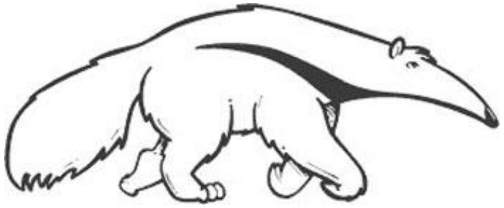
# Introduction to Machine Learning: Improve Performance by Observation

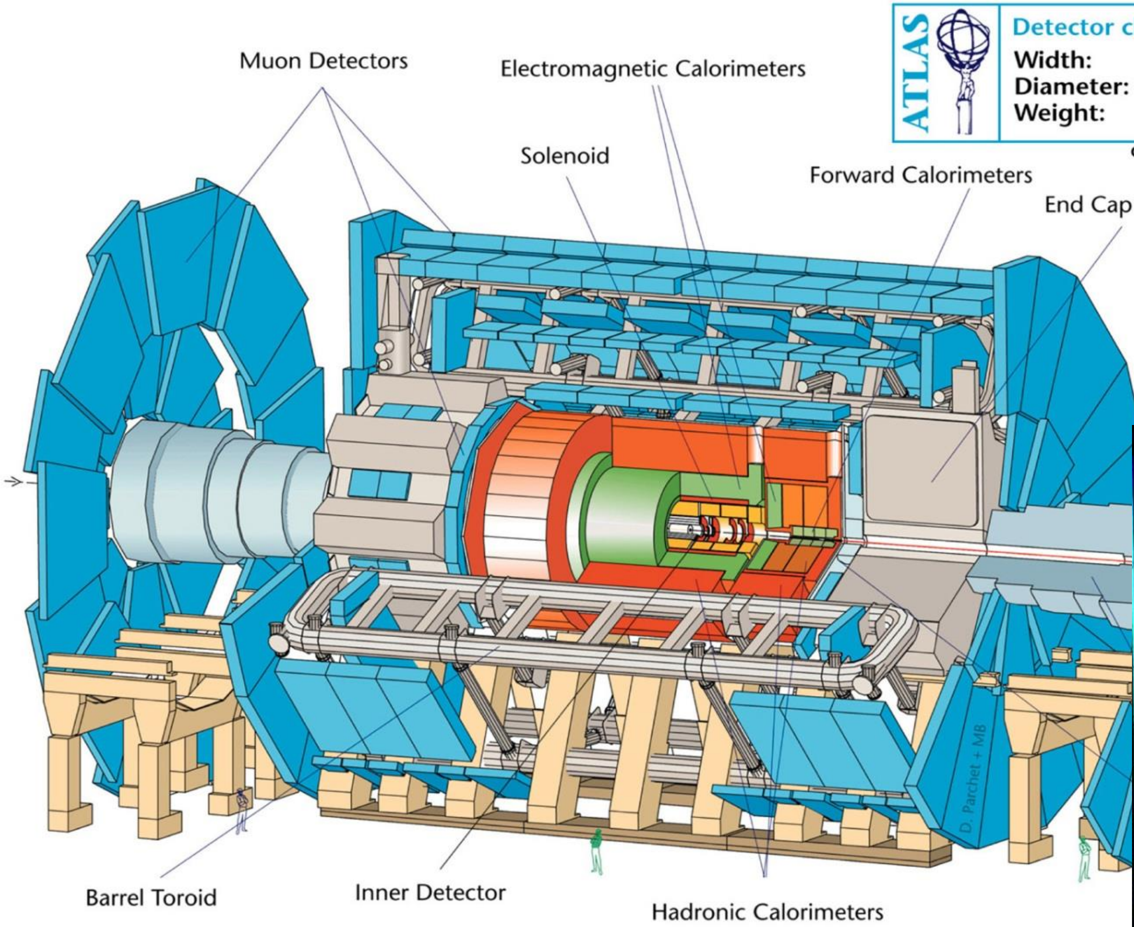
CS171, Winter Quarter, 2019
Introduction to Artificial Intelligence
Surmeet Kaur Jhajj

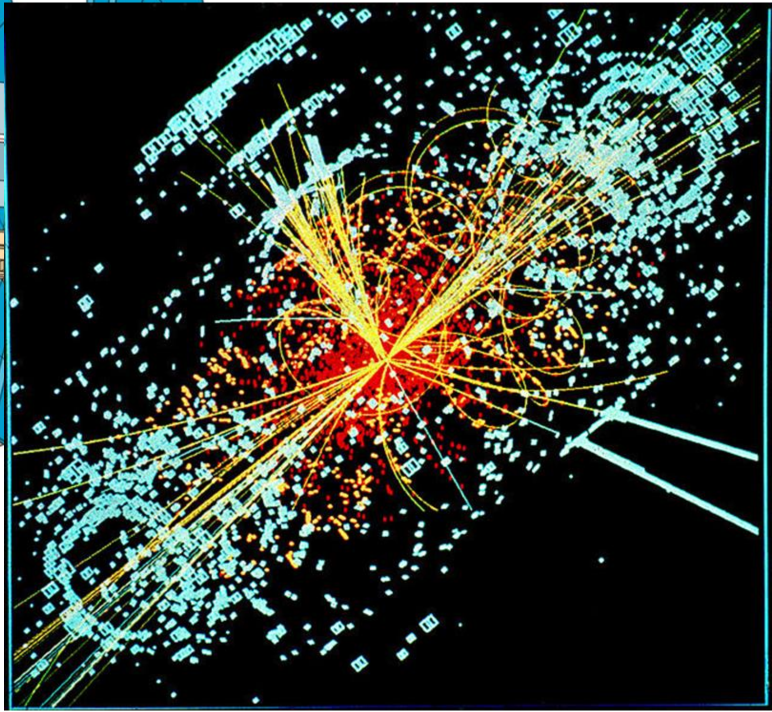


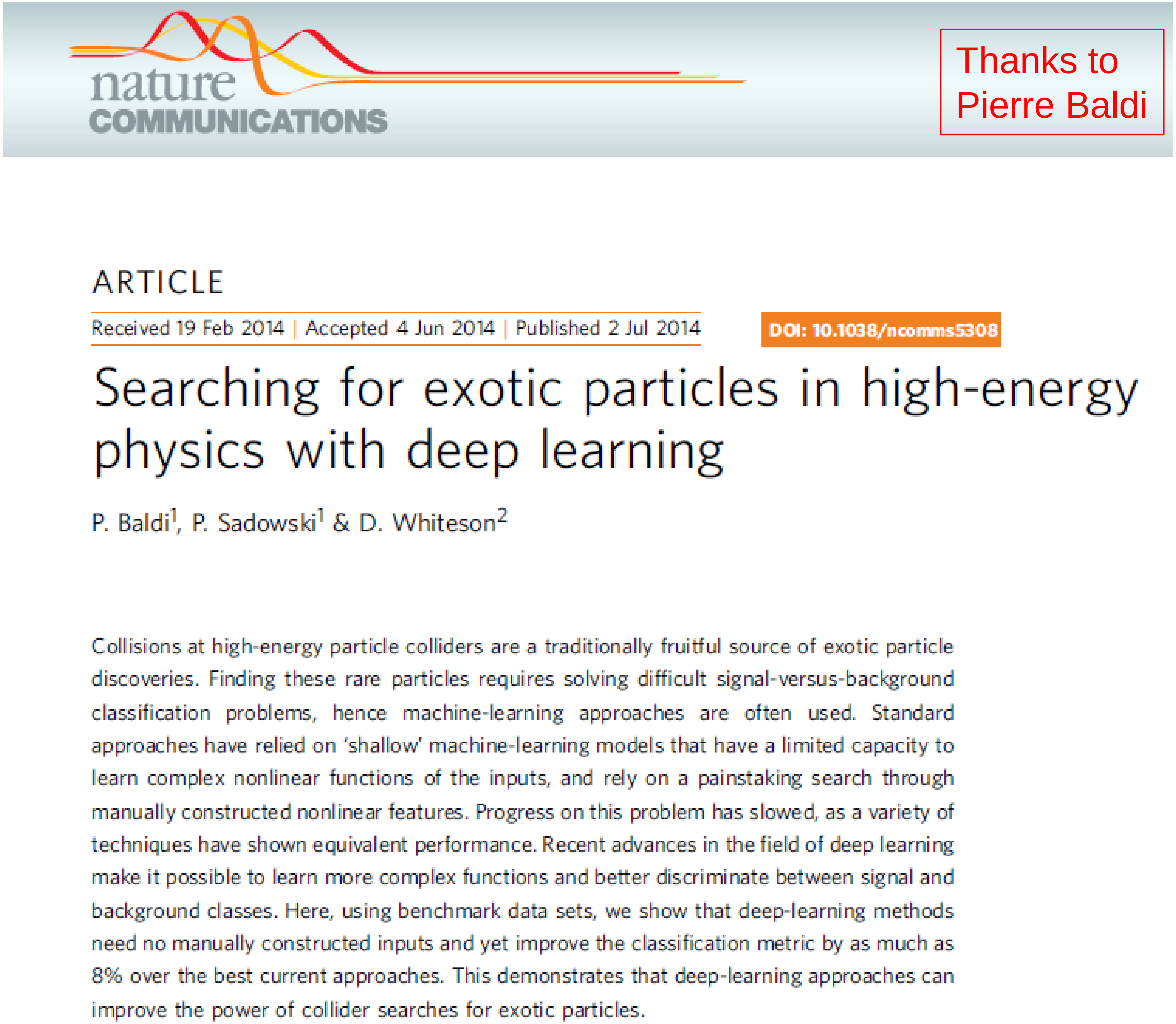
**Read Beforehand:** R&N Ch. 18.1-18.4

# Deep Learning in Physics: Searching for Exotic Particles

Thanks to Pierre Baldi







nature
COMMUNICATIONS

Thanks to
Pierre Baldi

ARTICLE

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# Searching for exotic particles in high-energy physics with deep learning

P. Baldi[1], P. Sadowski[1] & D. Whiteson[2]

Collisions at high-energy particle colliders are a traditionally fruitful source of exotic particle discoveries. Finding these rare particles requires solving difficult signal-versus-background classification problems, hence machine-learning approaches are often used. Standard approaches have relied on 'shallow' machine-learning models that have a limited capacity to learn complex nonlinear functions of the inputs, and rely on a painstaking search through manually constructed nonlinear features. Progress on this problem has slowed, as a variety of techniques have shown equivalent performance. Recent advances in the field of deep learning make it possible to learn more complex functions and better discriminate between signal and background classes. Here, using benchmark data sets, we show that deep-learning methods need no manually constructed inputs and yet improve the classification metric by as much as 8% over the best current approaches. This demonstrates that deep-learning approaches can improve the power of collider searches for exotic particles.

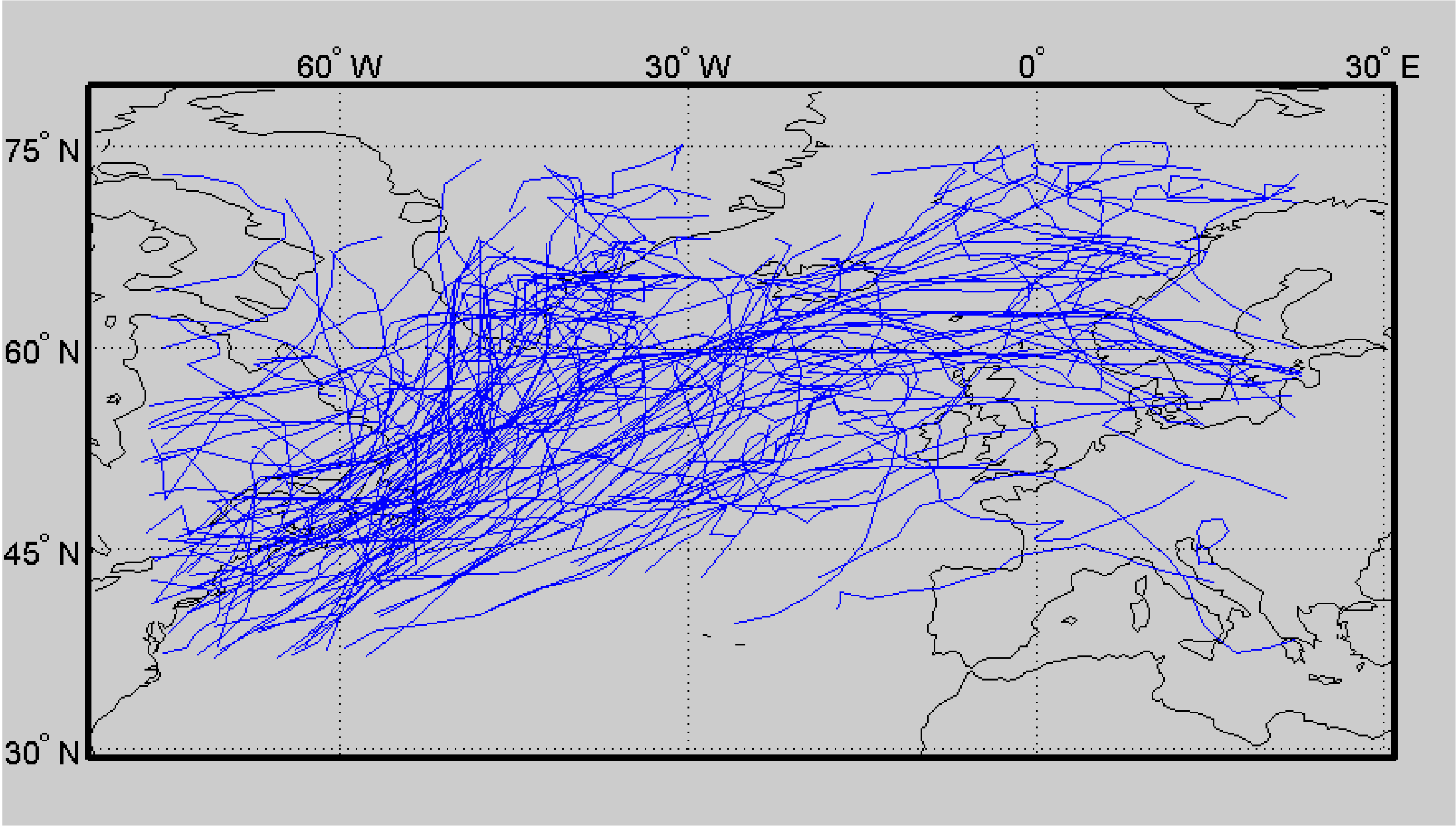
Daniel Whiteson

Peter Sadowski

Thanks to Padhraic Smyth

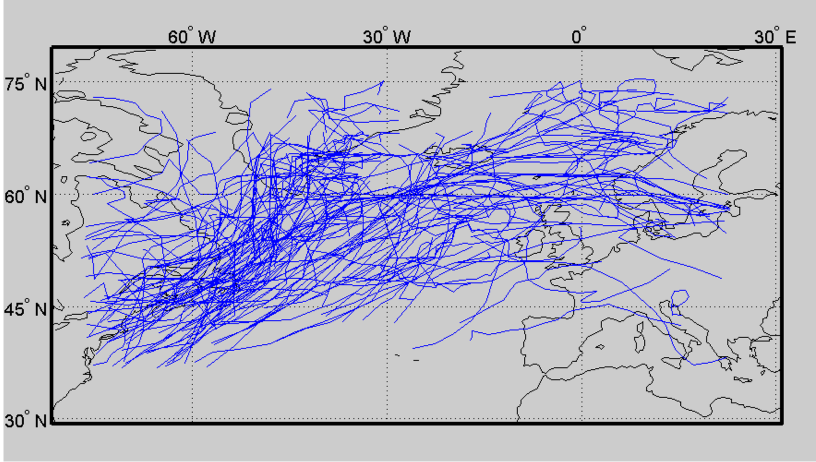
# Application to Extra-Tropical Cyclones

