CS 412 Intro. to Data Mining

Chapter 7. Classification: Basic Concepts

Arindam Banerjee, Computer Science, UIUC, Fall 2021

Chapter 8. Classification: Basic Concepts

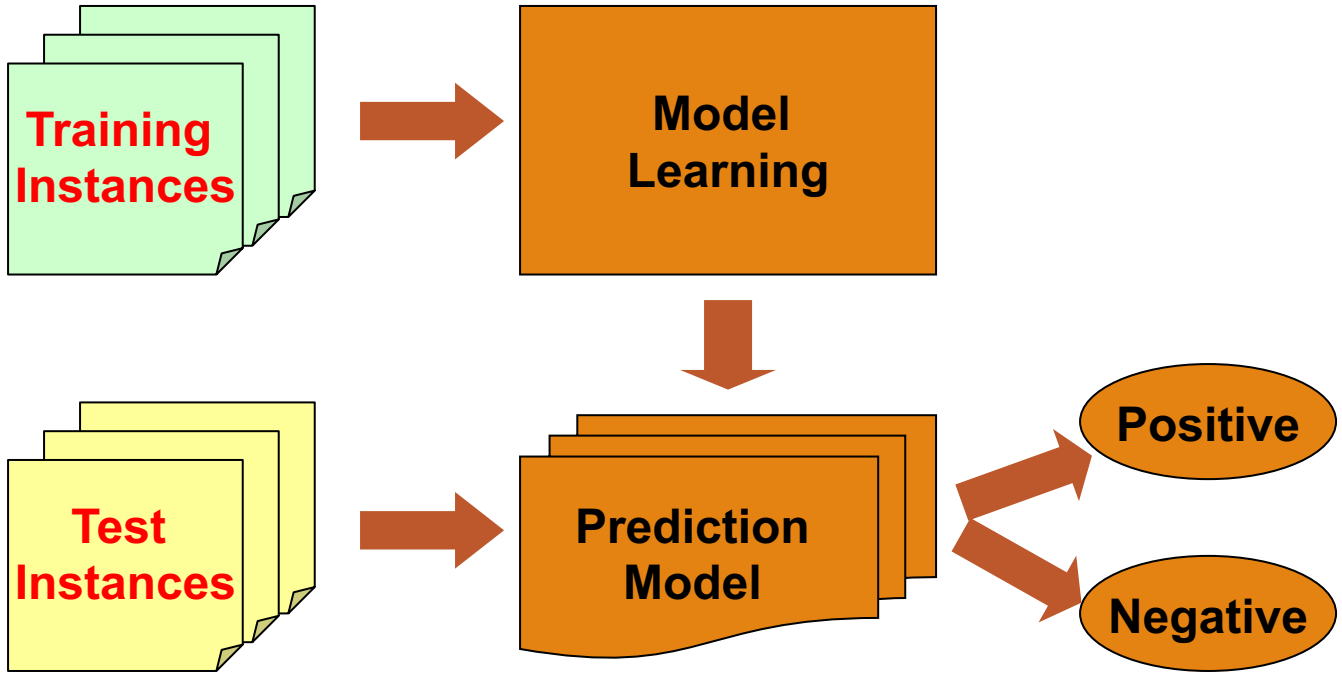
- Classification: Basic Concepts
- Decision Tree Induction
- Bayes Classification Methods
- Linear Classifier
- Model Evaluation and Selection
- Lazy Learning
- Ensemble Methods
- Imbalanced Data Sets
- Summary

Supervised vs. Unsupervised Learning (1)

- Supervised learning (classification)
  - Supervision: The training data such as observations or measurements are accompanied by **labels** indicating the classes which they belong to
  - New data is classified based on the models built from the training set

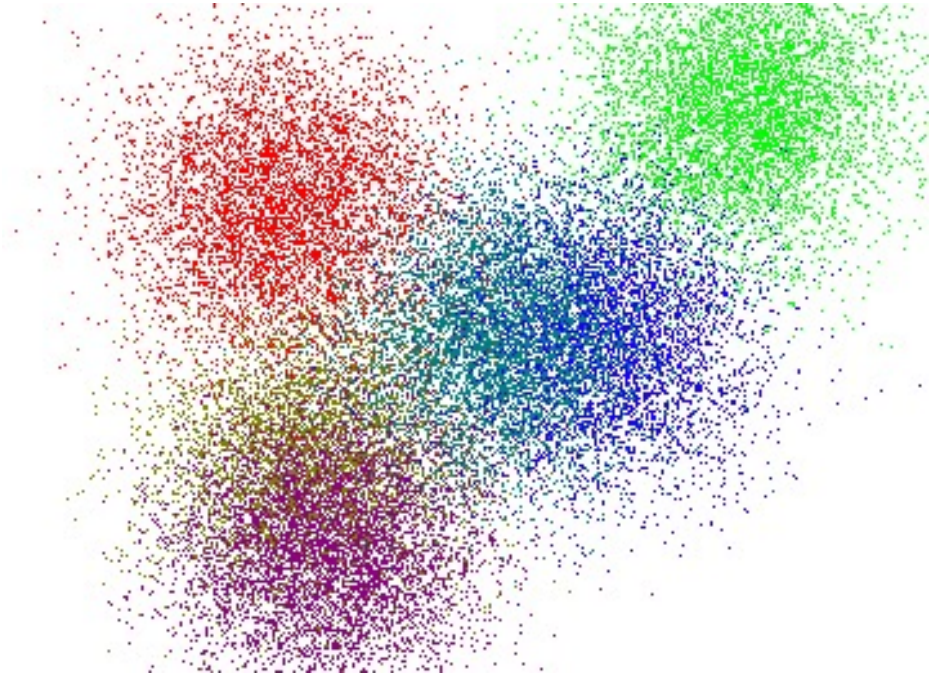
Training Data with class label:

Outlook	Temp	Humidity	Windy	Play Golf
Rainy	Hot	High	False	No
Rainy	Hot	High	True	No
Overcast	Hot	High	False	Yes
Sunny	Mild	High	False	Yes
Sunny	Cool	Normal	False	Yes
Sunny	Cool	Normal	True	No
Overcast	Cool	Normal	True	Yes
Rainy	Mild	High	False	No



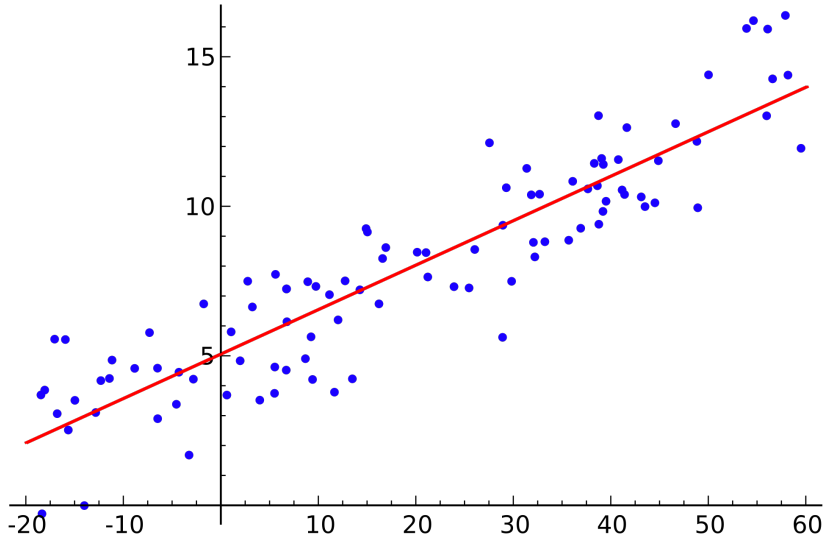
Supervised vs. Unsupervised Learning (2)

- Unsupervised learning (clustering)
  - The class labels of training data are **unknown**
  - Given a set of observations or measurements, establish the possible existence of classes or clusters in the data



Prediction Problems: Classification vs. Numeric Prediction

- Classification
  - Predict **categorical class labels** (discrete or nominal)
  - Construct a model based on the training set and the **class labels** (the values in a classifying attribute) and use it in classifying new data
- Numeric prediction
  - Model **continuous-valued functions** (i.e., predict unknown or missing values)



Prediction Problems: Classification vs. Numeric Prediction

- Typical applications of classification
  - Credit/loan approval
  - Medical diagnosis: if a tumor is cancerous or benign
  - Fraud detection: if a transaction is fraudulent
  - Web page categorization: which category it is

Classification—Model Construction, Validation and Testing

- **Model Construction and Training**
  - Model: Represented as decision trees, rules, mathematical formulas, or other forms
  - Assumption: Each sample belongs to a predefined class /**class label**
  - Training Set: The set of samples used for model construction

