Tulane University

More Machine Learning - Classification

Nicholas Mattei, *Tulane University*

CMPS3660 – Introduction to Data Science – Fall 2019

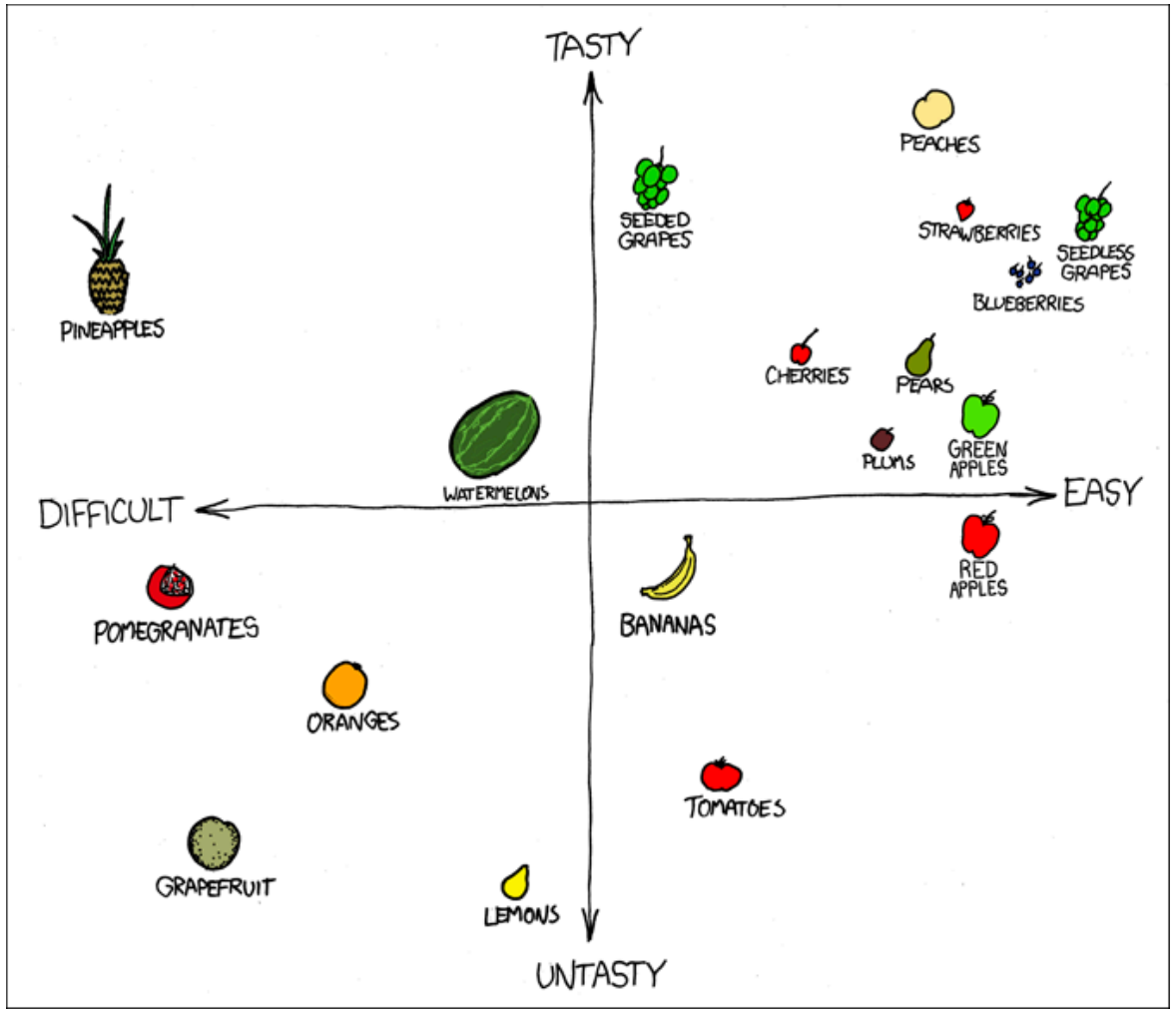
https://rebrand.ly/TUDataScience

Thanks to Bart Selman [Cornell] and Zico Kolter [CMU]

Many Thanks
Slides based off Introduction to Data Science from John P. Dickerson - https://cmsc320.github.io/

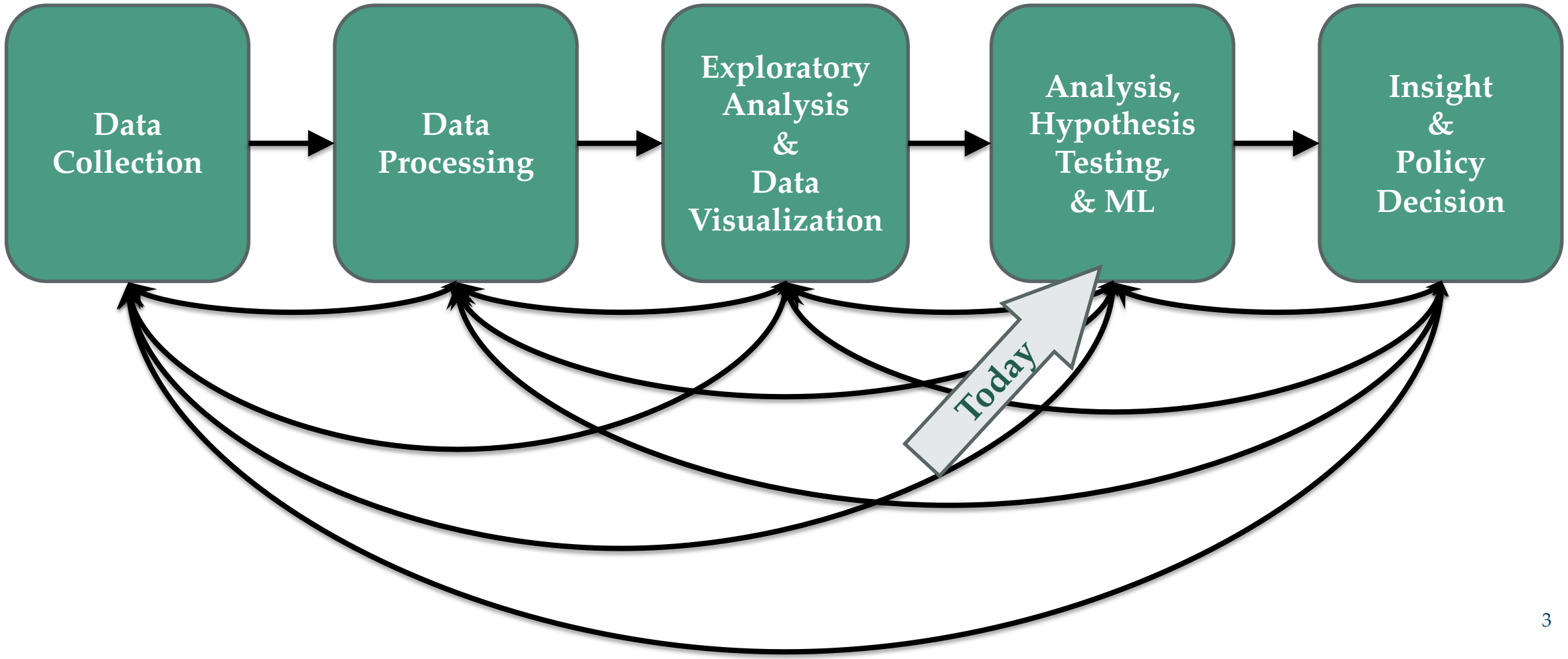
Announcements

- Lab 10 – Missing SQRT
- Lab 11 -- Clarification
- Thursday – Milestone 2 return and schedule, will talk about presentation.
- Classification and Decision Trees!



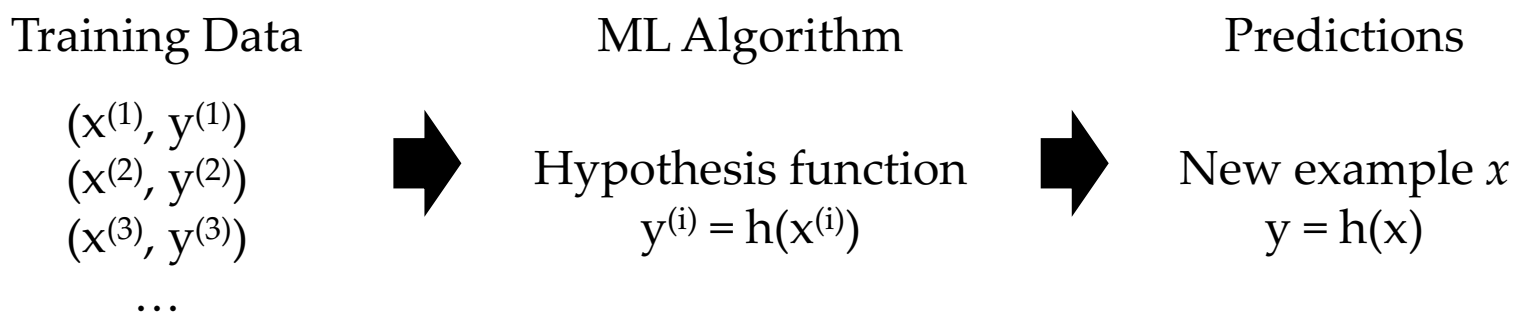
https://xkcd.com/388/

The Data LifeCycle



Machine learning

- We used a linear model to classify input documents
- The model parameters θ were given to us a priori
- (Nick created them by hand.)
- Typically, we cannot specify a model by hand.
- Supervised machine learning provides a way to automatically infer the predictive model from labeled data.



Terminology

- Input features: $x^{(i)} \in \mathbb{R}^n, i = 1, \ldots, m$

	I	like	hate	cats
$x^{(1)T}$ =	1	1	0	1
$x^{(2)T}$ =	1	0	1	1

- Outputs:
- $y^{(i)} \in \{0, 1\}$ = { hates_cats, likes_cats } $y^{(i)} \in \mathcal{Y}, i = 1, \ldots, m$

- Model parameters:

$$\theta \in \mathbb{R}^n$$

θ^T =	0	-1	1	-0.1	0	1	-1	0.5	1

Terminology

- Hypothesis function: $h_\theta : \mathbb{R}^n \to y$
- E.g., linear classifiers predict outputs using:

$$h_\theta(x) = \theta^T x = \sum_{j=1}^{n} \theta_j \cdot x_j$$

- Loss function: $\ell : y \times y \to \mathbb{R}_+$
- Measures difference between a prediction and the true output
- E.g., squared loss:
- E.g., hinge loss:

$$\ell(\hat{y}, y) = (\hat{y} - y)^2$$

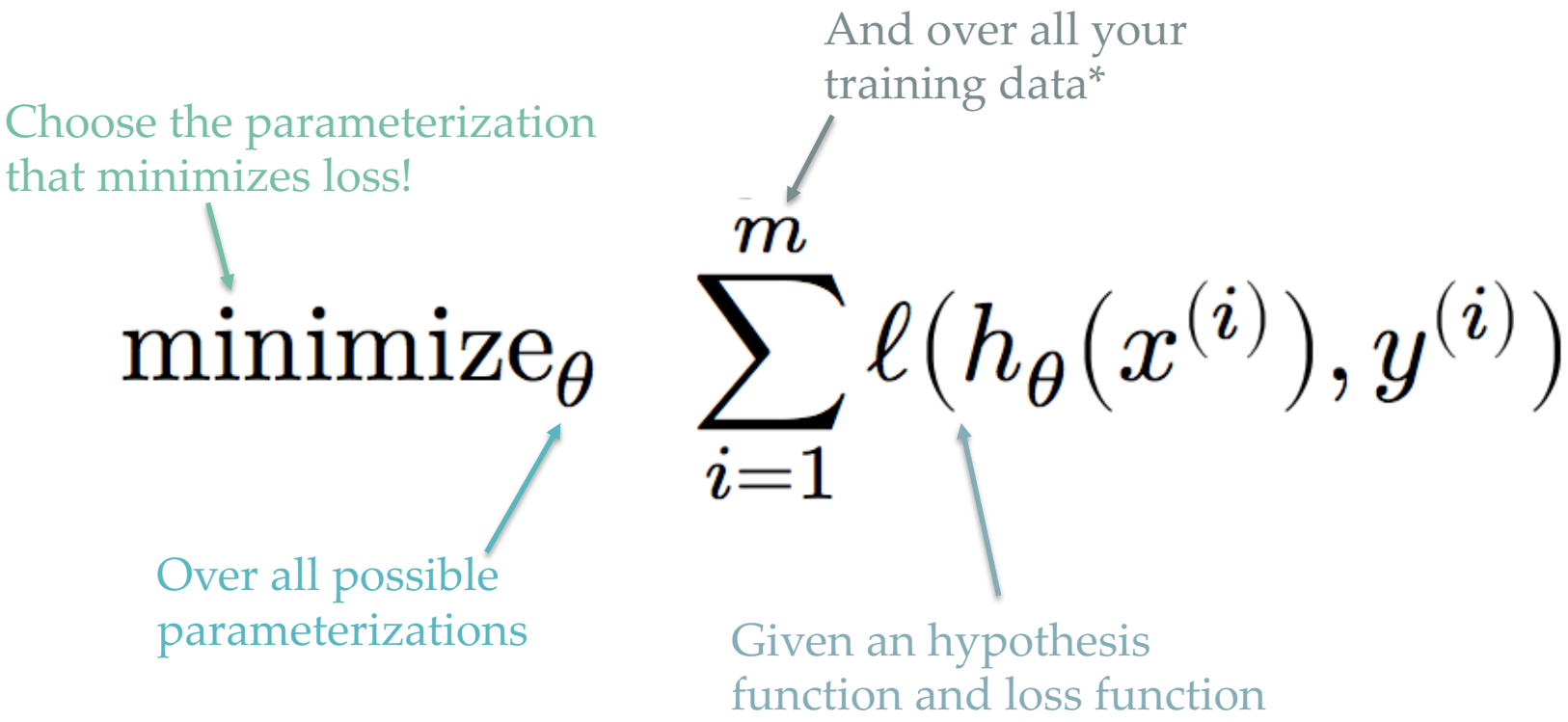
$$\ell(y) = \max(0, 1 - t \cdot y)$$

Output t = {-1,+1} based on -1 or +1 class label

Classifier score y

The canonical Machine learning problem

- At the end of the day, we want to learn a hypothesis function that predicts the actual outputs well.



*Not actually what we want – want it over the world of inputs – will discuss later …

How do I machine learn?

1. What is the hypothesis function?
   - Domain knowledge and EDA can help here.
2. What is the loss function?
   - We've discussed two already: squared and absolute.
3. How do we solve the optimization problem?
   - (We talked about gradient descent in class, but if you are interested, take ML next semester!)

First GIS result for "optimization"

Classification tasks

Regression tasks: predicting real-valued quantity $y \in \mathbb{R}$

Classification tasks: predicting *discrete-valued* quantity y

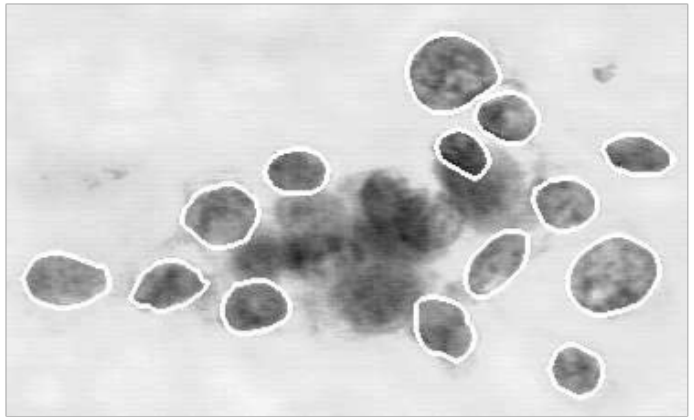
Binary classification: $y \in \{-1, +1\}$

Multiclass classification: $y \in \{1,2, \ldots, k\}$

Example: breast cancer classification

Well-known classification example: using machine learning to diagnose whether a breast tumor is benign or malignant [Street et al., 1992]

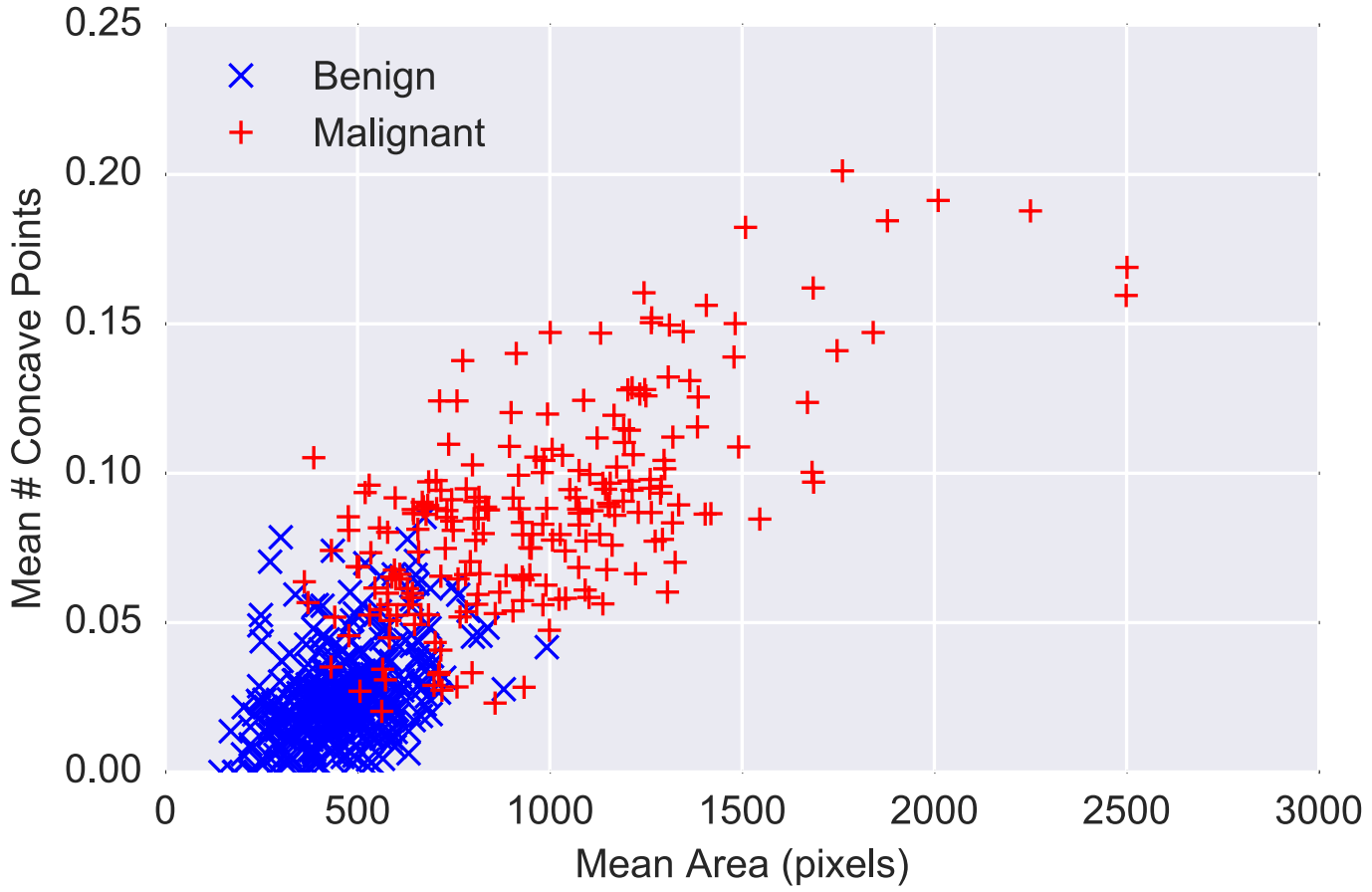
Setting: doctor extracts a sample of fluid from tumor, stains cells, then outlines several of the cells (image processing refines outline)



System computes features for each cell such as area, perimeter, concavity, texture (10 total); computes mean/std/max for all features

