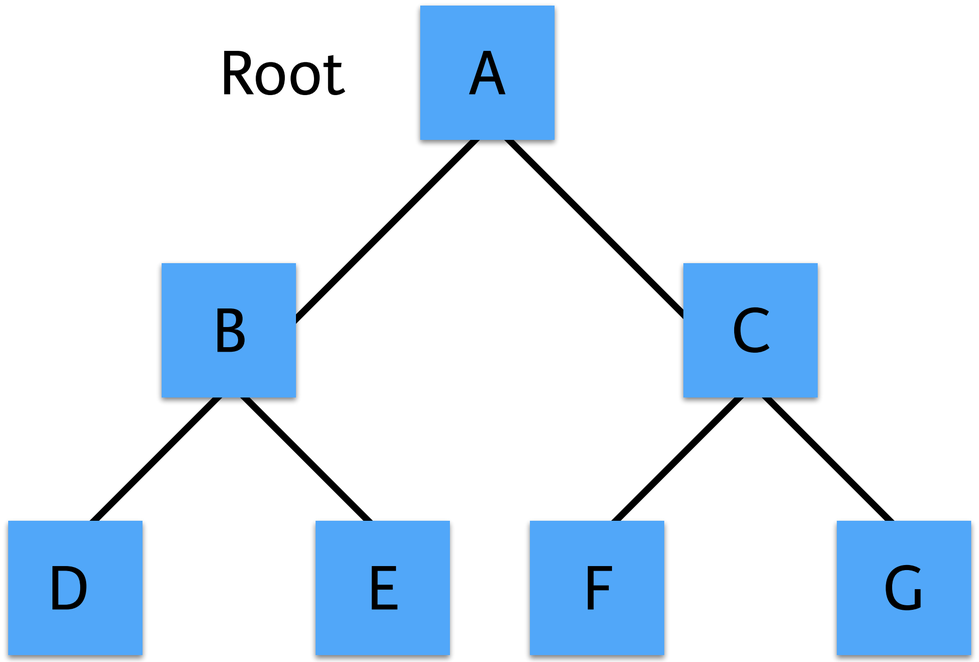


Define the tree

Edges



Define the tree



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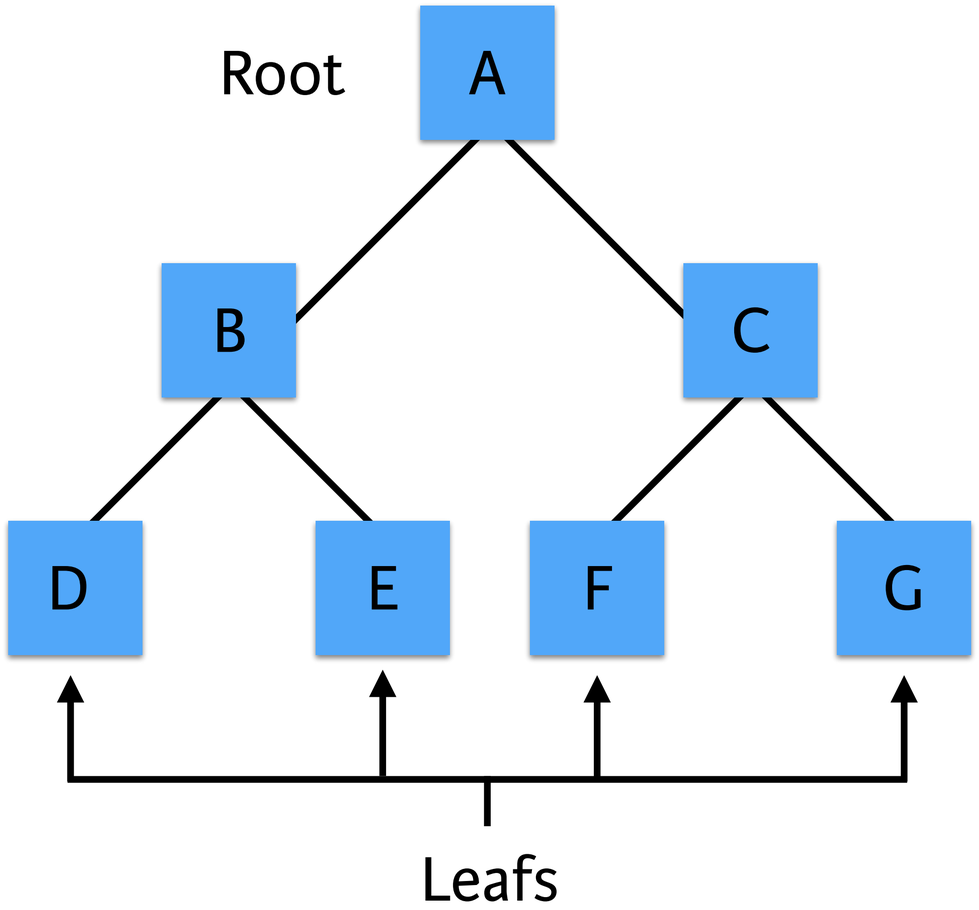

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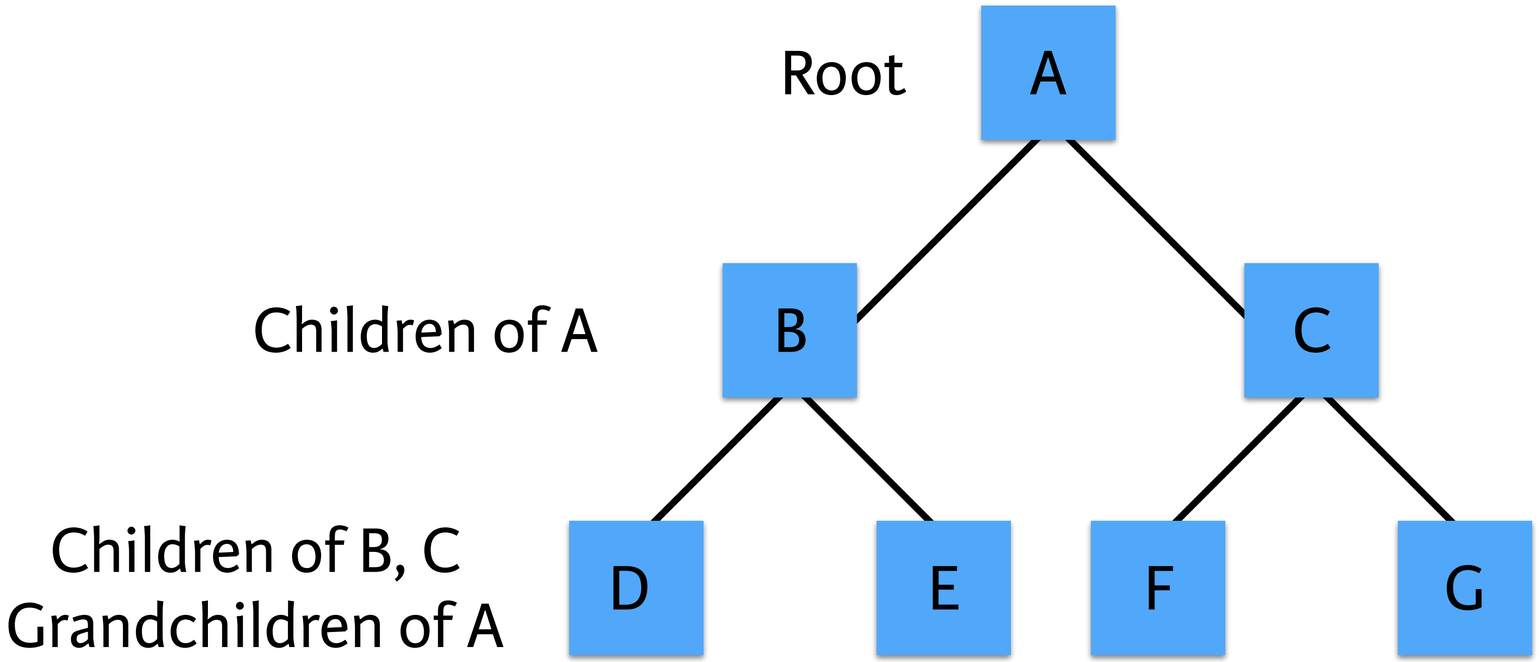