Classification—Model Construction, Validation and Testing

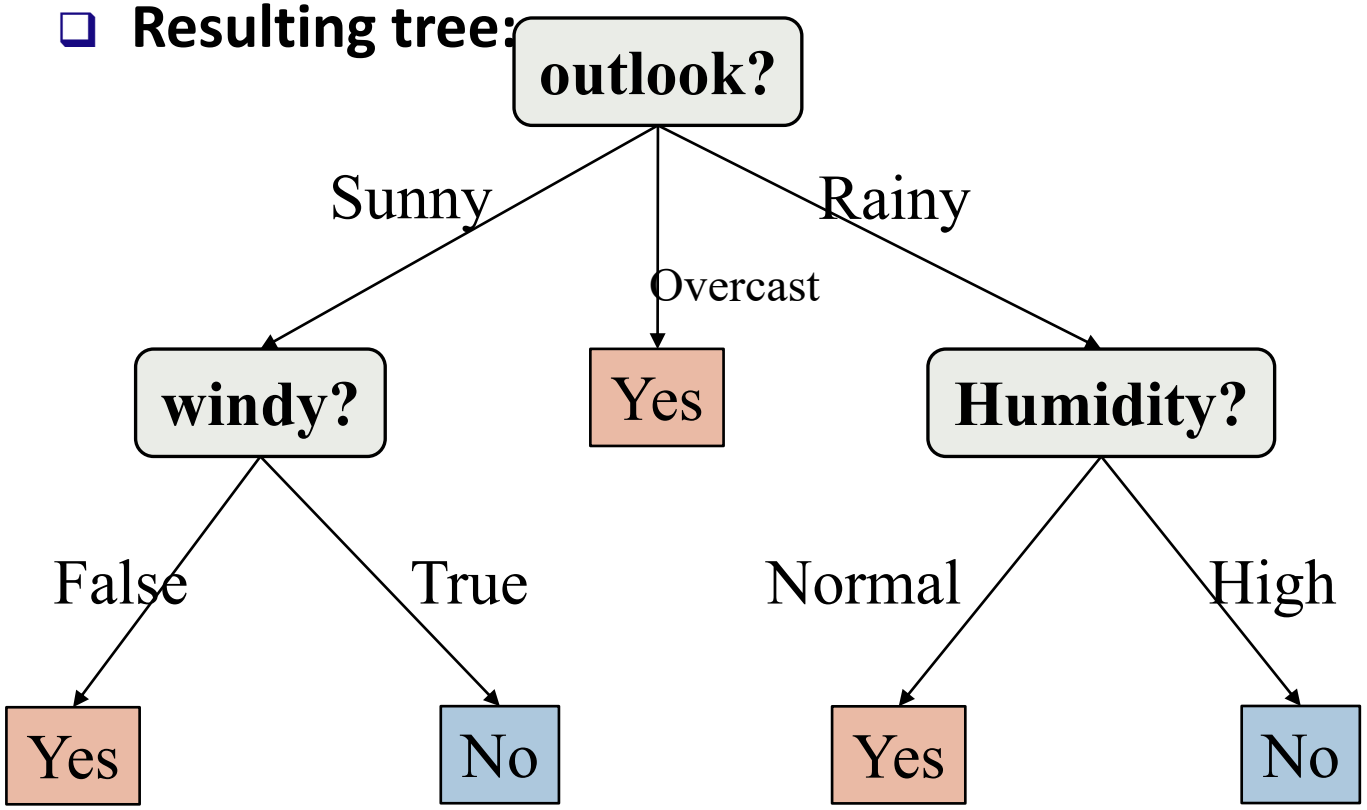
- **Model Validation and Testing**:
  - **Test:** Estimate accuracy of the model
    - The known label of test sample VS. the classified result from the model
    - *Accuracy:* % of test set samples that are correctly classified by the model
    - Test set is independent of training set
  - **Validation**: If *the test set* is used to select or refine models, it is called **validation** (or development) **(test) set**
- **Model Deployment:** If the accuracy is acceptable, use the model to classify new data

Chapter 8. Classification: Basic Concepts

- Classification: Basic Concepts
- Decision Tree Induction
- Bayes Classification Methods
- Linear Classifier
- Model Evaluation and Selection
- Imbalanced Data Sets
- Additional Concepts on Classification
- Summary

Decision Tree Induction: An Example

- **Decision tree construction**:
  - A top-down, recursive, divide-and-conquer process
- **Resulting tree:**



Training data set: Play Golf?

Outlook	Temp	Humidity	Windy	Play Golf
Rainy	Hot	High	False	No
Rainy	Hot	High	True	No
Overcast	Hot	High	False	Yes
Sunny	Mild	High	False	Yes
Sunny	Cool	Normal	False	Yes
Sunny	Cool	Normal	True	No
Overcast	Cool	Normal	True	Yes
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Rainy	Cool	Normal	False	Yes
Sunny	Mild	Normal	False	Yes
Rainy	Mild	Normal	True	Yes
Overcast	Mild	High	True	Yes
Overcast	Hot	Normal	False	Yes
Sunny	Mild	High	True	No

https://www.saedsayad.com/decision_tree.htm

Decision Tree Induction: Algorithm

- Basic algorithm
  - Tree is constructed in a **top-down, recursive, divide-and-conquer manner**
  - At start, all the training examples are at the root
  - Examples are partitioned recursively based on selected attributes
  - On each node, attributes are selected based on the training examples on that node, and a heuristic or statistical measure (e.g., **information gain, Gini index**)

Decision Tree Induction: Algorithm

- Conditions for stopping partitioning
  - All samples for a given node belong to the same class
  - There are no remaining attributes for further partitioning
  - There are no samples left
- Prediction
  - **Majority voting** is employed for classifying the leaf

How to Handle Continuous-Valued Attributes?

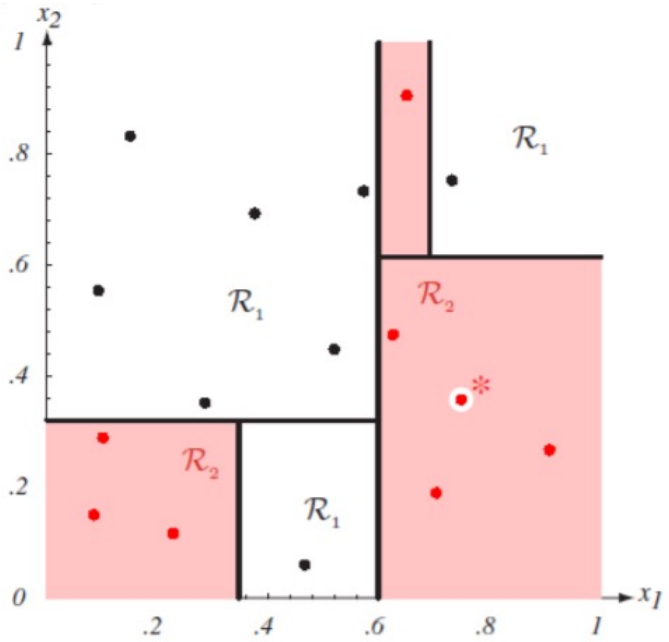
- Method 1: Discretize continuous values and treat them as categorical values
  - E.g., age: < 20, 20..30, 30..40, 40..50, > 50
- Method 2: Determine the ***best split point*** for continuous-valued attribute A
  - Sort:, e.g. 15, 18, 21, 22, 24, 25, 29, 31, …
  - *Possible split point:* $(a_i+a_{i+1})/2$
    - e.g., (15+18)/2 = 16.5, 19.5, 21.5, 23, 24.5, 27, 30, …
  - The point with the *maximum information gain* for A is selected as the **split-point** for A
- Split: Based on split point P
  - The set of tuples in D satisfying A ≤ P vs. those with A > P

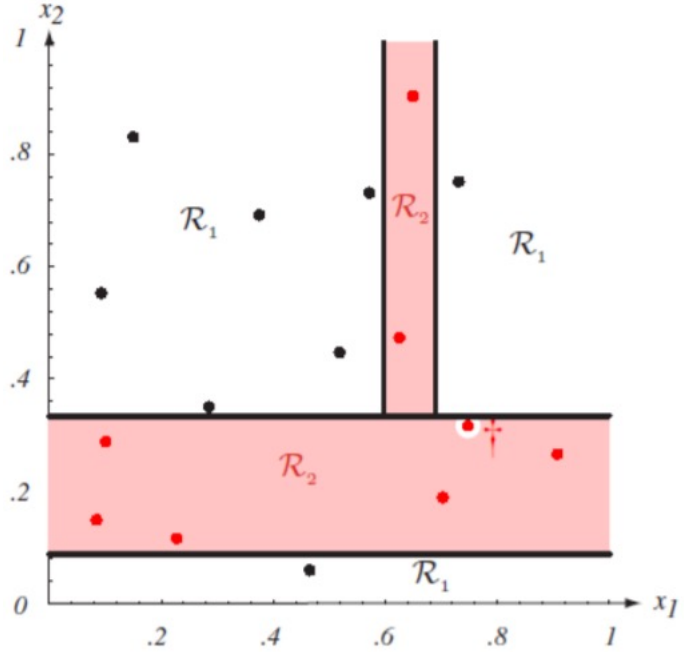
Pros and Cons

- Pros
  - Easy to explain (even for non-expert)
  - Easy to implement (many software)
  - Efficient
  - Can tolerate missing data
  - White box
  - No need to normalize data
  - Non-parametric: No assumption on data distribution, no assumption on attribute independency
  - Can work on various attribute types

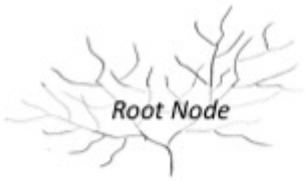
Pros and Cons

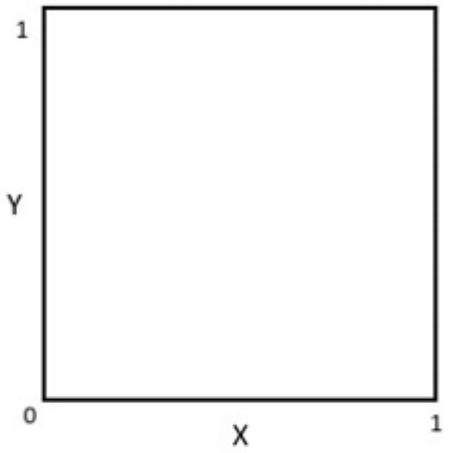
- Cons
  - Unstable. Sensitive to noise
  - Accuracy may be not good enough (depending on your data)
  - The optimal splitting is NP. Greedy algorithms are used
  - Overfitting





Overview





Example

Examples described by attribute values (Boolean, discrete, continuous, etc.)