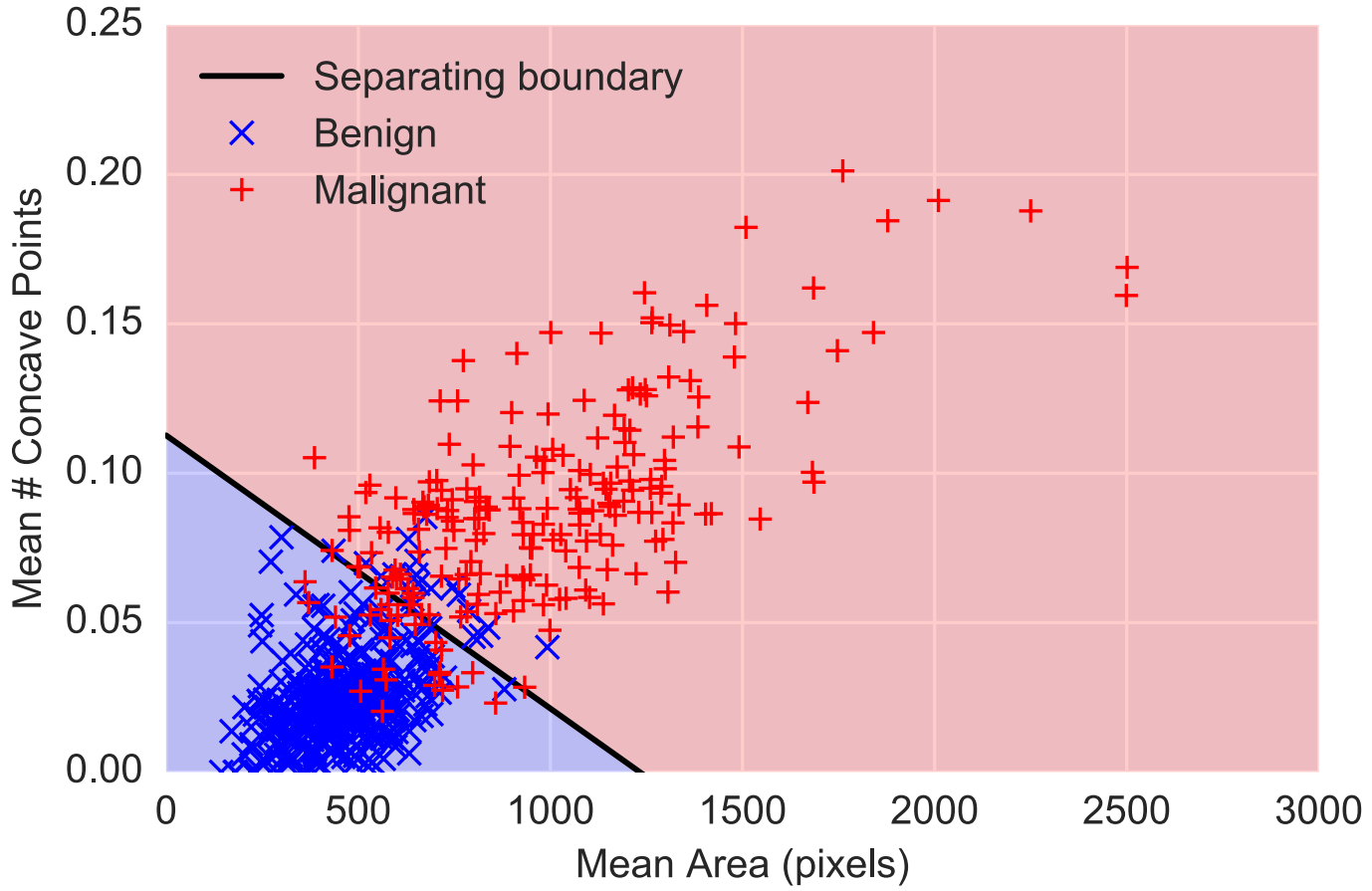
Example: breast cancer classification

Plot of two features: mean area vs. mean concave points, for two classes



Linear classification example

Linear classification ≡ “drawing line separating classes”



Formal setting

Input features: $x^{(i)} \in \mathbb{R}^n, i = 1, \ldots, m$

$$\text{E.g.: } x^{(i)} = \begin{bmatrix} \text{Mean\_Area}^{(i)} \\ \text{Mean\_Concave\_Points}^{(i)} \\ 1 \end{bmatrix}$$

Outputs: $y^{(i)} \in \mathcal{Y},\ i = 1, \ldots, m$

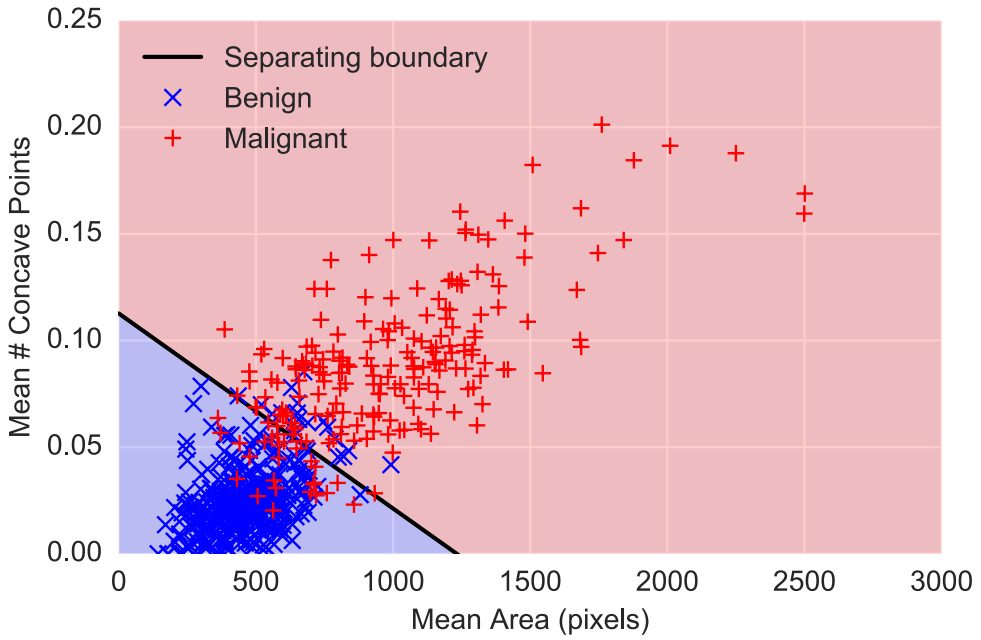
$$\text{E.g.: } y^{(i)} \in \{-1\ (\text{benign}), +1\ (\text{malignant})\}$$

Model parameters: $\theta \in \mathbb{R}^n$

Hypothesis function: $h_\theta : \mathbb{R}^n \to \mathbb{R}$, aims for same *sign* as the output (informally, a measure of *confidence* in our prediction)

$$\text{E.g.: } h_\theta(x) = \theta^T x, \qquad \hat{y} = \text{sign}(h_\theta(x))$$

Understanding linear classification diagrams



Color shows regions where the $h_\theta(x)$ is positive

Separating boundary is given by the equation $h_\theta(x) = 0$

Machine learning optimization

With this notation, the "canonical" machine learning problem is written in the exact same way

$$\underset{\theta}{\text{minimize}} \sum_{i=1}^{m} \ell\big(h_\theta\big(x^{(i)}\big), y^{(i)}\big)$$

Unlike least squares, there is not an analytical solution to the zero gradient condition for most classification losses

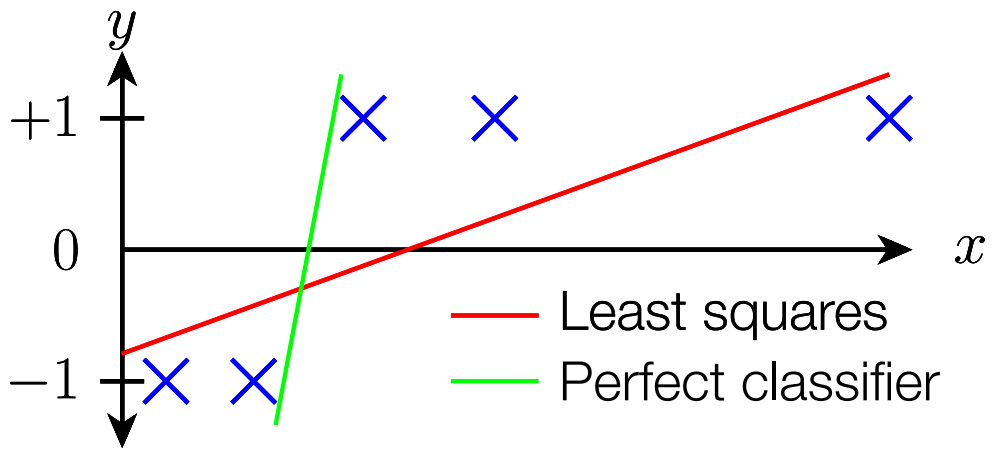
Instead, we solve these optimization problems using gradient descent (or a alternative optimization method, but we'll only consider gradient descent here)

$$\text{Repeat: } \theta := \theta - \alpha \sum_{i=1}^{m} \nabla_\theta \ell\big(\, h_\theta\big(x^{(i)}\big), y^{(i)}\big)$$

Loss functions for classification

How do we define a loss function $\ell: \mathbb{R} \times \{-1, +1\} \to \mathbb{R}_+$?

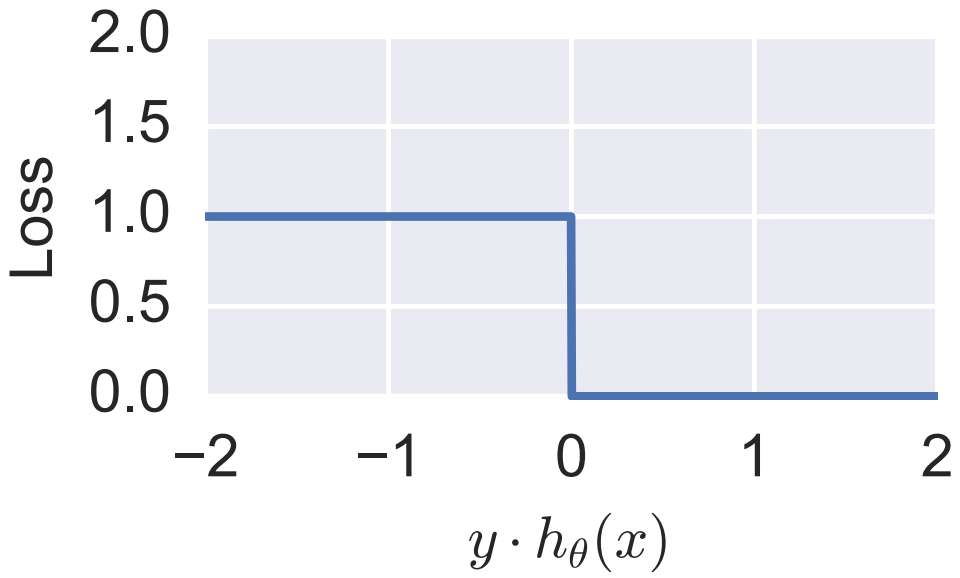
What about just using squared loss?



0/1 loss (i.e. error)

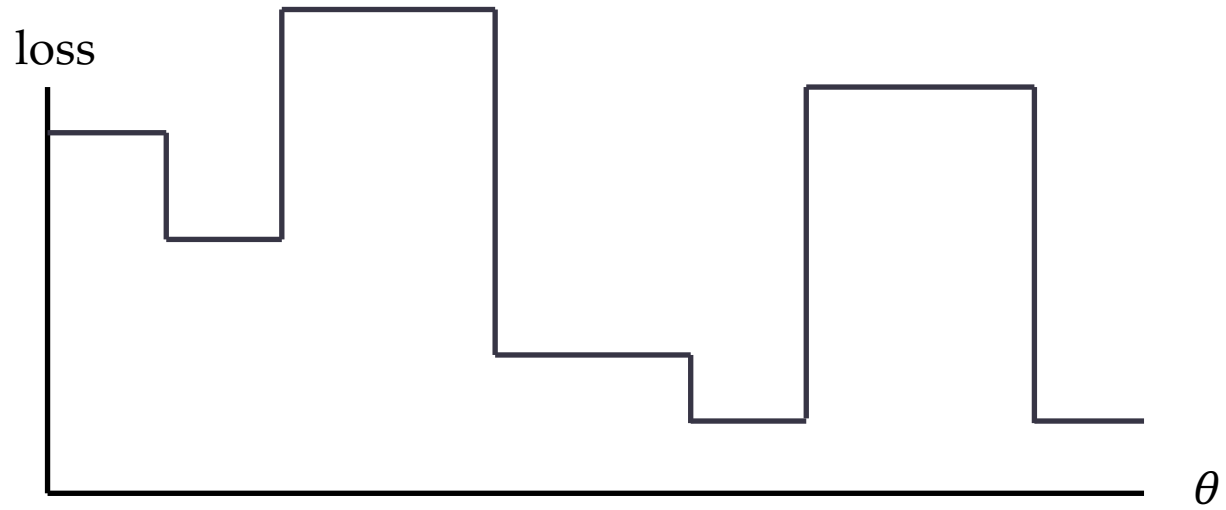
The loss we would like to minimize (0/1 loss, or just “error”):

$$\ell_{0/1}(h_\theta(x), y) = \begin{cases} 0 & \text{if } \operatorname{sign}\big(h_\theta(x)\big) = y \\ 1 & \text{otherwise} \end{cases}$$
$$= \mathbf{1}\{y \cdot h_\theta(x) \leq 0\}$$



Minimizing 0/1 loss in a single dimension

$$\sum_{i=1}^{n} 1\left[y^{(i)} \cdot \langle \theta, x^{(i)} \rangle \leq 0\right]$$



Each time we change θ such that the example is right (wrong) the loss will increase (decrease)

(Recall: y in {-1, +1})

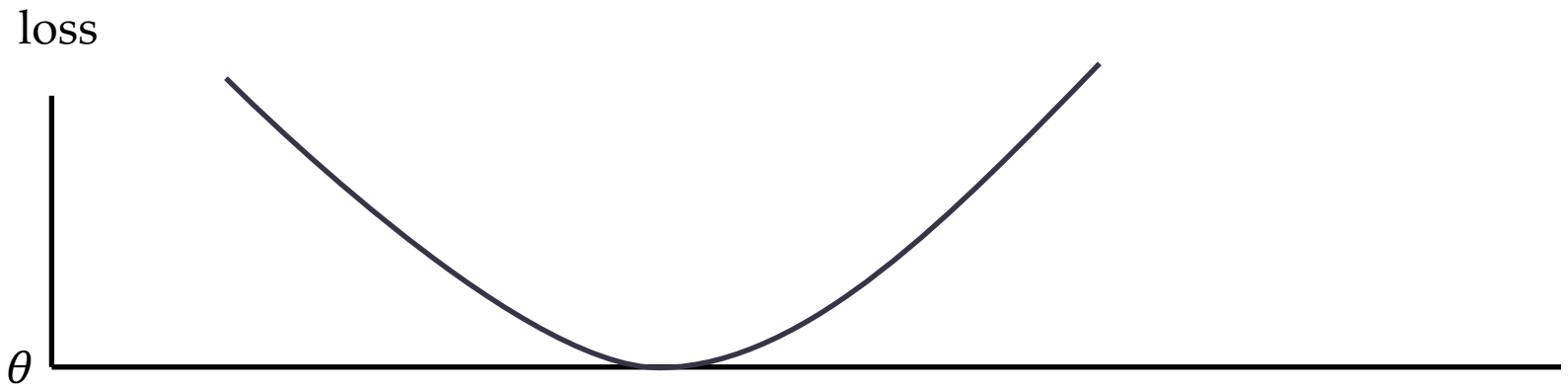
Minimizing 0/1 loss over all θ

$$\arg\min_{\theta} \sum_{i=1}^{n} 1\left[y^{(i)} \cdot \langle \theta, x^{(i)} \rangle \leq 0\right]$$

- This is NP-hard.
- Small changes in any θ can have large changes in the loss (the change isn't continuous)
- There can be many local minima
- At any give point, we don't have much information to direct us towards any minima
- Maybe we should consider other loss functions.

(Recall: y in {-1, +1})

Desirable properties

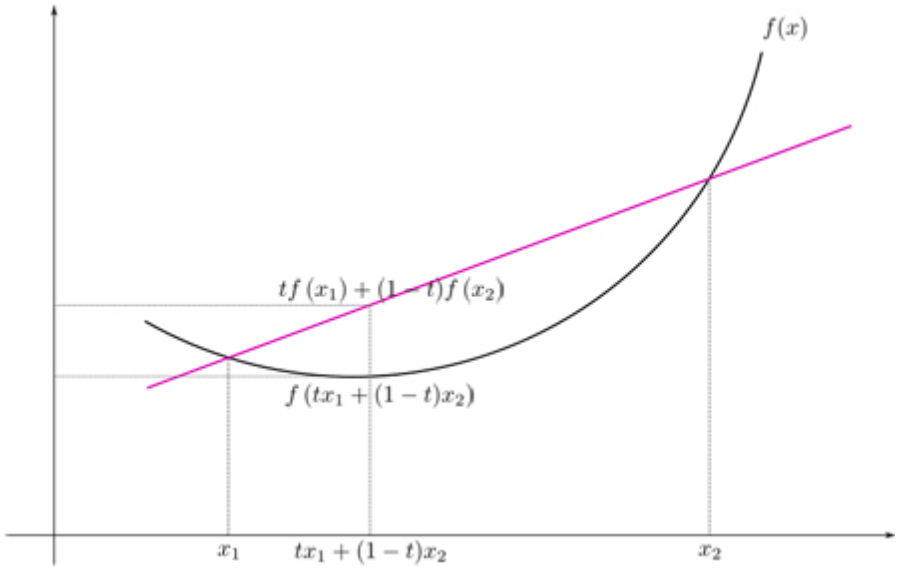


- What are some desirable properties of a loss function????????
- Continuous so we get a local indication of the direction of minimization
- Only one (i.e., global) minimum

Convex functions

- "A function is convex if the line segment between any two points on its graph lies above it."
- Formally, given function *f* and two points x, y:

$$f(\lambda \mathbf{x} + (1-\lambda)\mathbf{y}) \leq \lambda f(\mathbf{x}) + (1-\lambda) f(\mathbf{y}) \quad \forall \lambda \in [0,1]$$



Surrogate loss functions

- For many applications, we really would like to minimize the 0/1 loss
- A surrogate loss function is a loss function that provides an upper bound on the actual loss function (in this case, 0/1)
- We'd like to identify convex surrogate loss functions to make them easier to minimize
- Key to a loss function is how it scores the difference between the actual label y and the predicted label y'

Surrogate loss functions

- 0/1 loss: $\ell(\hat{y}, y) = \mathbf{1}\left[y\hat{y} \leq 0\right]$
- Any ideas for surrogate loss functions ??????????
  Want: a function that is continuous and convex and upper bounds the 0/1 loss.

- Hinge: $\ell(\hat{y}, y) = \max(0, 1 - y\hat{y})$

- Exponential: $\ell(\hat{y}, y) = e^{-y\hat{y}}$

- Squared: $\ell(\hat{y}, y) = (y - \hat{y})^2$

- What do each of these penalize?????????

(Recall: y in {-1, +1})

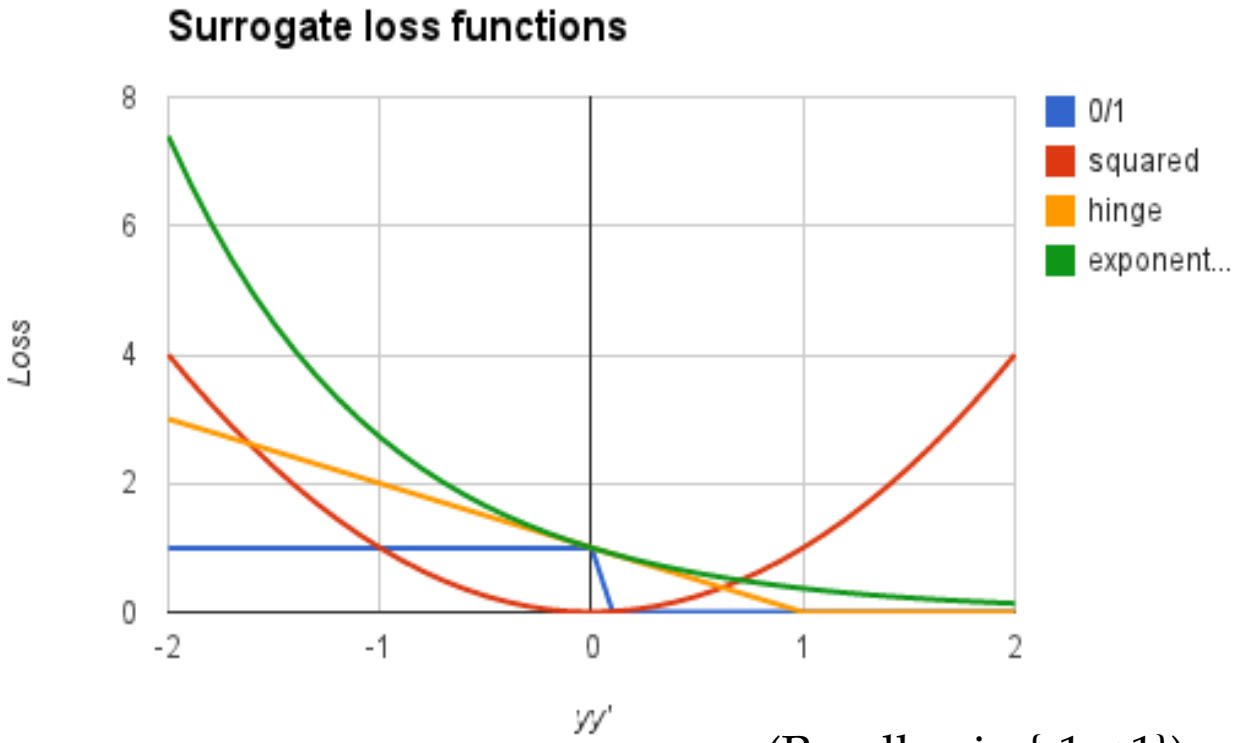
Surrogate loss functions

0/1 loss: $\ell(\hat{y}, y) = \mathbf{1}\left[y\hat{y} \leq 0\right]$

Hinge: $\ell(\hat{y}, y) = \max(0, 1 - y\hat{y})$

Exponential: $\ell(\hat{y}, y) = e^{-y\hat{y}}$

Squared loss: $\ell(\hat{y}, y) = (y - \hat{y})^2$



(Recall: y in {-1, +1})

Some ML algorithms

Name	Hypothesis Function	Loss Function	Optimization Approach
Least squares	Linear	Squared	Analytical or GD
Linear regression	Linear	Squared	Analytical or GD
Support Vector Machine (SVM)	Linear, Kernel	Hinge	Analytical or GD
Perceptron	Linear	Perceptron criterion (~Hinge)	Perceptron algorithm, others
Neural Networks	Composed nonlinear	Squared, Hinge	SGD
Decision Trees	Hierarchical halfplanes	Many	Greedy
Naïve Bayes	Linear	Joint probability	#SAT

Follow the white rabbit: https://en.wikipedia.org/wiki/List_of_machine_learning_concepts

The canonical Machine learning problem

- At the end of the day, we want to learn a hypothesis function that predicts the actual outputs well.