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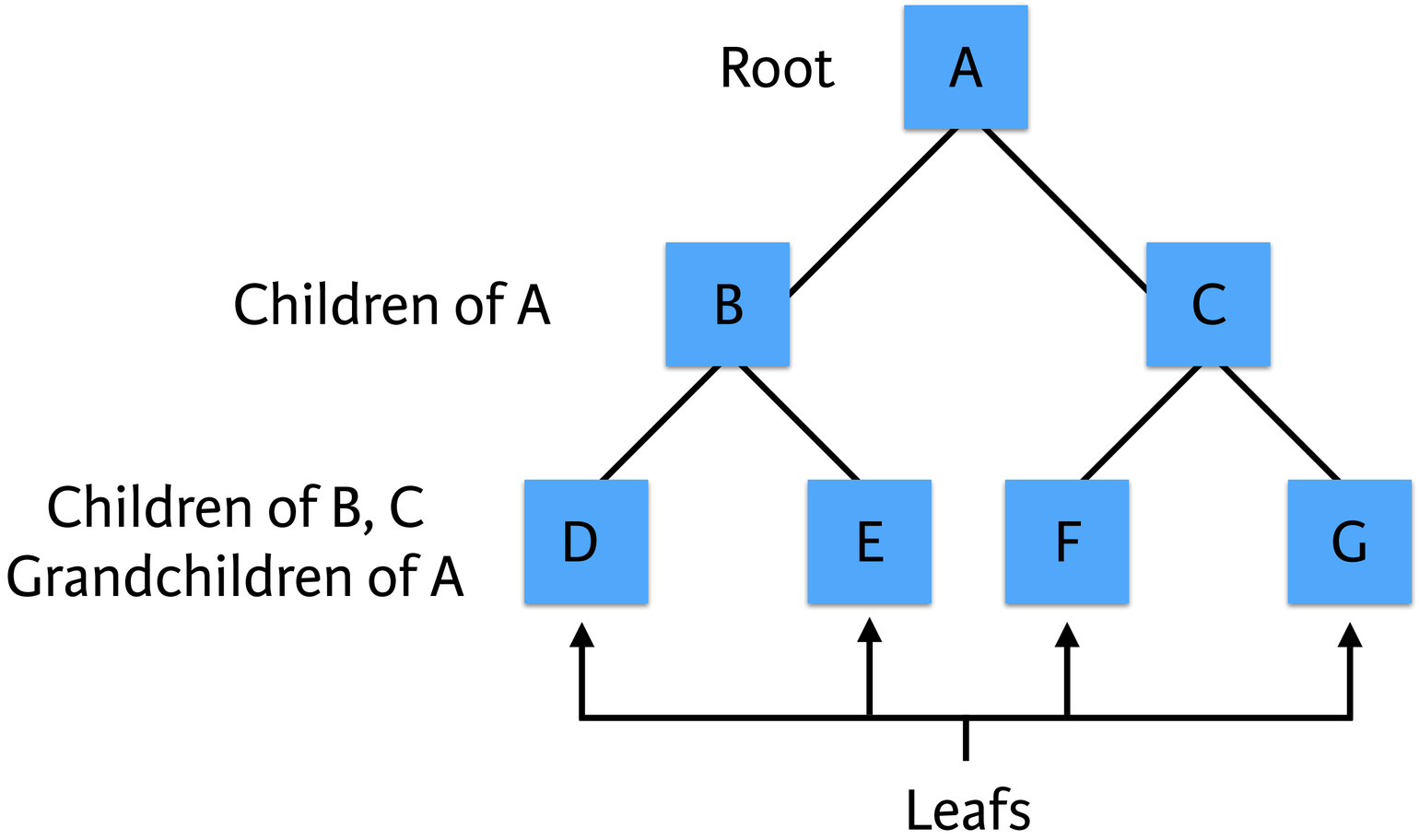
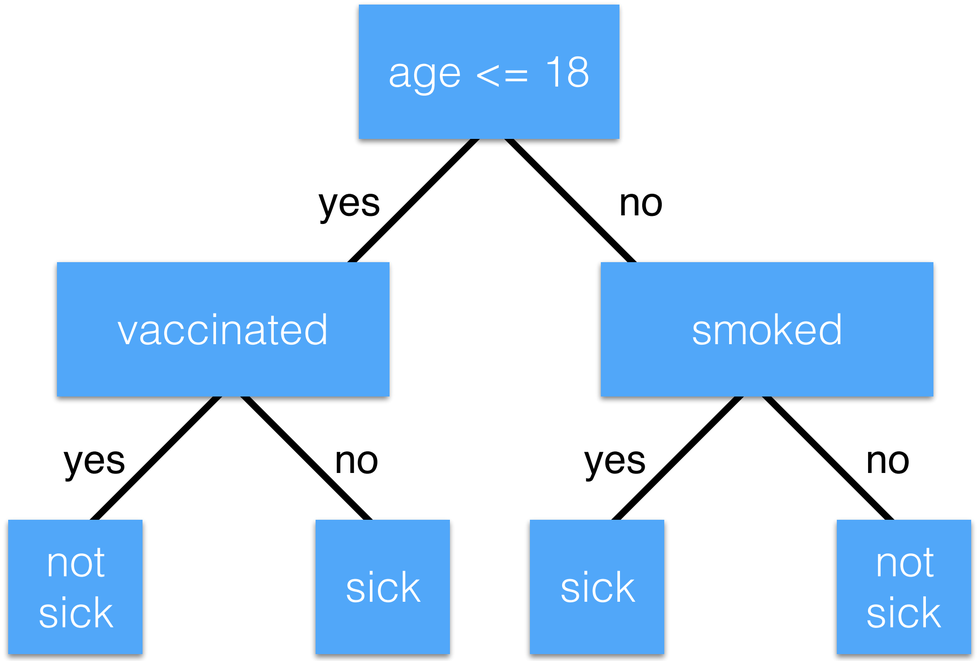
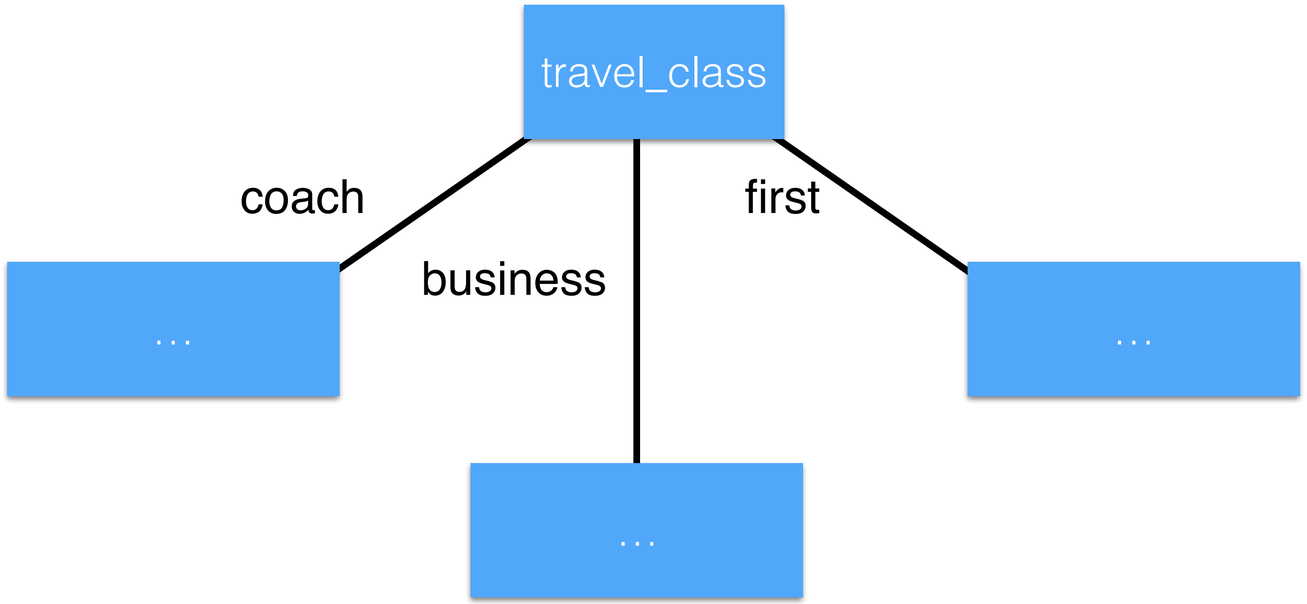


Questions to ask



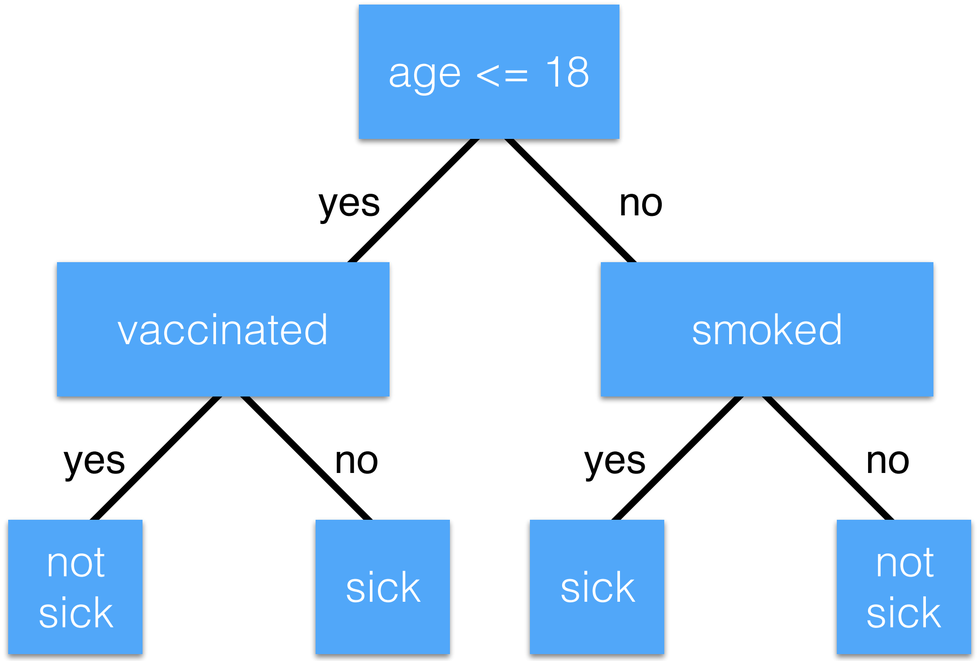
Categorical feature

- Can be a feature **test** on itself
- travel_class: coach, business or first



Classifying with the tree

Observation: patient of 40 years, vaccinated and didn't smoke



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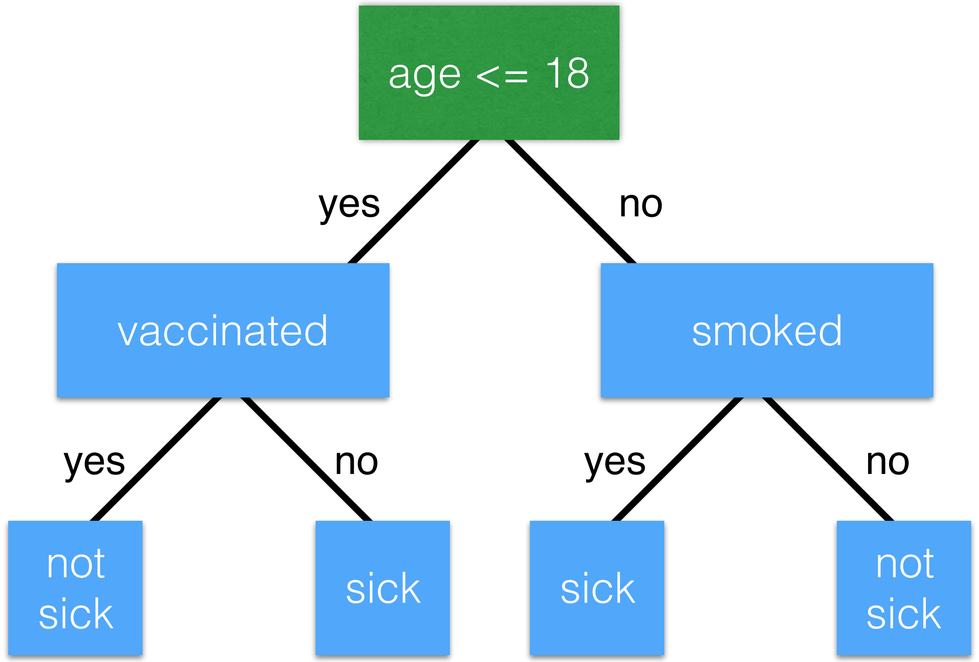

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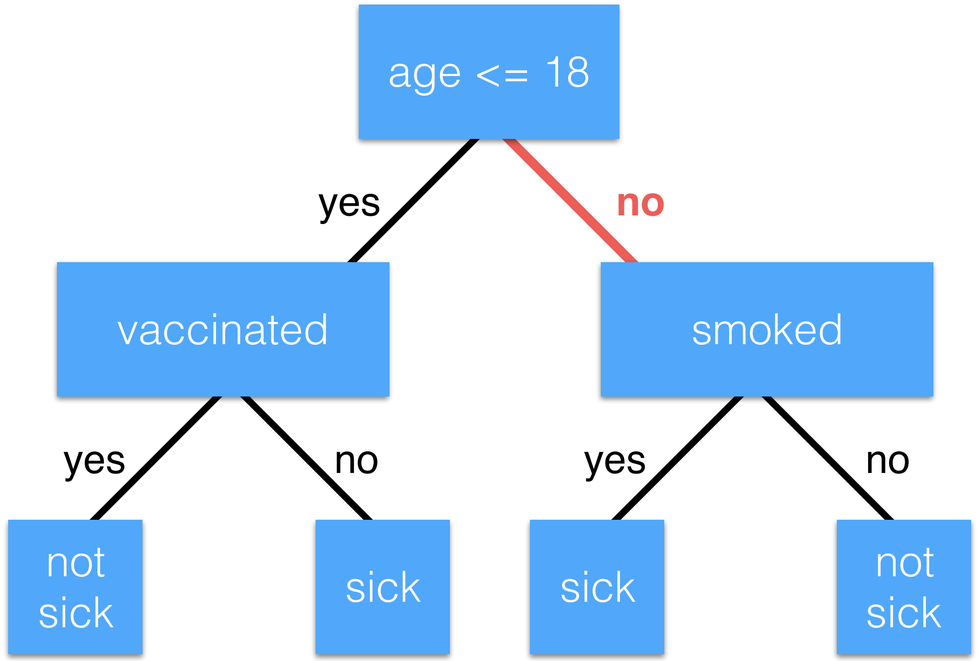