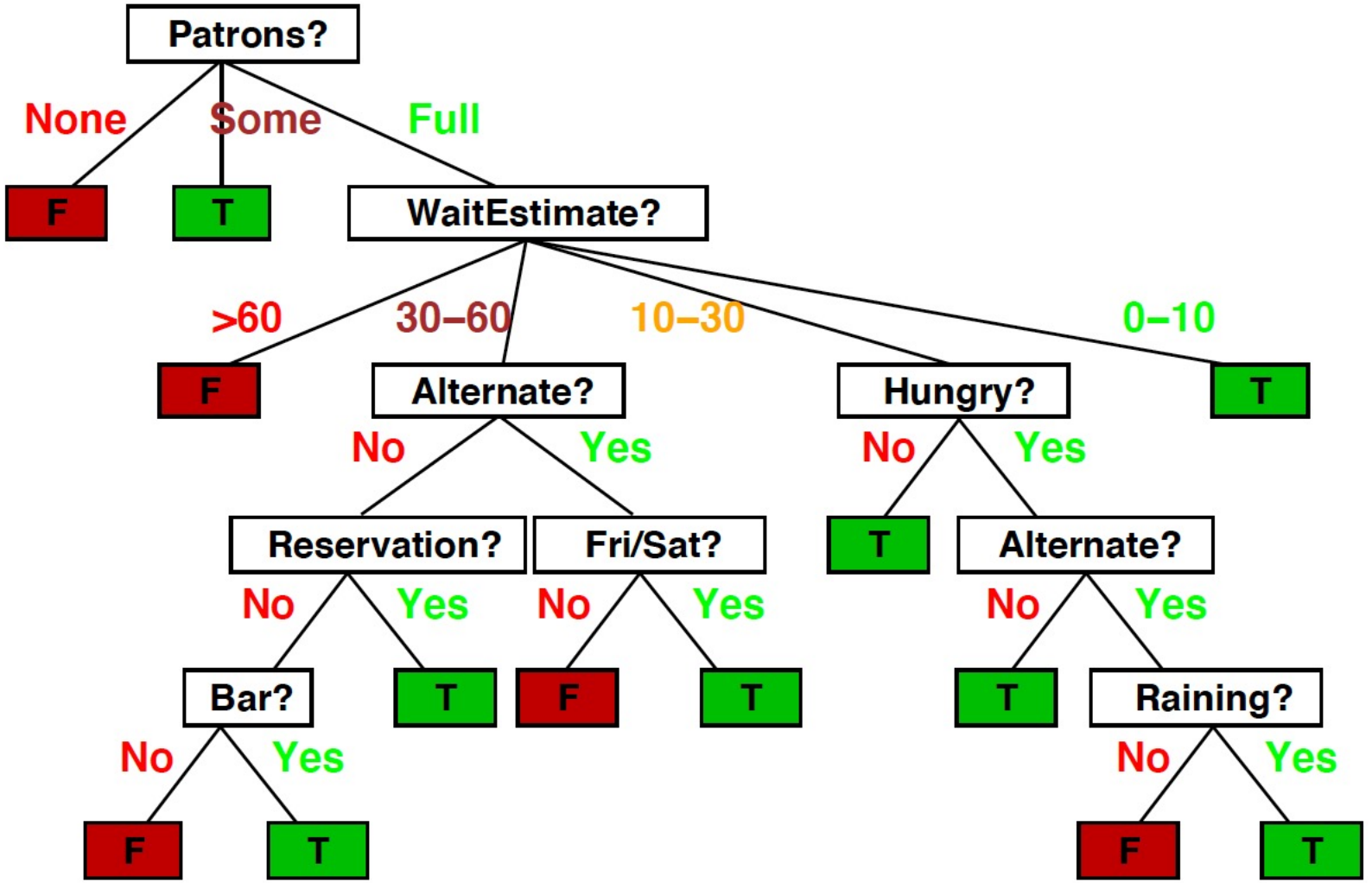
Example	*Attributes*										*Target*
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	WillWait
X_1	T	F	F	T	Some	$$$	F	T	French	0–10	T
X_2	T	F	F	T	Full	$	F	F	Thai	30–60	F
X_3	F	T	F	F	Some	$	F	F	Burger	0–10	T
X_4	T	F	T	T	Full	$	F	F	Thai	10–30	T
X_5	T	F	T	F	Full	$$$	F	T	French	>60	F
X_6	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

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

Example

- Problem: Decide whether to wait for a table at a restaurant, based on the following attributes:
  - Alternate: is there an alternative restaurant nearby?
  - Bar: is there a comfortable bar area to wait in?
  - Fri/Sat: is today Friday or Saturday?
  - Hungry: are we hungry?
  - Patrons: number of people in the restaurant (None, Some, Full)
  - Price: price range ($, $$, $$$)
  - Raining: is it raining outside?
  - Reservation: have we made a reservation?
  - Type: kind of restaurant (French, Italian, Thai, Burger)
  - WaitEstimate: estimated waiting time (0-10, 10-30, 30-60, $>$ 60)

Example: Decision Tree

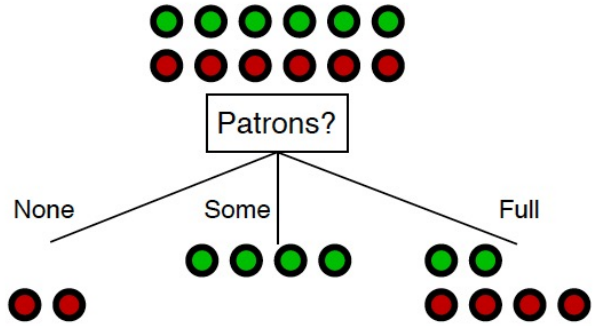


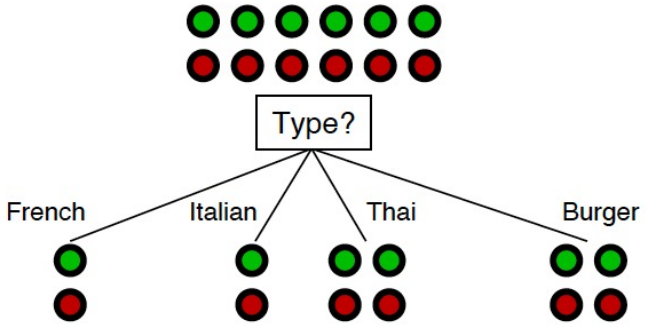
Example: Decision Tree Construction

Aim: Find a small tree consistent with the training examples

Recursively choose "most significant" attribute as root of (sub)tree

Good attribute splits the examples (ideally) into "pure" subsets





Patrons? is a better choice

—gives *information* about the classification

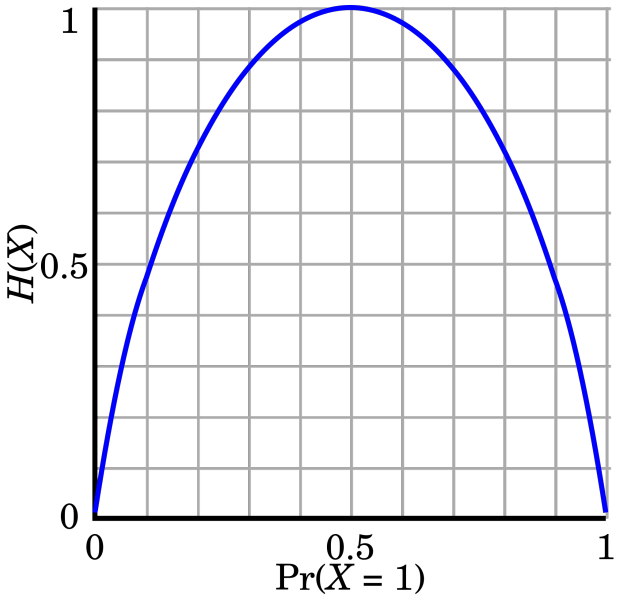
Splitting Measures: Information Gain

- Entropy (Information Theory)
  - A measure of uncertainty associated with a random number
  - Calculation: For a discrete random variable Y taking m distinct values $\{y_1, y_2, \ldots, y_m\}$

$$H(Y) = -\sum_{i=1}^{m} p_i \log(p_i) \quad where\ p_i = P(Y = y_i)$$

  - Interpretation
    - Higher entropy → higher uncertainty
    - Lower entropy → lower uncertainty
- Conditional entropy

$$H(Y|X) = \sum_{x} p(x) H(Y|X = x)$$



m = 2

Information Gain: An Attribute Selection Measure

- Select the attribute with the highest information gain (used in typical decision tree induction algorithm: ID3/C4.5)
- Let p_i be the probability that an arbitrary tuple in D belongs to class C_i, estimated by $|C_{i,D}|/|D|$
- Expected information (entropy) needed to classify a tuple in D:

$$Info(D) = -\sum_{i=1}^{m} p_i \log_2(p_i)$$

- Information needed (after using A to split D into v partitions) to classify D:

$$Info_A(D) = \sum_{j=1}^{v} \frac{|D_j|}{|D|} \times Info(D_j)$$

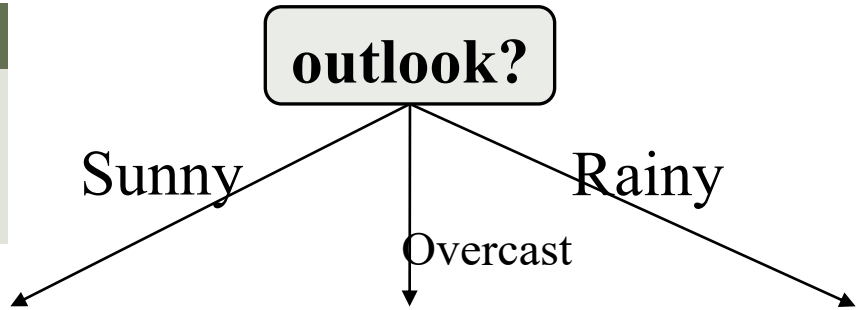
- Information gained by branching on attribute A

$$Gain(A) = Info(D) - Info_A(D)$$

Example: Attribute Selection with Information Gain

Outlook	Temp	Humidity	Windy	Play Golf
Rainy	Hot	High	False	No
Rainy	Hot	High	True	No
Overcast	Hot	High	False	Yes
Sunny	Mild	High	False	Yes
Sunny	Cool	Normal	False	Yes
Sunny	Cool	Normal	True	No
Overcast	Cool	Normal	True	Yes
Rainy	Mild	High	False	No
Rainy	Cool	Normal	False	Yes
Sunny	Mild	Normal	False	Yes
Rainy	Mild	Normal	True	Yes
Overcast	Mild	High	True	Yes
Overcast	Hot	Normal	False	Yes
Sunny	Mild	High	True	No

outlook	yes	no	I(yes, no)
rainy	2	3	0.971
overcast	4	0	0
sunny	3	2	0.971



$$Info(D) = I(9,5) = -\frac{9}{14}\log_2(\frac{9}{14}) - \frac{5}{14}\log_2(\frac{5}{14}) = 0.940$$

$$Info_{outlook}(D) = \frac{5}{14}I(2,3) + \frac{4}{14}I(4,0) + \frac{5}{14}I(3,2) = 0.694$$

$\frac{5}{14}I(2,3)$ means "outlook=rainy" has 5 out of 14 samples, with 2 yes'es and 3 no's. Hence $Gain(outlook) = Info(D) - Info_{outlook}(D) = 0.246$

Example: Attribute Selection with Information Gain

Outlook	Temp	Humidity	Windy	Play Golf
Rainy	Hot	High	False	No
Rainy	Hot	High	True	No
Overcast	Hot	High	False	Yes
Sunny	Mild	High	False	Yes
Sunny	Cool	Normal	False	Yes
Sunny	Cool	Normal	True	No
Overcast	Cool	Normal	True	Yes
Rainy	Mild	High	False	No
Rainy	Cool	Normal	False	Yes
Sunny	Mild	Normal	False	Yes
Rainy	Mild	Normal	True	Yes
Overcast	Mild	High	True	Yes
Overcast	Hot	Normal	False	Yes
Sunny	Mild	High	True	No

Temp	Yes	No	I(Yes, No)
Hot	2	2	?
Mild	4	2	?
Cool	3	1	?

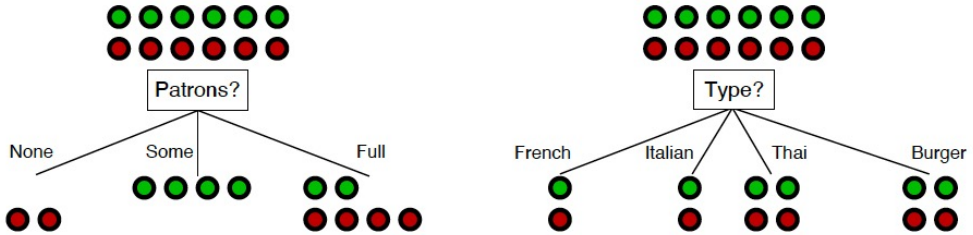
Windy	Yes	No	I(Yes, No)
True	?	?	?
False	?	?	?

Humidity	Yes	No	I(Yes, No)
Normal	6	1	?
High	3	4	?

Similarly, we can get

$$Gain(Temp) = 0.029,$$
$$Gain(humidity) = 0.151,$$
$$Gain(Windy) = 0.048$$

Example: Attribute Selection with Information Gain



- Patrons:
  - $H(X) = -6/12 \log_2 6/12 - 6/12 \log_2 6/12 = 1$
  - $H(X|None) = -0/2 \log_2 0/2 - 2/2 \log_2 2/2 = 0$
  - $H(X|Some) = -4/4 \log_2 4/4 - 0/4 \log_2 0/4 = 0$
  - $H(X|Full) = -2/6 \log_2 2/6 - 4/6 \log_2 4/6 = 0.9183$
  - $H(X) - H(X|Y) = 1 - 6/12(0.9183) = 0.5409$
- Type:
  - $H(X) = -6/12 \log_2 6/12 - 6/12 \log_2 6/12 = 1$
  - $H(X|French) = H(X|Italian) = -1/2 \log_2 1/2 - 1/2 \log_2 1/2 = 1$
  - $H(X|Thai) = H(X|Burger) = -2/4 \log_2 2/4 - 2/4 \log_2 2/4 = 1$
  - $H(X) - H(X|Y) = 1 - 2/12(1) - 2/12(1) - 4/12(1) - 4/12(1) = 0$
- Choose the attribute that maximizes information gain: Patrons?

Gain Ratio: A Refined Measure for Attribute Selection

- Information gain measure is biased towards attributes with a large number of values (e.g. ID)
- Gain ratio: Overcomes the problem (as a normalization to information gain)

$$SplitInfo_A(D) = -\sum_{j=1}^{v} \frac{|D_j|}{|D|} \times \log_2\left(\frac{|D_j|}{|D|}\right)$$

  - GainRatio(A) = Gain(A)/SplitInfo(A)
  - The attribute with the maximum gain ratio is selected as the splitting attribute
  - Gain ratio is used in a popular algorithm C4.5 (a successor of ID3) by R. Quinlan
- Example
  - $\text{SplitInfo}_{\text{temp}}(\text{D}) = -\frac{4}{14}\log_2\frac{4}{14} - \frac{6}{14}\log_2\frac{6}{14} - \frac{4}{14}\log_2\frac{4}{14} = 1.557$
  - GainRatio(temp) = 0.029/1.557 = 0.019

Another Measure: Gini Index

- Gini index (or Gini impurity): Used in CART, and also in IBM IntelligentMiner
- CART is a binary tree
- If a data set D contains examples from n classes, gini index, $gini(D)$ is defined as
  - $gini(D) = 1 - \sum_{j=1}^{n} p_j^2$
    - p_j is the relative frequency of class j in D
- What is the range of Gini index?
  - The minimum= 0, meaning pure
  - The maximum=? What is the case that Gini index reach the maximum?

Another Measure: Gini Index

- If a data set D is split on A into two subsets D_1 and D_2, the $gini$ index $gini(D)$ is defined as
  - $gini_A(D) = \frac{|D_1|}{|D|} gini(D_1) + \frac{|D_2|}{|D|} gini(D_2)$
- Reduction in Impurity:
  - $\Delta gini(A) = gini(D) - gini_A(D)$
- The attribute provides the smallest $gini_{split}(D)$ (or the largest reduction in impurity) is chosen to split the node (*For binary tree, need to enumerate all the possible splitting points for each attribute*)

Computation of Gini Index

- Example: D has 9 tuples in play_golf= “yes” and 5 in “no”

$$gini(D) = 1 - \left(\frac{9}{14}\right)^2 - \left(\frac{5}{14}\right)^2 = 0.459$$

- Suppose the attribute temp partitions D into 10 in D_1: {cool, mild} and 4 in D_2
  - $gini_{temp \in \{cool,mild\}}(D) = \frac{10}{14} gini(D_1) + \frac{4}{14} gini(D_2)$

$$= \frac{10}{14}\left(1 - \left(\frac{7}{10}\right)^2 - \left(\frac{3}{10}\right)^2\right) + \frac{4}{14}\left(1 - \left(\frac{2}{4}\right)^2 - \left(\frac{2}{4}\right)^2\right)$$

$$= 0.443$$

  - $Gini_{\{cool,hot\}}$ is 0.458; $Gini_{\{mild,hot\}}$ is 0.450
  - Thus, split on the {cool,mild} (and {hot}) since it has the lowest Gini index

Outlook	Temp	Humidity	Windy	Play Golf
Rainy	Hot	High	False	No
Rainy	Hot	High	True	No
Overcast	Hot	High	False	Yes
Sunny	Mild	High	False	Yes
Sunny	Cool	Normal	False	Yes
Sunny	Cool	Normal	True	No
Overcast	Cool	Normal	True	Yes
Rainy	Mild	High	False	No
Rainy	Cool	Normal	False	Yes
Sunny	Mild	Normal	False	Yes
Rainy	Mild	Normal	True	Yes
Overcast	Mild	High	True	Yes
Overcast	Hot	Normal	False	Yes
Sunny	Mild	High	True	No