Choose the parameterization that minimizes loss!

And over all your training data*

$$\text{minimize}_\theta \sum_{i=1}^{m} \ell\left(h_\theta\left(x^{(i)}\right), y^{(i)}\right)$$

Over all possible parameterizations

Given an hypothesis function and loss function

*Not actually what we want – want it over the world of inputs – will discuss later …

Big Picture of Learning

- Learning can be seen as fitting a function to the data. We can consider
- different target functions and therefore different hypothesis spaces.
- Examples:
- Propositional if-then rules
- Decision Trees
- First-order if-then rules
- First-order logic theory
- Linear functions
- Polynomials of degree at most k
- Neural networks
- Java programs
- Turing machine
- Etc

A learning problem
is realizable if its hypothesis space
contains the true function.

Tradeoff between expressiveness of
a hypothesis space and the
complexity of finding simple, consistent hypotheses
within the space.

Decision Tree Learning

Task:

- Given: collection of examples *(x, f(x))*
- Return: a function *h* (*hypothesis*) that approximates *f*
- *h is a decision tree*

- **Input:** an object or situation described by a set of attributes (or features)
- **Output:** a "decision" – the predicts output value for the input.

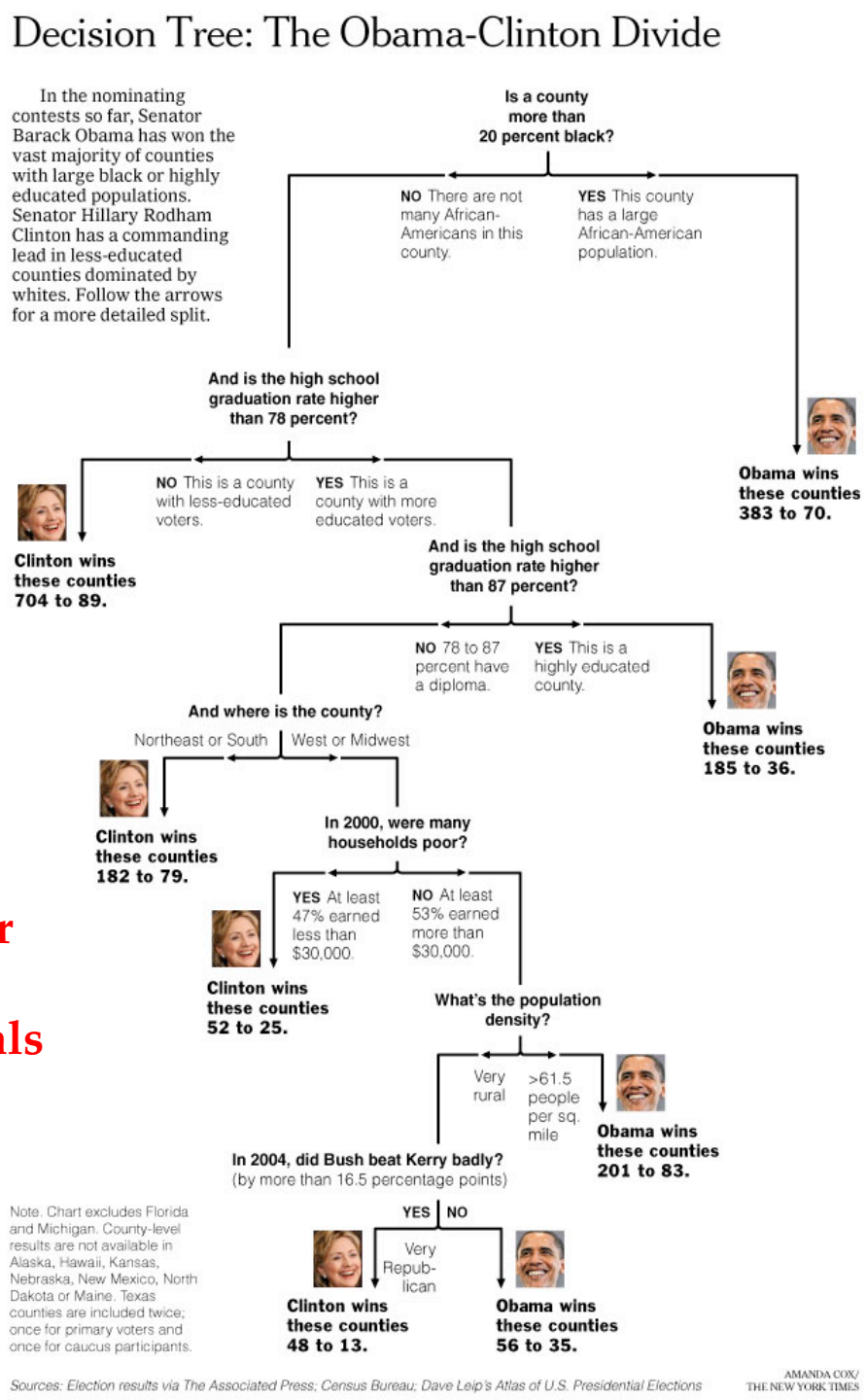
- The input attributes and the outputs can be discrete or continuous.

- We will focus on decision trees for Boolean classification:
- each example is classified as positive or negative.

Can we learn
how counties vote?

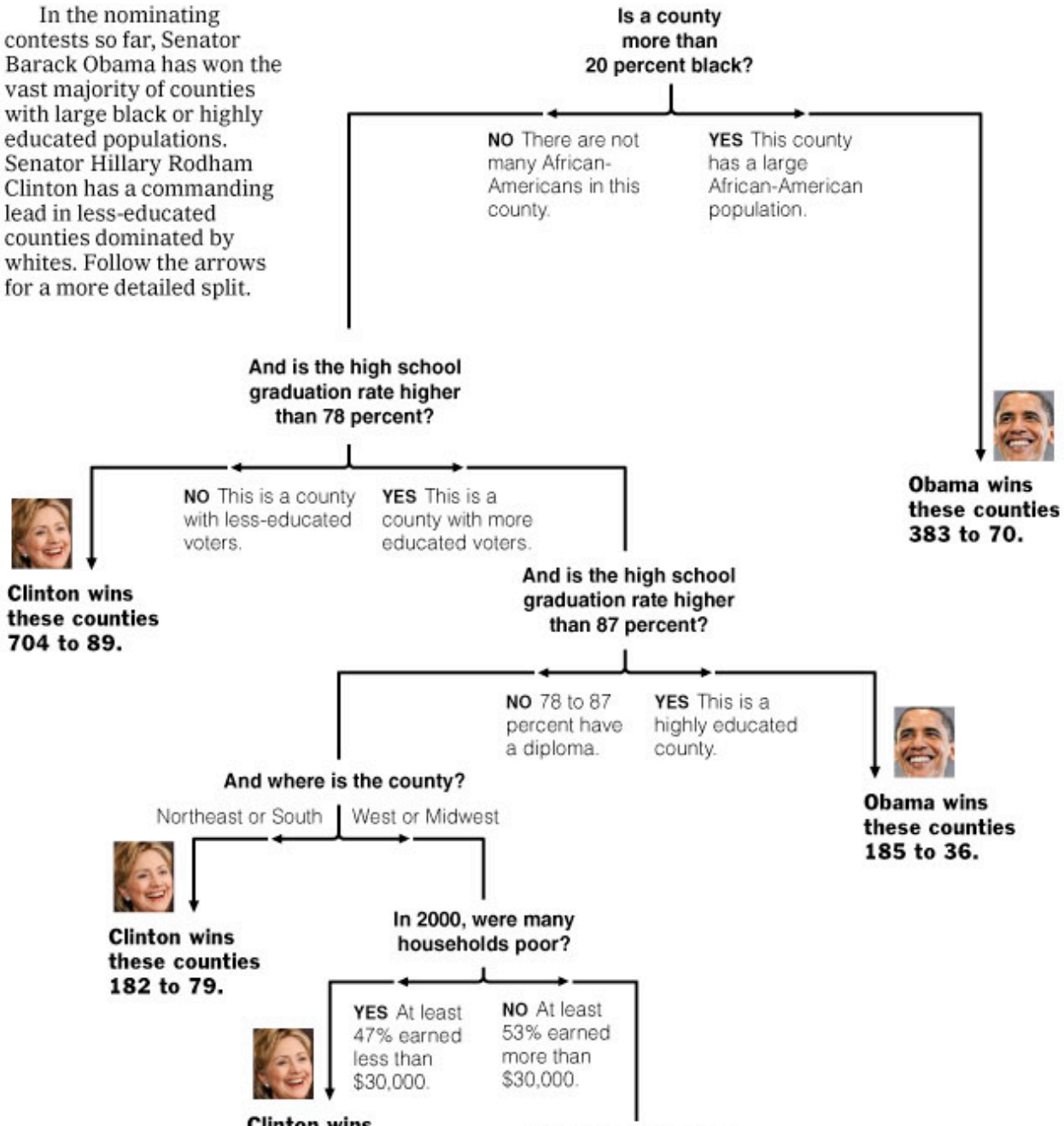
New York Times
April 16, 2008

Decision Trees:
a sequence of tests.
Representation very natural for humans.
Style of many "How to" manuals and trouble-shooting procedures.

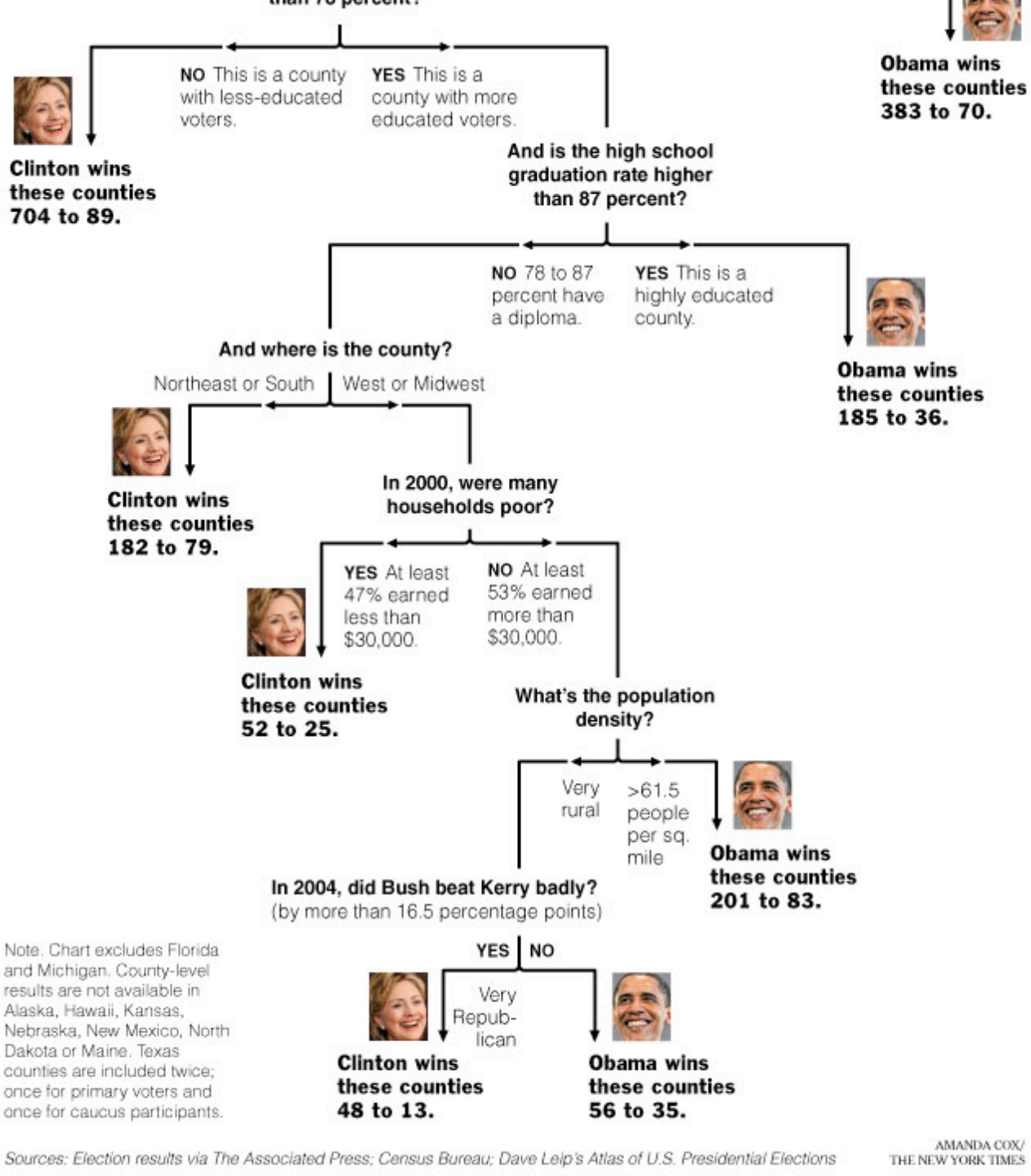


Decision Tree: The Obama-Clinton Divide

In the nominating contests so far, Senator Barack Obama has won the vast majority of counties with large black or highly educated populations. Senator Hillary Rodham Clinton has a commanding lead in less-educated counties dominated by whites. Follow the arrows for a more detailed split.



Note: order of tests matters (in general)! When not?



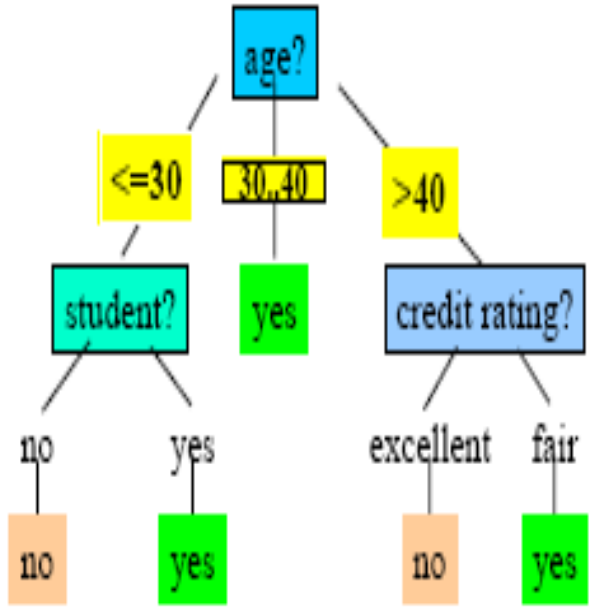
Tulane University

Decision tree learning approach can construct tree (with test thresholds) from example counties.

Decision Tree

- A tree with two types of nodes:
  - Decision nodes
  - Leaf nodes
  -
- Decision node: Specifies a choice or test of some attribute with 2 or more alternatives;
  - every decision node is part of a path to a leaf node
- Leaf node: Indicates classification of an example

- Decision Tree example (is a customer going to buy a computer or not):



Inductive Learning Example

Food (3)	Chat (2)	Fast (2)	Price (3)	Bar (2)	BigTip
great	yes	yes	normal	no	yes
great	no	yes	normal	no	yes
mediocre	yes	no	high	no	no
great	yes	yes	normal	yes	yes

Etc.

Instance Space X: Set of all possible objects described by attributes (often called features).

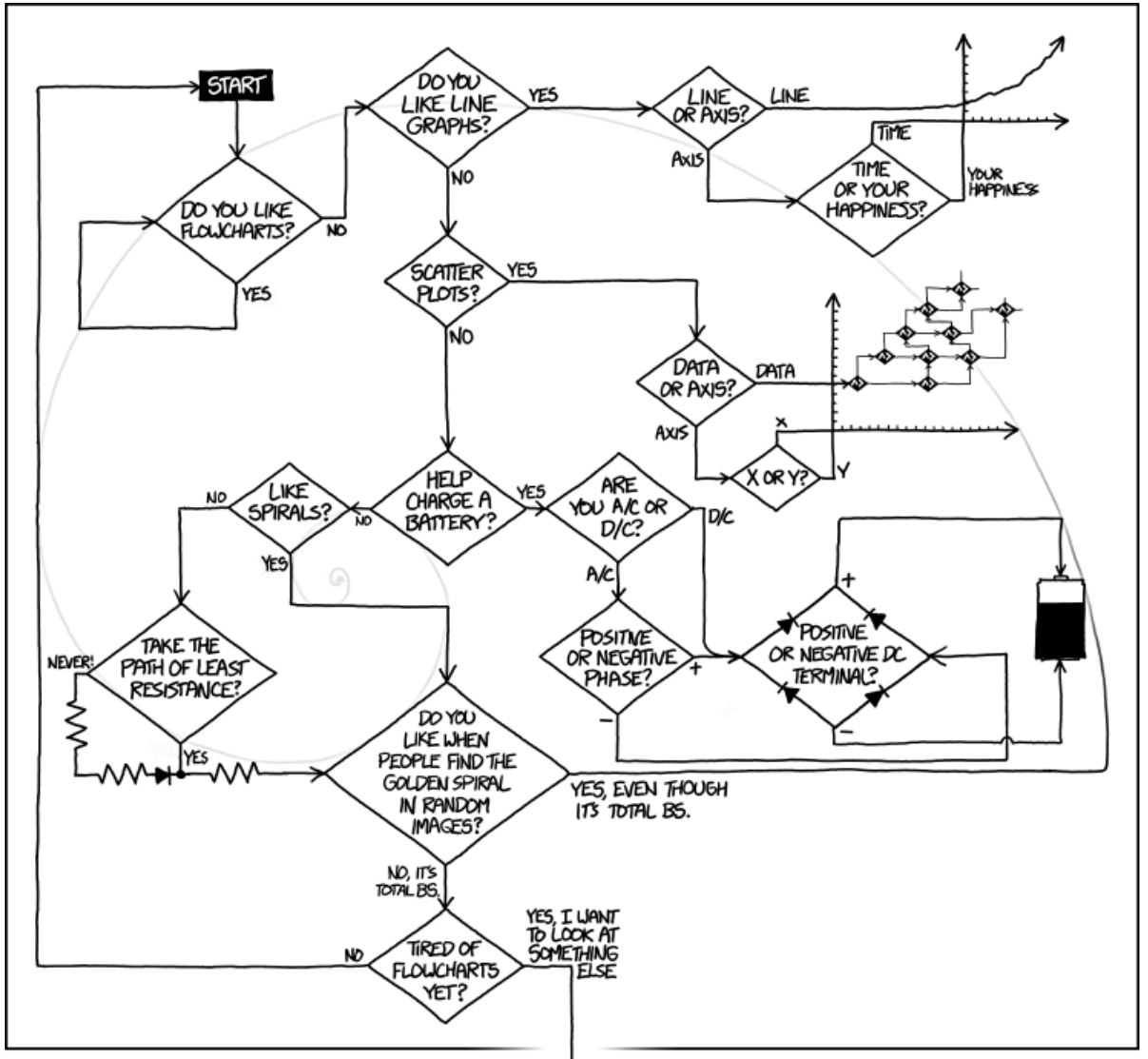
Target Function f: Mapping from Attributes to Target Feature (often called label) (f is unknown)

Hypothesis Space H: Set of all classification rules h_i we allow.