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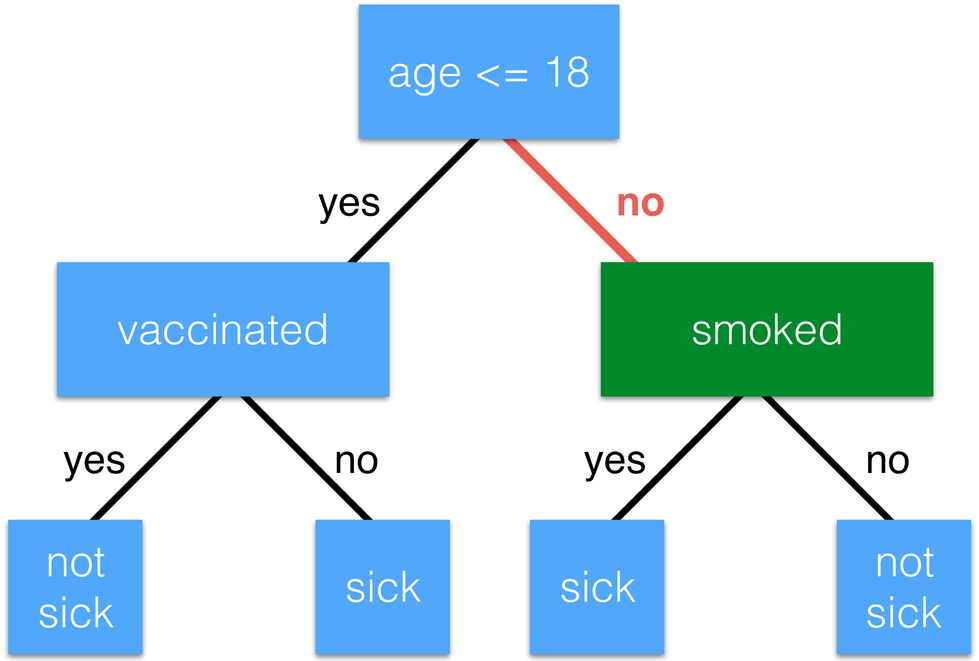

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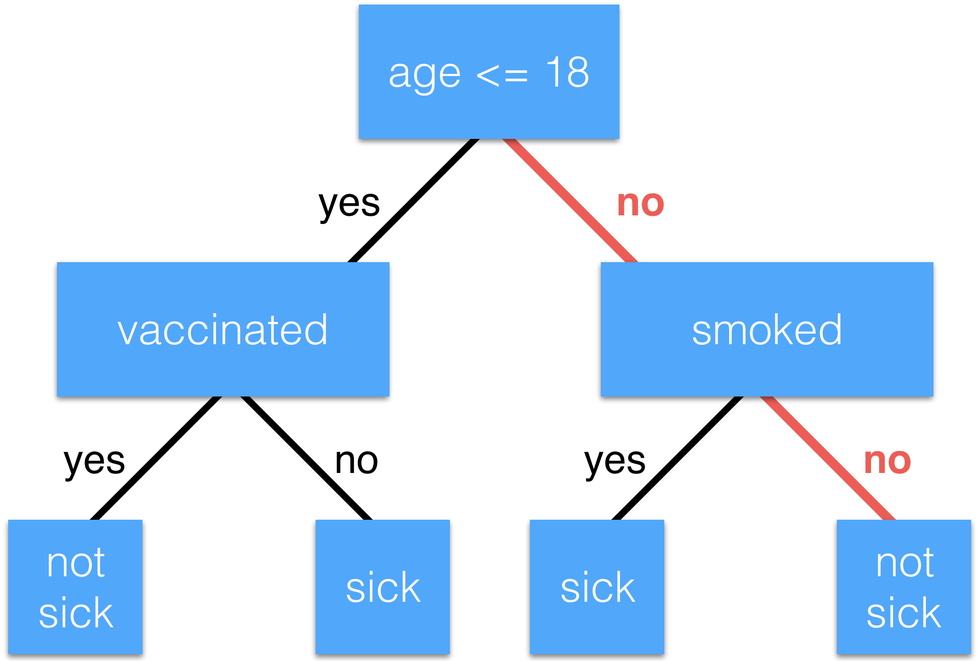

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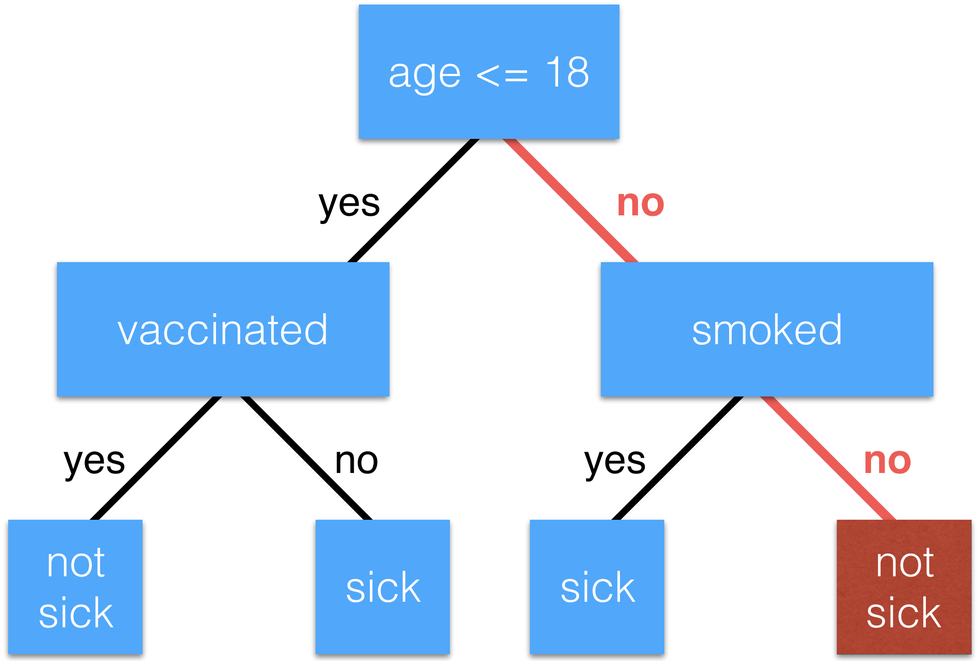
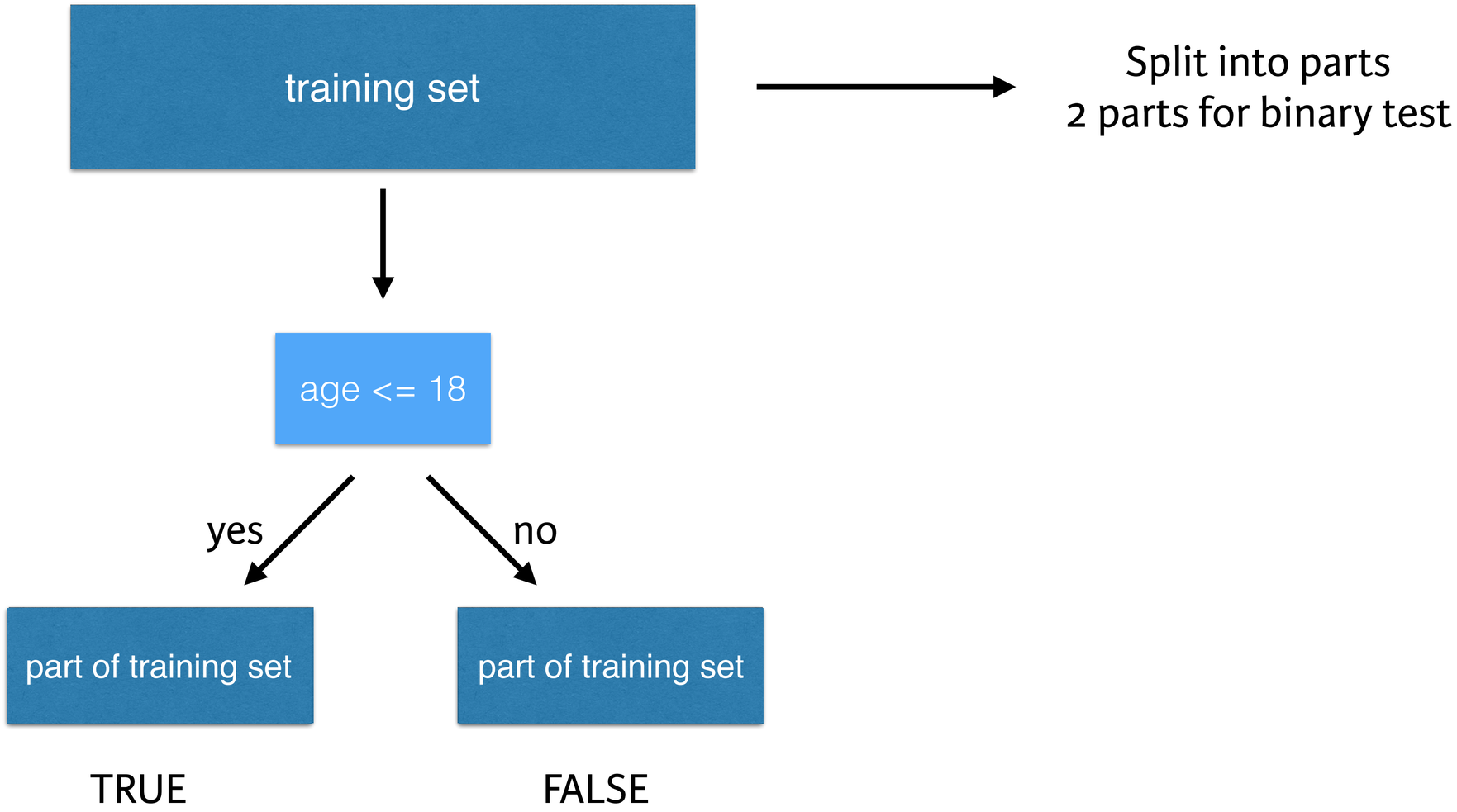
Observation: patient of 40 years, vaccinated and didn't smoke