Comparing Three Attribute Selection Measures

- The three measures, in general, return good results but
  - **Information gain**:
    - biased towards multivalued attributes
  - **Gain ratio**:
    - tends to prefer unbalanced splits in which one partition is much smaller than the others
  - **Gini index**:
    - biased to multivalued attributes
    - has difficulty when # of classes is large
    - tends to favor tests that result in equal-sized partitions and purity in both partitions

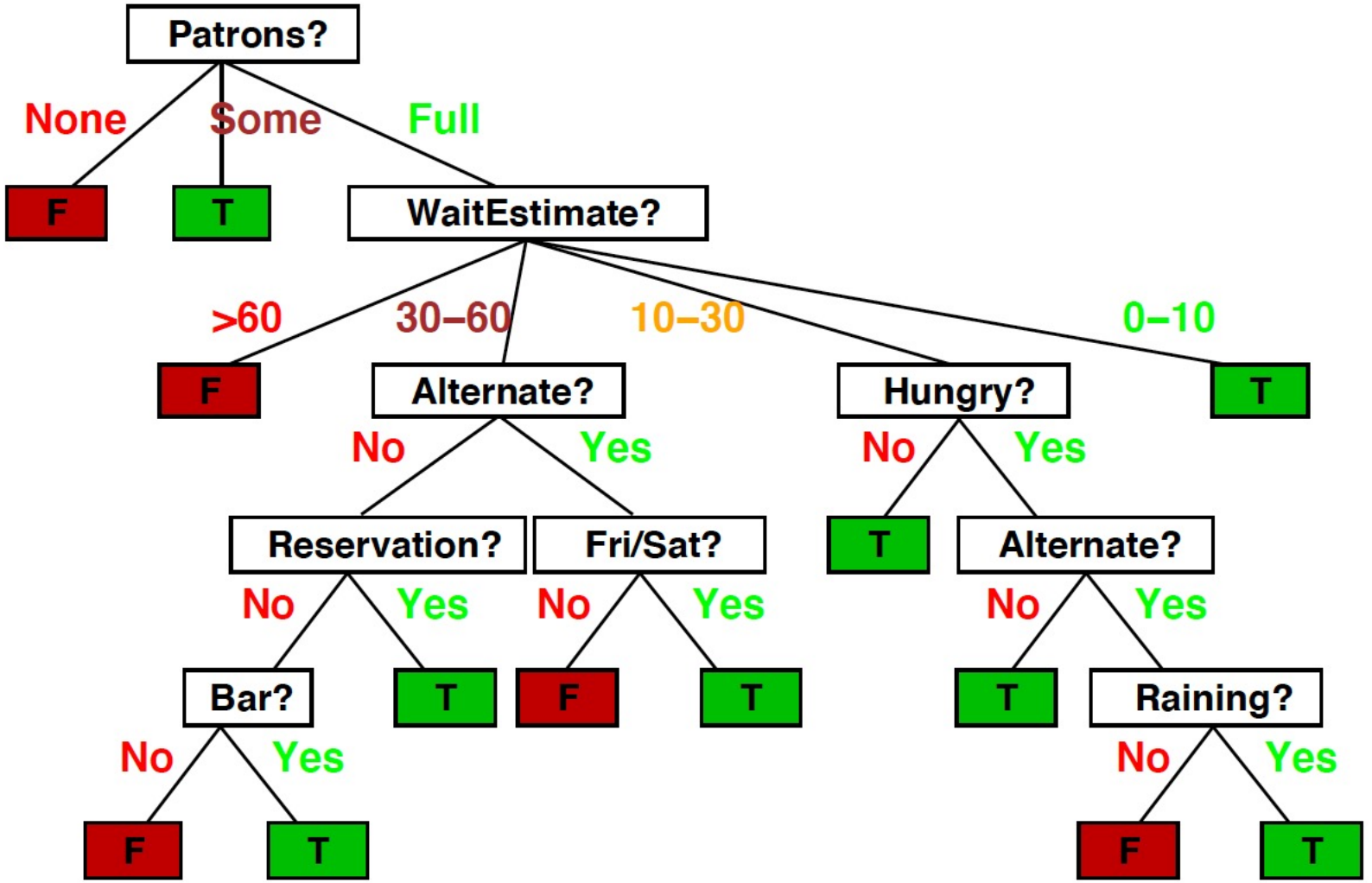
Comparing Three Attribute Selection Measures

- In reality
- Theoretical comparison between the gini index and information gain criteria
- It only matters in 2% of the cases.
- Entropy might be a little slower to compute (because of the logarithm).

Other Attribute Selection Measures

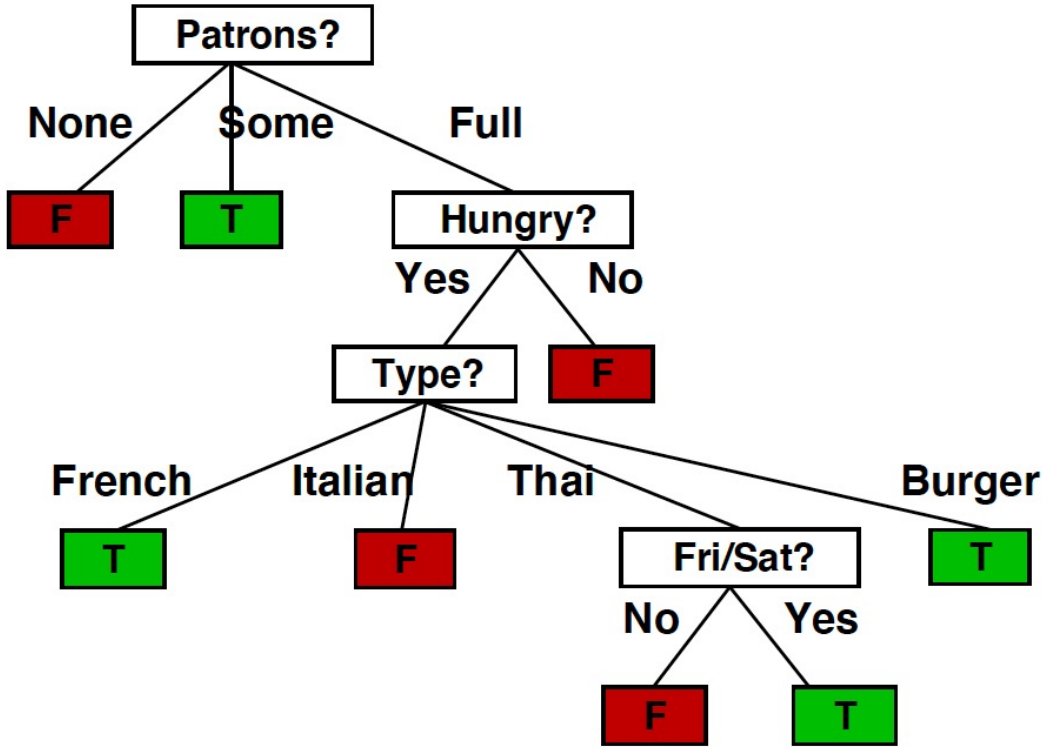
- Minimal Description Length (MDL) principle
  - Philosophy: The simplest solution is preferred
  - The best tree as the one that requires the fewest # of bits to both (1) encode the tree, and (2) encode the exceptions to the tree
- CHAID: a popular decision tree algorithm, measure based on χ^2 test for independence
- Multivariate splits (partition based on multiple variable combinations)
  - CART: finds multivariate splits based on a linear combination of attributes
- There are many other measures proposed in research and applications
  - E.g., G-statistics, C-SEP
- Which attribute selection measure is the best?
  - Most give good results, none is significantly superior than others

Example: Decision Tree



Example: Smaller Decision Tree

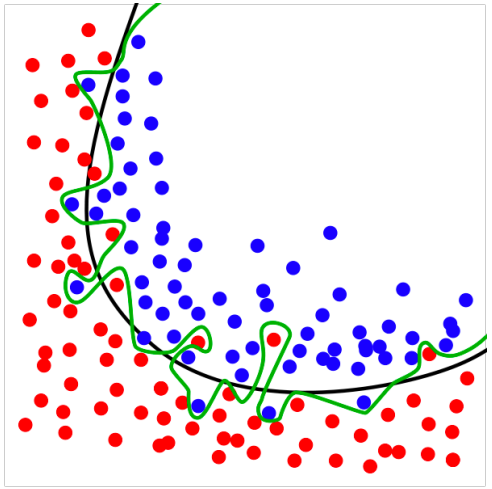
- Decision tree learned from the 12 examples:

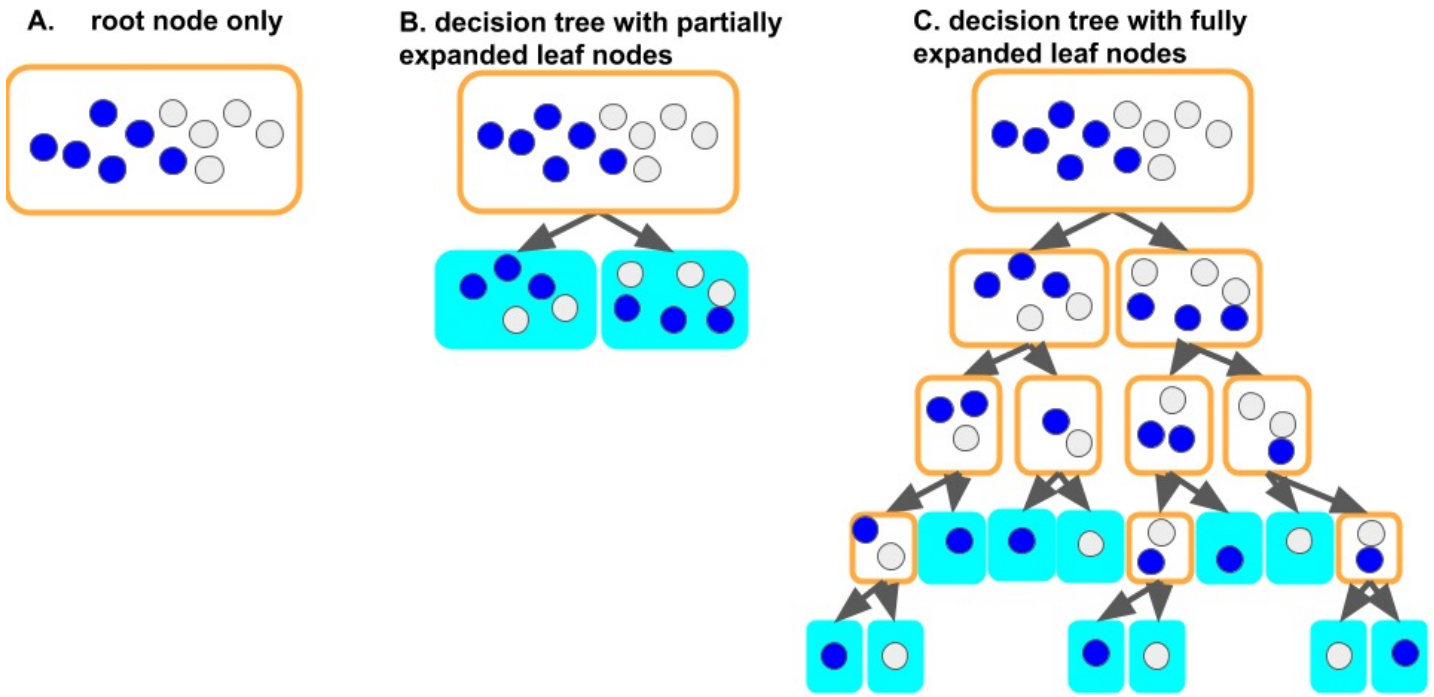


- Substantially simpler than "true" tree
  - More complex hypothesis is not justified by a small dataset

Overfitting and Tree Pruning

- Overfitting:
  - Too many branches, some may reflect anomalies due to noise or outliers
  - Poor accuracy for unseen samples





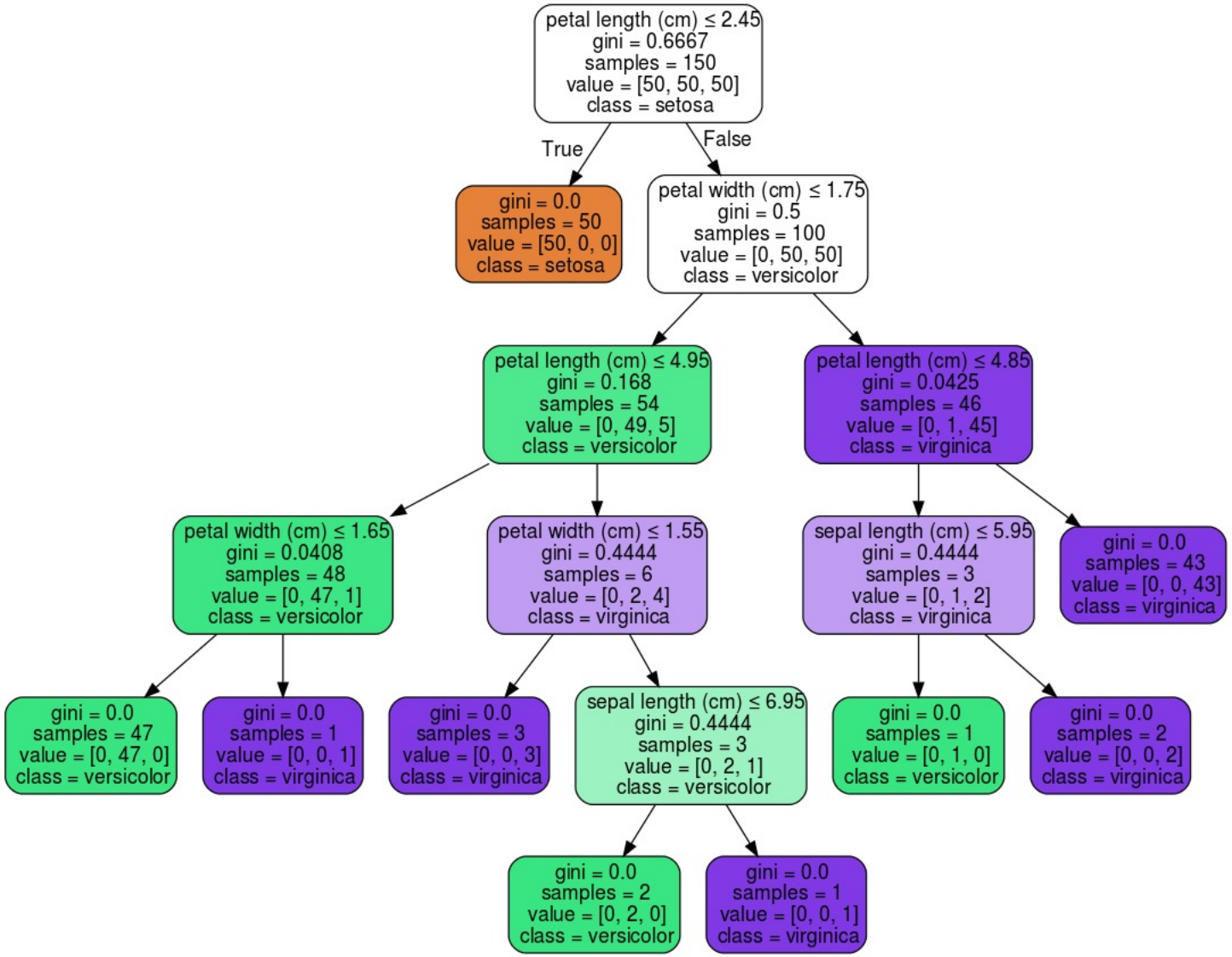
Overfitting and Tree Pruning

- Two approaches to avoid overfitting
  - Errors: use a cross-validation to compute
  - Pre-pruning (Early stop): Error does not decrease *significantly* -> stop splitting
    - Efficient but prone to under-fit (stop too early)
  - Post-pruning: After the full tree is constructed, prune back to the point where the cross-validation error is minimum
    - Extra computations but mathematically rigorous
  - Can be used alone, in combination, or not at all
    - For different purposes (accuracy, efficiency, interpretability)