Training Data D: Set of instances labeled with Target Feature

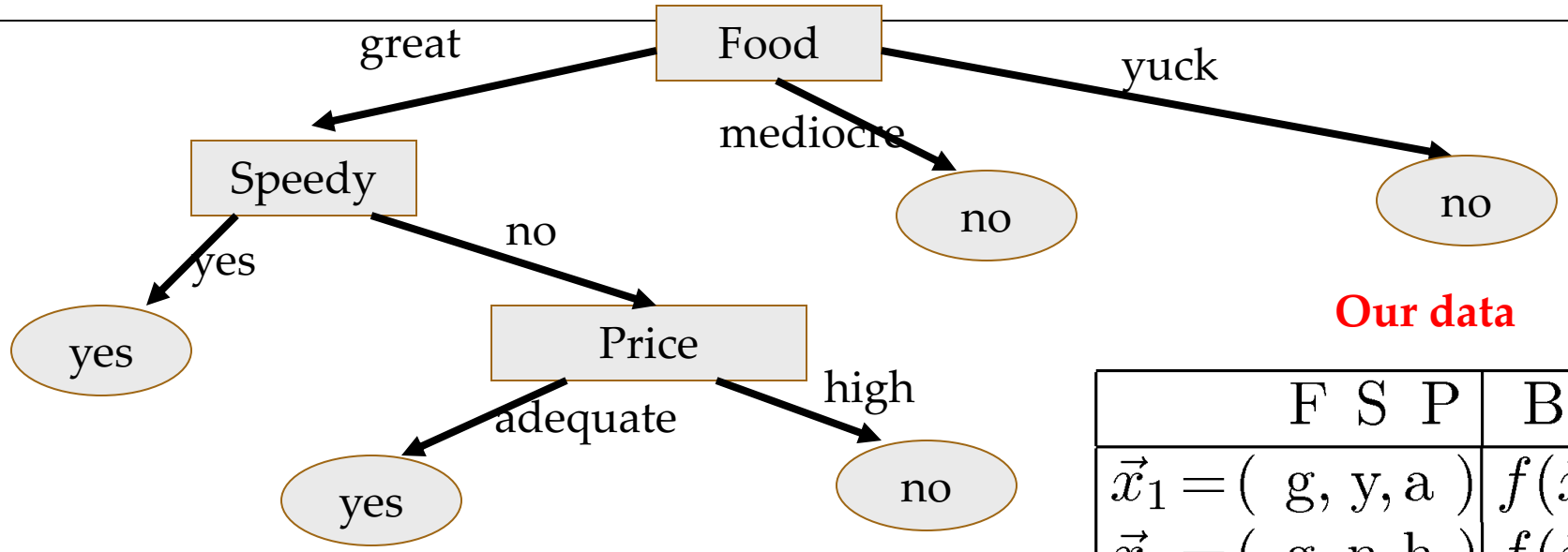
Announcements

- Lab 11 Review
- Final Presentation Schedule
- Milestone 2 / Optional Lab 12 / Questions Announcement.
- Tuesday (Last) Lecture Survey?
- (More) Classification and Decision Trees!



https://xkcd.com/1488/

Decision Tree Example: "BigTip"



Our data

	F	S	P	BigTip
$\vec{x}_1 = (\ $	g,	y,	a $)$	$f(\vec{x}_1) = 1$
$\vec{x}_2 = (\ $	g,	n,	h $)$	$f(\vec{x}_2) = 0$
$\vec{x}_3 = (\ $	g,	y,	h $)$	$f(\vec{x}_3) = 1$
$\vec{x}_4 = (\ $	g,	n,	a $)$	$f(\vec{x}_4) = 1$
$\vec{x}_5 = (\ $	m,	y,	a $)$	$f(\vec{x}_5) = 0$
$\vec{x}_6 = (\ $	y,	y,	a $)$	$f(\vec{x}_6) = 0$
$\vec{x}_7 = (\ $	g,	y,	a $)$	$f(\vec{x}_7) = 1$
$\vec{x}_8 = (\ $	g,	y,	h $)$	$f(\vec{x}_8) = 1$
$\vec{x}_9 = (\ $	m,	y,	a $)$	$f(\vec{x}_9) = 0$
$\vec{x}_{10} = (\ $	g,	y,	a $)$	$f(\vec{x}_{10}) = 1$

Is the decision tree we learned consistent?

Yes, it agrees with all the examples!

Data: Not all 2x2x3 = 12 tuples
Also, some repeats! These are literally "observations."

Learning decision trees: An example

- **Problem: decide whether to wait for a table at a restaurant. What attributes would you use?**

- Attributes used by R&N
  1. Alternate: is there an alternative restaurant nearby?
  2. Bar: is there a comfortable bar area to wait in?
  3. Fri/Sat: is today Friday or Saturday?
  4. Hungry: are we hungry?
  5. Patrons: number of people in the restaurant (None, Some, Full)
  6. Price: price range ($, $$, $$$)
  7. Raining: is it raining outside?
  8. Reservation: have we made a reservation?
  9. Type: kind of restaurant (French, Italian, Thai, Burger)
  10. WaitEstimate: estimated waiting time (0-10, 10-30, 30-60, >60)

Goal predicate: WillWait?

What about restaurant name?

It could be great for generating a small tree but …

It doesn't generalize!

Attribute-based representations

- Examples described by attribute values (Boolean, discrete, continuous)
- E.g., situations where I will/won't wait for a table:

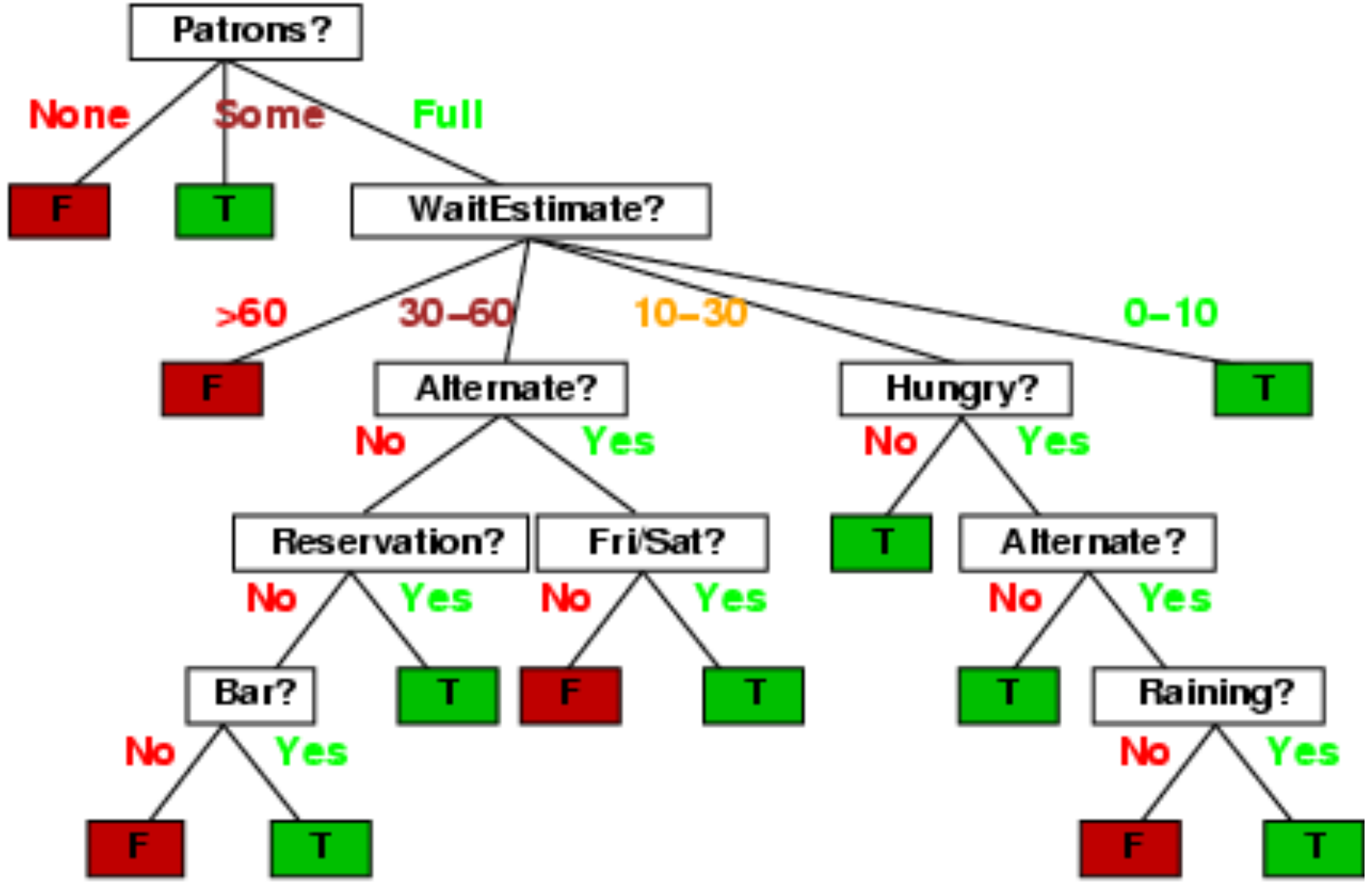
Example	Attributes										Target
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*Wait*
X_1	T	F	F	T	Some	$$$	F	T	French	0–10	T
X_2	T	F	F	T	Full	$	F	F	Thai	30–60	F
X_3	F	T	F	F	Some	$	F	F	Burger	0–10	T
X_4	T	F	T	T	Full	$	F	F	Thai	10–30	T
X_5	T	F	T	F	Full	$$$	F	T	French	>60	F
X_6	F	T	F	T	Some	$$	T	T	Italian	0–10	T
X_7	F	T	F	F	None	$	T	F	Burger	0–10	F
X_8	F	F	F	T	Some	$$	T	T	Thai	0–10	T
X_9	F	T	T	F	Full	$	T	F	Burger	>60	F
X_{10}	T	T	T	T	Full	$$$	F	T	Italian	10–30	F
X_{11}	F	F	F	F	None	$	F	F	Thai	0–10	F
X_{12}	T	T	T	T	Full	$	F	F	Burger	30–60	T

12 examples
6 +
6 -

- Classification of examples is positive (T) or negative (F)

Decision trees

- One possible representation for hypotheses
- E.g., here is a tree for deciding whether to wait:



Expressiveness of Decision Trees

Any particular decision tree hypothesis for WillWait goal predicate can be seen as a disjunction of a conjunction of tests, i.e., an assertion of the form:

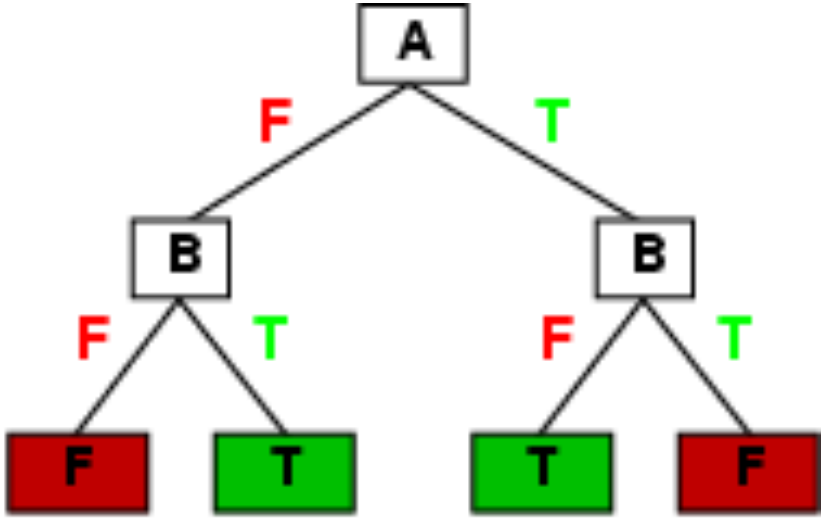
$$\forall s \;\; \text{WillWait}(s) \leftrightarrow (P1(s) \vee P2(s) \vee \ldots \vee Pn(s))$$

Where each condition Pi(s) is a conjunction of tests corresponding to the path from the root of the tree to a leaf with a positive outcome.

Expressiveness

- Decision trees can express any Boolean function of the input attributes.
- E.g., for Boolean functions, truth table row → path to leaf:

A	B	A xor B
F	F	F
F	T	T
T	F	T
T	T	F



Number of Distinct Decision Trees

- How many distinct decision trees with *10* Boolean attributes?
- = number of Boolean functions with 10 propositional symbols

Input features	Output
0 0 0 0 0 0 0 0 0 0	0/1
0 0 0 0 0 0 0 0 0 1	0/1
0 0 0 0 0 0 0 0 1 0	0/1
0 0 0 0 0 0 0 1 0 0	0/1
…	
1 1 1 1 1 1 1 1 1 1	0/1

How many entries does this table have? 2^{10}

So how many Boolean functions with 10 Boolean attributes are there, given that each entry can be 0/1?

$= 2^{2^{10}}$

Hypothesis spaces

- How many distinct decision trees with *n* Boolean attributes?
- = number of Boolean functions

- = number of distinct truth tables with 2^n rows

$= 2^{2^n}$

E.g. how many Boolean functions on 6 attributes? A lot…

- **With 6 Boolean attributes, there are 18,446,744,073,709,551,616 possible trees!**

Many calculators can't handle 10 attributes ☺!

There are even more decision trees! (see later)

Decision tree learning Algorithm

- Decision trees can express any Boolean function.
- Goal: Finding a decision tree that agrees with training set.
- We could construct a decision tree that has one path to a leaf for each example, where the path tests sets each attribute value to the value of the example.

What is the problem with this from a learning point of view?

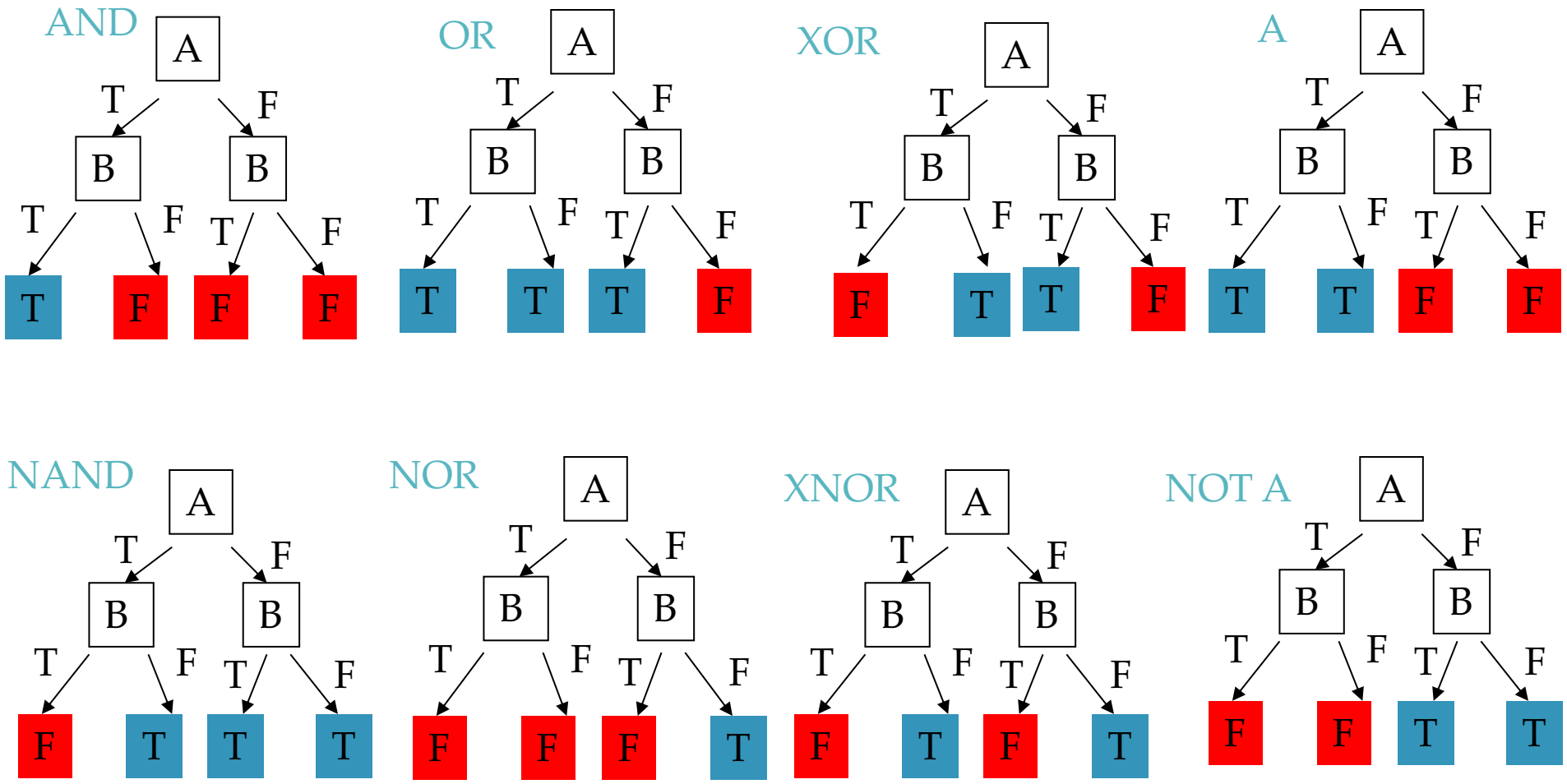
Problem: This approach would just memorize example. How to deal with new examples? It doesn't generalize!

(But sometimes hard to avoid --- e.g. parity function, 1, if an even number of inputs, or majority function, 1, if more than half of the inputs are 1).

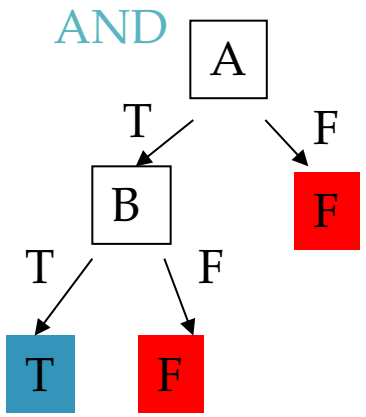
We want a compact/smallest tree.
But finding the smallest tree consistent with the examples is NP-hard!

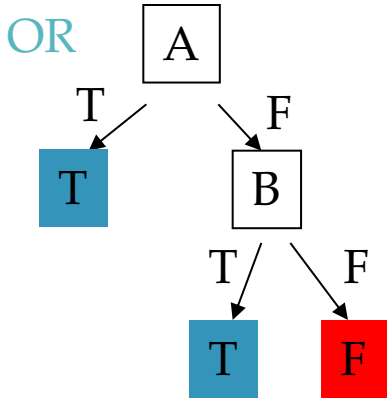
- Overall Goal: get a good classification with a small number of tests.

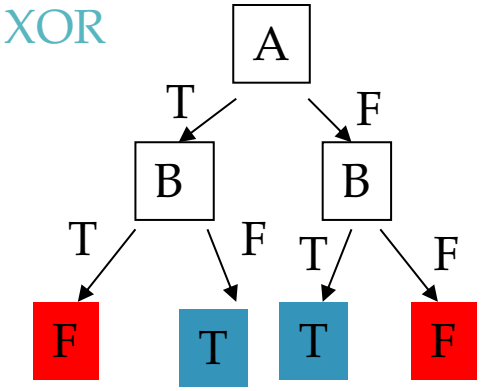
Expressiveness: Boolean Function with 2 attributes → 2^{2^2} DTs

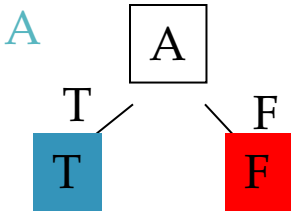


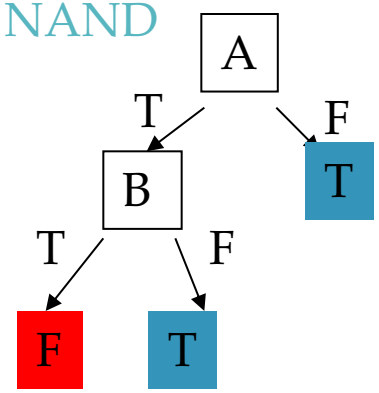
Expressiveness: 2 attribute → 2^{2^2} DTs