Gaffney et al, *Climate Dynamics*, 2007

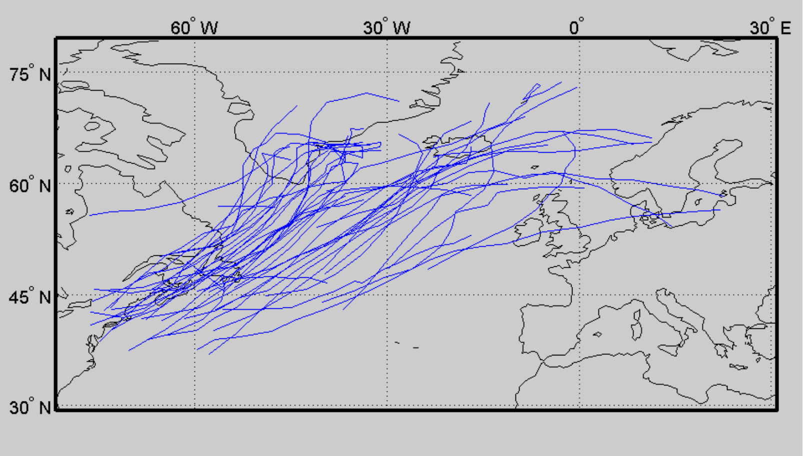


Thanks to
Padhraic Smyth

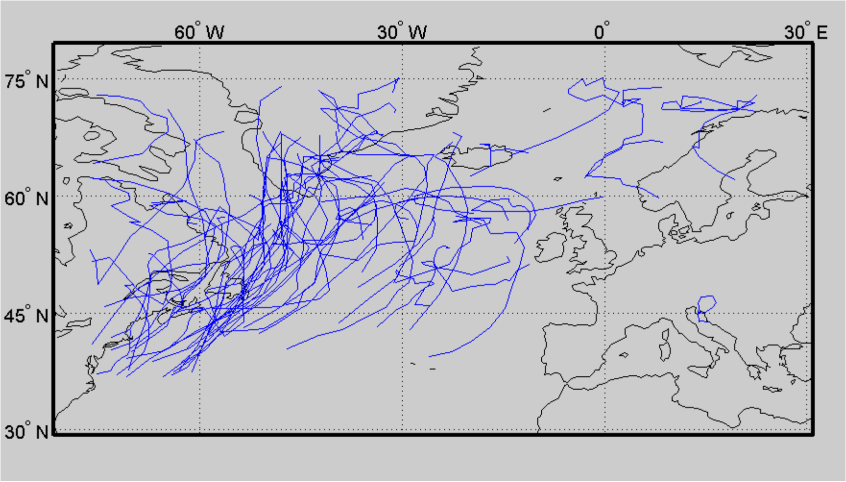
## Original Data



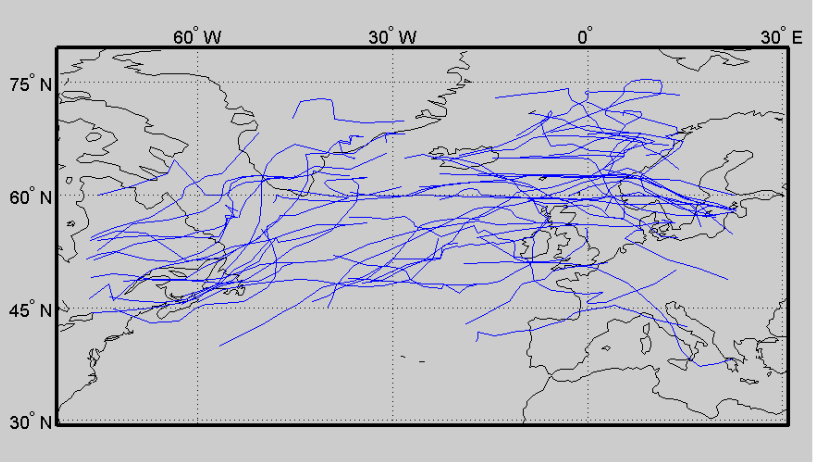
## Iceland Cluster



## Greenland Cluster



## Horizontal Cluster



# *Handwritten Hangul recognition using deep convolutional neural networks*

Thanks to Xiaohui Xie

**In-Jung Kim & Xiaohui Xie**

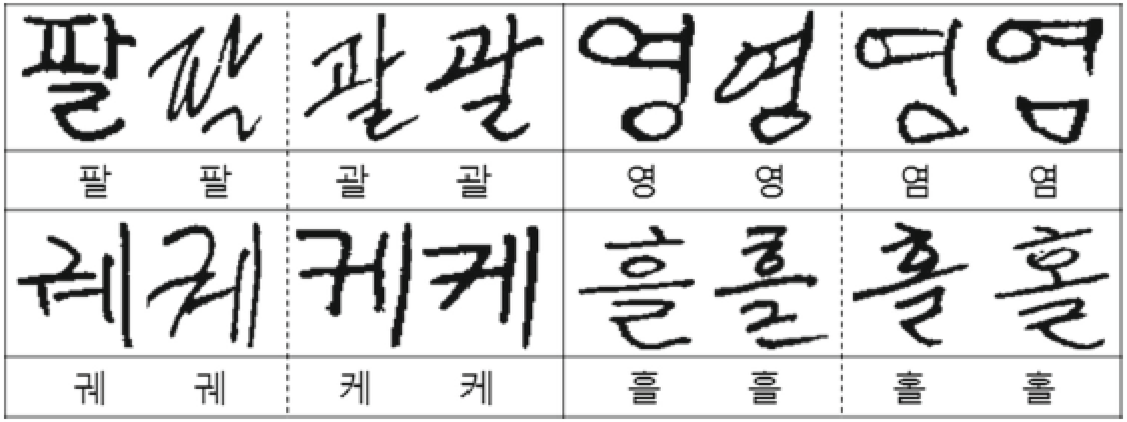


**Fig. 1** Examples of Hangul characters

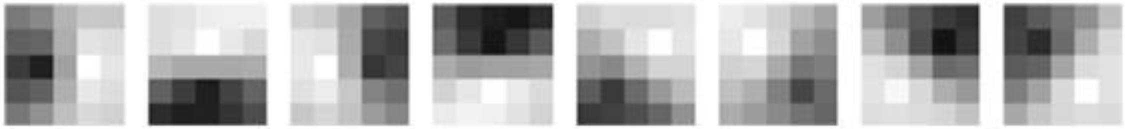


Fig. 4 Edge operators used to initialize convolution masks of the bottom layer

Thanks to Xiaohui Xie

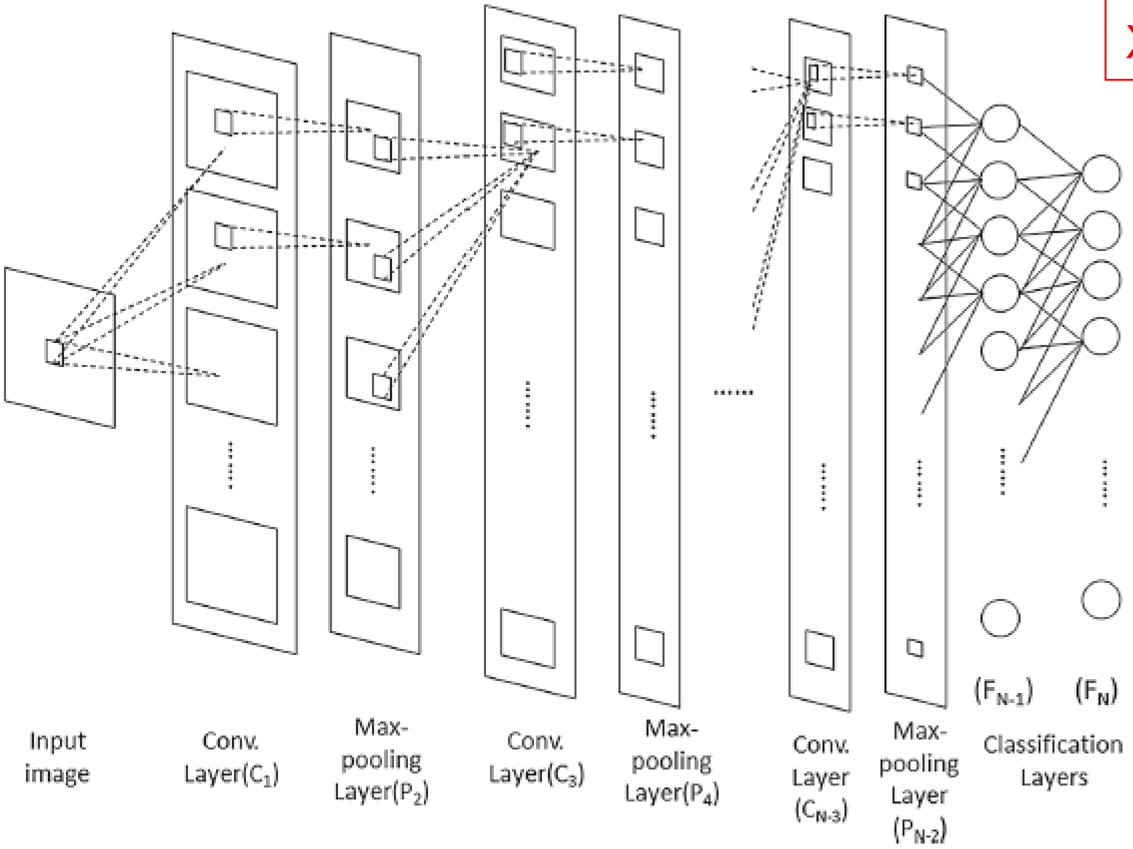


Fig. 2 The overall architecture of the DCNN used by us, which includes an input layer, multiple alternating convolution and max-pooling layers, and two fully connected classification layers. *N* denotes the total number of layers in the network

# AI vs ML

- More specific and broadly applied
- Predictions and decisions
- EG : email spam detection
- Difficult to identify and write a set of rules so need computer to identify

# Automated Learning

- Why learn?
  - Key hallmark of intelligence
  - Take real data → get feedback → improve performance → repeat
  - Check out USC Autonomous Flying Vehicle Project!

- Types of learning
  - **Supervised learning:** learn mapping, attributes → target
    - Classification: target variable is discrete (e.g., spam email)
    - Regression: target variable is real-valued (e.g., stock market)

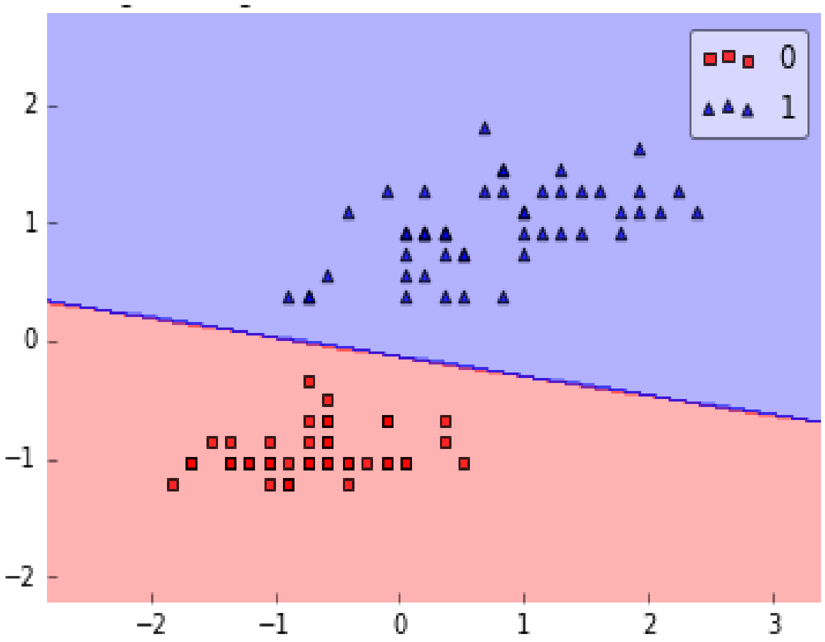
  - **Unsupervised learning:** understand hidden data structure
    - Clustering: group data into "similar" groups
    - Latent space embedding: learn a simple data representation

  - **Other types of learning**
    - Reinforcement learning: e.g., game-playing agent
    - Learning to rank, e.g., document ranking in Web search
    - And many others….

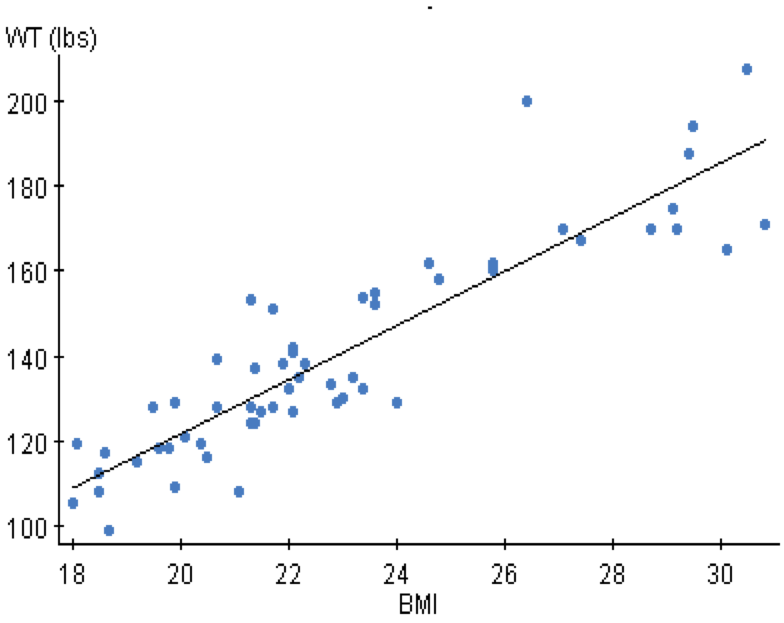
# Supervised Learning

- Use supervised learning – training data is given with correct output
- We write program to  reproduce this output with new test data
- Eg : face detection
- Classification : face detection, spam email
- Regression : Netflix guesses how much you will rate the movie

Classification Graph



Regression Graph



# Unsupervised and semi-supervised

- To understand data, it’s structure – similarity, relation to each other etc
- Semisupervised – supervised and then is a specific signal to predict but some examples do not have the target that needs to be predicted
- Medical – a lot of data but few outputs

# Terminology

- Attributes
  - Also known as features, variables, independent variables, covariates
- Target Variable
  - Also known as goal predicate, dependent variable, …
- Classification
  - Also known as discrimination, supervised classification, …
- Error function
  - Also known as objective function, loss function, …

# Inductive or Supervised learning

- Let x = input vector of attributes (feature vectors)