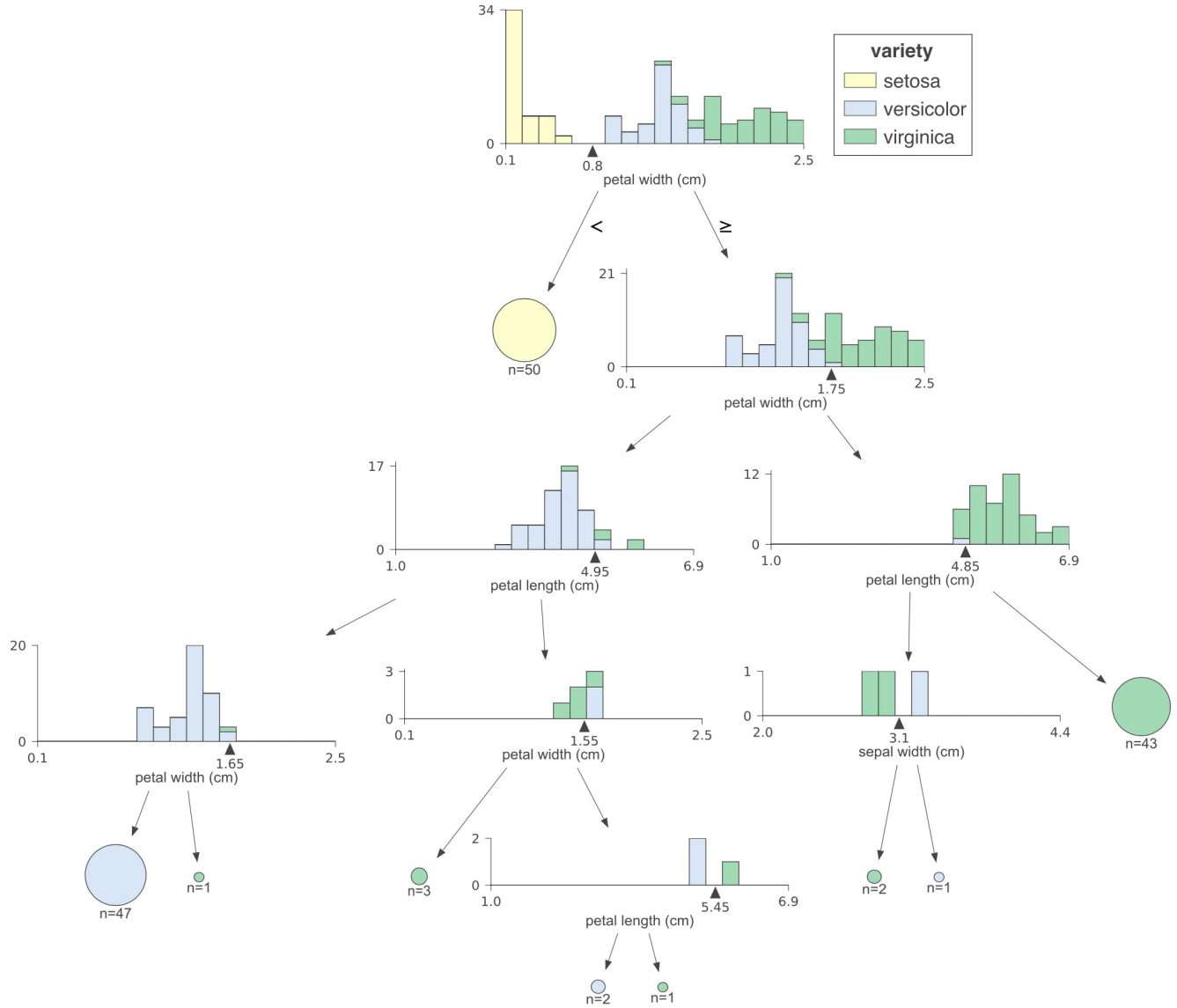
Classification in Large Databases

- Scalability: Classifying data sets with **millions** of examples and hundreds of attributes with **reasonable speed**
- Why is decision tree induction popular?
  - Relatively fast learning speed
  - Convertible to simple and easy to understand classification rules
  - Easy to be adapted to database system implementations (e.g., using SQL)
  - Comparable classification accuracy with other methods
  - Easy to ensemble, i.e., random forests, xgboost

Visualization of a Decision Tree (in scikit-learn)



Visualization of a Decision Tree



Chapter 8. Classification: Basic Concepts

- Classification: Basic Concepts
- Decision Tree Induction
- Bayes Classification Methods
- Linear Classifier
- Model Evaluation and Selection
- Lazy Learning
- Ensemble Methods
- Imbalanced Data Sets
- Summary

Bayes' Theorem: Basics

- Total probability Theorem:

$$p(B) = \sum_i p(B|A_i)p(A_i)$$

- Bayes' Theorem:

$$p(H|\mathbf{X}) = \frac{p(\mathbf{X}|H)P(H)}{p(\mathbf{X})} \propto p(\mathbf{X}|H)\,P(H)$$

posteriori probability — What we should choose

likelihood — What we just see

prior probability — What we knew previously

- **X:** a data sample ("*evidence*")
- H: X belongs to class C

Prediction can be done based on Bayes' Theorem:

Classification is to derive the maximum posteriori

Bayes' Theorem Example 1: Cancer Tests

	Cancer (1%)	No Cancer (99%)
Test Pos	80%	9.6%
Test Neg	20%	90.4%

- Only 1% people have cancer
- How accurate is the test?
  - 80%? 99%? 1%?

	Cancer (1%)	No Cancer (99%)
Test Pos	True Pos 1% x 80% = .008	False Pos 99% x 9.6% = .09504
Test Neg	False Neg 1% x 20% = .002	True Neg 99% x 90.4% = .89496

- $P(X,H) = P(X|H)P(H)$
- Chance of true positive is thus

1%*80% = 0.008

- According to Bayes' Theorem, $P(H|X) = P(X|H)P(H)/P(X)$, the chance of having a cancer given positive test results is

True pos / (True pos + False pos) = 0.008 / (0.008+0.09504) = 7.76%

- The Theorem lets us correct for the skewness introduced by false positives

Bayes' Theorem Example 2: Picnic Day

- The morning is cloudy ☹
- What is the chance of rain? P(Rain | Cloud) = ?
- 50% of all rainy days start off cloudy. P(Cloud | Rain) = 50%
- Cloudy mornings are common (40% of days start cloudy) P(Cloud) = 40%
- This is usually a dry month (only 3 of 30 days tend to be rainy) P(Rain) = 10%

P(Rain | Cloud) = P(Rain) P(Cloud | Rain) / P(Cloud) = 10% * 50% / 40% = 12.5%

- Again, the chance of rain is probably not as high as expected ☺
- Bayes' Theorem allows us to tell back and forth between posterior and likelihood

(*e.g.*, P(Rain | Cloud) and P(Cloud | Rain)), tests and reality, which is the most important trick in Bayesian Inference

Bayes' Theorem: Multiple Steps

- Usually more than one hypothesis: H_1, H_2, …, H_m

$$p(H_i|X) = \frac{p(X|H_i)p(H_i)}{p(X)}$$

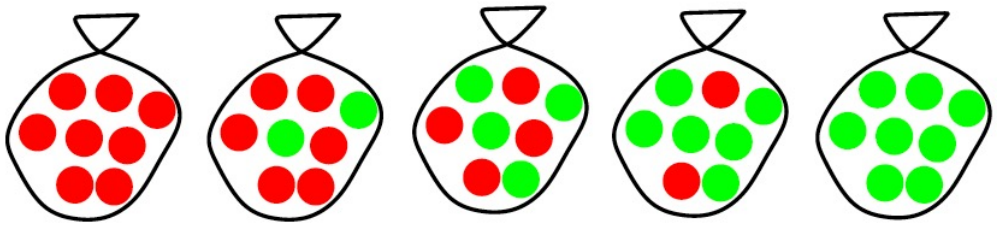
- Observations (evidence) over multiple steps: X_1, X_2,…,X_T

$$p(H_i|X_1) = \frac{p(X_1|H_i)p(H_i)}{p(X_1)}$$

Example: Bayes' Theorem, Multiple Steps

Suppose there are five kinds of bags of candies:

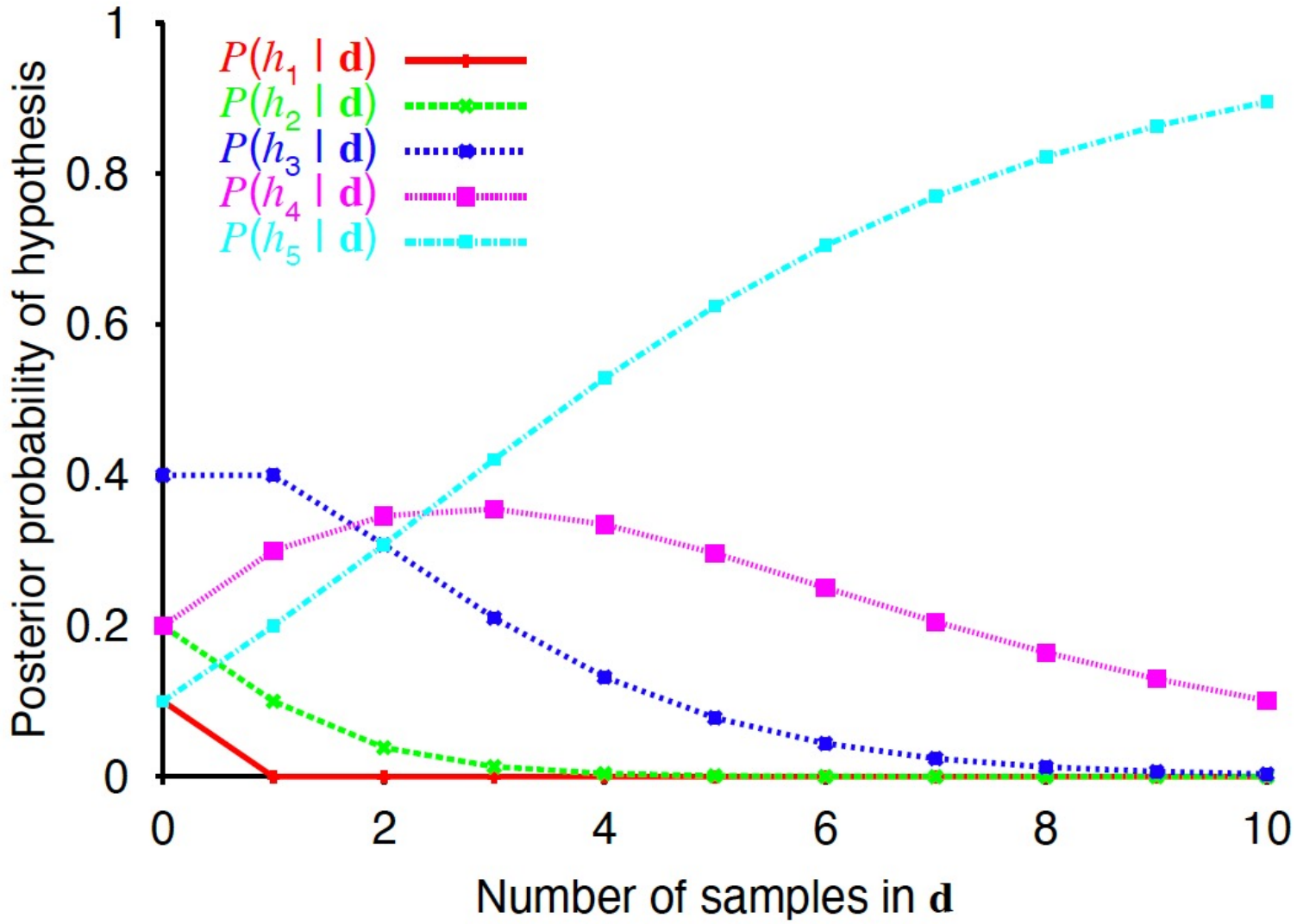
- 10% are h_1: 100% cherry candies
- 20% are h_2: 75% cherry candies + 25% lime candies
- 40% are h_3: 50% cherry candies + 50% lime candies
- 20% are h_4: 25% cherry candies + 75% lime candies
- 10% are h_5: 100% lime candies