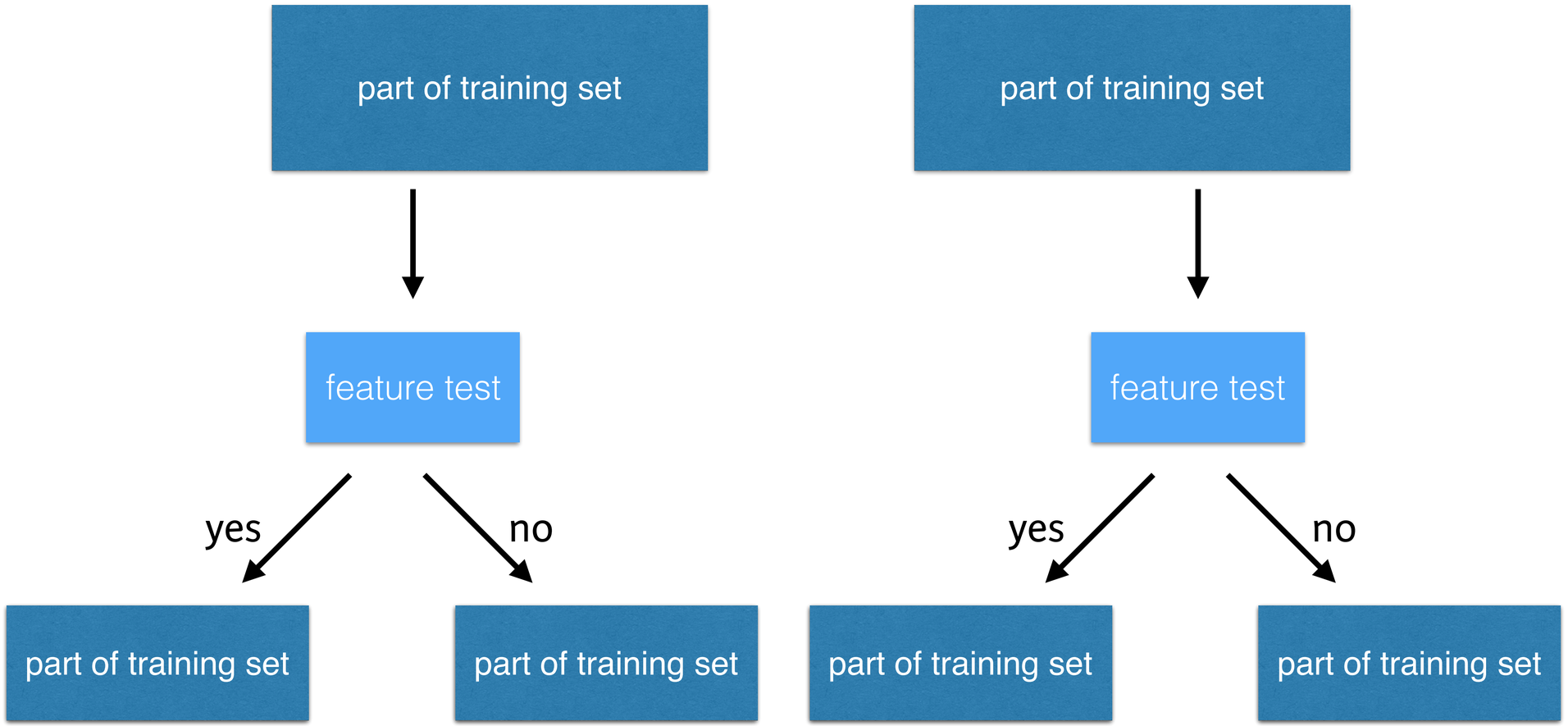


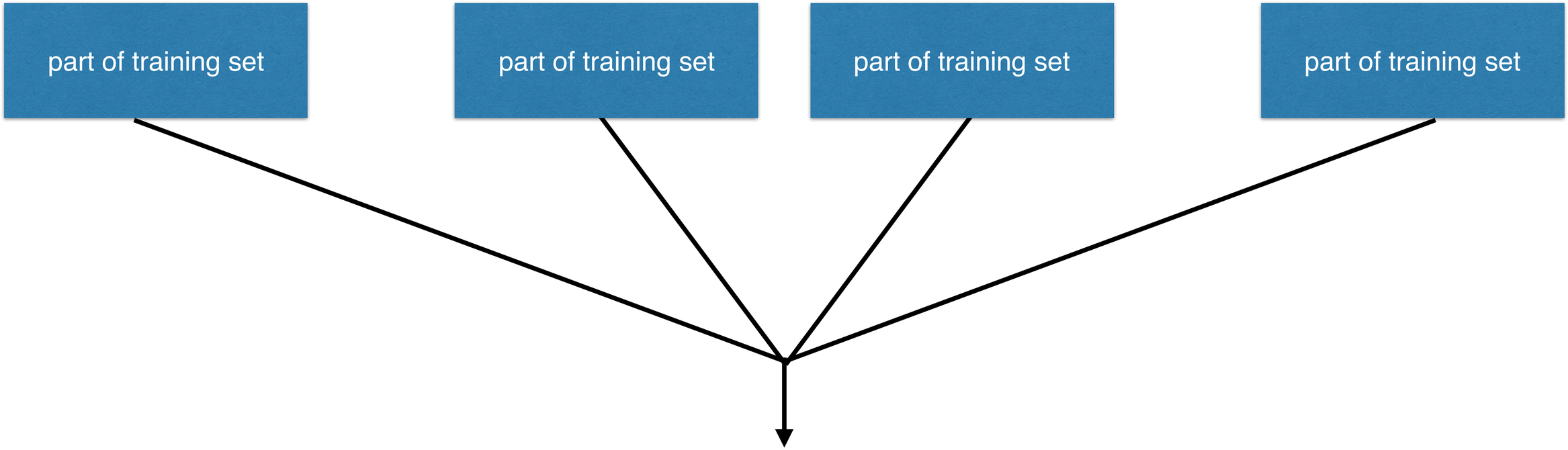
Prediction: not sick

Learn a tree

- Use **training** set
- Come up with queries (feature tests) at each node


training set
Split into parts
2 parts for binary test
age <= 18
yes
no
part of training set
part of training set
TRUE
FALSE

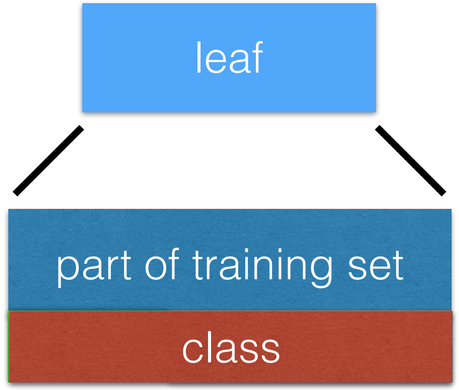

part of training set
feature test
yes
no
part of training set
part of training set
part of training set
feature test
yes
no
part of training set
part of training set



keep splitting until **leafs** contain small portion of **training set**

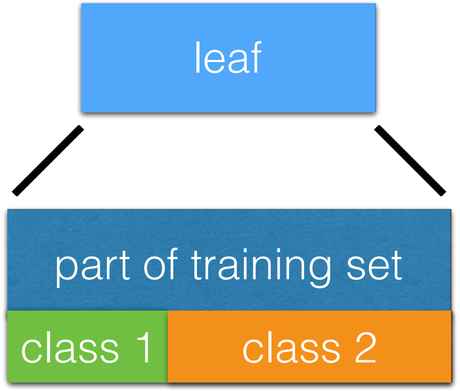
Learn the tree

- **Goal**: end up with **pure** leafs — leafs that contain observations of one particular class



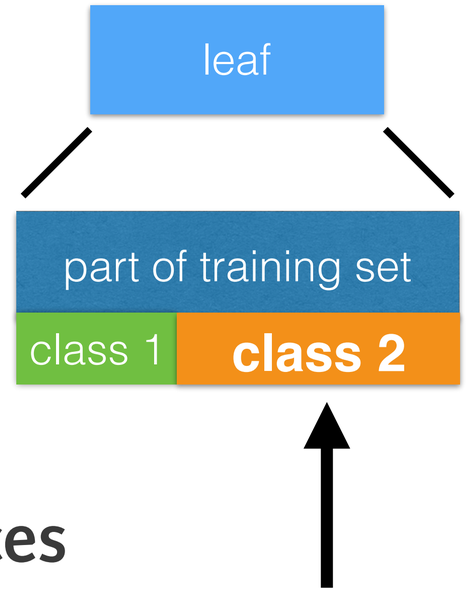
Learn the tree

- **Goal**: end up with **pure** leafs — leafs that contain observations of one particular class
- In **practice**: almost never the case — noise
- When classifying **new instances**
    - end up in **leaf**



Learn the tree

- **Goal**: end up with **pure** leafs — leafs that contain observations of one particular class
- In **practice**: almost never the case — noise
- When classifying **new instances**
    - end up in **leaf**
    - assign class of **majority** of **training instances**



Learn the tree

- At each node
  - Iterate over different feature tests
  - Choose the best one
- Comes down to two parts
  - **Make** list of **feature tests**
  - **Choose** test with **best split**

Construct list of tests

- **Categorical** features
  - Parents/grandparents/... didn't use the test yet
- **Numerical** features
  - Choose **feature**
  - Choose **threshold**

Choose best feature test

- More complex
- Use **splitting criteria** to decide which test to use
- **Information gain** ~ entropy

Information gain

- Information gained from **split** based on **feature test**
- **Test** leads to nicely divided **classes**
  -> high **information gain**
- **Test** leads to scrambled **classes**
  -> low **information gain**
- **Test** with highest information gain will be chosen

Pruning

- **Number of nodes** influences chance on overfit
- Restrict size — higher **bias**
  - Decrease chance on **overfit**
  - **Pruning** the tree

INTRODUCTION TO MACHINE LEARNING

Let’s practice!

INTRODUCTION TO MACHINE LEARNING

k-Nearest Neighbors

Instance-based learning

- **Save training set** in memory
- No real model like **decision tree**
- **Compare** unseen instances to training set
- **Predict** using the **comparison** of **unseen data** and the **training set**

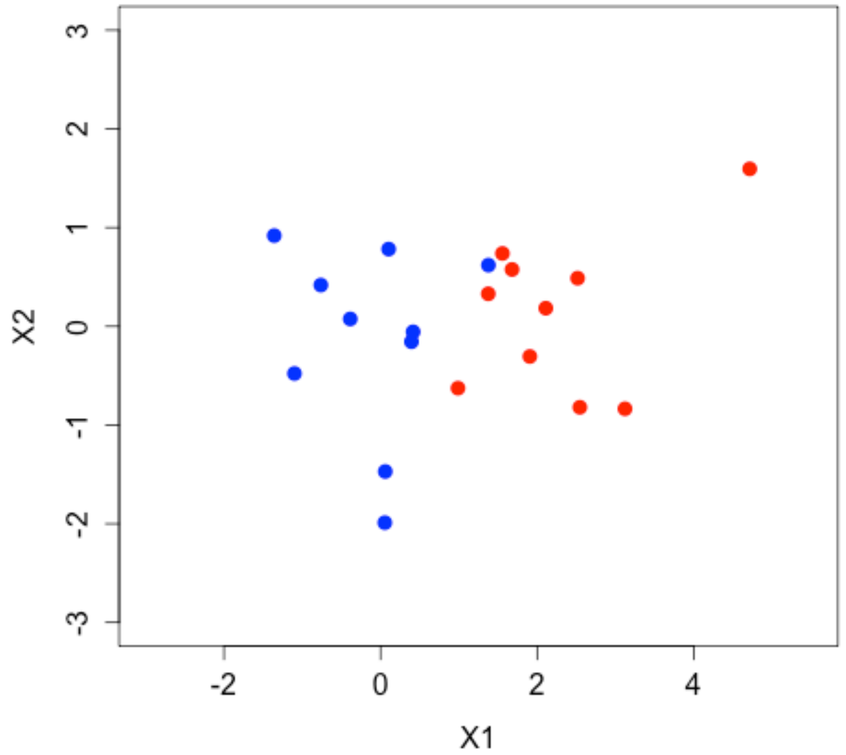
k-Nearest Neighbor

- Form of **instance-based learning**
- Simplest form: 1-Nearest Neighbor or Nearest Neighbor