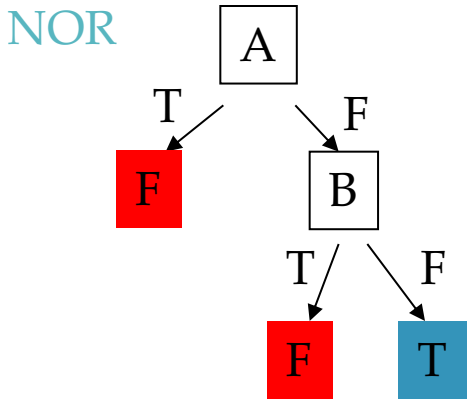


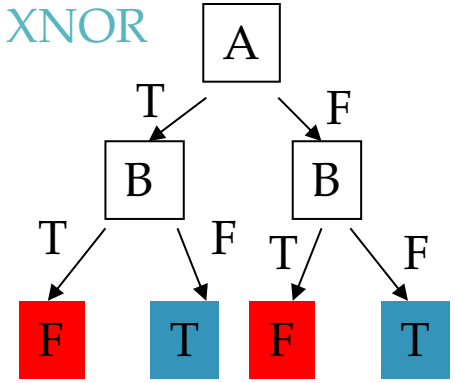


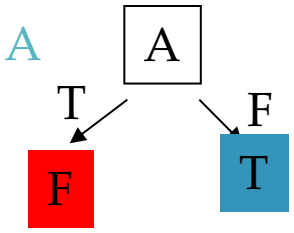






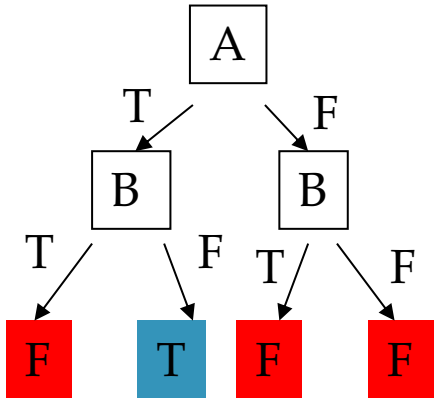




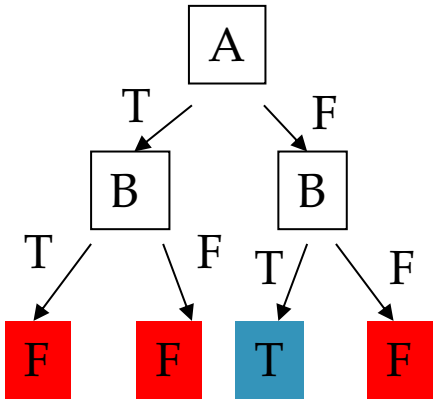


Expressiveness: 2 attribute → 2^{2^2} DTs

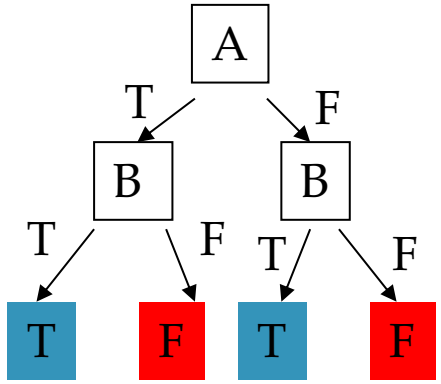
A AND-NOT B



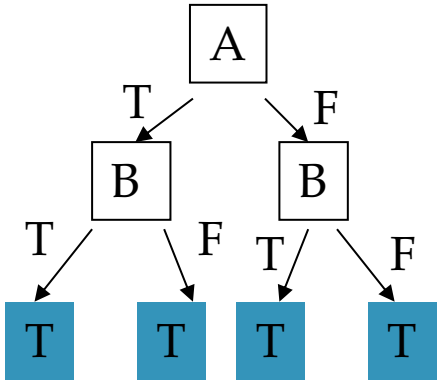
NOT A AND B



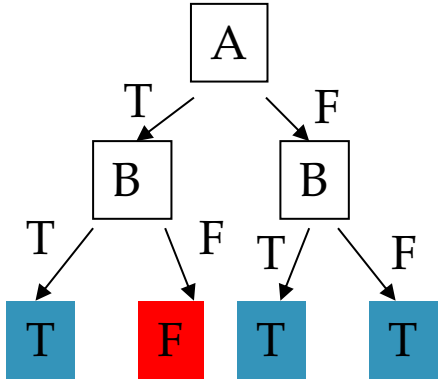
B



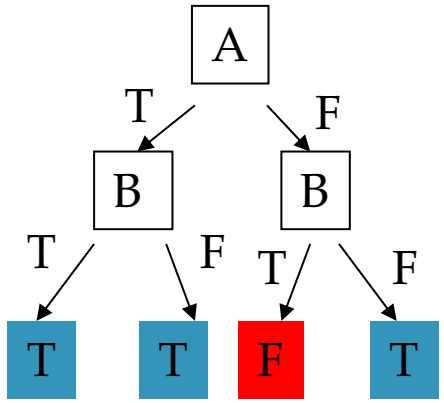
TRUE



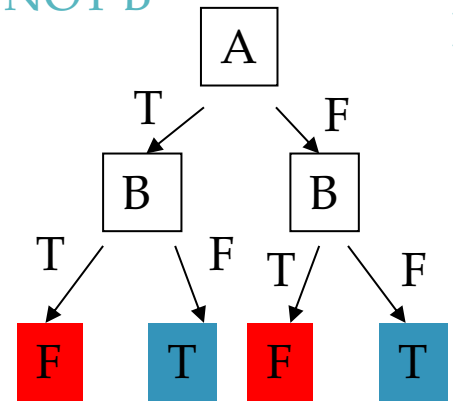
A OR NOT B



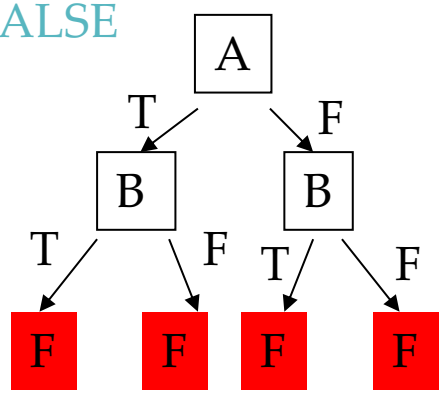
NOR A OR B



NOT B

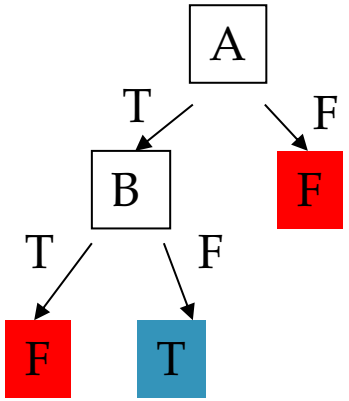


FALSE

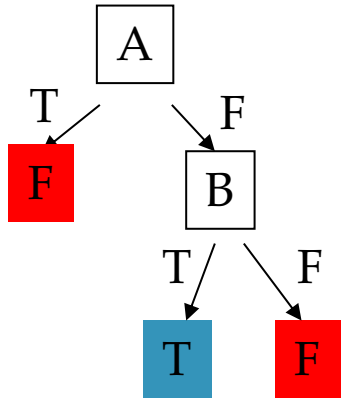


Expressiveness: 2 attribute → 2^{2^2} DTs

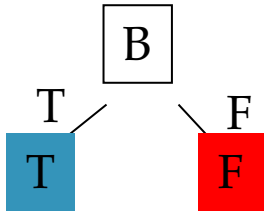
A AND-NOT B



NOT A AND B

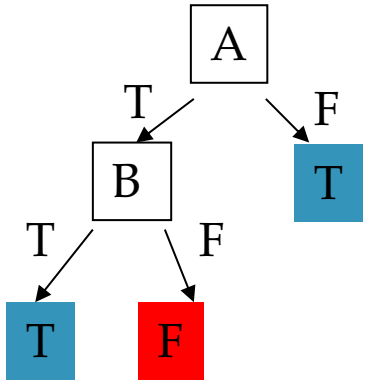


B

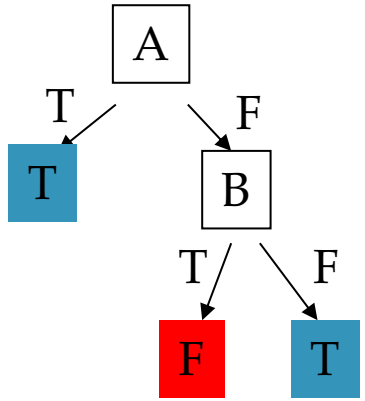


TRUE

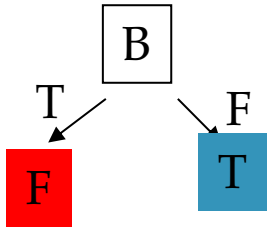
A OR NOT B



NOR A OR B



NOT B



FALSE

Basic DT Learning Algorithm

- Goal: find a *small* tree consistent with the training examples

"most significant"
In what sense?

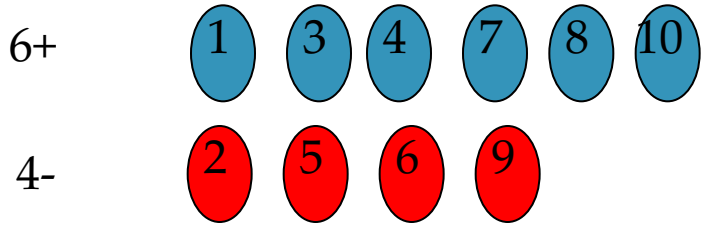
- Idea: (recursively) choose "most significant" attribute as root of (sub)tree;
- Use a top-down greedy search through the space of possible decision trees.
- Greedy because there is no backtracking. It picks highest values first.

- Variations of known algorithms ID3, C4.5 (Quinlan -86, -93)

- Top-down greedy construction
  - Which attribute should be tested?
    - Heuristics and Statistical testing with current data (ID3 Iterative Dichotomiser 3)
  - Repeat for descendants

Big Tip Example

10 examples:



Attributes:
- Food with values g,m,y
- Speedy? with values y,n
- Price, with values a, h

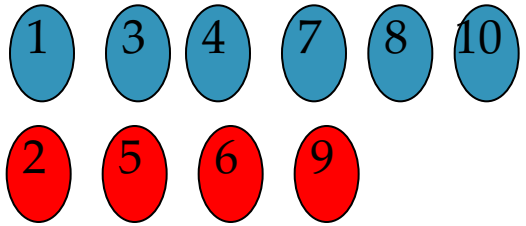
Let's build our decision tree starting with the attribute Food, (3 possible values: g, m, y).

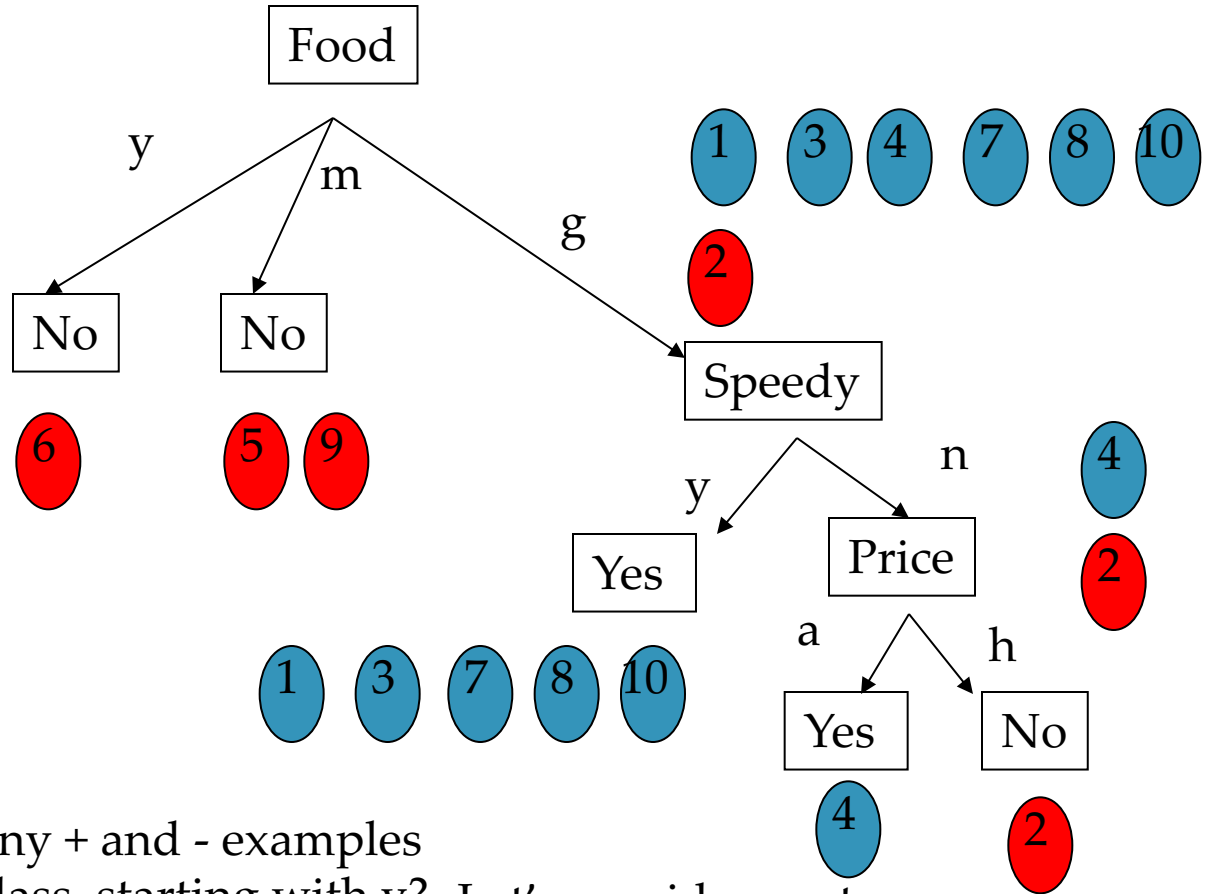
	F S P	BigTip
$\vec{x}_1$	(g, y, a)	$f(\vec{x}_1)=1$
$\vec{x}_2$	(g, n, h)	$f(\vec{x}_2)=0$
$\vec{x}_3$	(g, y, h)	$f(\vec{x}_3)=1$
$\vec{x}_4$	(g, n, a)	$f(\vec{x}_4)=1$
$\vec{x}_5$	(m, y, a)	$f(\vec{x}_5)=0$
$\vec{x}_6$	(y, y, a)	$f(\vec{x}_6)=0$
$\vec{x}_7$	(g, y, a)	$f(\vec{x}_7)=1$
$\vec{x}_8$	(g, y, h)	$f(\vec{x}_8)=1$
$\vec{x}_9$	(m, y, a)	$f(\vec{x}_9)=0$
$\vec{x}_{10}$	(g, y, a)	$f(\vec{x}_{10})=1$

Top-Down Induction of Decision Tree: Big Tip Example

Tulane University

Node "done" when uniform label or "no further uncertainty."

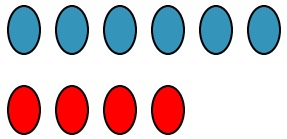




How many + and - examples per subclass, starting with y?

Let's consider next the attribute Speedy

10 examples:



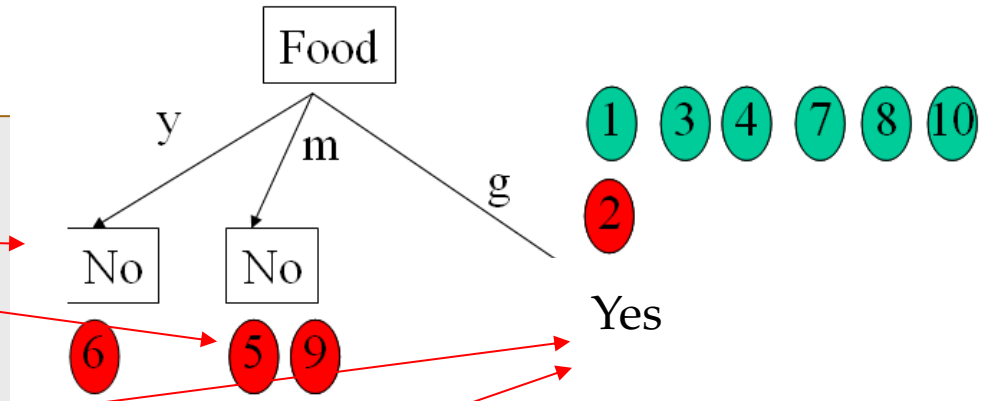
6+

4-

	F S P	BigTip
$\vec{x}_1$	(g, y, a)	$f(\vec{x}_1)=1$
$\vec{x}_2$	(g, n, h)	$f(\vec{x}_2)=0$
$\vec{x}_3$	(g, y, h)	$f(\vec{x}_3)=1$
$\vec{x}_4$	(g, n, a)	$f(\vec{x}_4)=1$
$\vec{x}_5$	(m, y, a)	$f(\vec{x}_5)=0$
$\vec{x}_6$	(y, y, a)	$f(\vec{x}_6)=0$
$\vec{x}_7$	(g, y, a)	$f(\vec{x}_7)=1$
$\vec{x}_8$	(g, y, h)	$f(\vec{x}_8)=1$
$\vec{x}_9$	(m, y, a)	$f(\vec{x}_9)=0$
$\vec{x}_{10}$	(g, y, a)	$f(\vec{x}_{10})=1$

Top-Down Induction of DT (simplified)

- TDIDF(D,c_{def})
- **IF(all examples in D have same class c)**
  - Return leaf with class c (or class c_{def}, if D is empty)
- **ELSE IF(no attributes left to test)**
  - Return leaf with class c of majority in D
- **ELSE**
  - Pick A as the "best" decision attribute for next node
  - FOR each value v_i of A create a new descendent of node
    - $D_i = \{(\vec{x}, y) \in D : \text{attribute A of } \vec{x} \text{ has value } v_i\}$
    - Subtree t_i for v_i is TDIDF(D_i,c_{def})
  - RETURN tree with A as root and t_i as subtrees



Training Data: $D = \{(\vec{x}_1, y_1), \ldots, (\vec{x}_n, y_n)\}$

Picking the Best Attribute to Split

- Ockham's Razor:
  - All other things being equal, choose the simplest explanation
- Decision Tree Induction:
  - Find the smallest tree that classifies the training data correctly
- Problem
  - Finding the smallest tree is computationally hard ☹!
- Approach
  - Use heuristic search (greedy search)

Key Heuristics:

- Pick attribute that *maximizes information (Information Gain)* ⟵
  i.e. "most informative"
- Other statistical tests

Attribute-based representations

- Examples described by attribute values (Boolean, discrete, continuous)
- E.g., situations where I will/won't wait for a table:

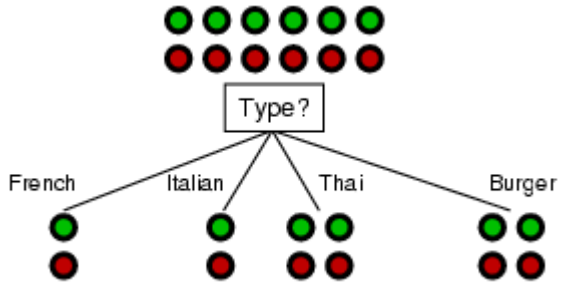
Example	Attributes										Target
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*Wait*
X_1	T	F	F	T	Some	$$$	F	T	French	0–10	T
X_2	T	F	F	T	Full	$	F	F	Thai	30–60	F
X_3	F	T	F	F	Some	$	F	F	Burger	0–10	T
X_4	T	F	T	T	Full	$	F	F	Thai	10–30	T
X_5	T	F	T	F	Full	$$$	F	T	French	>60	F
X_6	F	T	F	T	Some	$$	T	T	Italian	0–10	T
X_7	F	T	F	F	None	$	T	F	Burger	0–10	F
X_8	F	F	F	T	Some	$$	T	T	Thai	0–10	T
X_9	F	T	T	F	Full	$	T	F	Burger	>60	F
X_{10}	T	T	T	T	Full	$$$	F	T	Italian	10–30	F
X_{11}	F	F	F	F	None	$	F	F	Thai	0–10	F
X_{12}	T	T	T	T	Full	$	F	F	Burger	30–60	T

12 examples
6 +
6 -

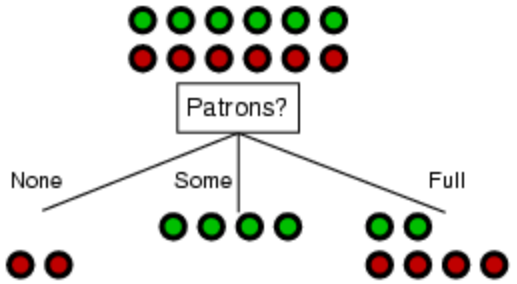
- Classification of examples is positive (T) or negative (F)

Choosing an attribute: Information Gain

Goal: trees with short paths to leaf nodes



Is this a good attribute to split on?



Which one should we pick?

A perfect attribute would ideally divide the examples into sub-sets that are all positive or all negative…
i.e. maximum information gain.

Information Gain

- Most useful in classification
  - how to measure the 'worth' of an attribute ***information gain***
  - how well attribute separates examples according to their classification
- Next
  - precise definition for gain

→ measure from Information Theory

Shannon and Weaver 49

One of the most successful and impactful mathematical theories known.

Information

- "Information" answers questions.
  - The more clueless I am about a question, the more information
    - the **answer** to the question contains.

- Example – fair coin → prior <0.5,0.5>
-
- By definition Information of the prior (or entropy of the prior):
- $I(P1,P2) = - P1 \log_2(P1) - P2 \log_2(P2) =$
- $I(0.5,0.5) = -0.5 \log_2(0.5) - 0.5 \log_2(0.5) = 1$

- **We need 1 bit to convey the outcome of the flip of a fair coin.**

Scale: 1 bit = answer to Boolean question with prior <0.5, 0.5>

- **Why does a biased coin have less information?**
- **(How can we code the outcome of a biased coin sequence?)**

Information (or Entropy)

- Information in an answer given possible answers v_1, v_2, … v_n:

$$I(P(v_1), \ldots, P(v_n)) = \sum_{i=1}^{n} -P(v_i) \ log_2(P(v_i))$$

— $v_1, \ldots, v_n$ possible answers
— $P(v_i)$ probabibilty of answer v_i

(Also called entropy of the prior.)