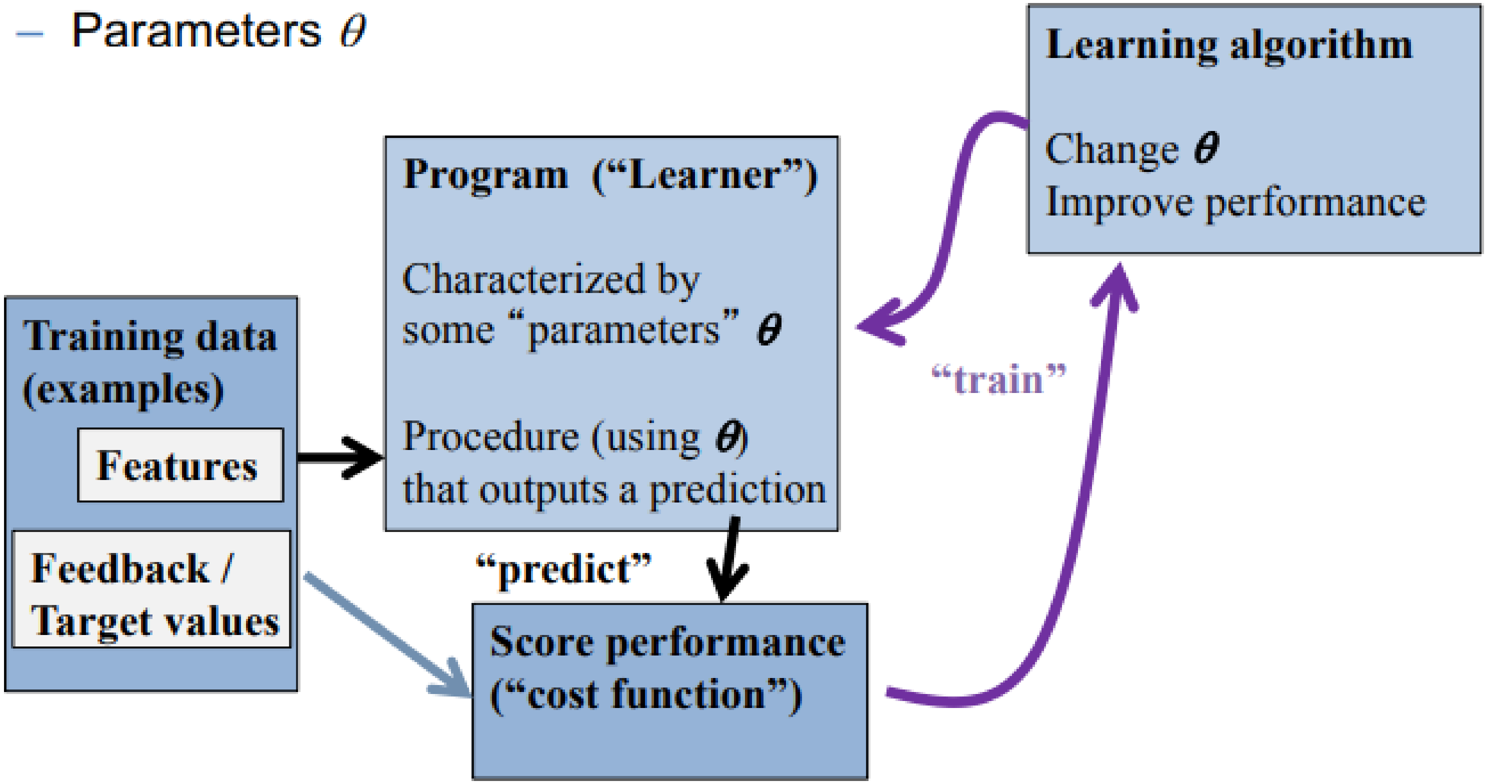
- Let f(x) = target label
  - The implicit mapping from x to f(x) is unknown to us
  - We only have training data pairs, D = {**x**, **f(x)**} available

- We want to learn a mapping from x to f(x)
  - Our hypothesis function is h(x, θ)
  - h(x, θ) ≈ f(x) for all training data points x
  - θ are the parameters of our predictor function h

- Examples:
  - $h(x, \theta) = \text{sign}(\theta_1 x_1 + \theta_2 x_2 + \theta_3)$ (perceptron)
  - $h(x, \theta) = \theta_0 + \theta_1 x_1 + \theta_2 x_2$ (regression)
  - $h_k(x) = (x_1 \wedge x_2) \vee (x_3 \wedge \neg x_4)$

Thanks to Prof. Alex Ihler

- Targets $y$
- Predictions $\hat{y} = f(x\ ;\ \theta)$
- Parameters $\theta$



Learning algorithm
Change $\boldsymbol{\theta}$
Improve performance
Program ("Learner")
Characterized by some "parameters" $\boldsymbol{\theta}$
Procedure (using $\boldsymbol{\theta}$) that outputs a prediction
"train"
Training data (examples)
Features
Feedback / Target values
"predict"
Score performance ("cost function")

# Empirical Error Functions

- $E(h) = \Sigma_x$ distance$[h(x, \theta) , f(x)]$

  Sum is over all training pairs in the training data D

  Examples:

  distance = squared error if h and f are real-valued (regression)

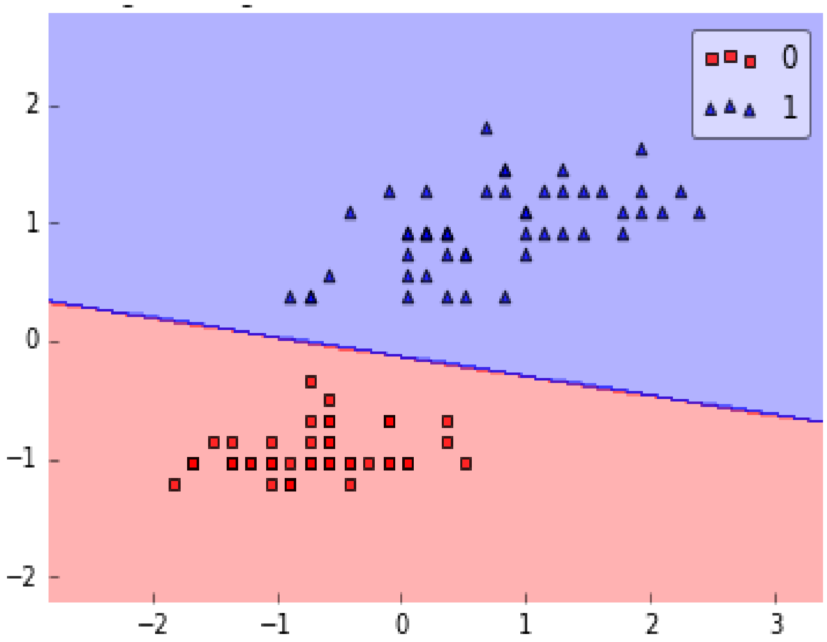
  distance = delta-function if h and f are categorical (classification)

  In learning, we get to choose

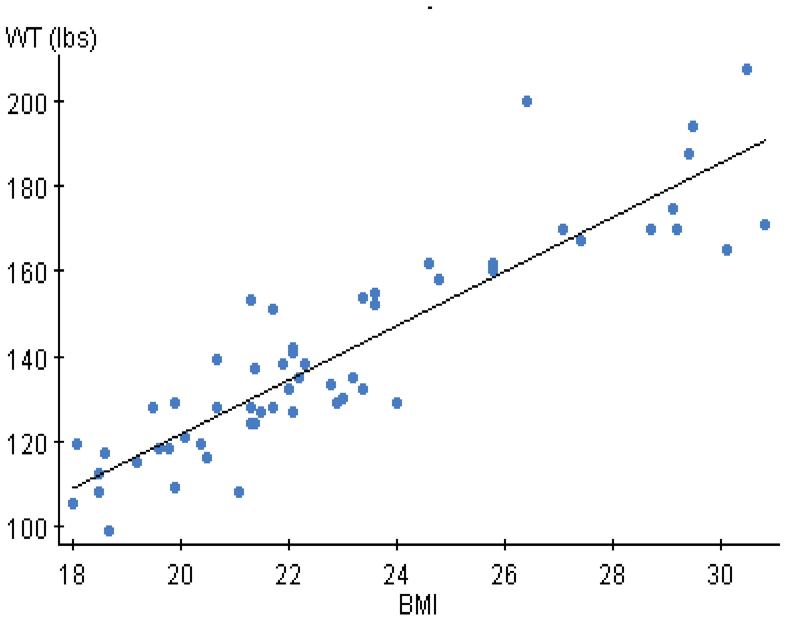
  1. what class of functions h(..) we want to learn
     – potentially a huge space! ("hypothesis space")

  2. what error function/distance we want to use
     - should be chosen to reflect real "loss" in problem
     - but often chosen for mathematical/algorithmic convenience

Classification Graph



Regression Graph



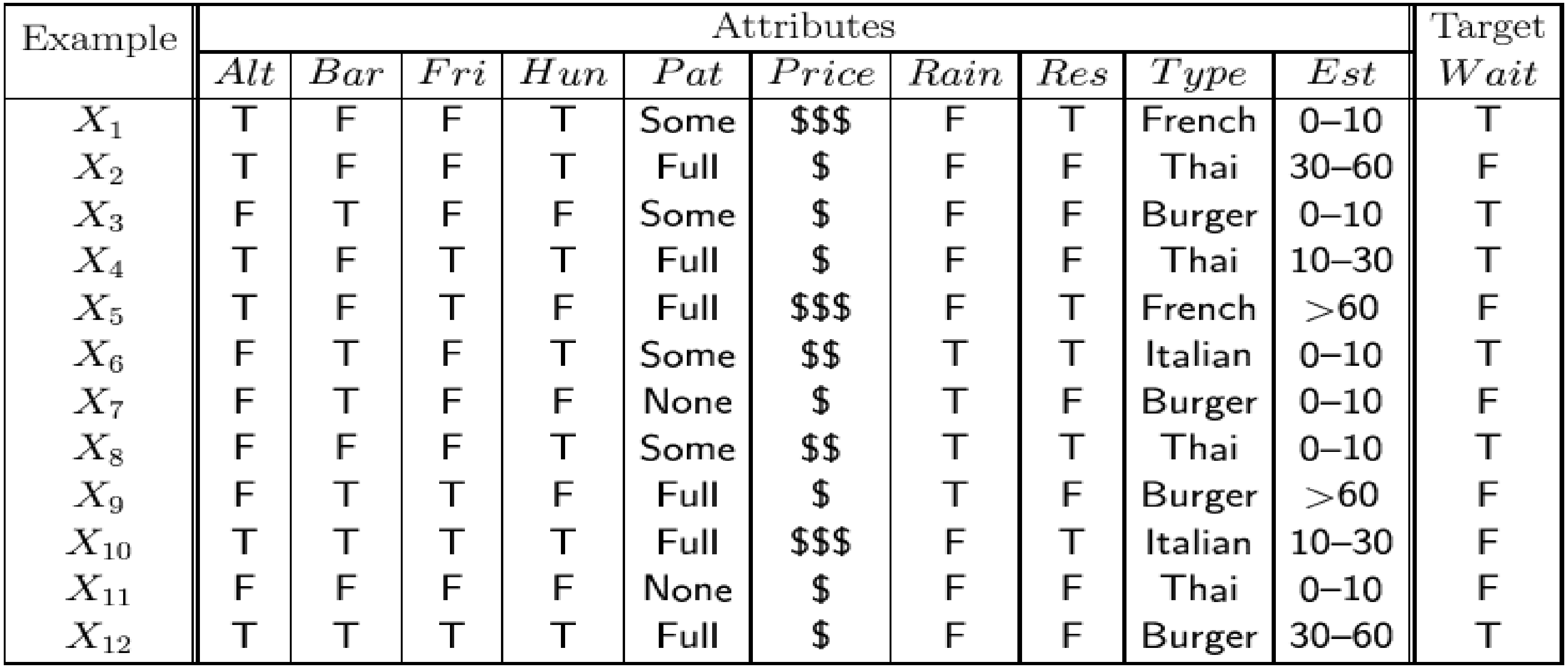
## Simple illustrative learning problem

Problem:

Decide whether to wait for a table at a restaurant, based on the following attributes:

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)

# Training Data for Supervised Learning

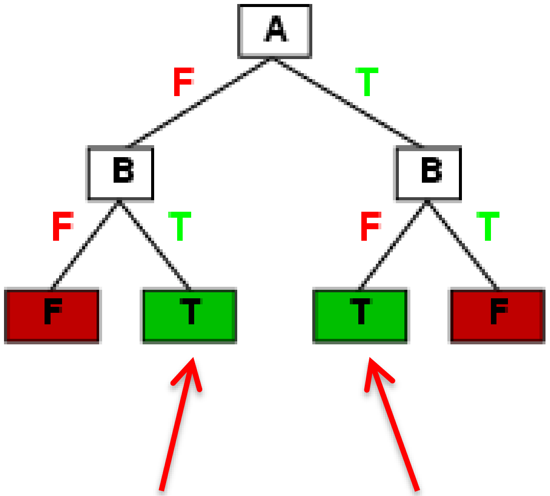


| Example | Attributes | | | | | | | | | | Target |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | *Alt* | *Bar* | *Fri* | *Hun* | *Pat* | *Price* | *Rain* | *Res* | *Type* | *Est* | *Wait* |
| $X_1$ | T | F | F | T | Some | $$$ | F | T | French | 0–10 | T |
| $X_2$ | T | F | F | T | Full | $ | F | F | Thai | 30–60 | F |
| $X_3$ | F | T | F | F | Some | $ | F | F | Burger | 0–10 | T |
| $X_4$ | T | F | T | T | Full | $ | F | F | Thai | 10–30 | T |
| $X_5$ | T | F | T | F | Full | $$$ | 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 |

# Decision Tree Representations

- Decision trees are fully expressive
  - Can represent any Boolean function (in DNF)
  - Every path in the tree could represent 1 row in the truth table
  - Might yield an exponentially large tree
    - Truth table is of size $2^d$, where d is the number of attributes

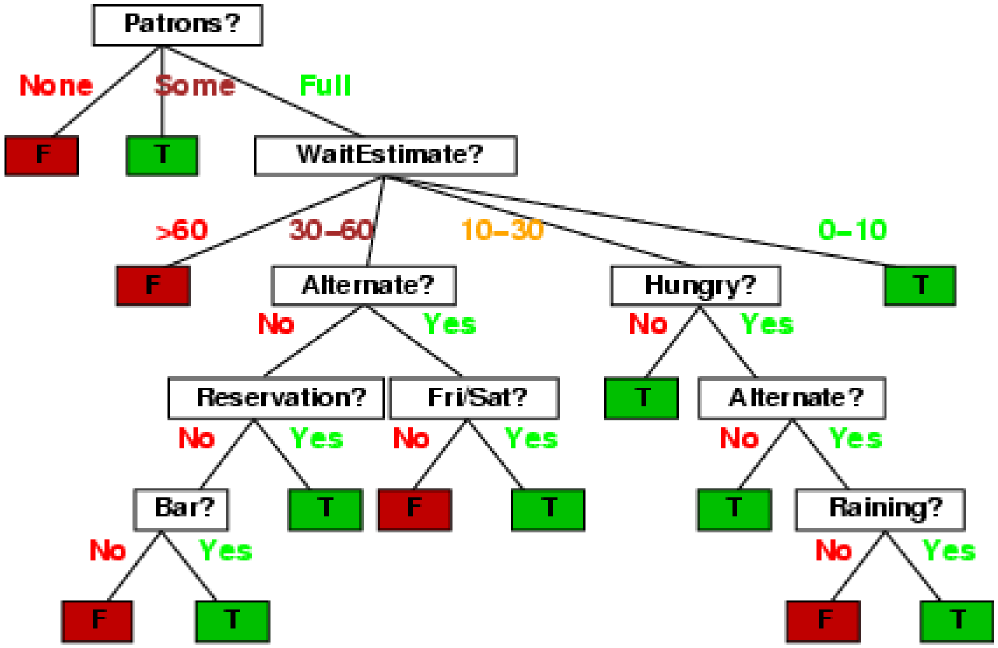
| A | B | A xor B |
|---|---|---|
| F | F | F |
| F | T | T |
| T | F | T |
| T | T | F |



**A xor B = ( ¬ A ∧ B ) ∨ ( A ∧ ¬ B )** in DNF

# Decision Tree Learning

- Constrain h(..) to be a decision tree
  - This is the R&N tree for the Restaurant Wait problem:



# Decision Tree Representations

- Decision trees are DNF representations
  - often used in practice → often result in compact approximate representations for complex functions
  - E.g., consider a truth table where most of the variables are irrelevant to the function

- Simple DNF formulae can be easily represented
  - E.g., $f = (A \land B) \lor (\neg A \land D)$
  - DNF = disjunction of conjunctions

- Trees can be very inefficient for certain types of functions
  - Parity function: 1 only if an even number of 1's in the input vector
    - Trees are very inefficient at representing such functions
  - Majority function: 1 if more than ½ the inputs are 1's
    - Also inefficient

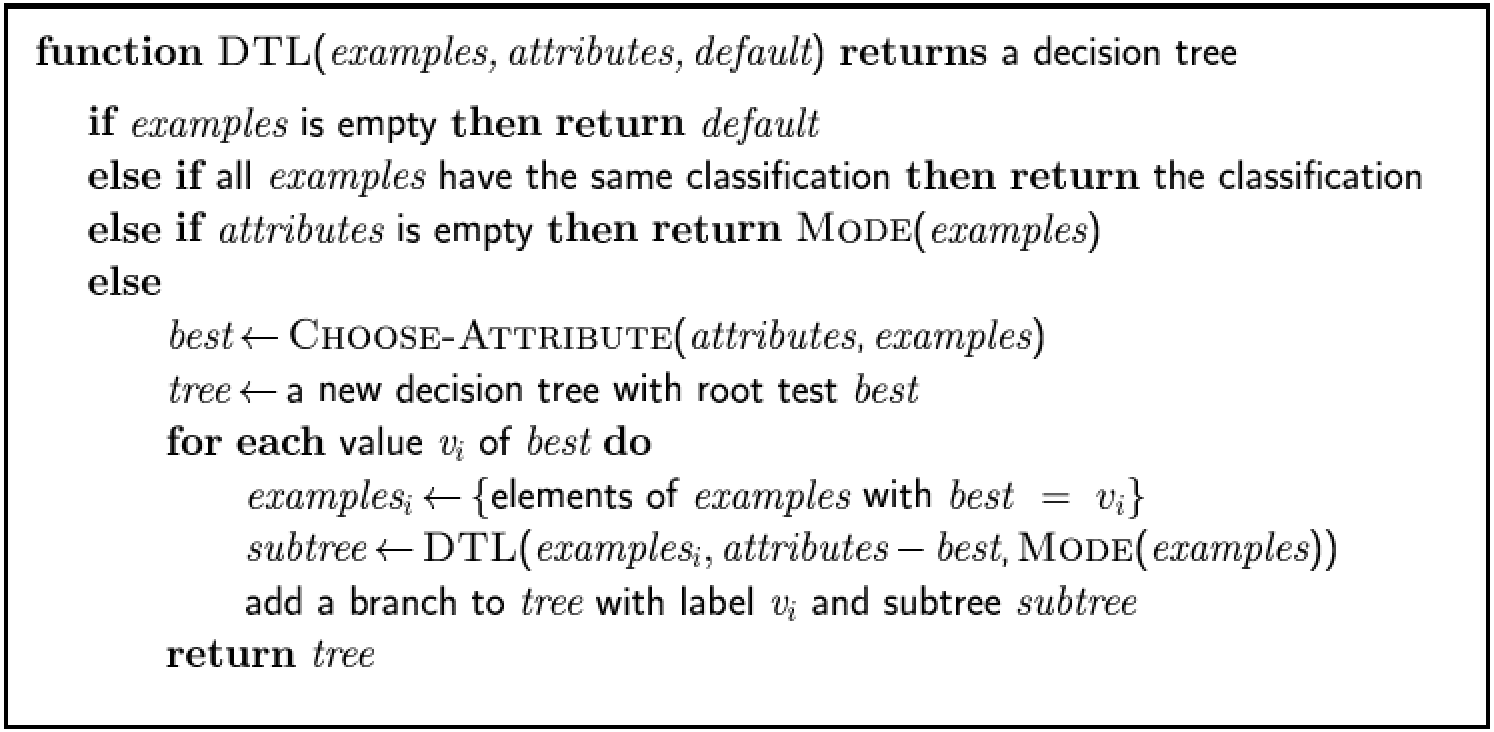
# Decision Tree Learning

- Find the smallest decision tree consistent with the n examples
  - Unfortunately this is provably intractable to do optimally

- Greedy heuristic search used in practice:
  - Select root node that is "best" in some sense
  - Partition data into 2 subsets, depending on root attribute value
  - Recursively grow subtrees
  - Different termination criteria
    - For noiseless data, if all examples at a node have the same label then declare it a leaf and backup
    - For noisy data it might not be possible to find a "pure" leaf using the given attributes
      - we'll return to this later – but a simple approach is to have a depth-bound on the tree (or go to max depth) and use majority vote

- We have talked about binary variables up until now, but we can trivially extend to multi-valued variables

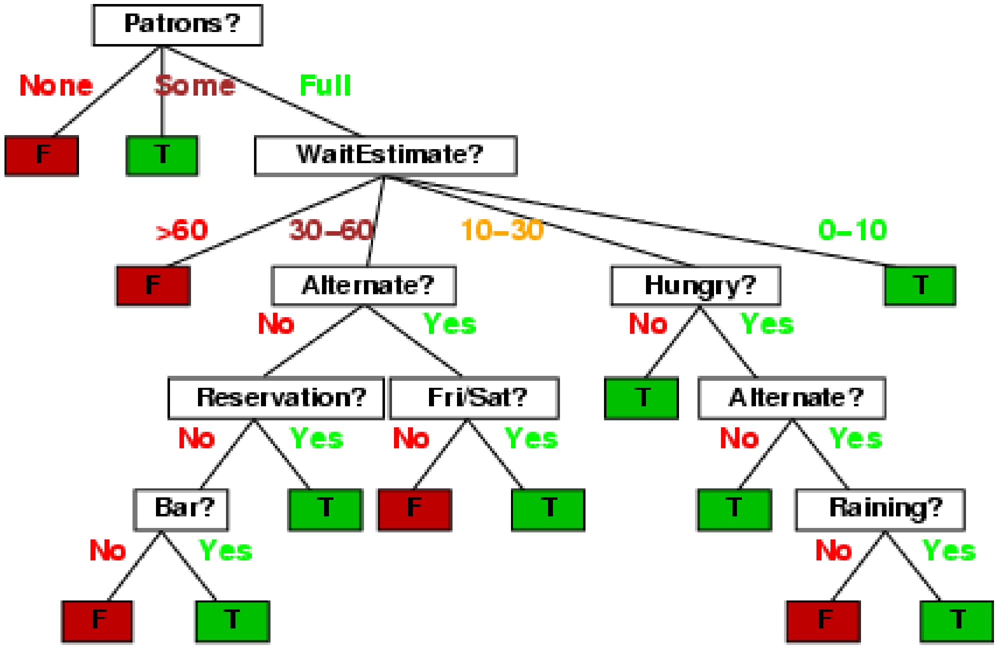
# Pseudocode for Decision tree learning



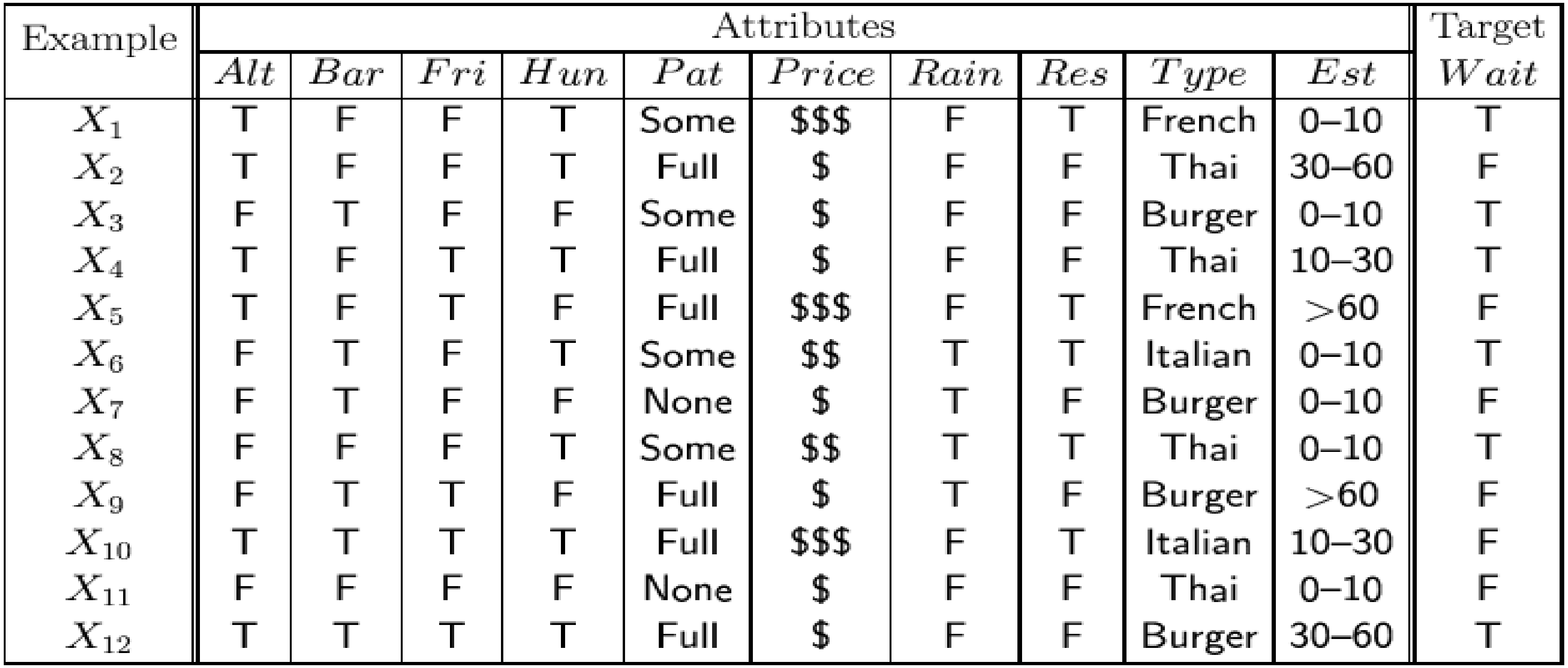
```
function DTL(examples, attributes, default) returns a decision tree

    if examples is empty then return default
    else if all examples have the same classification then return the classification
    else if attributes is empty then return MODE(examples)
    else
        best ← CHOOSE-ATTRIBUTE(attributes, examples)
        tree ← a new decision tree with root test best
        for each value $v_i$ of best do
            $examples_i$ ← {elements of examples with best $= v_i$}
            subtree ← DTL($examples_i$, attributes − best, MODE(examples))
            add a branch to tree with label $v_i$ and subtree subtree
        return tree
```

# Decision Tree Learning

- Constrain h(..) to be a decision tree
  - This is the R&N tree for the Restaurant Wait problem:



# Training Data for Supervised Learning



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|---|---|---|---|---|---|---|---|---|---|---|---|
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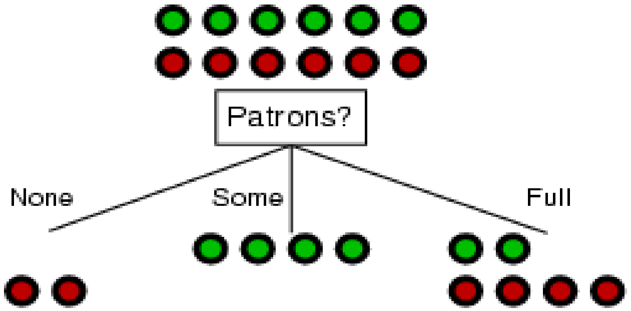
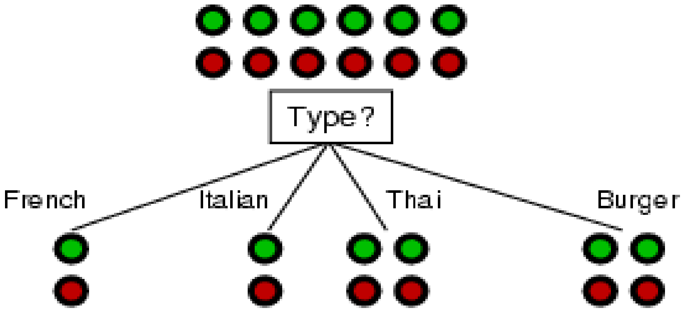
| $X_{12}$ | T | T | T | T | Full | $ | F | F | Burger | 30–60 | T |

# Choosing an attribute

- Idea: a good attribute splits the examples into subsets that are (ideally) "all positive" or "all negative"

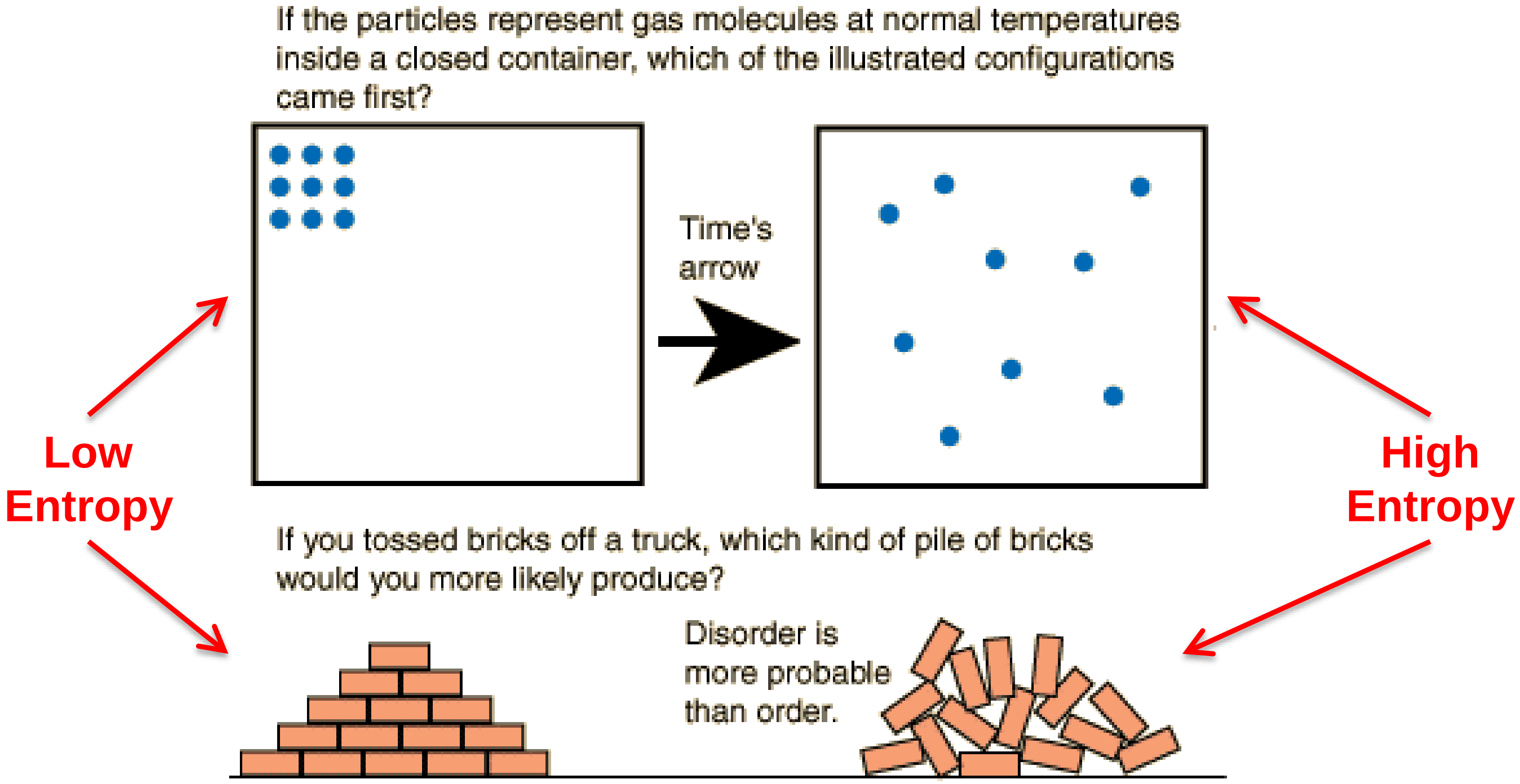




- *Patrons?* is a better choice
  - How can we quantify this?
  - One approach would be to use the classification error E directly (greedily)
    - Empirically it is found that this works poorly
  - **Much better is to use information gain (next slides)**
  - Other metrics are also used, e.g., Gini impurity, variance reduction
    - Often very similar results to information gain in practice

# Entropy and Information

- **“Entropy” is a measure of randomness**
  **= amount of disorder**



If the particles represent gas molecules at normal temperatures inside a closed container, which of the illustrated configurations came first?