Nearest Neighbor - example

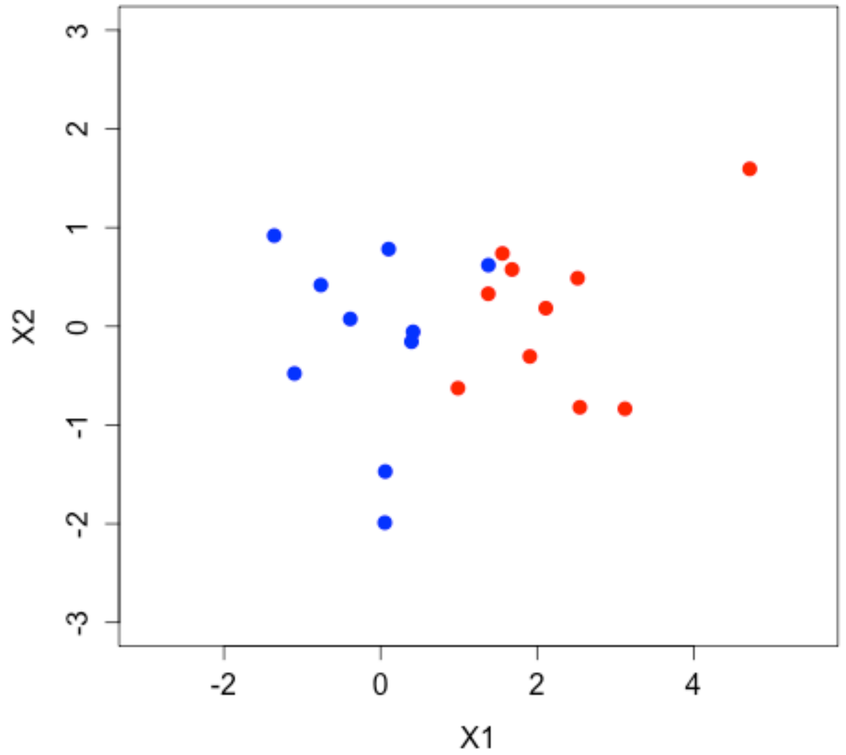
- **2 features**: X1 and X2
- **Class**: red or blue
- Binary classification

Nearest Neighbor - example



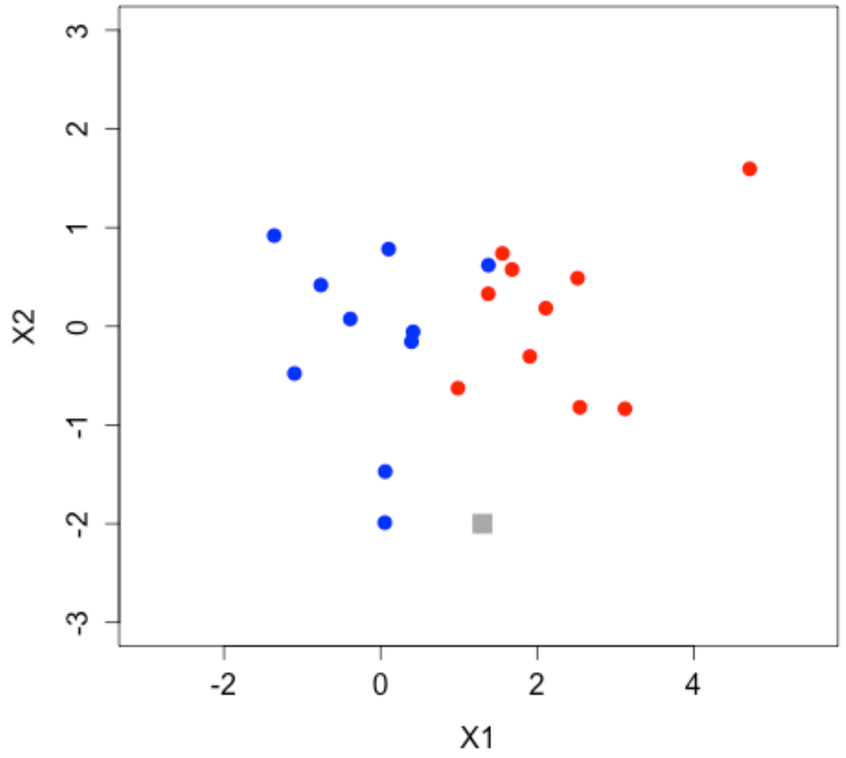
Nearest Neighbor - example

- Save complete **training set**



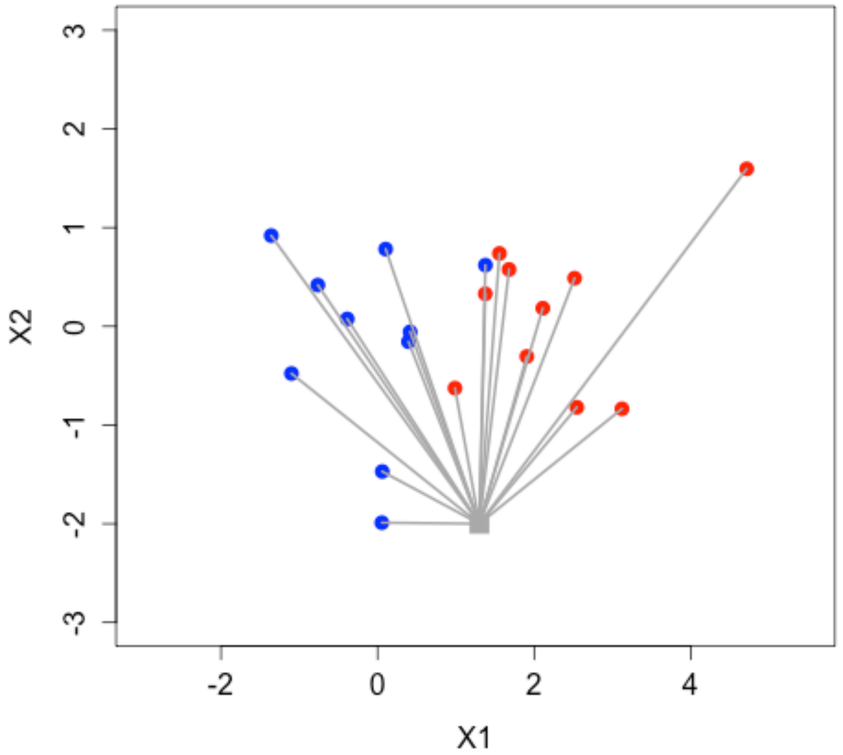
Nearest Neighbor - example

- Save complete training set
- Given: **unseen observation** with features $X = (1.3, -2)$



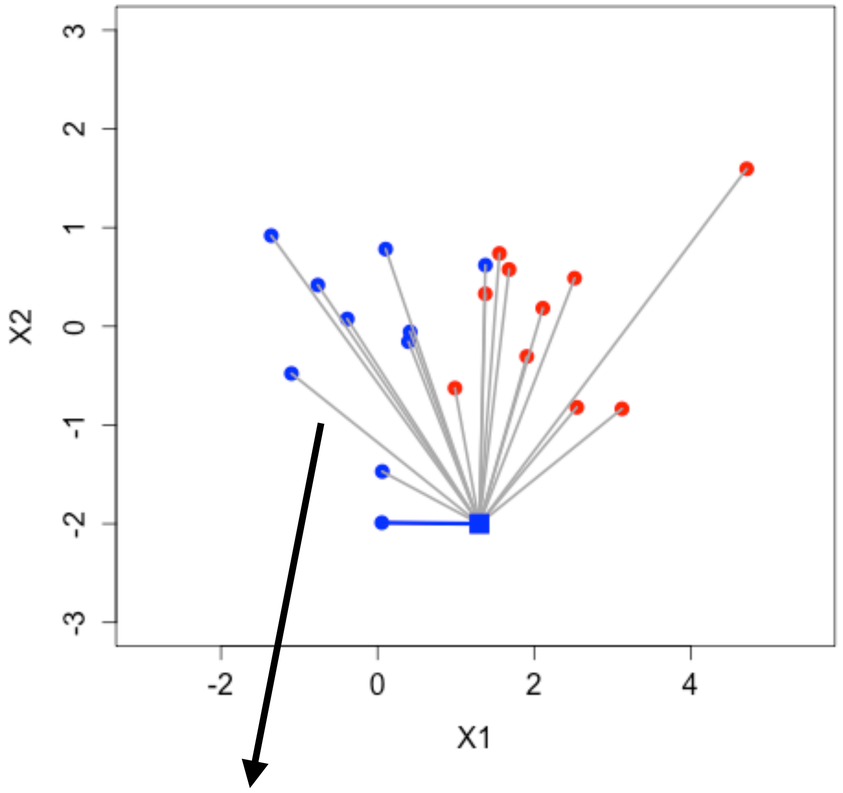
Nearest Neighbor - example

- Save complete training set
- Given: unseen observation with features $X = (1.3, -2)$
- **Compare** training set with new observation



Nearest Neighbor - example

- Save complete training set
- Given: unseen observation with features $X = (1.3, -2)$
- Compare training set with new observation
- Find **closest** observation — nearest neighbor — and assign **same class**



just Euclidean distance, nothing fancy

k-Nearest Neighbors

- **k** is the amount of neighbors
- If **k** = 5
  - Use 5 most similar observations (neighbors)
  - Assigned class will be the most represented class within the 5 neighbors

Distance metric

- **Important** aspect of k-NN

Distance metric

- **Important** aspect of k-NN
- **Euclidian** distance:

$$d_E(\mathbf{a}, \mathbf{b}) = \sqrt{\sum_{i=1}^{D} (a_i - b_i)^2}$$

Distance metric

- **Important** aspect of k-NN
- **Euclidian** distance:

$$d_E(\mathbf{a}, \mathbf{b}) = \sqrt{\sum_{i=1}^{D} (a_i - b_i)^2}$$

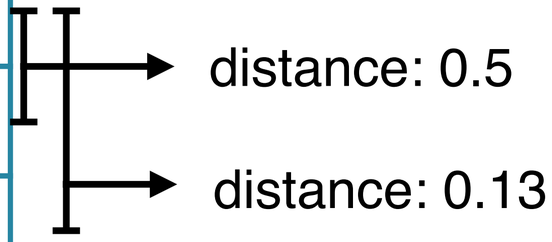
- **Manhattan** distance:

$$d_M(\mathbf{a}, \mathbf{b}) = \sum_{i=1}^{D} |a_i - b_i|$$

Scaling - example

- Dataset with
  - **2 features**: weight and height
  - **3 observations**

	height (m)	weight (kg)
1	1.83	80
2	1.83	80.5
3	1.70	80

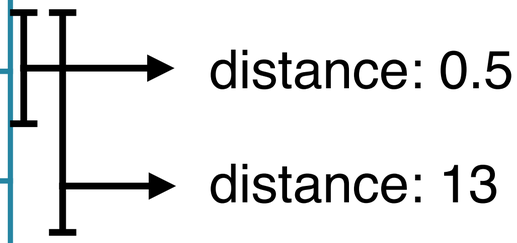


Scaling - example

- Dataset with
  - **2 features**: weight and height
  - **3 observations**

Scale influences distance!

	height (cm)	weight (kg)
1	**183**	80
2	**183**	80.5
3	**170**	80



Scaling

- **Normalize** all features
- e.g. **rescale** values between 0 and 1
- Gives **better** measure of **real distance**
- Don’t forget to scale **new observations**

Categorical features

- How to **use** in distance metric?
- **Dummy** variables
- **1** categorical features with **N** possible outcomes to **N** binary features (2 outcomes)

Dummy variables — Example

mother tongue: Spanish, Italian or French

mother_tongue		spanish	italian	french
Spanish		1	0	0
Italian		0	1	0
Italian	→	0	1	0
Spanish		1	0	0
French		0	0	1
French		0	0	1
French		0	0	1

INTRODUCTION TO MACHINE LEARNING

Let’s practice!