Example – biased coin → prior <1/100,99/100>

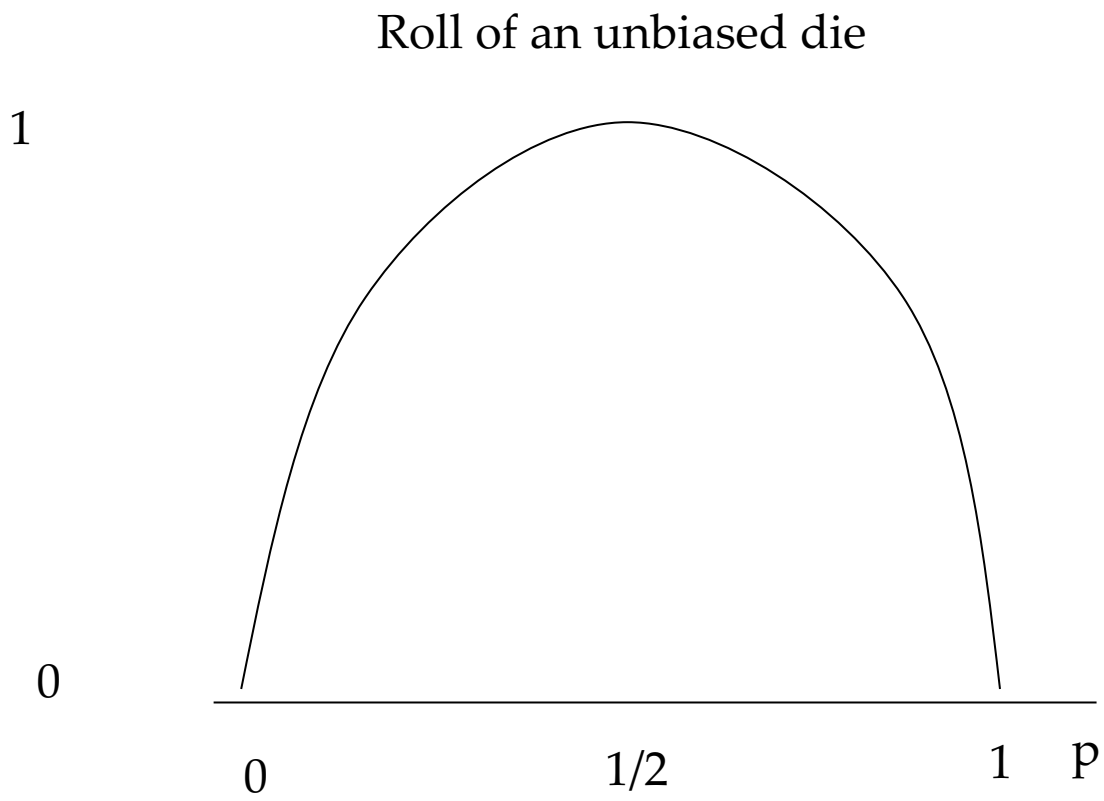
I(1/100,99/100) = -1/100 $\log_2$(1/100) –99/100 $\log_2$(99/100)
= 0.08 bits (so not much information gained from "answer.")

Example – fully biased coin → prior <1,0>

I(1,0) = -1 $\log_2$(1) – 0 $\log_2$(0) = 0 bits
0 $\log_2$(0) =0

i.e., no uncertainty left in source!

Shape of Entropy Function



The more uniform the probability distribution,
the greater is its entropy.

Information or Entropy

- Information or Entropy measures the "randomness" of an arbitrary collection of examples.

- We don't have exact probabilities but our training data provides an estimate of the probabilities of positive vs. negative examples given a set of values for the attributes.
- For a collection S, entropy is given as:

- $$I(\frac{p}{p+n}, \frac{n}{p+n}) = -\frac{p}{p+n}\ log_2(\frac{p}{p+n}) - \frac{n}{p+n}\ log_2(\frac{n}{p+n})$$

- For a collection S having positive and negative examples

- p - # positive examples;
- n - # negative examples

Attribute-based representations

Tulane University

- Examples described by attribute values (Boolean, discrete, continuous)
- E.g., situations where I will/won't wait for a table:

Example	Attributes										Target
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*Wait*
X_1	T	F	F	T	Some	$$$	F	T	French	0–10	T
X_2	T	F	F	T	Full	$	F	F	Thai	30–60	F
X_3	F	T	F	F	Some	$	F	F	Burger	0–10	T
X_4	T	F	T	T	Full	$	F	F	Thai	10–30	T
X_5	T	F	T	F	Full	$$$	F	T	French	>60	F
X_6	F	T	F	T	Some	$$	T	T	Italian	0–10	T
X_7	F	T	F	F	None	$	T	F	Burger	0–10	F
X_8	F	F	F	T	Some	$$	T	T	Thai	0–10	T
X_9	F	T	T	F	Full	$	T	F	Burger	>60	F
X_{10}	T	T	T	T	Full	$$$	F	T	Italian	10–30	F
X_{11}	F	F	F	F	None	$	F	F	Thai	0–10	F
X_{12}	T	T	T	T	Full	$	F	F	Burger	30–60	T

12 examples
6 +
6 -

What's the entropy of this collection of examples?

- Classification of examples is positive (T) or negative (F)
- p = n = 6; I(0.5,0.5) = -0.5 log2(0.5) –0.5 log2(0.5) = 1

So, we need 1 bit of info to classify a randomly picked example, assuming no other information is given about the example.

Choosing an attribute: Information Gain

- Intuition: Pick the attribute that reduces the entropy (the uncertainty) the most.

- So we measure the information gain after testing a given attribute A:

$$Gain(A) = I(\frac{p}{p+n}, \frac{n}{p+n}) - Remainder(A)$$

Remainder(A) → gives us the remaining uncertainty after getting info on attribute A.

Choosing an attribute: Information Gain

- Remainder(A)
- → gives us the amount information we still need after testing on A.
- Assume A divides the training set E into E_1, E_2, … E_v, corresponding to the different v distinct values of A.
- Each subset E_i has p_i positive examples and n_i negative examples.
- So for total information content, we need to weigh the contributions of the different subclasses induced by A

Weight (relative size) of each subclass

$$Remainder(A) = \sum_{i=1}^{v} \frac{p_i+n_i}{p+n} \; I\left(\frac{p_i}{p_i+n_i}, \frac{n_i}{p_i+n_i}\right)$$

Choosing an attribute: Information Gain

- Measures the expected reduction in entropy. The higher the Information Gain (IG), or just Gain, with respect to an attribute A , the more is the expected reduction in entropy.

Weight of each subclass

$$Gain(S, A) = Entropy(S) - \sum_{v \in Values(A)} \frac{|S_v|}{|S|} Entropy(S_v)$$

- where Values(A) is the set of all possible values for attribute A,
- S_v is the subset of S for which attribute A has value v.

Interpretations of Gain

- Gain(S,A)
  - expected reduction in entropy caused by knowing A
  - information provided about the target function value given the value of A
  - number of bits saved in the coding a member of S knowing the value of A

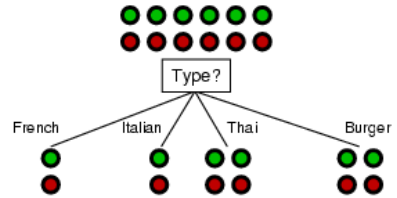
Used in ID3 (Iterative Dichotomiser 3) Ross Quinlan

Information gain

- For the training set, $p = n = 6$, $I(6/12, 6/12) = 1$ bit
- Consider the attributes *Type* and *Patrons*:

What if we used attribute "example label" uniquely specifying the answer? Info gain? Issue?

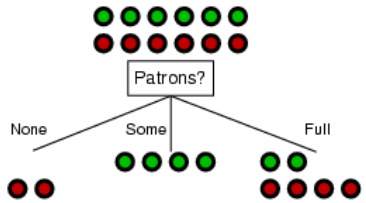
High branching: can correct with "info gain ratio"



Info gain?

$$IG(Type) = 1 - [\frac{2}{12} I(\frac{1}{2}, \frac{1}{2}) + \frac{2}{12} I(\frac{1}{2}, \frac{1}{2}) + \frac{4}{12} I(\frac{2}{4}, \frac{2}{4}) + \frac{4}{12} I(\frac{2}{4}, \frac{2}{4})] = 0 \text{ bits}$$

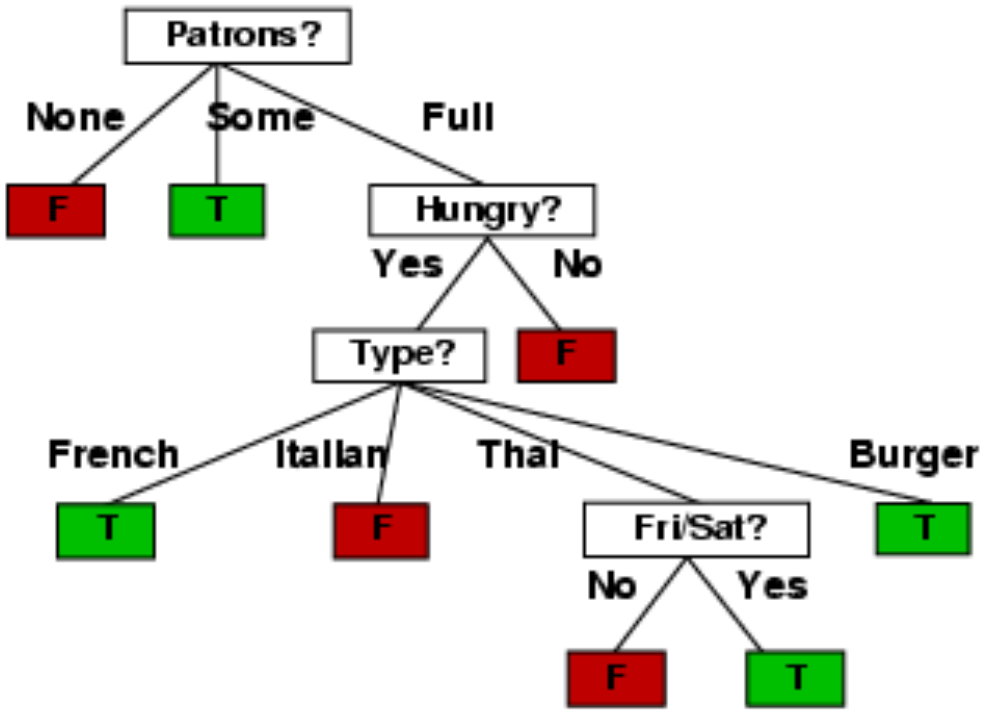
$$IG(Patrons) = 1 - [\frac{2}{12} I(0,1) + \frac{4}{12} I(1,0) + \frac{6}{12} I(\frac{2}{6}, \frac{4}{6})] = .0541 \text{ bits}$$



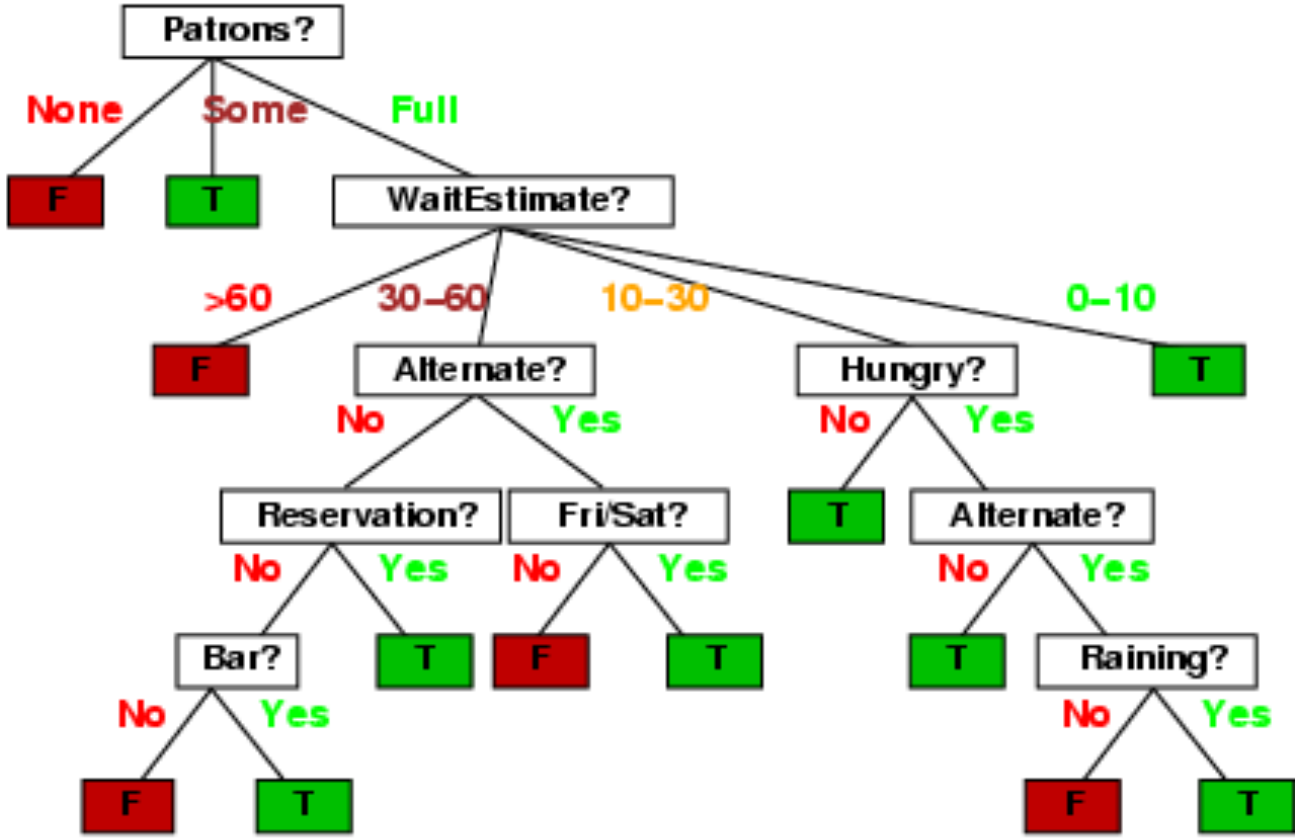
- ***Patrons* has the highest IG of all attributes and so is chosen by the DTL algorithm as the root.**

Example contd.

- Decision tree learned from the 12 examples:



"personal R&N Tree"



Substantially simpler than "true" tree -- but a more complex hypothesis isn't justified from just the data.

Inductive Bias

- Roughly: prefer
  - shorter trees over deeper/more complex ones
    - E.g., Occam's Razor
  - ones with high gain attributes near root

- Difficult to characterize precisely
  - attribute selection heuristics
  - interacts closely with given data

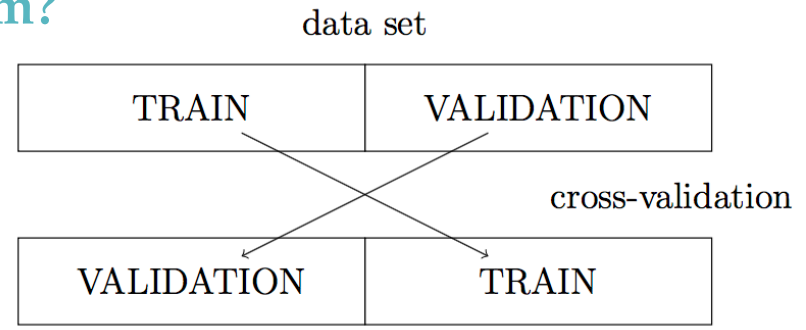
Evaluation Methodology General for Machine Learning

Evaluation Methodology

How to evaluate the quality of a learning algorithm, i.e.,:

How good are the hypotheses produced by the learning algorithm?

How good are they at classifying unseen examples?



- Standard methodology **("Holdout Cross-Validation")**:
  1. Collect a large set of examples.
  2. Randomly divide collection into two disjoint sets: **training set** and **test set**.
  3. Apply learning algorithm to training set generating hypothesis *h*
  4. Measure performance of *h* w.r.t. test set (a form of cross-validation)

     → measures generalization to unseen data

- **Important: keep the training and test sets disjoint! "No peeking"!**
- ***Note: The first two questions about any learning result: Can you describe***
- ***your training and your test set? What's your error on the test set?***

Peeking

- Example of peeking:

- We generate four different hypotheses –
  for example by using different criteria to pick the next attribute to branch on.

- We test the performance of the four different hypothesis on the test set and we select the best hypothesis.

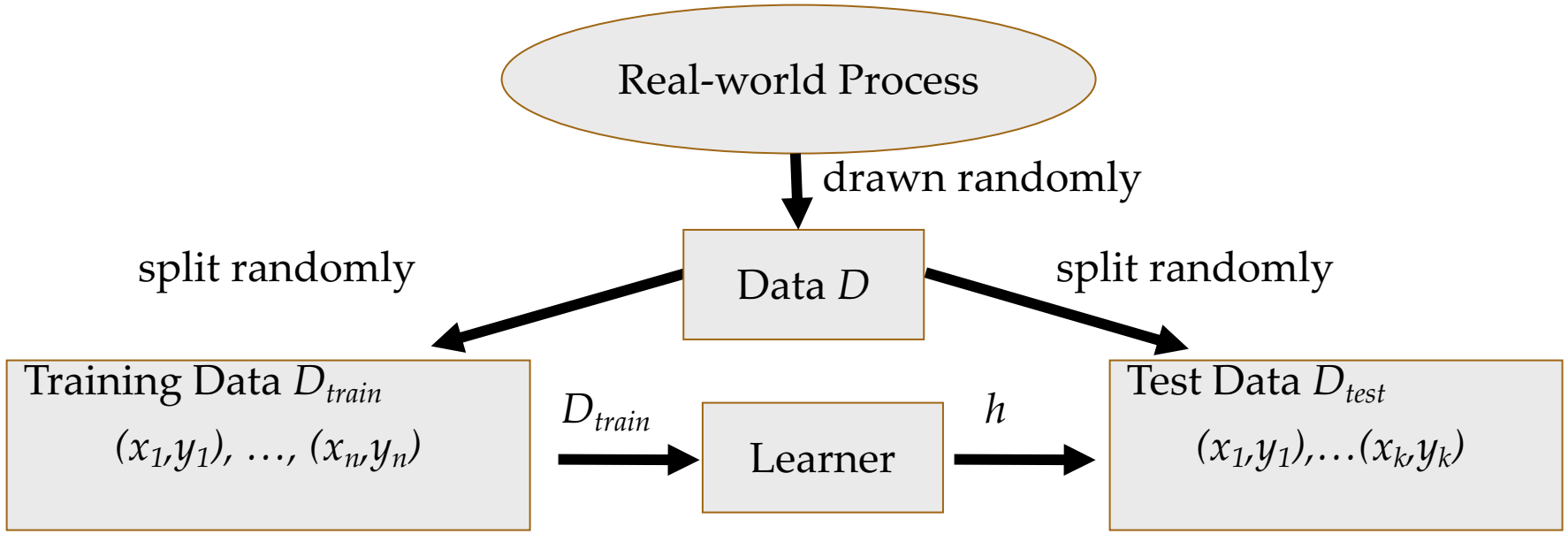
Voila: Peeking occurred! Why?

The hypothesis was selected on the basis of its performance on the **test set**,
so information about the test set has leaked into the learning algorithm.

So a new (separate!) test set would be required!

Note: In competitions, such as the "Netflix $1M challenge," test set is not revealed to the competitors. (Data is held back.)

Test/Training Split



Measuring Prediction Performance

Tulane University

Definition: *The* **training error** $Err_{D_{train}}(h)$ *on training data* $D_{train} = ((\vec{x}_1, y_1), ..., (\vec{x}_n, y_n))$ *of a hypothesis* h *is* $Err_{D_{train}}(h) = \frac{1}{n}\sum_{i=1}^{n} \Delta(h(\vec{x}_i), y_i)$.

Definition: *The* **test error** $Err_{D_{test}}(h)$ *on test data* $D_{test} = ((\vec{x}_1, y_1), ..., (\vec{x}_k, y_k))$ *of a hypothesis* h *is* $Err_{D_{test}}(h) = \frac{1}{k}\sum_{i=1}^{k} \Delta(h(\vec{x}_i), y_i)$.

Definition: *The* **prediction/generalization/true error** $Err_P(h)$ *of a hypothesis* h *for a learning task* $P(X, Y)$ *is*

$$Err_P(h) = \sum_{\vec{x} \in X, y \in Y} \Delta(h(\vec{x}), y) P(X = \vec{x}, Y = y).$$

Definition: *The* zero/one-loss function $\Delta(a, b)$ *returns* 1 *if* $a \neq b$ *and* 0 *otherwise.*

Performance Measures

- Error Rate
  - Fraction (or percentage) of false predictions
- Accuracy
  - Fraction (or percentage) of correct predictions
- Precision/Recall

  Example: binary classification problems (classes pos/neg)
  - Precision: Fraction (or percentage) of correct predictions among all examples predicted to be positive
  - Recall: Fraction (or percentage) of correct predictions among all real positive examples

  (Can be generalized to multi-class case.)

Types of Error

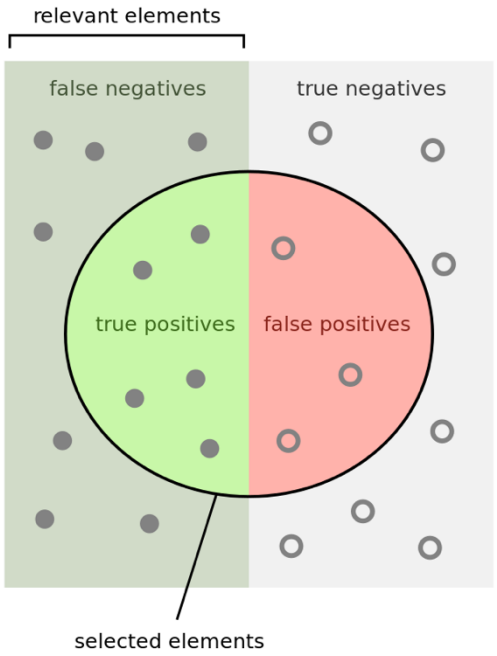
- We can make errors in different directions in classification.
- Say we have 13 animals and we are trying to classify them.