If you tossed bricks off a truck, which kind of pile of bricks would you more likely produce?

Disorder is more probable than order.

https://www.youtube.com/watch?v=ZsY4WcQOrfk

# Entropy, H(p), with only 2 outcomes

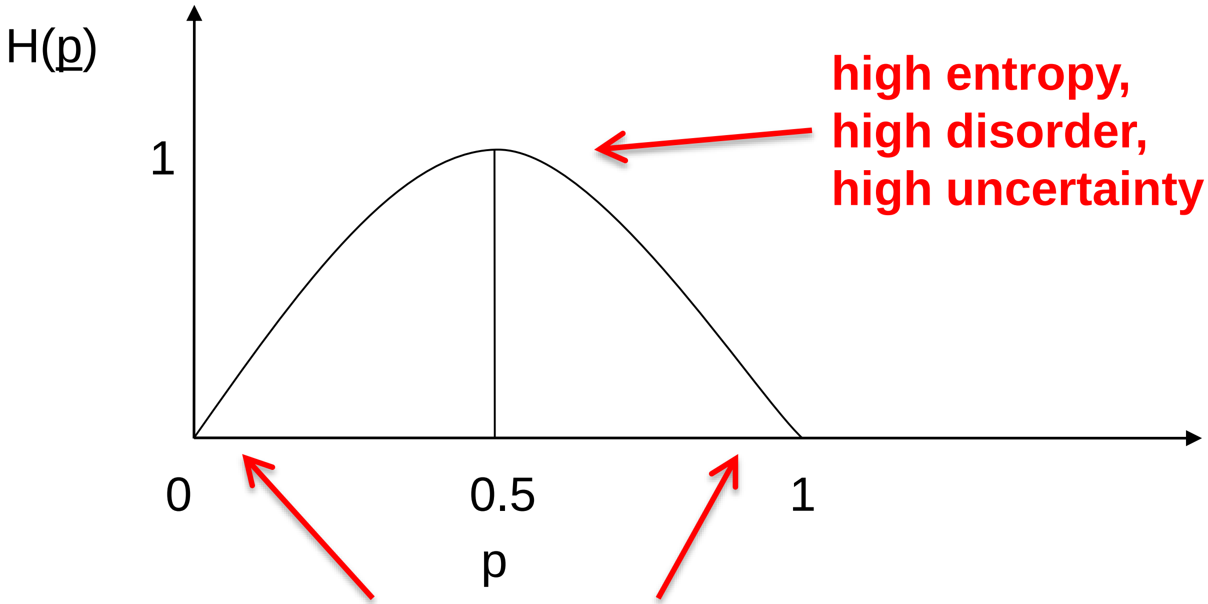
Consider 2 class problem:

p = probability of class #1,

1 – p = probability of class #2

In binary case:

$$H(p) = -\,p \log p \;-\; (1-p) \log (1-p)$$



high entropy,
high disorder,
high uncertainty

Low entropy, low disorder, low uncertainty

# Entropy and Information

- “Entropy” is a measure of randomness
  - How long a message does it take to communicate a result to you?
  - Depends on the probability of the outcomes; more predictable = shorter message

- Communicating fair coin tosses
  - Output: H H T H T T T H H H H T …
  - Sequence takes n bits – each outcome totally unpredictable

- Communicating my daily lottery results
  - Output: 0 0 0 0 0 0 …
  - Most likely to take one bit – I lost every day.
  - Small chance I’ll have to send more bits (won & when)

| | |
|---|---|
| **Lost:** | **0** |
| **Won 1:** | **1(when)0** |
| **Won 2:** | **1(when)1(when)0** |

- More predictable takes less length to communicate because it’s less random
  - Use a few bits for the most likely outcome, more for less likely ones

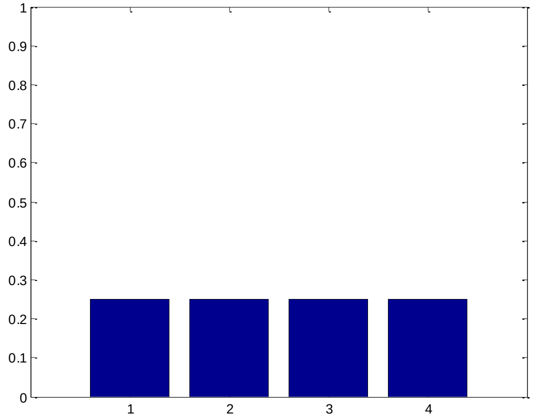
# Entropy and Information

- **Entropy $H(X) = E[\log 1/P(X)] = \sum_{x \in X} P(x) \log 1/P(x)$**

  **$= -\sum_{x \in X} P(x) \log P(x)$**

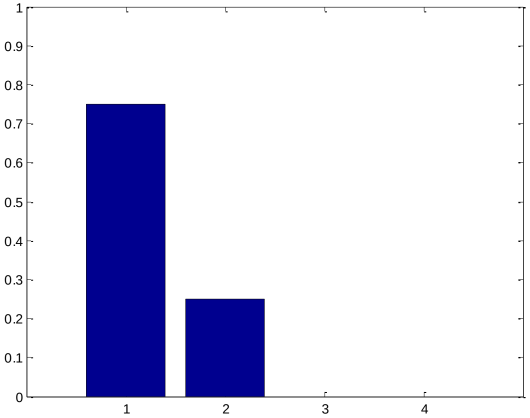
  - Log base two, units of entropy are "bits"
  - If only two outcomes: $H(p) = -p \log(p) - (1-p) \log(1-p)$

- Examples:

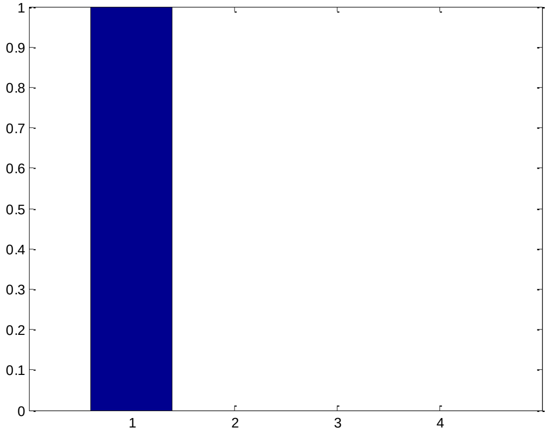


**H(x) = .25 log 4 + .25 log 4 +**
**.25 log 4 + .25 log 4**
**= log 4 = 2 bits**

**Max entropy for 4 outcomes**



**H(x) = .75 log 4/3 + .25 log 4**
**= 0.8133 bits**



**H(x) = 1 log 1**
**= 0 bits**

**Min entropy**

# Information Gain

- H(P) = current entropy of class distribution P at a particular node,
  before further partitioning the data

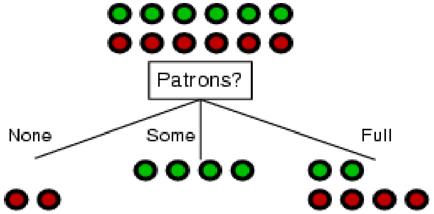
- H(P | A) = conditional entropy given attribute A
  = weighted average entropy of conditional class distribution,
  after partitioning the data according to the values in A

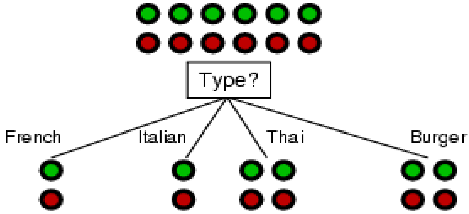
- Gain(A) = H(P) – H(P | A)
  - Sometimes written IG(A) = InformationGain(A)

- Simple rule in decision tree learning
  - **At each internal node, split on the node with the largest information gain [or equivalently, with smallest H(P|A) ]**

- Note that by definition, conditional entropy can't be greater than the entropy, so Information Gain must be non-negative

# Root Node Example





For the training set, *6 positives, 6 negatives, H(6/12, 6/12) = 1* bit

positive (p)

negative (1-p)

H(6/12,6/12) = -(6/12)*log2(6/12)-(6/12)*log2(6/12) = 1

Consider the attributes *Patrons* and *Type:*

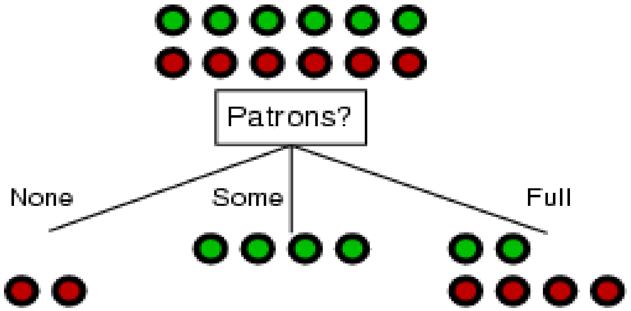
$$IG(\text{Patrons}) = 1 \ - \ [\frac{2}{12}H(0,1) + \frac{4}{12}H(1,0) + \frac{6}{12}H(\frac{2}{6},\frac{4}{6})] \quad = 0.541 \text{ bits}$$

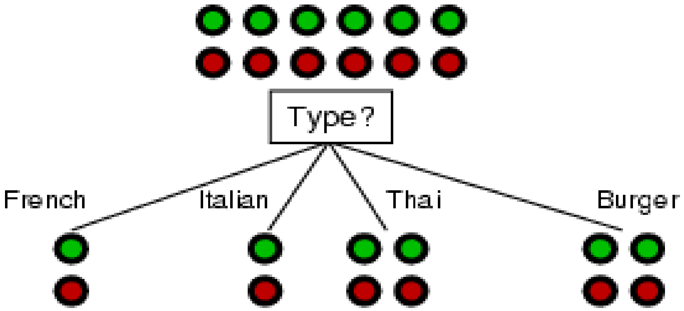
$$IG(\text{Type}) = 1 - [\frac{2}{12}H(\frac{1}{2},\frac{1}{2}) + \frac{2}{12}H(\frac{1}{2},\frac{1}{2}) + \frac{4}{12}H(\frac{2}{4},\frac{2}{4}) + \frac{4}{12}H(\frac{2}{4},\frac{2}{4})] \quad = 0 \text{ bits}$$

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

Information gain is then repeatedly applied at internal nodes until all leaves contain only examples from one class or the other

# Choosing an attribute



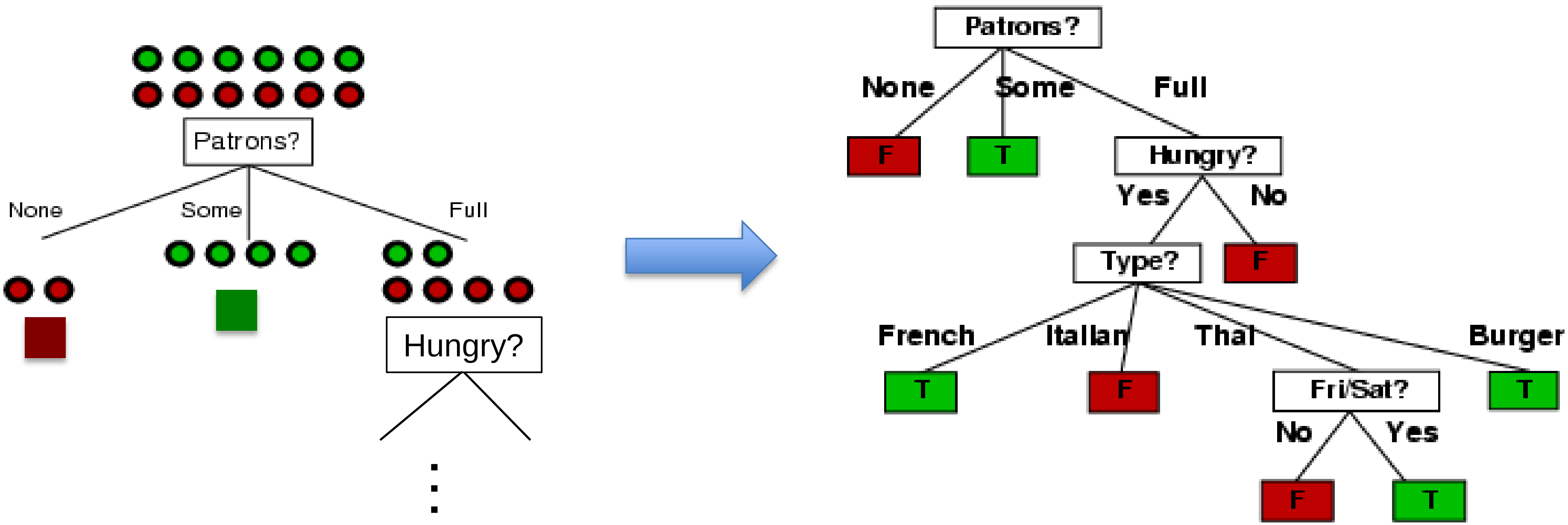


IG(Patrons) = 0.541 bits

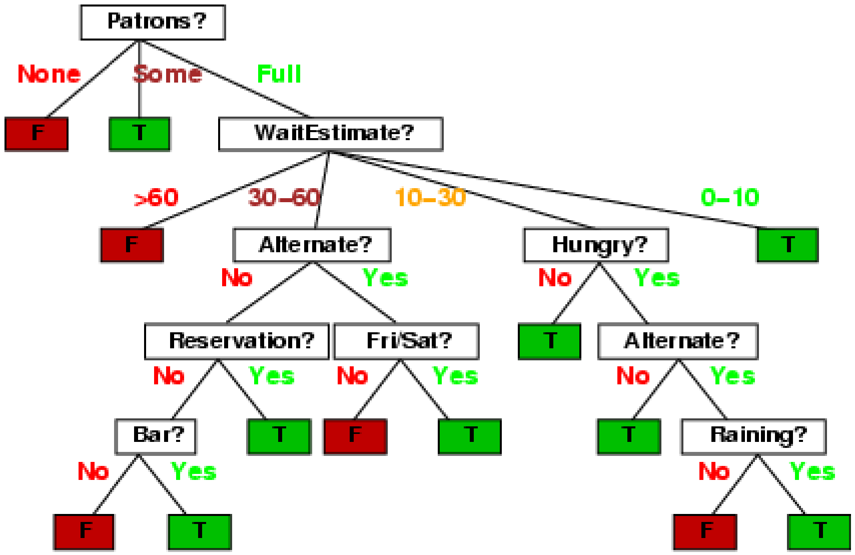
IG(Type) = 0 bits

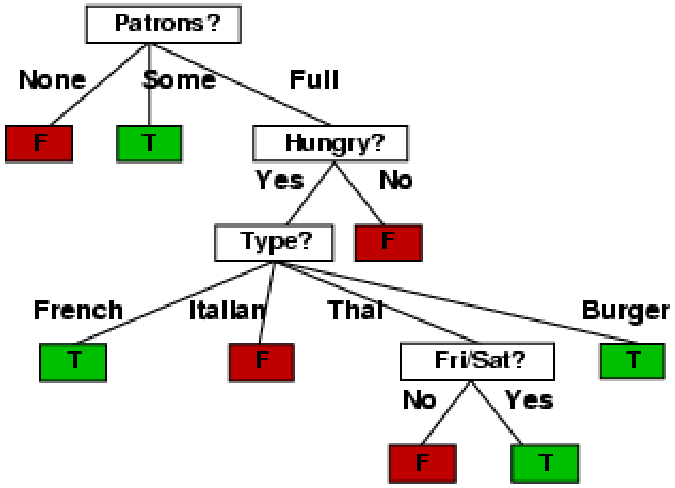
# Decision Tree Learned

- Decision tree learned from the 12 examples:



# R&N Tree (left) versus Learned Tree (right)





# Assessing Performance

Training data performance is typically optimistic

e.g., error rate on training data

Reasons?