INTRODUCTION TO MACHINE LEARNING

Introducing: The ROC curve

Introducing

- Very **powerful** performance measure
- For **binary classification**
- **R**eiceiver **O**perator **C**haracteristic Curve (ROC Curve)

Probabilities as output

- Used **decision trees** and **k-NN** to predict **class**
- They can also output **probability** that instance belongs to **class**

Probabilities as output - example

- **Binary classification**

- Decide whether patient is **sick** or **not sick** → **decision function!**
- Define **probability threshold** from which you decide patient to be **sick**

Decision tree:

New patient: 70%

30%

higher than 50% classify as

Avoid sending sick patient home: lower threshold to 30%

More

patients classified as

but also

More

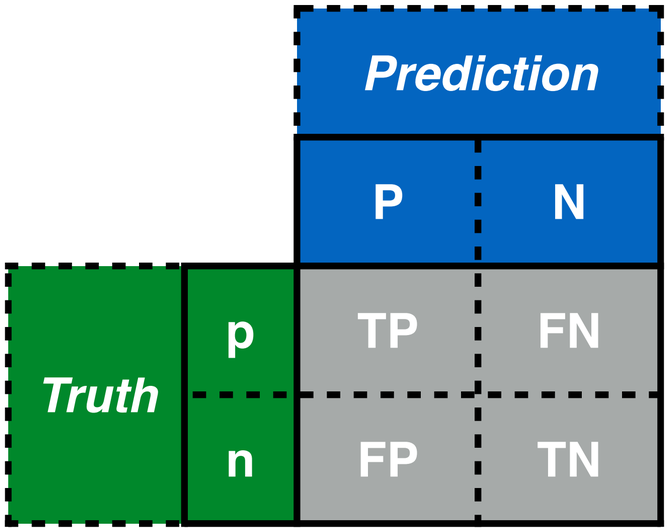
patients classified as

Confusion matrix

- Other **performance measure** for **classification**
- Important to construct the **ROC curve**

Confusion matrix

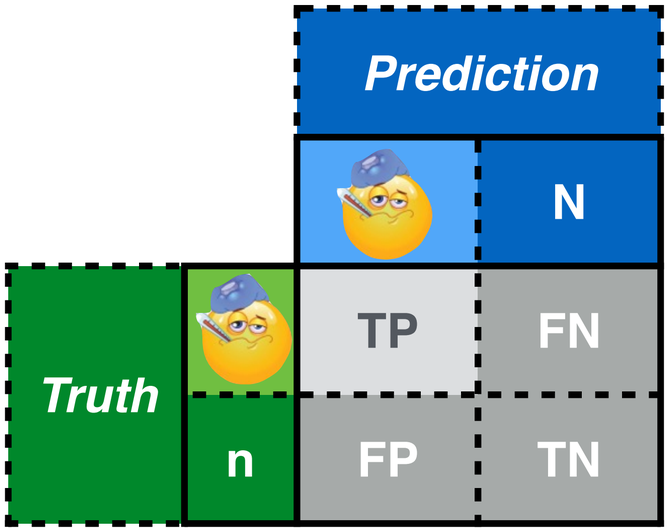
- Binary classifier: positive or negative (1 or 0)



Confusion matrix

- Binary classifier: positive or negative (1 or 0)

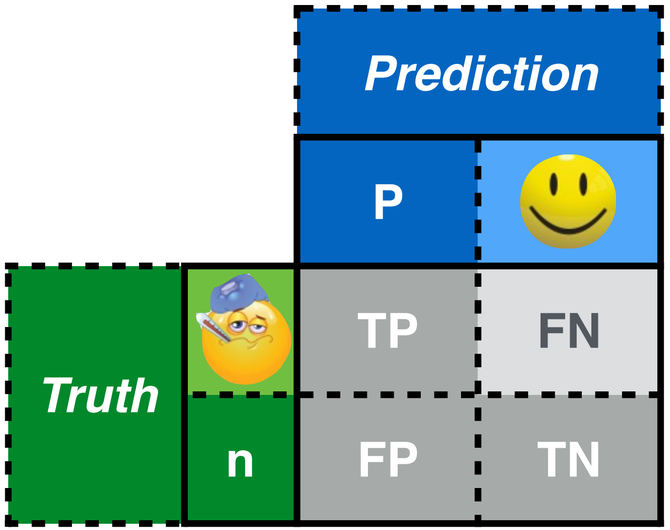
True Positives
Prediction: P
Truth: P



Confusion matrix

- Binary classifier: positive or negative (1 or 0)

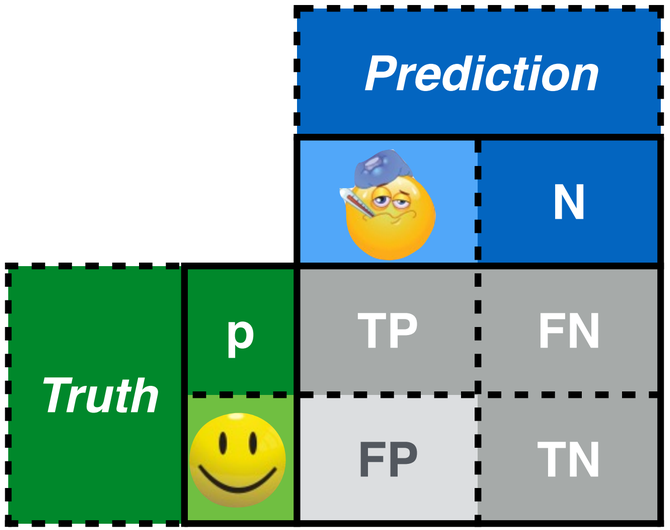
False Negatives
Prediction: N
Truth: P



Confusion matrix

- Binary classifier: positive or negative (1 or 0)

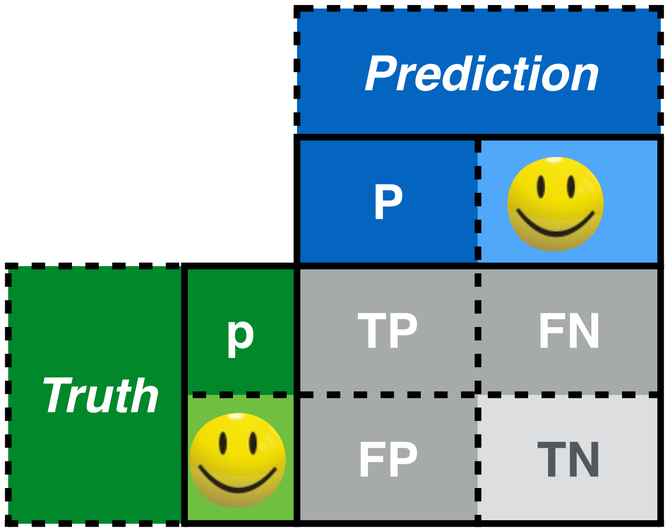
False Positives
Prediction: P
Truth: N



Confusion matrix

- Binary classifier: positive or negative (1 or 0)

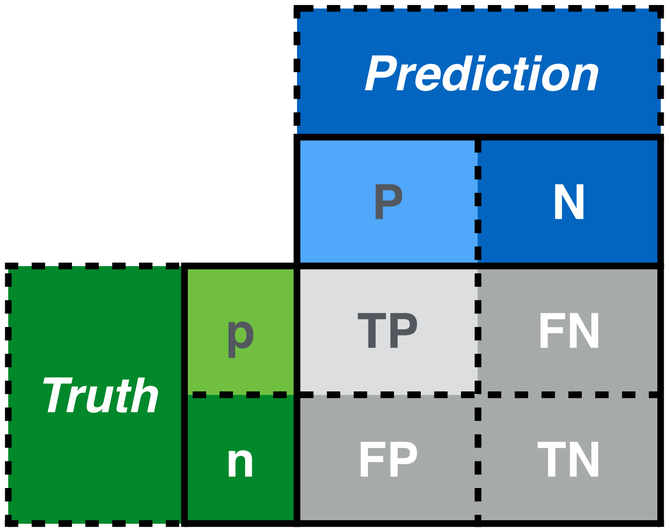
True Negatives
Prediction: N
Truth: N



Ratios in the confusion matrix

- True positive rate (TPR) = recall
- False positive rate (FPR)

TPR
TP/(TP+FN)



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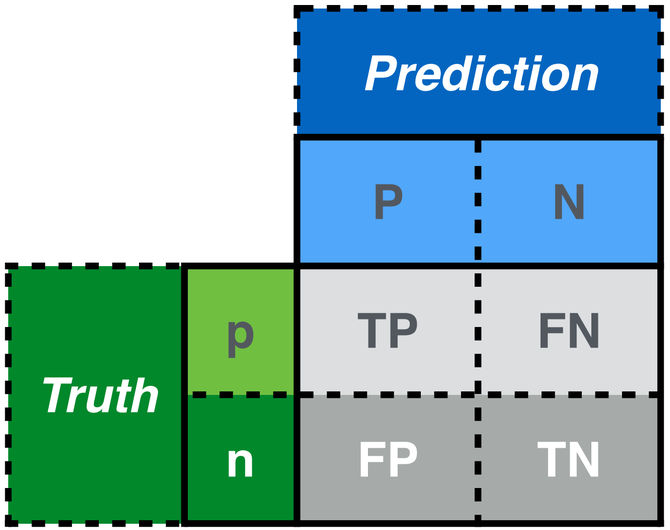

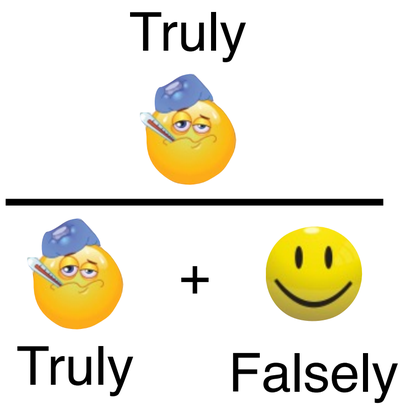

Ratios in the confusion matrix

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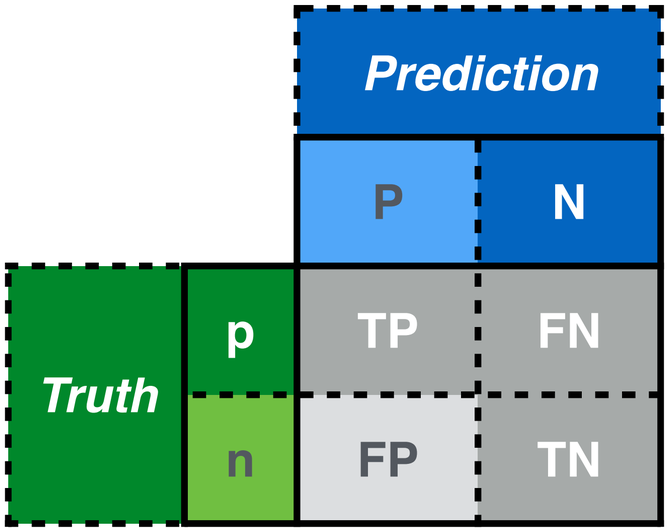
- False positive rate (FPR)

FPR
FP/(FP+TN)