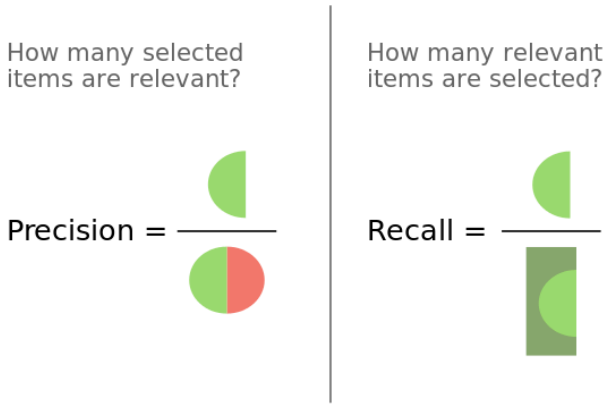
		Actual class	
		Cat	Dog
Predicted class	Cat	5	2
	Dog	3	3

		Predicted Class: Positive	Predicted Class: Negative	
Actual Class	Positive	True Positive (TP)	False Negative (FN) **Type II Error**	**Sensitivity** $\frac{TP}{(TP+FN)}$
	Negative	False Positive (FP) **Type I Error**	True Negative (TN)	**Specificity** $\frac{TN}{(TN+FP)}$
		Precision $\frac{TP}{(TP+FP)}$	**Negative Predictive Value** $\frac{TN}{(TN+FN)}$	**Accuracy** $\frac{TP+TN}{(TP+TN+FP+FN)}$

Precision Versus Recall:

- Precision P:
  #correct positive results / #positive results returned
- Recall R:
  #correct positive results / #all possible positive results



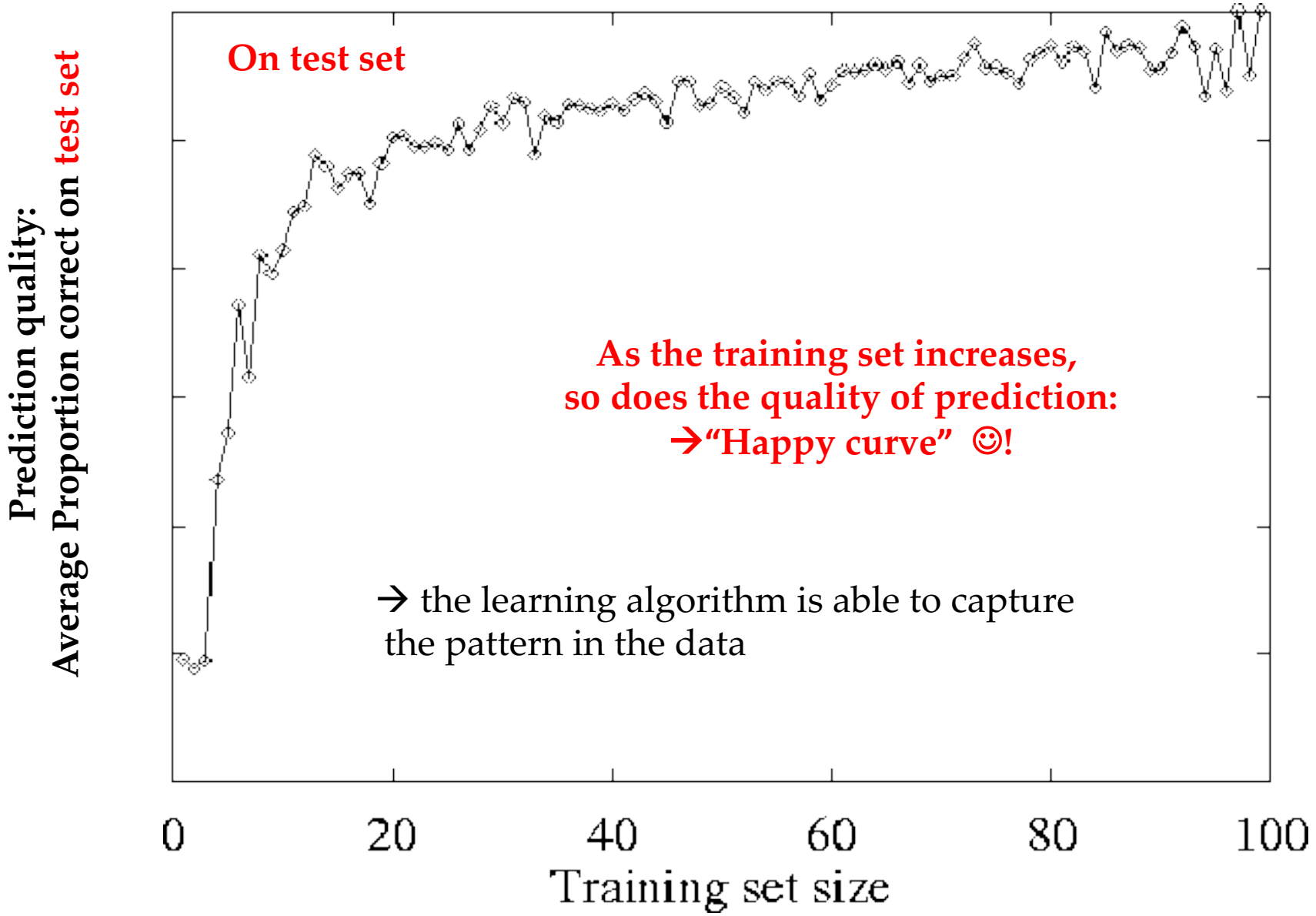


Learning Curve Graph

- Learning curve graph
- average prediction quality –

  proportion correct on test set –
- as a function of the size of the training set..

Restaurant Example: Learning Curve



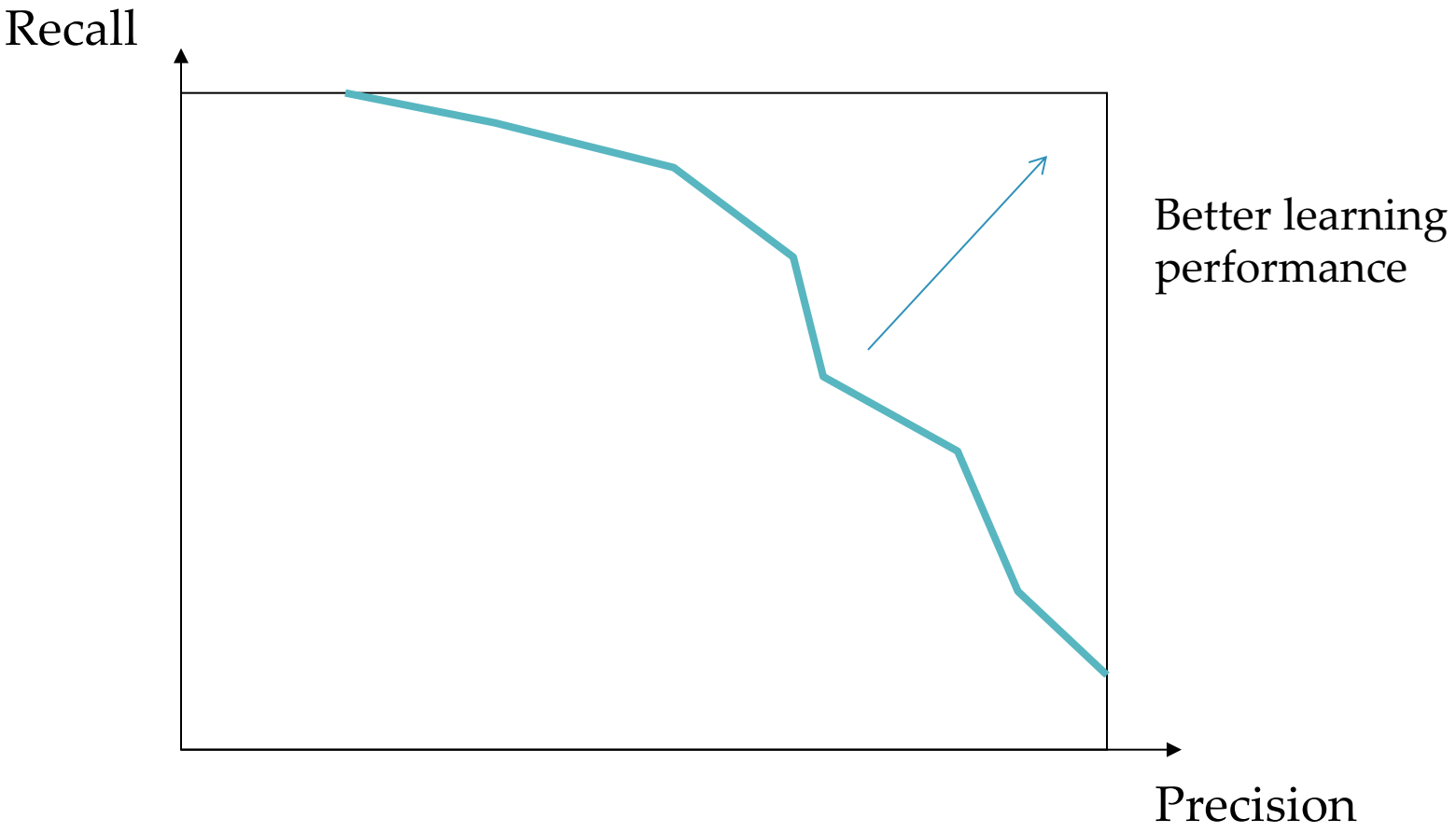
Precision vs. Recall

- **Precision**
  - # of true positives / (# true positives + # false positives)
- **Recall**
  - # of true positives / (# true positives + # false negatives)

- A precise classifier is selective
- A classifier with high recall is inclusive

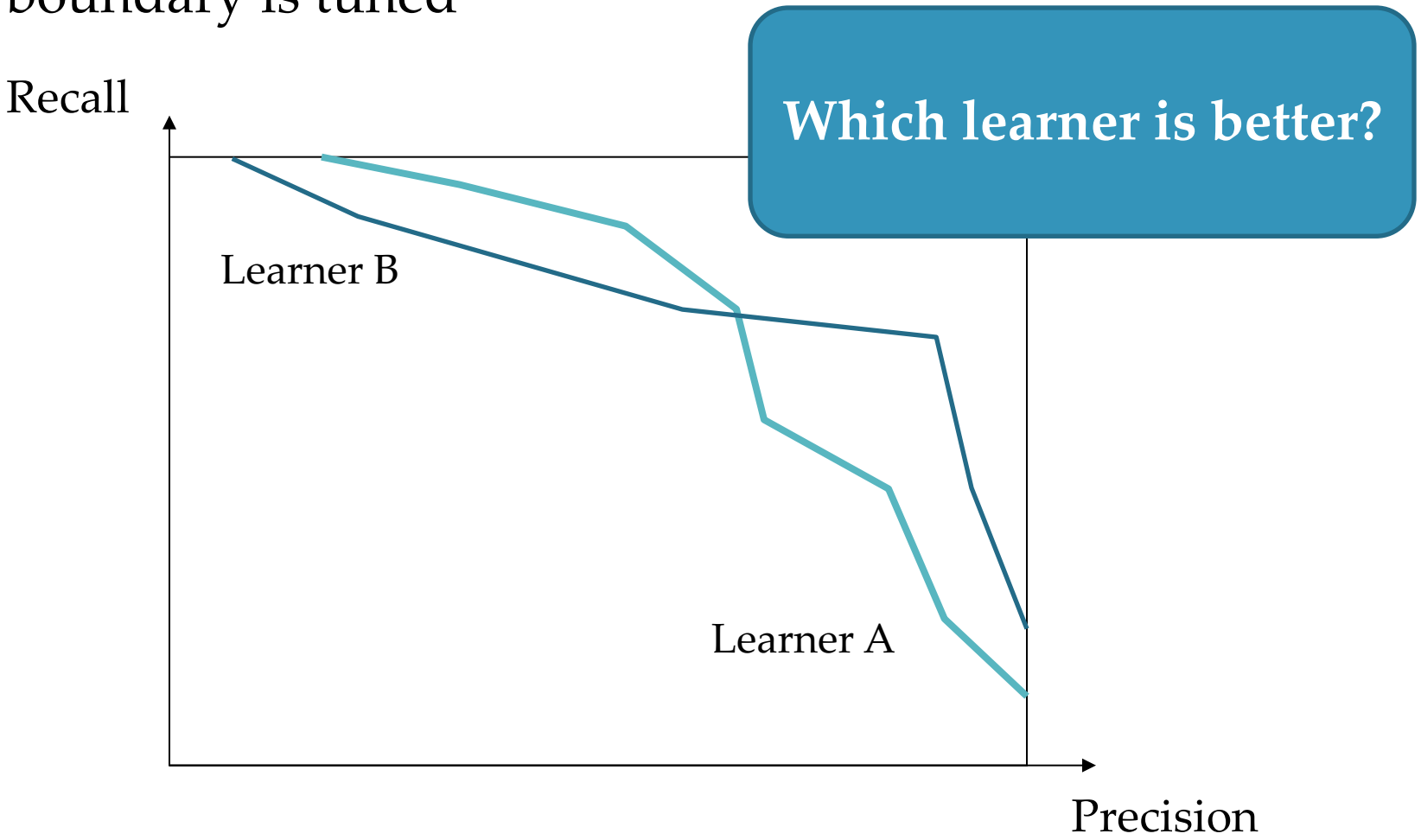
Precision-Recall curves

Measure Precision vs Recall as the classification boundary is tuned



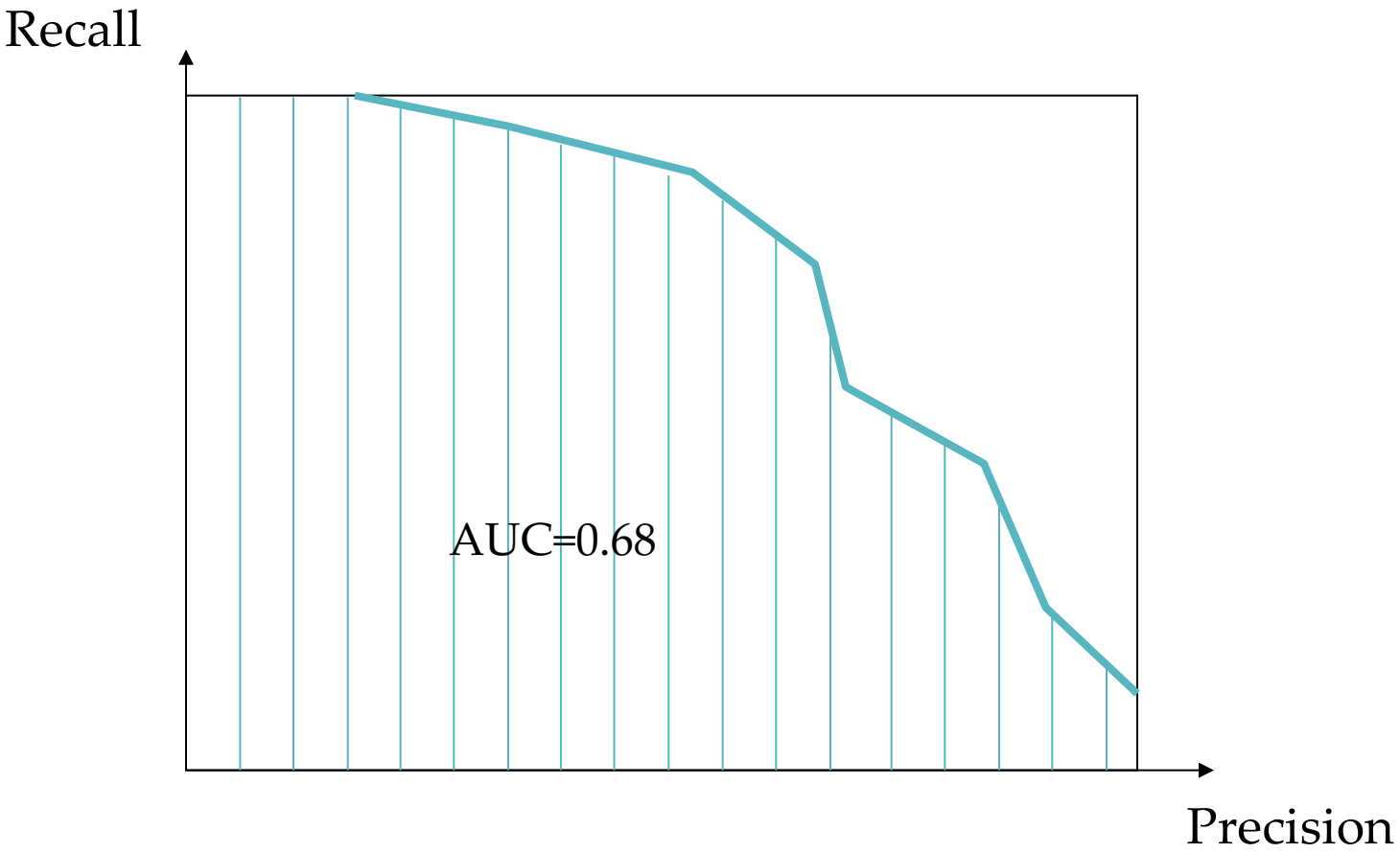
Precision-Recall curves

Measure Precision vs Recall as the classification boundary is tuned



Area Under Curve

AUC-PR: measure the area under the precision-recall curve



AUC metrics

- A single number that measures "overall" performance across multiple thresholds
  - Useful for comparing many learners
  - "Smears out" PR curve
- Note training / testing set dependence

F-Score

- F-Score F:
  weighted average of the precision and recall of a test
- F_1: (harmonic) mean of precision and recall:

$$F_1 = 2 \cdot \frac{1}{\frac{1}{\text{recall}} + \frac{1}{\text{precision}}} = 2 \cdot \frac{\text{precision} \cdot \text{recall}}{\text{precision} + \text{recall}}$$

- Can be parameterized to attach higher importance to recall:

$$F_\beta = (1 + \beta^2) \cdot \frac{\text{precision} \cdot \text{recall}}{(\beta^2 \cdot \text{precision}) + \text{recall}}$$

How well does it work?

- Many case studies have shown that decision trees are at least as accurate as human experts.
  - A study for diagnosing breast cancer had humans correctly classifying the examples 65% of the time, and the decision tree classified 72% correct.
  - British Petroleum designed a decision tree for gas-oil separation for offshore oil platforms that replaced an earlier rule-based expert system.
  - Cessna designed an airplane flight controller using 90,000 examples and 20 attributes per example.