- classifier may not have enough data to fully learn the concept (but on training data we don’t know this)
- for noisy data, the classifier may overfit the training data

In practice we want to assess performance “out of sample”

how well will the classifier do on new unseen data? This is the true test of what we have learned (just like a classroom)

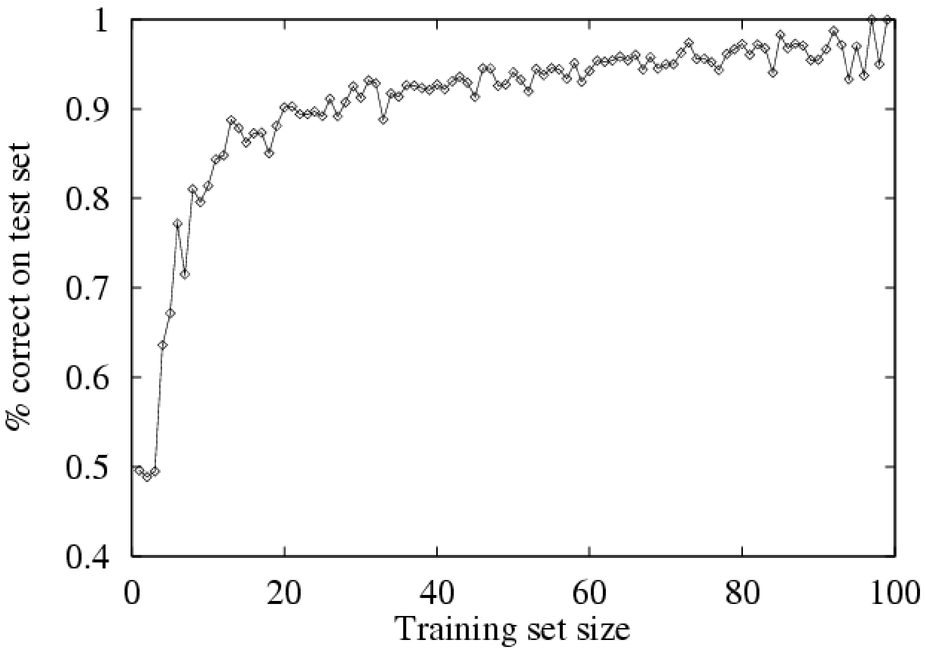
With large data sets we can partition our data into 2 subsets, train and test

- build a model on the training data
- assess performance on the test data

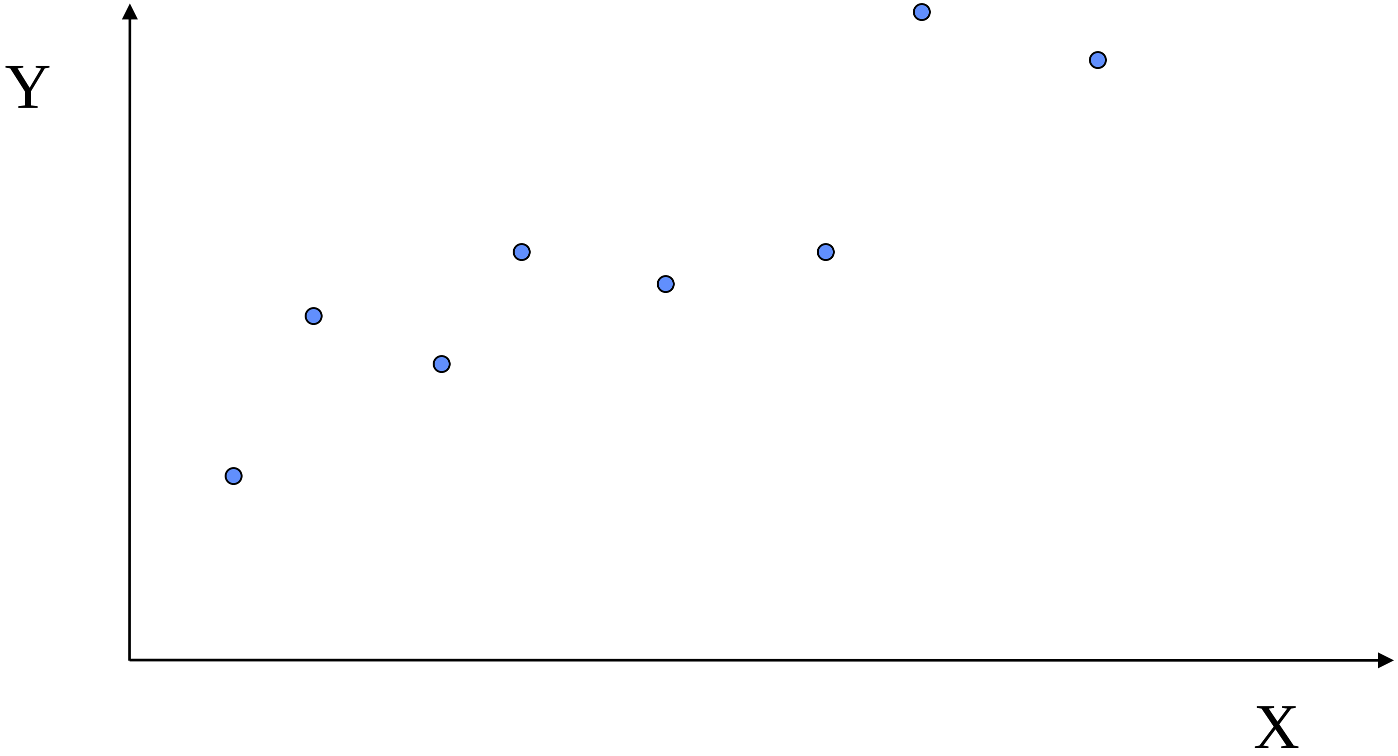
# Example of Test Performance

Restaurant problem

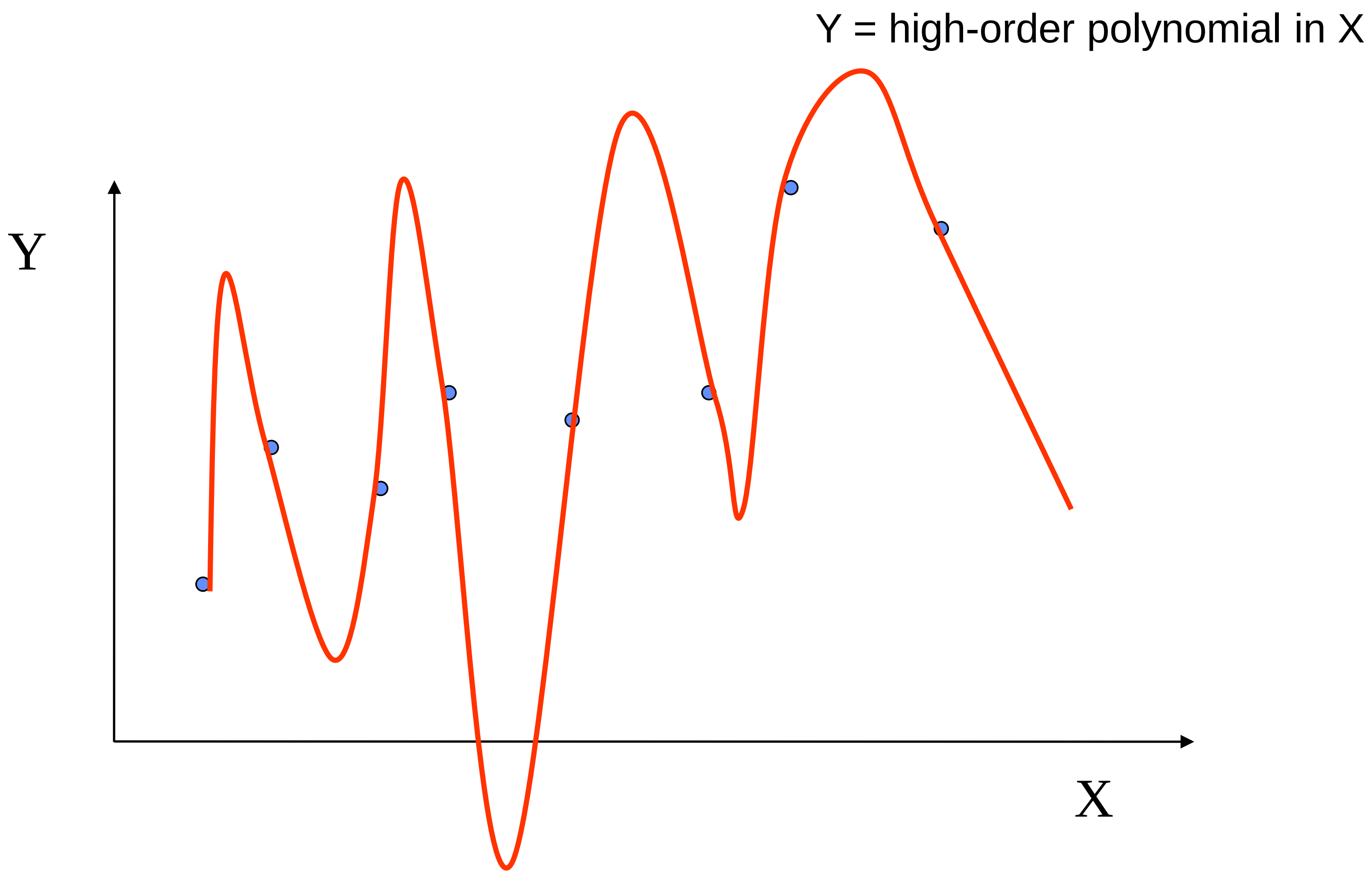
- simulate 100 data sets of different sizes
- train on this data, and assess performance on an independent test set
- learning curve = plotting accuracy as a function of training set size
- typical “diminishing returns” effect (some nice theory to explain this)