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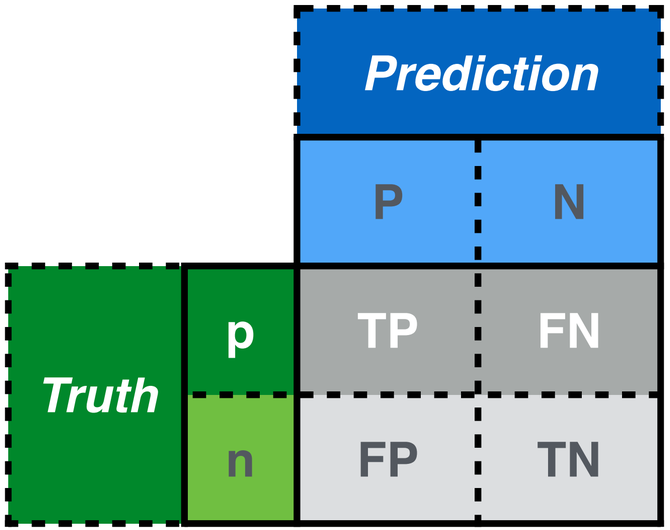
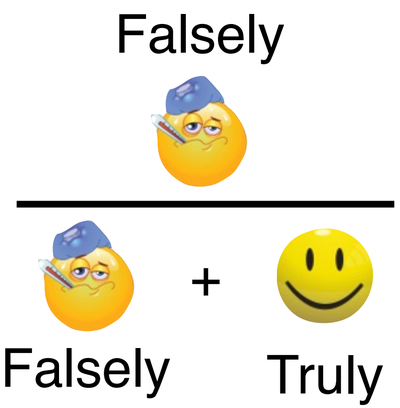
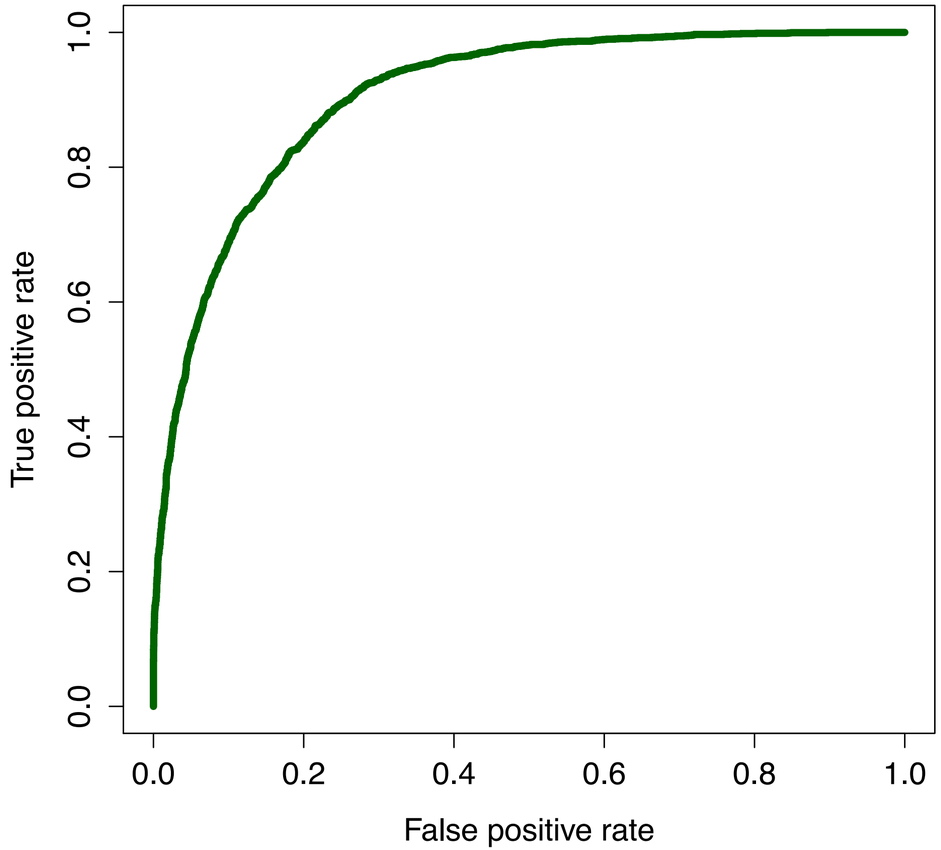




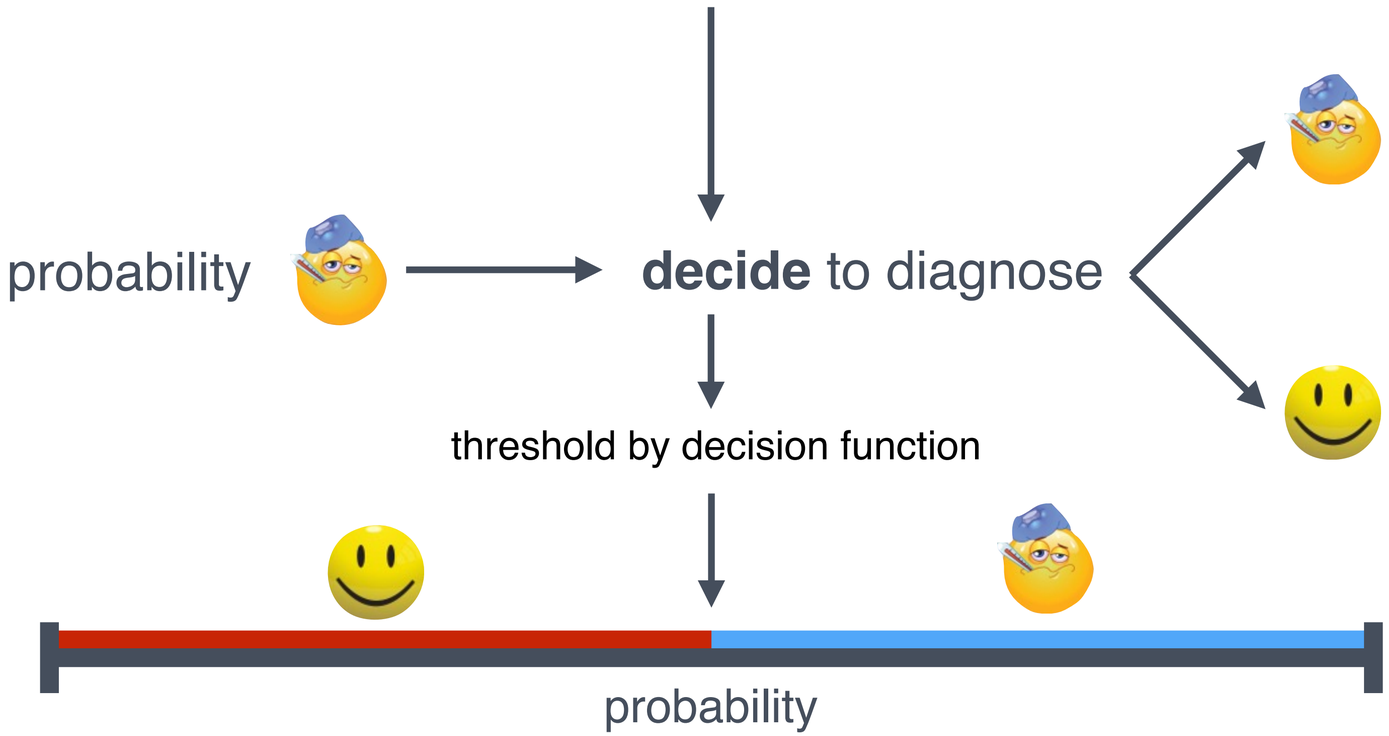
ROC curve

- **Horizontal axis:** FPR
- **Vertical axis:** TPR
- How to **draw** the **curve**?



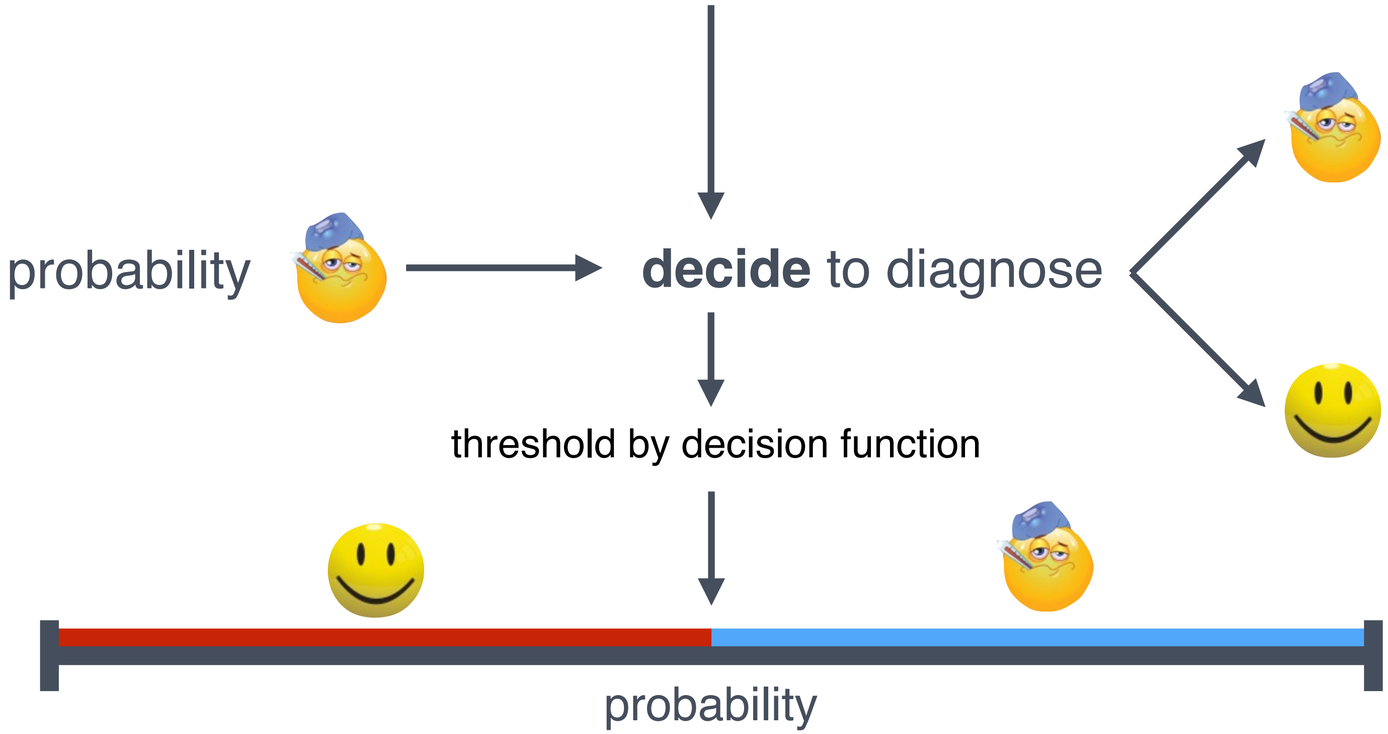
Draw the curve

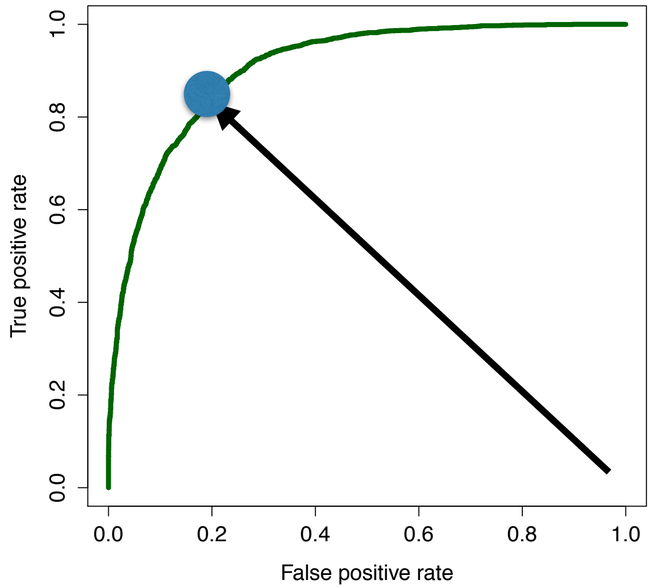
- Need classifier which **outputs probabilities**
- The **decision function**