Summary

- Decision tree learning is a particular case of supervised learning,
- For supervised learning, the aim is to find a simple hypothesis approximately consistent with training examples
- Decision tree learning using information gain
- Learning performance = prediction accuracy measured on test set

Decision Trees in Scikit

```
from sklearn.datasets import load_iris
from sklearn import tree

# Load a common dataset, fit a decision tree to it
iris = load_iris()
clf = tree.DecisionTreeClassifier()
clf = clf.fit(iris.data, iris.target)
```

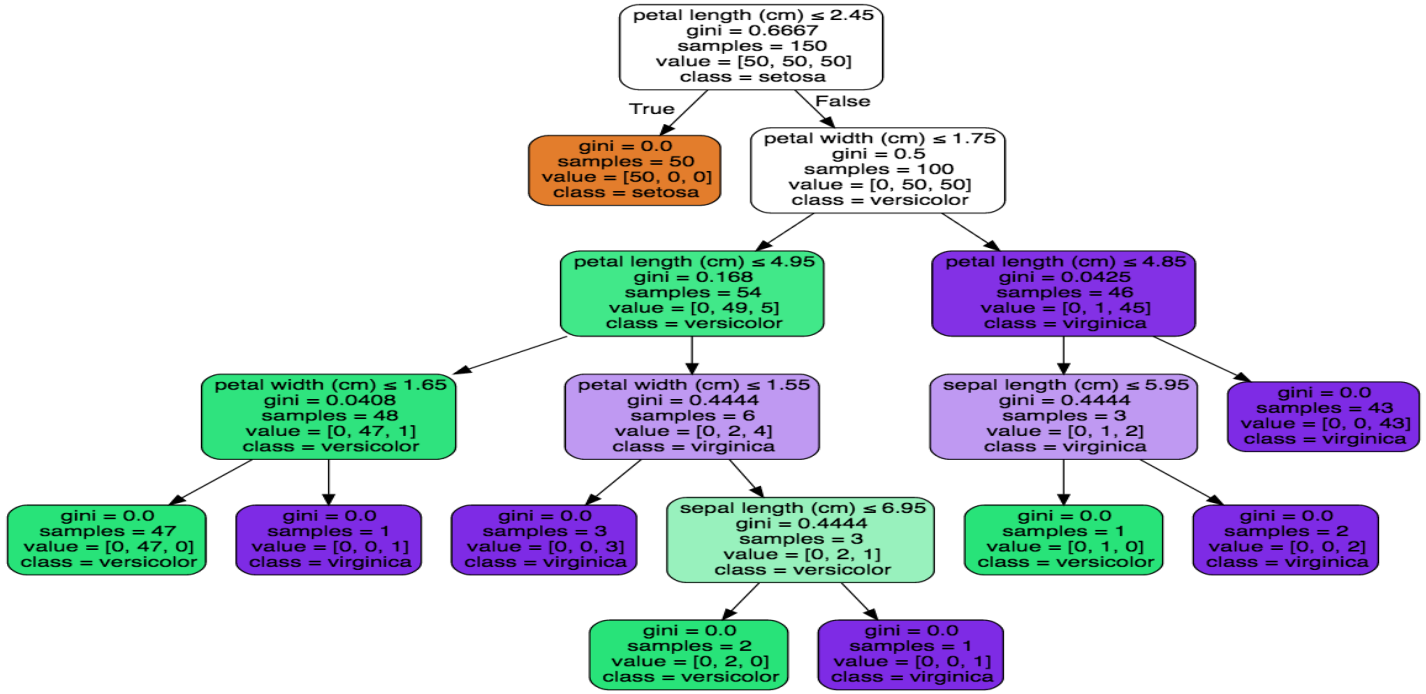
- Trains a decision tree using default parameters (attribute chosen to split on either Gini or entropy, no max depth, etc)

```
# Predict most likely class
clf.predict([[2., 2.]])
```

```
# Predict PDF over classes (%training samples in leaf)
clf.predict_proba([[2., 2.]])
```

Visualizing a decision tree

```
from IPython.display import Image
dot_data = tree.export_graphviz(clf,
                out_file=None,
                feature_names=iris.feature_names,
                class_names=iris.target_names,
                filled=True, rounded=True)
graph = pydotplus.graph_from_dot_data(dot_data)
Image(graph.create_png())
```



Random Forests

- Decision trees are very interpretable, but may be brittle to changes in the training data, as well as noise
- Random forests are an ensemble method that:
- Resamples the training data;
- Builds many decision trees; and
- Averages predictions of trees to classify.
- This is done through bagging and random feature selection

Bagging

- Bagging: Bootstrap aggregation
- Resampling a training set of size n via the bootstrap:
- Sample with replacement n elements
- General scheme for random forests:

1. Create B bootstrap samples, $\{Z_1, Z_2, \ldots, Z_B\}$
2. Build B decision trees, $\{T_1, T_2, \ldots, T_B\}$, from $\{Z_1, Z_2, \ldots, Z_B\}$

- Classification/Regression:

1. Each tree T_j predicts class/value y_j
2. Return average $1/B \, \Sigma_{j=\{1,\ldots,B\}} \, y_j$ for regression,
   or majority vote for classification

Original training dataset (Z):

obs_id	ft_1	ft_2
1	12.2	puppy
2	34.5	dog
3	8.1	cat

B Bootstrap samples Z_j

Z_1 Z_2 Z_B

obs_id	ft_1	ft_2
3	8.1	cat
2	34.5	dog
3	8.1	cat

obs_id	ft_1	ft_2
1	12.2	puppy
2	34.5	dog
1	12.2	puppy

obs_id	ft_1	ft_2
1	12.2	puppy
1	12.2	puppy
3	8.1	cat

T_1 T_2 T_j T_B

Aggregate/Vote

Class estimate or predicted value

Random Attribute selection

- We get some randomness via bootstrapping
- We like this! Randomness increases the bias of the forest slightly at a huge decrease in variance (due to averaging)
-

We can further reduce correlation between trees by:

1. For each tree, at every split point …
2. … choose a random subset of attributes …
3. … then split on the "best" (entropy, Gini) within only that subset

Random forests in scikit-learn

```
from sklearn.ensemble import RandomForestClassifier

# Train a random forest of 10 default decision trees
X = [[0, 0], [1, 1]]
Y = [0, 1]
clf = RandomForestClassifier(n_estimators=10)
clf = clf.fit(X, Y)
```

- Can we get even more random?!
- Extremely randomized trees (`ExtraTreesClassifier`) do bagging, random attribute selection, but also:

1. At each split point, choose random splits
2. Pick the best of those random splits

- Similar bias/variance performance to RFs, but can be faster computationally

Extensions of the Decision Tree Learning Algorithm (Briefly)

- Noisy data
- Overfitting and Model Selection
- Cross Validation
- Missing Data (R&N, Section 18.3.6)
- Using gain ratios (R&N, Section 18.3.6)
- Real-valued data (R&N, Section 18.3.6)
- Generation of rules and pruning

Noisy data

- Many kinds of "noise" that could occur in the examples:
  - Two examples have same attribute/value pairs, but different classifications
    →report majority classification for the examples corresponding to the node deterministic hypothesis.
    →report estimated probabilities of each classification using the relative frequency (if considering stochastic hypotheses)
  - Some values of attributes are incorrect because of errors in the data acquisition process or the preprocessing phase
  - The classification is wrong (e.g., + instead of -) because of some error

One important reason why you don't want to "overfit" your learned model.

Overfitting

Ex.: Problem of trying to predict the roll of a die. The experiment data include:

Day of the week; (2) Month of the week; (3) Color of the die;

….

DTL may find an hypothesis that fits the data but with irrelevant attributes.

Some attributes are irrelevant to the decision-making process, e.g., color

of a die is irrelevant to its outcome but they are used to differentiate examples → Overfitting.

Overfitting means fitting the **training set** "too well"
→ **performance on the test set degrades.**

Example overfitting risk: Using restaurant name.

- If the hypothesis space has many dimensions because of a large number of attributes, we may find **meaningless regularity** in the data that is irrelevant to the true, important, distinguishing features.

  - **Fix by pruning to lower # nodes in the decision tree or put a limit on number of nodes created.**

  - **For example, if Gain of the best attribute at a node is below a threshold, stop and make this node a leaf rather than generating children nodes.**

Overfitting is a key problem in learning. There are formal results on the number of examples needed to properly train an hypothesis of a certain complexity ("number of parameters" or # nodes in DT). The more params, the more data is needed. We'll see some of this in our discussion of PAC learning.

Overfitting

- **Let's consider D, the entire distribution of data, and T, the training set.**

- **Hypothesis h ∈ H overfits D if**

  ∃ h'≠ h ∈ H such that

  $error_T(h) < error_T(h')$ but

  $error_D(h) > error_D(h')$

  Note: estimate error on full distribution by using test data set.

- **Data overfitting is the arguably the most common pitfall in machine learning**

- **Why?**

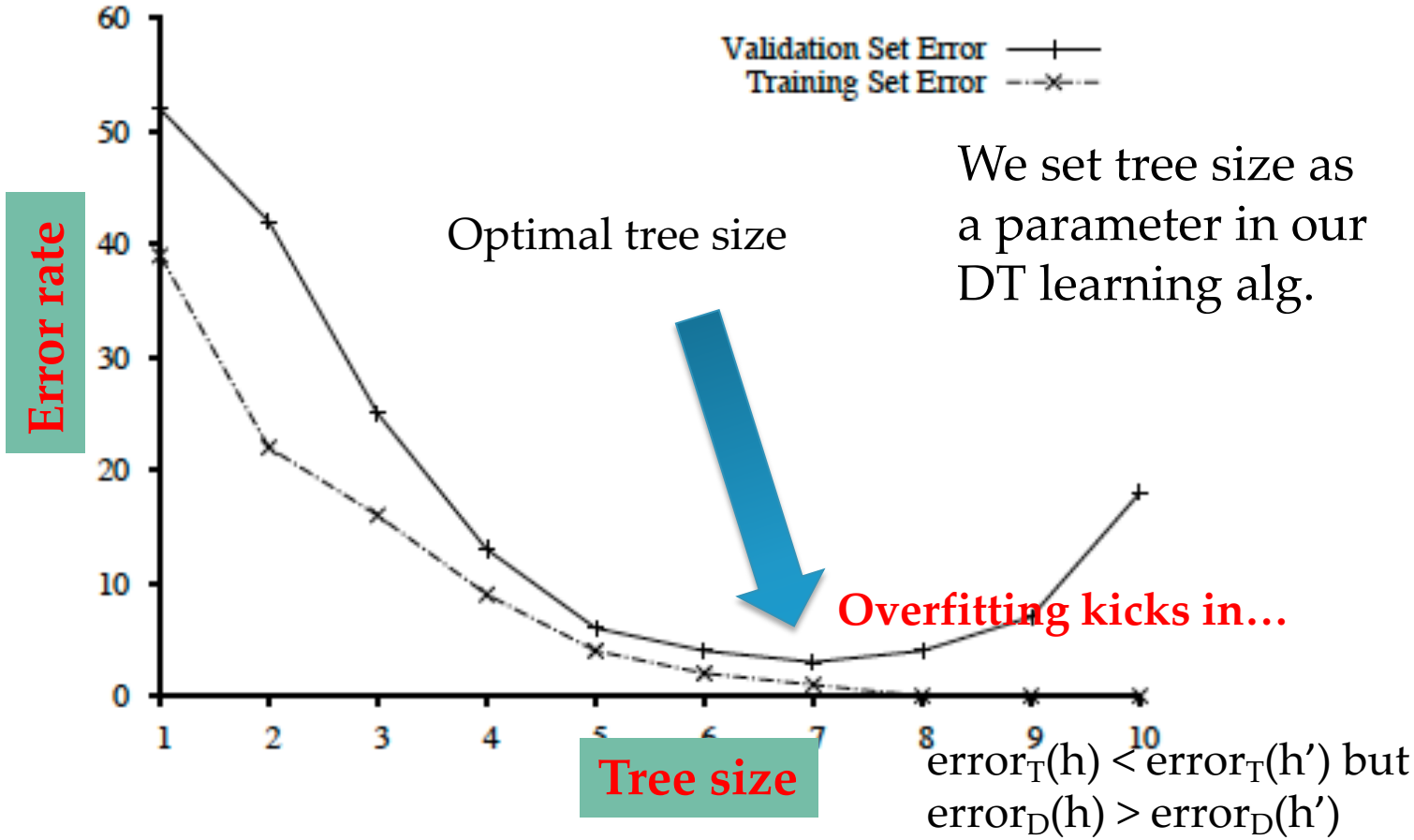
1) **Temptation to use as much data as possible to train on. ("Ignore test till end." Test set too small.) Data "peeking" not noticed.**

1) **Temptation to fit very complex hypothesis (e.g. large decision tree). In general, the larger the tree, the better the fit to the training data.**

- **It's hard to think of a better fit to the training data as a "worse"**
- **result. Often difficult to fit training data well, so it seems that**
- **"a good fit to the training data means a good result."**

Note: Modern "savior:" Massive amounts of data to train on! Somewhat characteristic of ML AI community vs. traditional statistics community. Anecdote: Netflix competition.

Key figure in machine learning



Optimal tree size

We set tree size as a parameter in our DT learning alg.

Overfitting kicks in…

$error_T(h) < error_T(h')$ but $error_D(h) > error_D(h')$

Note: with larger and larger trees, we just do better and better on the training set!

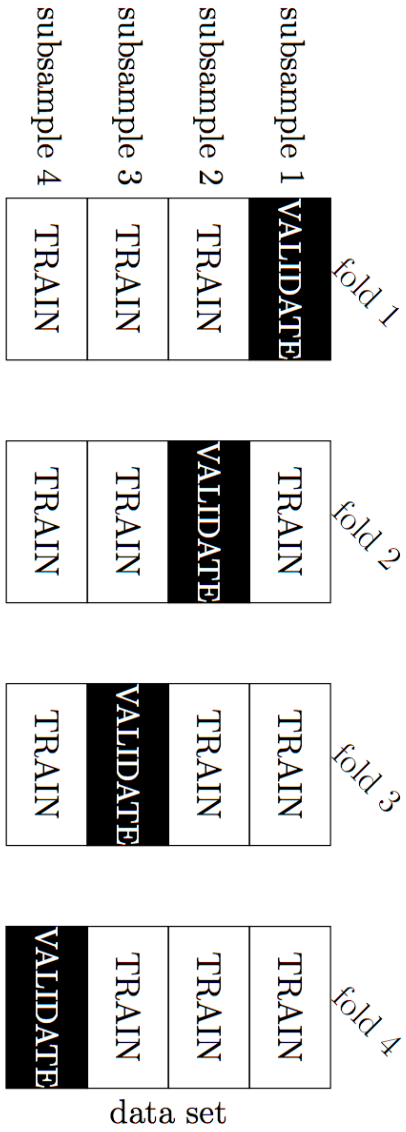
But note the performance on the validation set…

- **Procedure for finding the optimal tree size is called "model selection."**
- **See section 18.4.1 R&N and Fig. 18.8.**

- To determine validation error for each tree size, use k-fold cross-validation. (Uses the data better than "holdout cross-validation.")
- Uses "all data - test set" --- k times splits that set into a training
- set and a validation set.

- After right decision tree size is found from the error rate curve on
- validation data, train on all training data to get final decision tree
- (of the right size).

- Finally, evaluate tree on the test data (not used before) to get
- true generalization error (to unseen examples).

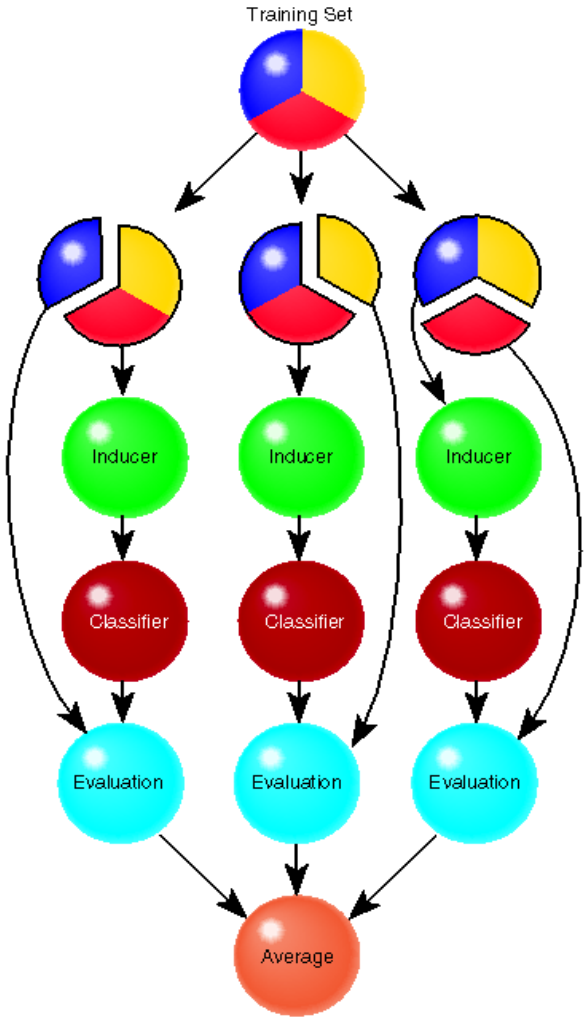


Cross Validation

Learner L is e.g. DT learner for "tree with 7 nodes" max.

A method for estimating the accuracy (or error) of a learner (using validation set).

CV(data S, alg L, int k)
  Divide S into k disjoint sets $\{ S_1, S_2, \ldots, S_k \}$
  For i = 1..k do
    Run L on $S_{-i} = S - S_i$
    obtain $L(S_{-i}) = h_i$
    Evaluate h_i on S_i
      $err_{S_i}(h_i) = 1/|S_i| \sum_{\langle x,y \rangle \in S_i} I(h_i(x) \neq y)$
  Return Average $1/k \sum_i err_{S_i}(h_i)$



Specific Techniques For Overfitting in DTs

- 1) **Decision tree pruning or grow only up to certain size.**
- **Prevent splitting on features that are not clearly relevant.**

- Testing of relevance of features --- "does split provide new information":
- statistical tests ---> Section 18.3.5 R&N χ^2 test.

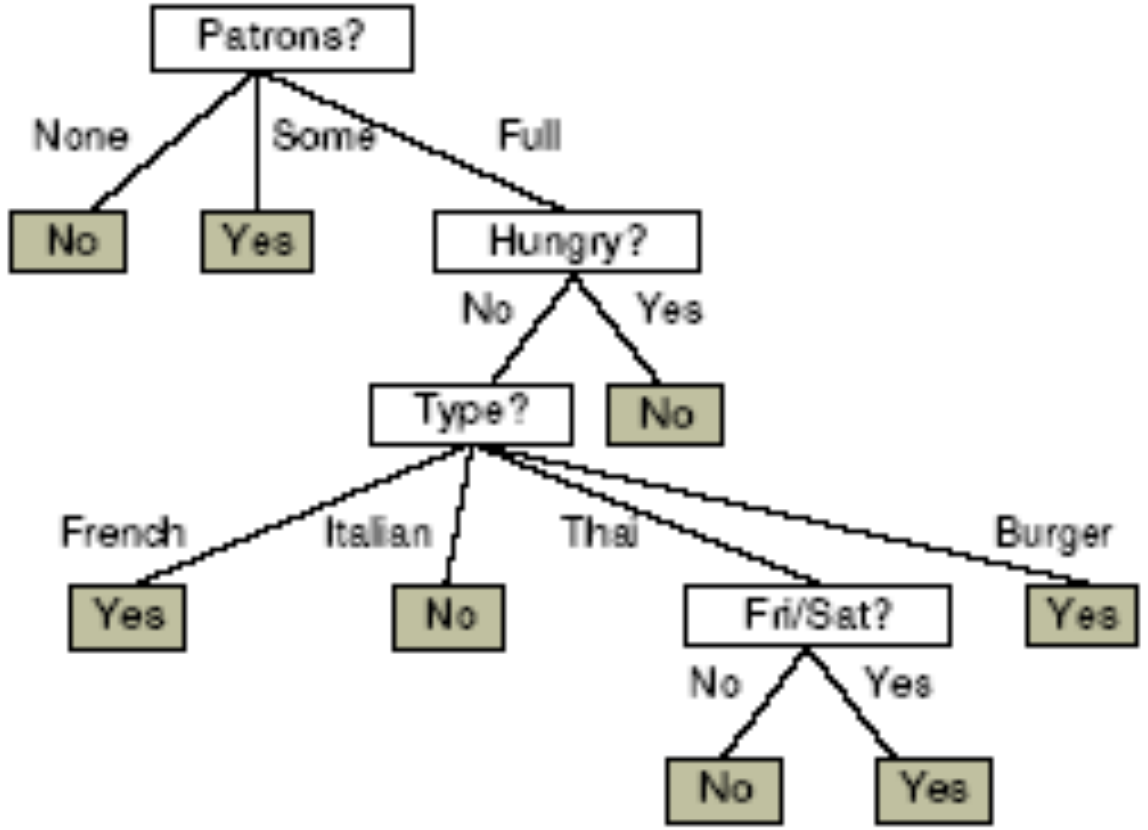
- **2) Grow full tree, then post-prune rule post-pruning**

- **3) MDL (minimal description length):**

minimize
size(tree) + size(misclassifications(tree))

Converting Trees to Rules

- Every decision tree corresponds to set of rules:
  - IF (Patrons = None)
    THEN WillWait = No
  - IF (Patrons = Full)
    & (Hungry = No)
    &(Type = French)
    THEN WillWait = Yes
  - ...
-



Fighting Overfitting: Using Rule Post-Pruning

1. Grow decision tree. Fit as much data as possible. Allow overfitting.

2. Convert tree to equivlent set of rules. One rule for each path from root to leaf.

3. Prune (generalize) each rule independently of others.
    1. I.e., delete preconditions that improve accuracy (greedy)

4. Sort final rules into desired sequence depending on accuracy.

5. Use ordered sequence for classification.

This is the strategy of the most successful commercial decision tree learning method (C4.5 — Quinlan 1993). Widely used in data mining.

What is advantage of rule representation over the decision tree?

Decision trees are a restricted from of general logical statements.

We can also describe our target function directly in first-order sentences.

Example:

$$\forall WillWait(r) \Leftrightarrow Patrons(r, Some)$$
$$\vee(Patrons(r, Full) \wedge \neg Hungry(r) \wedge Type(r, French))$$
$$\vee(Patrons(r, Full) \wedge \neg Hungry(r) \wedge Type(r, Thai) \wedge Fri/Sat(r$$
$$\vee(Patrons(r, Full) \wedge \neg Hungry(r) \wedge Type(r, Burger))$$

This is our **hyposthesis** H_r. In general, we search from among a space of hypotheses:

$$H_1 \vee H_2 \vee H_3 \vee \ldots \vee H_n.$$

Here's an **example** in logical form:

$$Alternate(X1) \wedge \neg Bar(X_1) \wedge \neg Fri/Sat(X_1) \wedge$$
$$Hungry(X_1) \wedge \ldots \wedge WillWait(X_1)$$

We can test if this example is **consistent** with our hyposthesis. If not, we may have to **generalize** or **specialize** our hypothesis:

Current-best-hypothesis search.

Summary: When to use Decision Trees

- Instances presented as attribute-value pairs
- Method of approximating discrete-valued functions
- Target function has discrete values: classification problems

- Robust to noisy data:
- Training data may contain
  - errors
  - missing attribute values
- Typical bias: prefer smaller trees (Ockham's razor)

Widely used, practical and easy to interpret results

- Inducing decision trees is one of the most widely used learning methods in practice
- Can outperform human experts in many problems

- Strengths include
  - Fast
  - simple to implement
  - human readable
  - can convert result to a set of easily interpretable rules
  - empirically valid in many commercial products
  - handles noisy data

Can be a legal requirement! Why?

- Weaknesses include:
  - "Univariate" splits/partitioning using only one attribute at a time so limits types of possible trees
  - large decision trees may be hard to understand
  - requires fixed-length feature vectors
  - non-incremental (i.e., batch method)