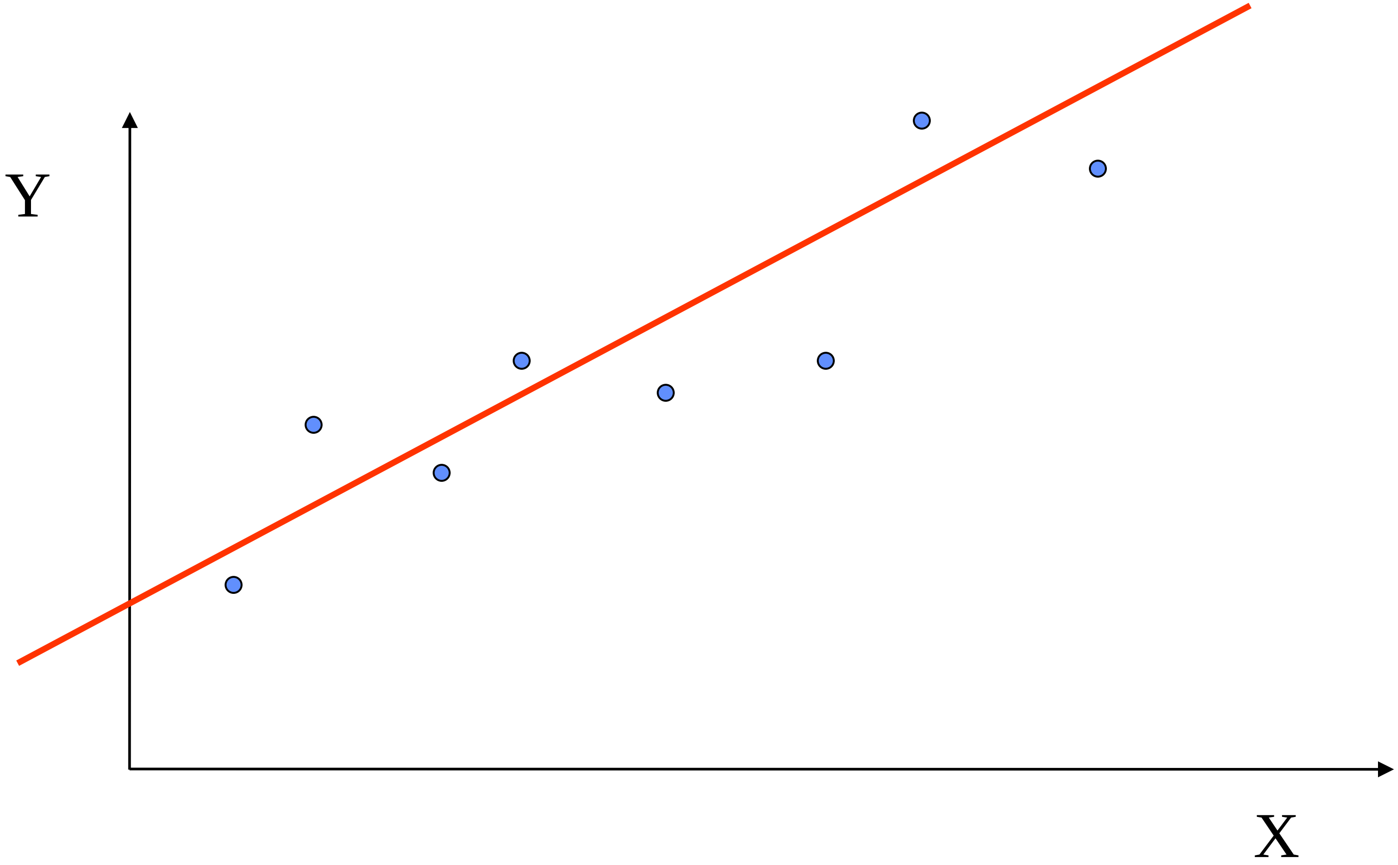
# Overfitting and Underfitting



# A Complex Model

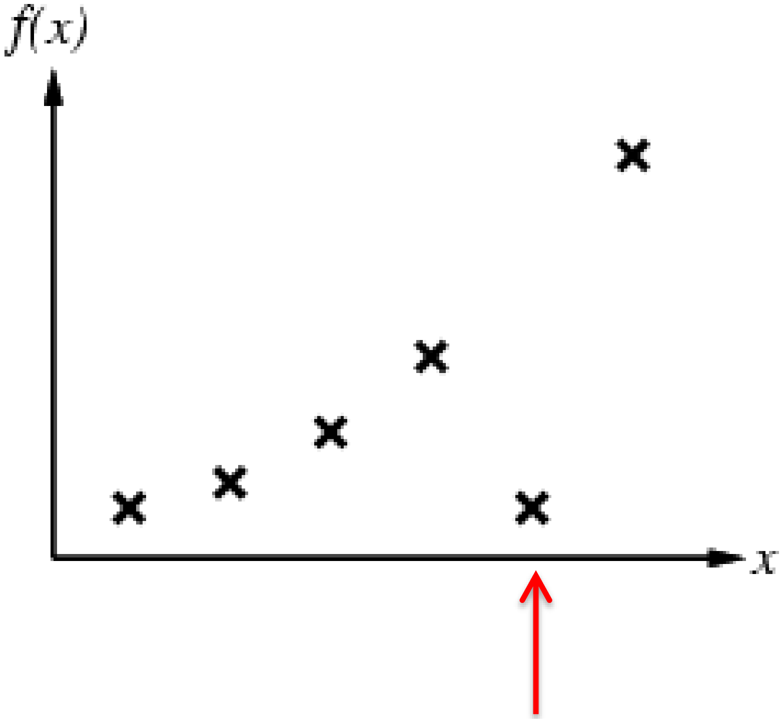


# A Much Simpler Model



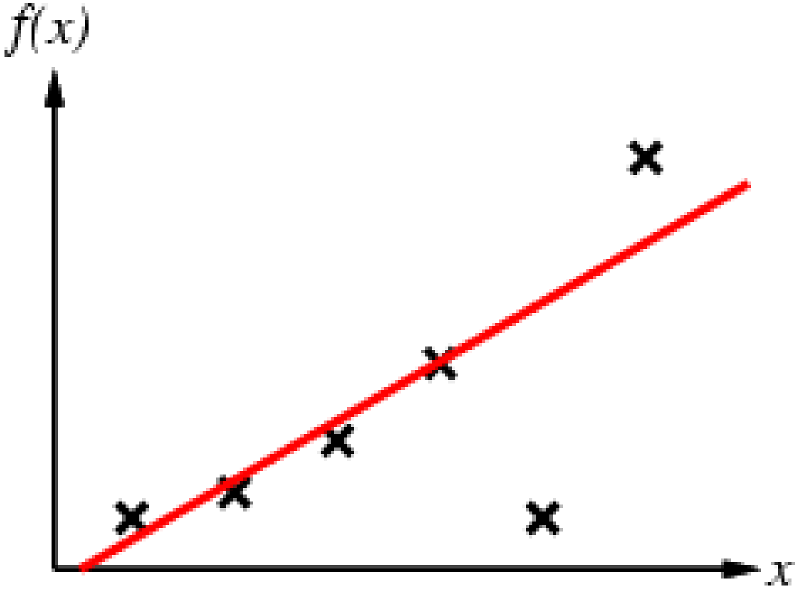
Y = a X + b + noise

# Example 2

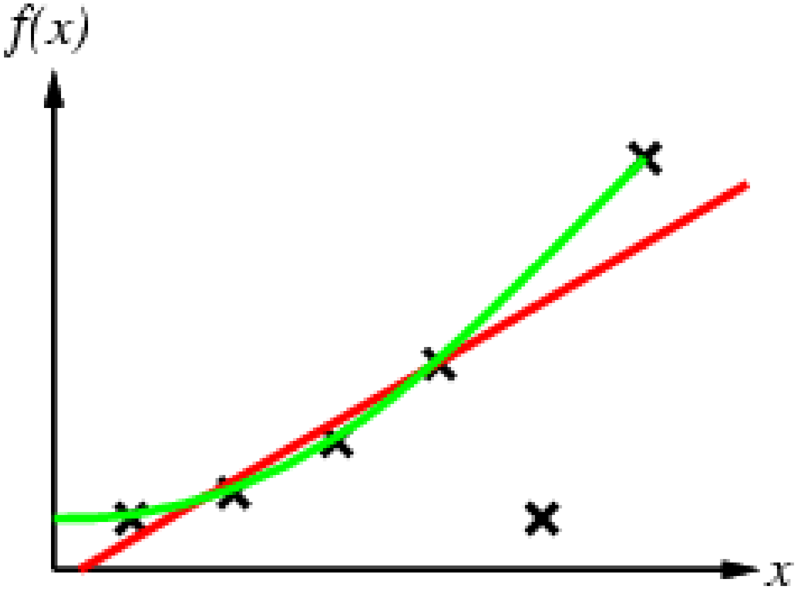


My biologist colleagues say, “Oh, that’s the sample that we dropped on the floor!”