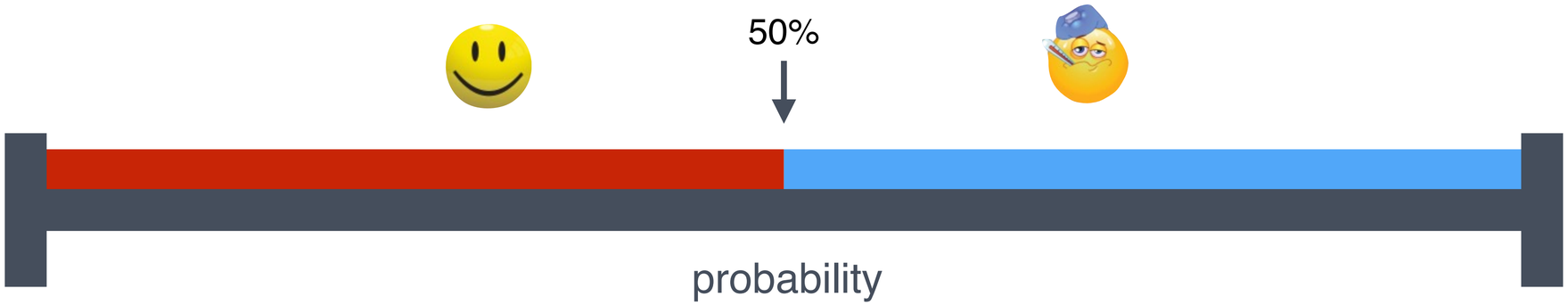
Draw the curve

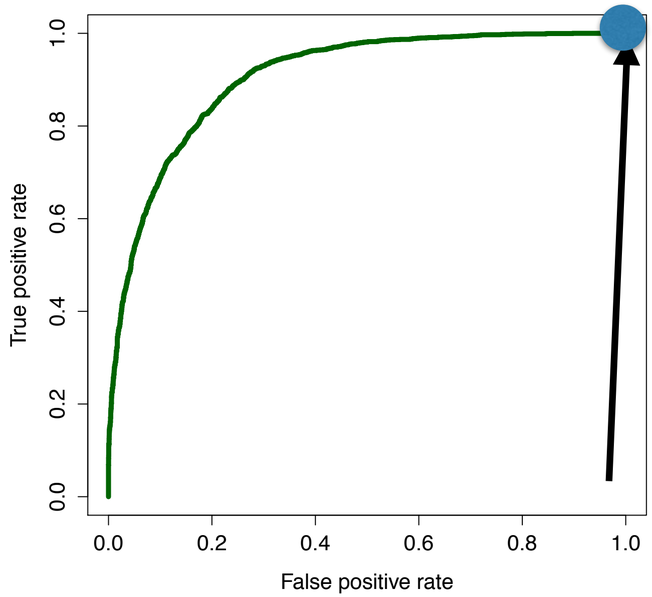
- Need classifier which **outputs probabilities**
- The **decision function**





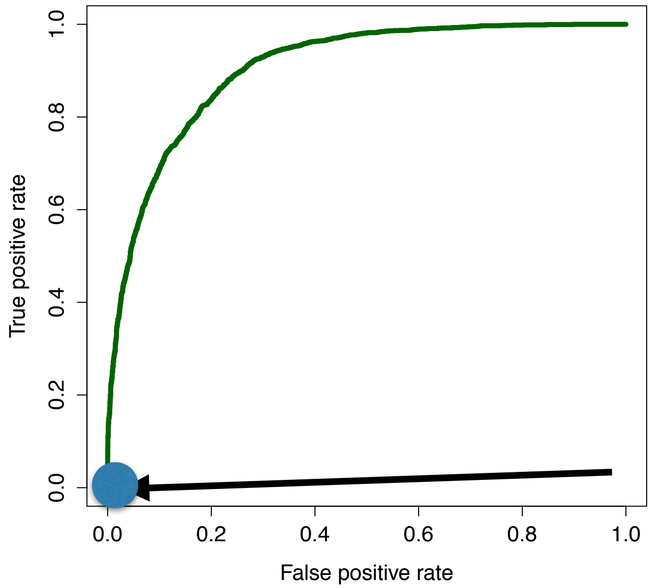
>=50%: sick
< 50%: healthy




True positive rate
0.0
0.2
0.4
0.6
0.8
1.0
False positive rate
0.0
0.2
0.4
0.6
0.8
1.0

all sick


0%
probability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0.0
0.2
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0.6
0.8
1.0
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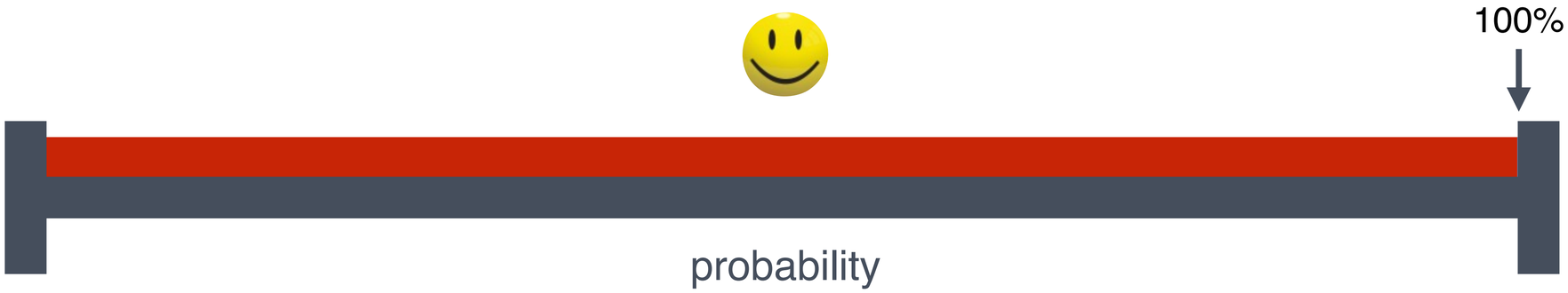
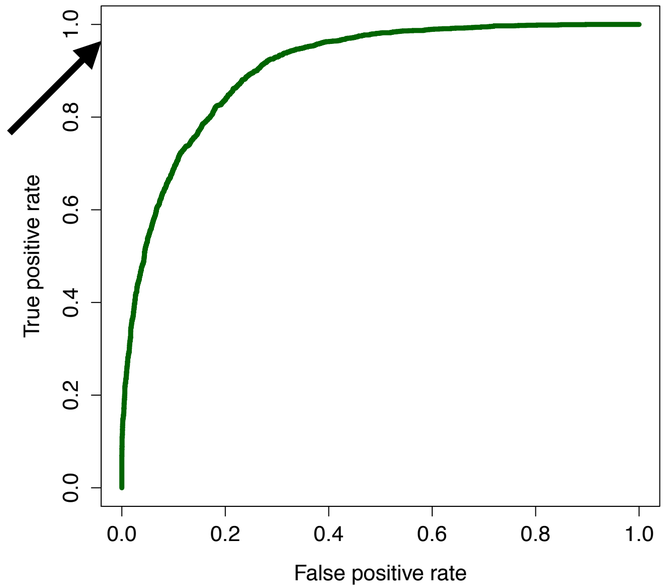
0.0
0.2
0.4
0.6
0.8
1.0

all healthy

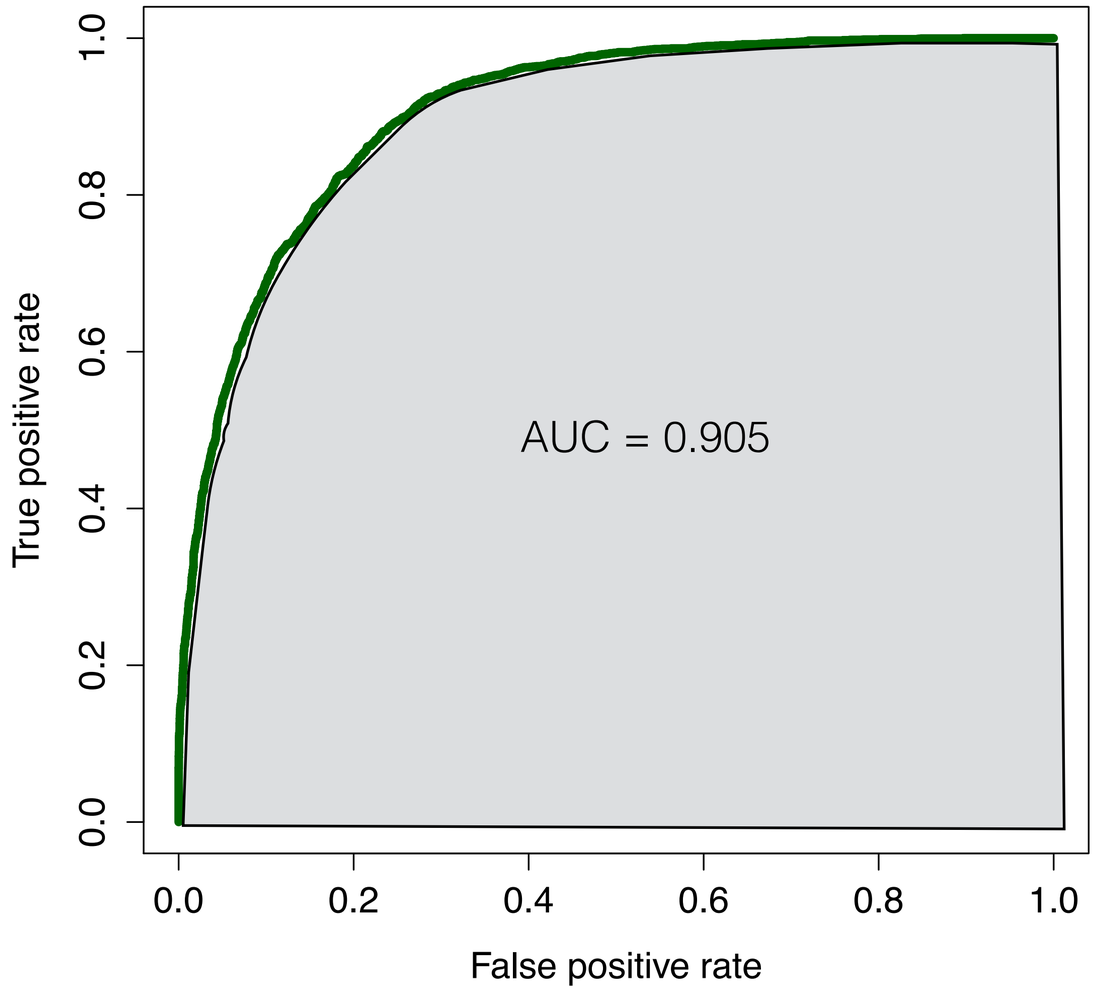

100%
probability

Interpreting the curve

- Is it a good curve?
- **Closer** to left upper corner = **better**
- Good classifiers have **big area under the curve**



> 0.9 = very good



Area under the curve (AUC)

INTRODUCTION TO MACHINE LEARNING

Let’s practice!