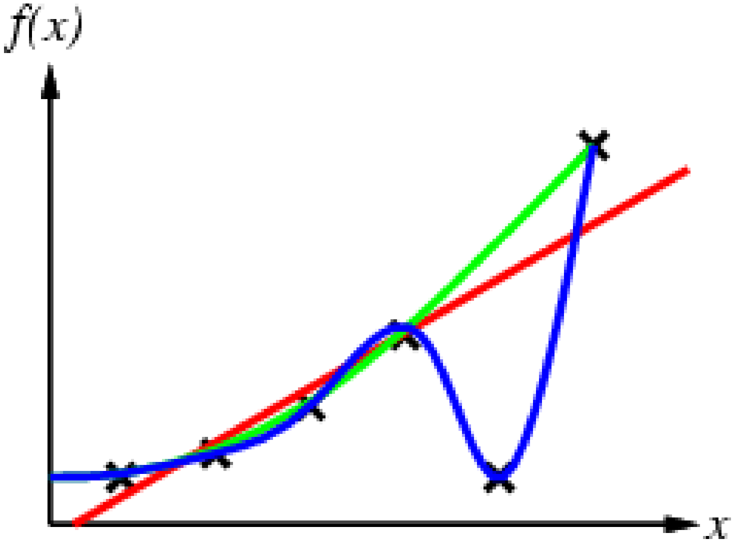
## Example 2



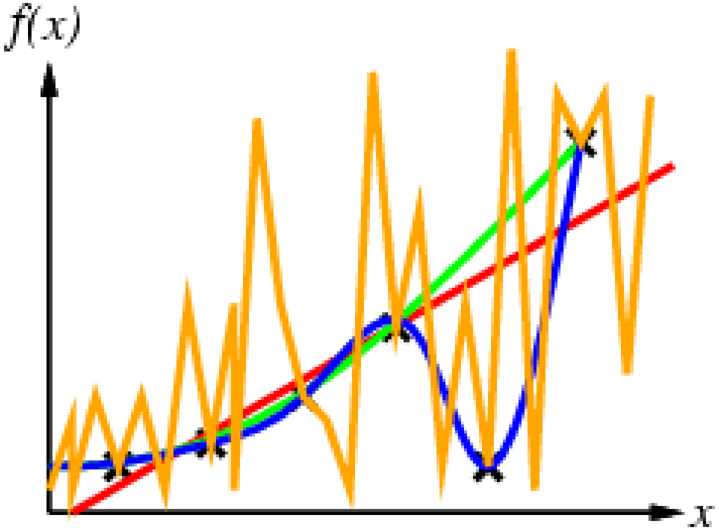
## Example 2



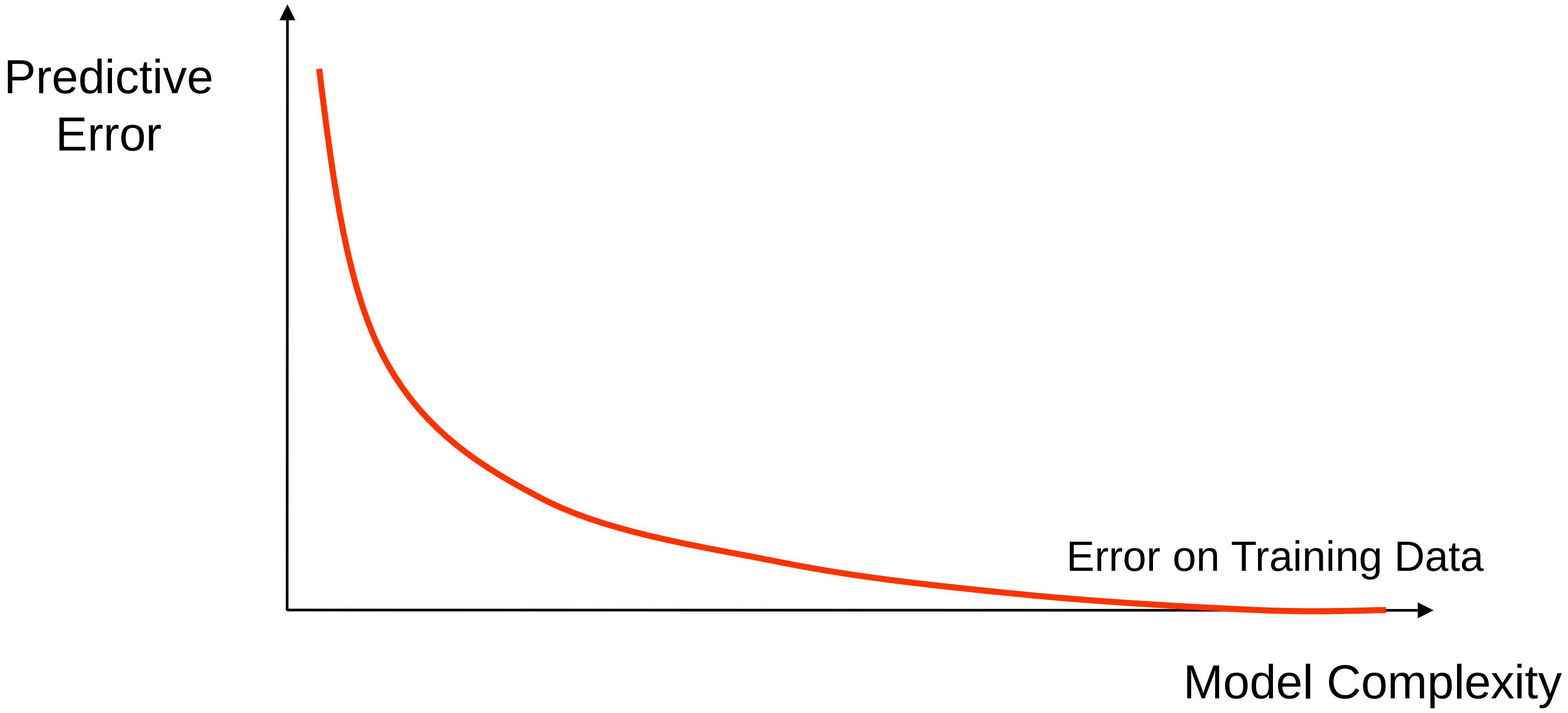
# Example 2



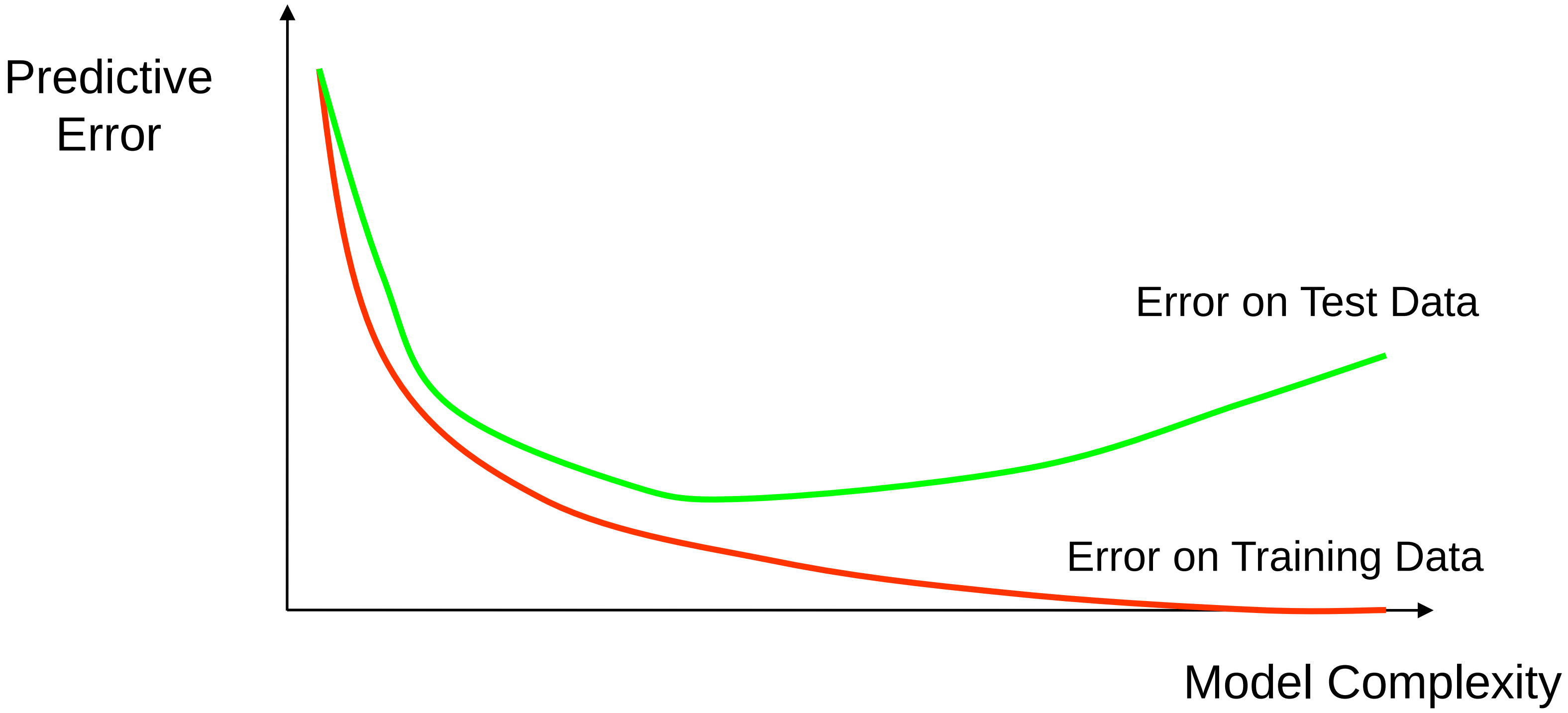
## Example 2



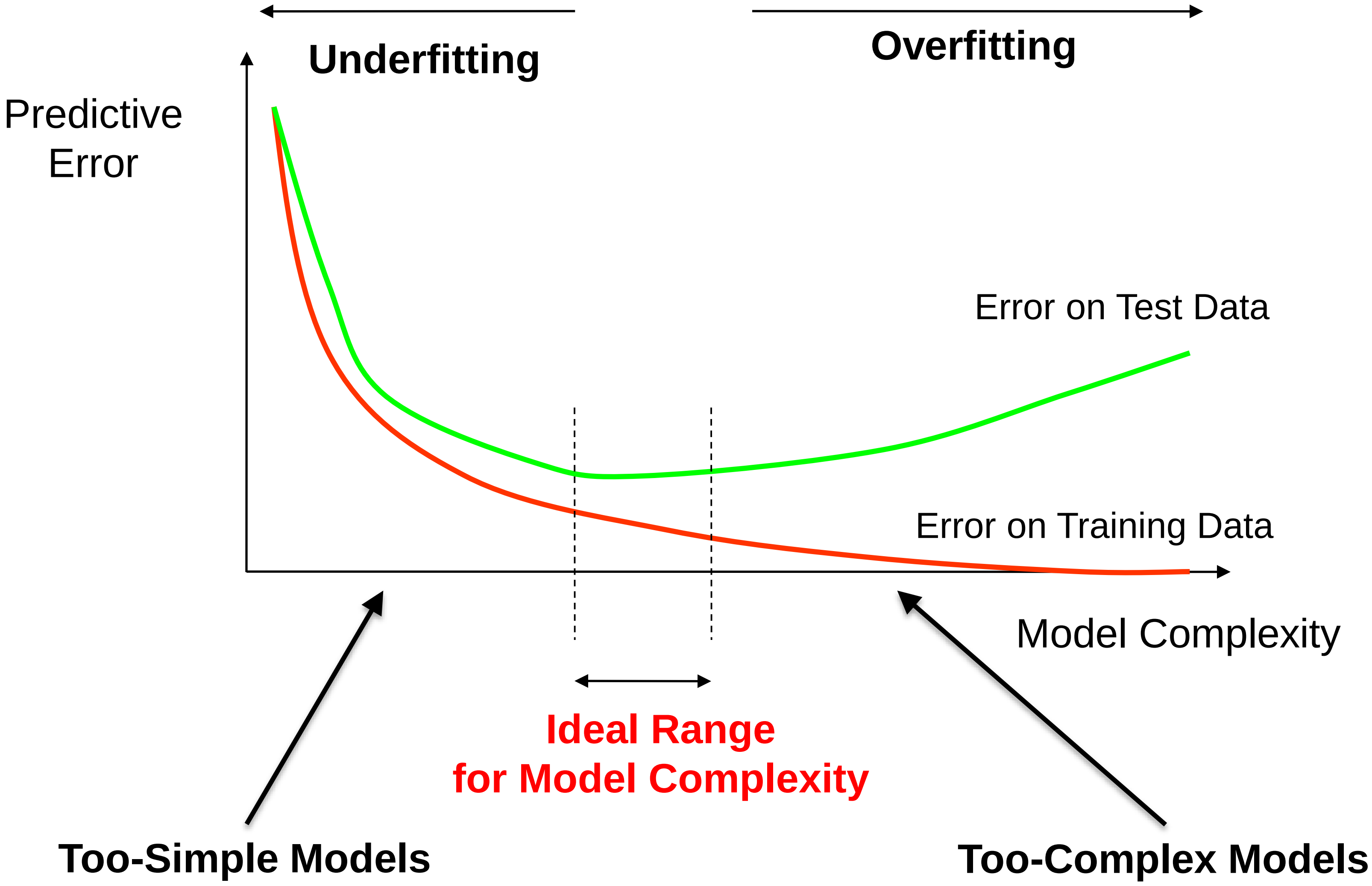
# How Overfitting affects Prediction



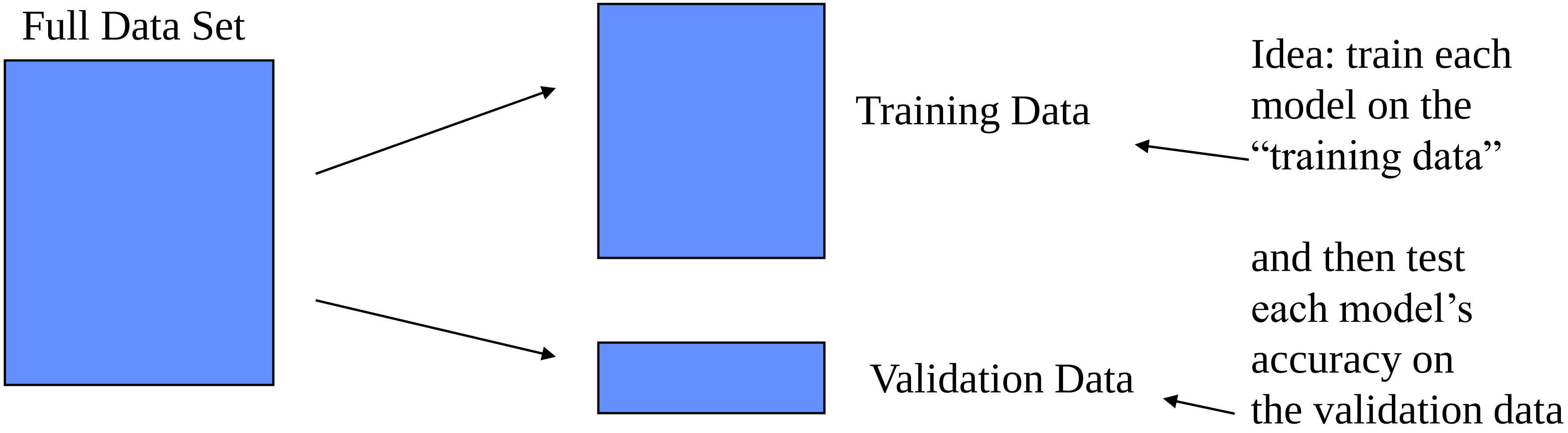
# How Overfitting affects Prediction



# How Overfitting affects Prediction



# Training and Validation Data



Full Data Set

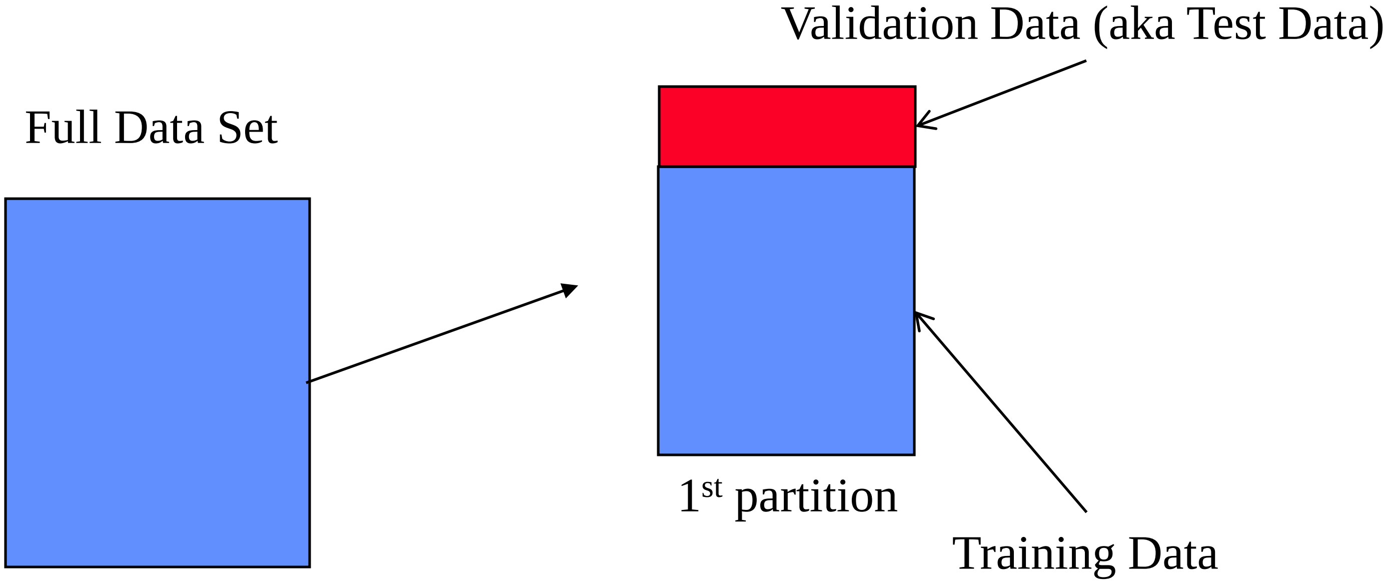
Training Data

Validation Data

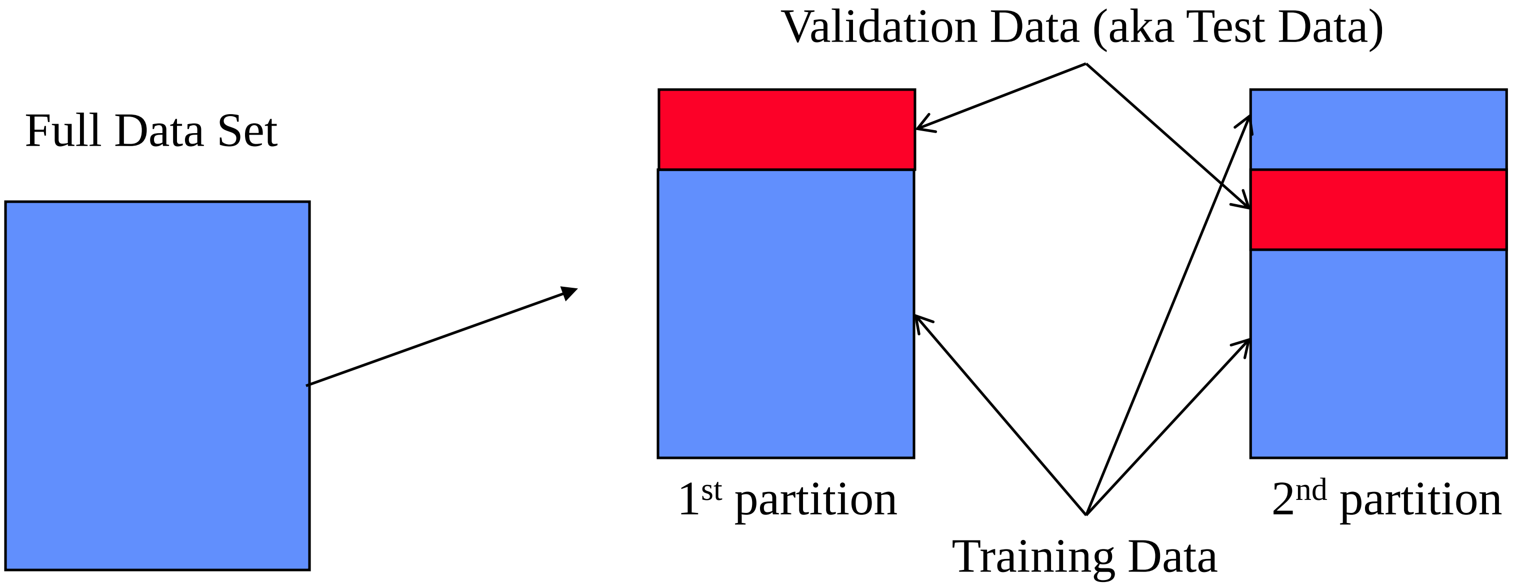
Idea: train each model on the "training data"

and then test each model's accuracy on the validation data

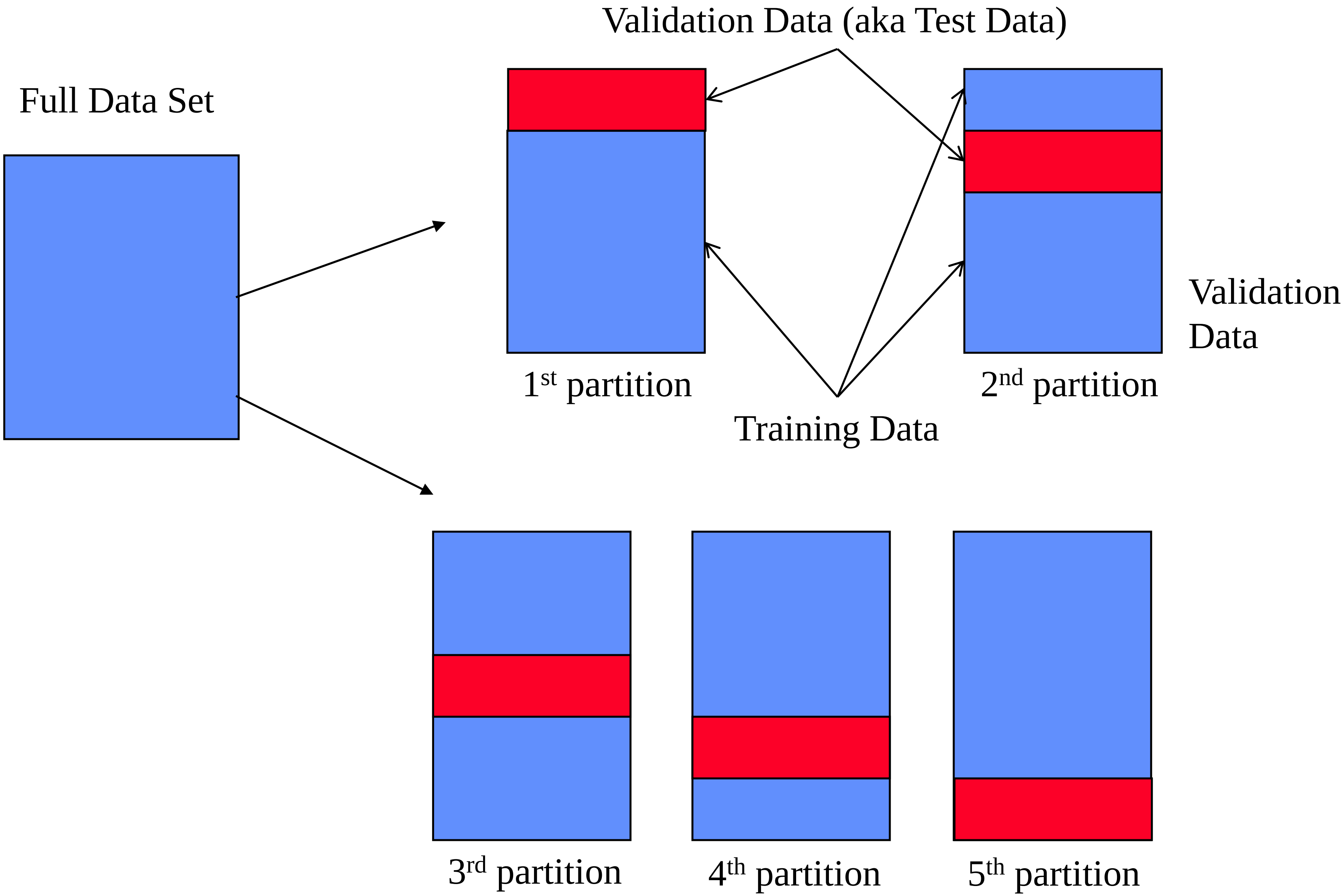
# Disjoint Validation Data Sets



# Disjoint Validation Data Sets



# Disjoint Validation Data Sets



Validation Data (aka Test Data)

Full Data Set

Validation Data

1st partition

2nd partition

Training Data

3rd partition

4th partition

5th partition

# More on Cross-Validation

- Notes
  - cross-validation generates an approximate estimate of how well the learned model will do on “unseen” data

  - by averaging over different partitions it is more robust than just a single train/validate partition of the data

  - “k-fold” cross-validation is a generalization
    - partition data into disjoint validation subsets of size n/k
    - train, validate, and average over the v partitions
    - e.g., k=10 is commonly used

  - k-fold cross-validation is approximately k times computationally more expensive than just fitting a model to all of the data

## The k-fold Cross-Validation Method

- Why just choose one particular 90/10 “split” of the data?
  - In principle we could do this multiple times
- “k-fold Cross-Validation” (e.g., k=10)
  - randomly partition our full data set into k disjoint subsets (each roughly of size n/k, n = total number of training data points)
    - for i = 1:10 (here k = 10)
      - train on 90% of data,
      - Acc(i) = accuracy on other 10%
    - end
    - Cross-Validation-Accuracy = $1/k \ \Sigma_i \ Acc(i)$
  - choose the method with the highest cross-validation accuracy
  - common values for k are 5 and 10
  - Can also do “leave-one-out” where k = n

## You will be expected to know

- Understand Attributes, Error function, Classification, Regression, Hypothesis (Predictor function)
- What is Supervised Learning?
- Decision Tree Algorithm
- Entropy
- Information Gain
- Tradeoff between train and test with model complexity
- Cross validation

# Summary

- Inductive learning
  - Error function, class of hypothesis/models {h}
  - Want to minimize E on our training data
  - Example: decision tree learning

- Generalization
  - Training data error is over-optimistic
  - We want to see performance on test data
  - Cross-validation is a useful practical approach

- Learning to recognize faces
  - Viola-Jones algorithm: state-of-the-art face detector, entirely learned from data, using boosting+decision-stumps