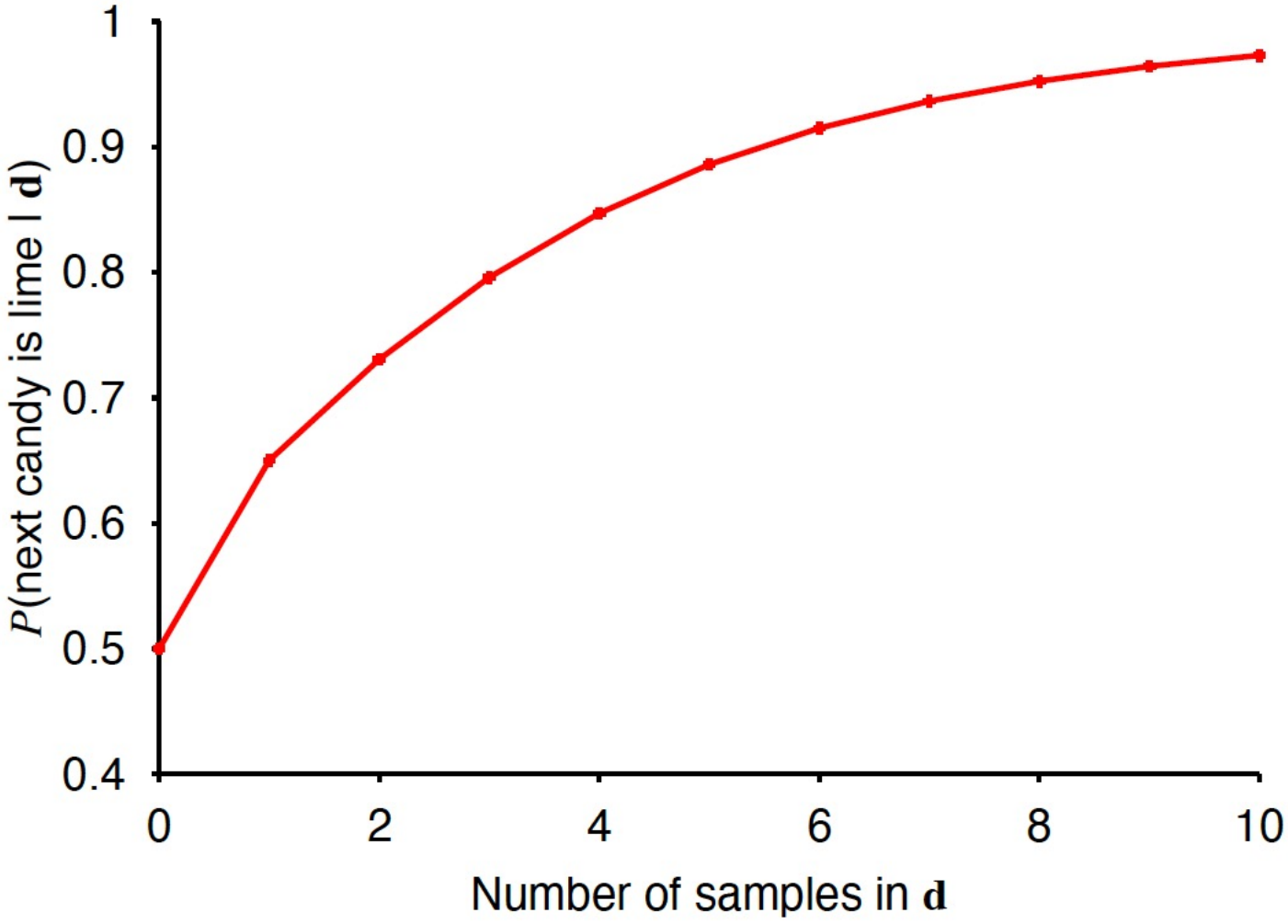
Then we observe candies drawn from some bag:

What kind of bag is it? What flavor will the next candy be?

Example: Bayes' Theorem, Multiple Steps



Example: Bayes' Theorem, Multiple Steps



Naïve Bayes Classifier: Making a Naïve Assumption

- Based on the Bayes' Theorem, we can derive a Bayes Classifier to compute the posterior probability of classifying an object X to a class C
  - $P(C|X) \propto P(X|C)P(C) = P(x1|C)P(x2|x1,C)...P(xn|x1,...,C)P(C)$
- A naïve assumption to simplify the complex dependencies: *features are conditionally independent!*
  - $P(C|X) \propto P(X|C)P(C) \approx P(x1|C)P(x2|C)...P(xn|C)P(C)$
- Super efficient: each feature only conditions on the class (boils down to sample counting)
- Achieves surprisingly comparable performance

Naïve Bayes Classifier: Categorical vs. Continuous Valued Features

- If feature x_k is categorical, $p(x_k = v_k|C_i)$ is the # of tuples in C_i with $x_k = v_k$, divided by $|C_{i,D}|$ (# of tuples of C_i in D)

$$p(X|C_i) = \prod_k p(x_k|C_i) = p(x_1|C_i) \cdot p(x_2|C_i) \cdots\cdots p(x_n|C_i)$$

- If feature x_k is continuous-valued, $p(x_k = v_k|C_i)$ is usually computed based on Gaussian distribution with a mean μ and standard deviation σ

$$p(x_k = v_k|C_i) = N\left(x_k|\mu_{C_i}, \sigma_{C_i}\right) = \frac{1}{\sqrt{2\pi}\sigma_{C_i}} e^{-\frac{\left(x-\mu_{C_i}\right)^2}{2\sigma^2}}$$

Naïve Bayes Classifier Example 1: Training Dataset

Class:
play golf= ‘yes’
play golf = ‘no’

Outlook	Temp	Humidity	Windy	Play Golf
Rainy	Hot	High	False	No
Rainy	Hot	High	True	No
Overcast	Hot	High	False	Yes
Sunny	Mild	High	False	Yes
Sunny	Cool	Normal	False	Yes
Sunny	Cool	Normal	True	No
Overcast	Cool	Normal	True	Yes
Rainy	Mild	High	False	No
Rainy	Cool	Normal	False	Yes
Sunny	Mild	Normal	False	Yes
Rainy	Mild	Normal	True	Yes
Overcast	Mild	High	True	Yes
Overcast	Hot	Normal	False	Yes
Sunny	Mild	High	True	No

Naïve Bayes Classifier Example *P(Yes / Sunny)*

$$P(x \mid c) = P(Sunny \mid Yes) = 3/9 = 0.33$$

Frequency Table		Play Golf	
		Yes	No
Outlook	Sunny	3	2
	Overcast	4	0
	Rainy	2	3

Likelihood Table		Play Golf		
		Yes	No	
Outlook	Sunny	3/9	2/5	5/14
	Overcast	4/9	0/5	4/14
	Rainy	2/9	3/5	5/14
		9/14	5/14	

$$P(x) = P(Sunny) = 5/14 = 0.36$$

$$P(c) = P(Yes) = 9/14 = 0.64$$

Posterior Probability:

$$P(c \mid x) = P(Yes \mid Sunny) = 0.33 \times 0.64 \div 0.36 = 0.60$$

Naïve Bayes Classifier Example: P(No | Sunny)

Frequency Table		Play Golf	
		Yes	No
Outlook	Sunny	3	2
	Overcast	4	0
	Rainy	2	3

$$P(x \mid c) = P(Sunny \mid No) = 2/5 = 0.4$$

		Play Golf		
		Yes	No	
Outlook	Sunny	3	2	5
	Overcast	4	0	4
	Rainy	2	3	5
		9	5	14

$$P(x) = P(Sunny) = 5/14 = 0.36$$

$$P(c) = P(No) = 5/14 = 0.36$$

Posterior Probability:

$$P(c \mid x) = P(No \mid Sunny) = 0.40 \times 0.36 \div 0.36 = 0.40$$

Naïve Bayes Classifier Example: Likelihood Tables

Frequency Table

		Play Golf	
		Yes	No
Outlook	Sunny	3	2
	Overcast	4	0
	Rainy	2	3

		Play Golf	
		Yes	No
Humidity	High	3	4
	Normal	6	1

		Play Golf	
		Yes	No
Temp.	Hot	2	2
	Mild	4	2
	Cool	3	1

		Play Golf	
		Yes	No
Windy	False	6	2
	True	3	3

Likelihood Table

		Play Golf	
		Yes	No
Outlook	Sunny	3/9	2/5
	Overcast	4/9	0/5
	Rainy	2/9	3/5

		Play Golf	
		Yes	No
Humidity	High	3/9	4/5
	Normal	6/9	1/5

		Play Golf	
		Yes	No
Temp.	Hot	2/9	2/5
	Mild	4/9	2/5
	Cool	3/9	1/5

		Play Golf	
		Yes	No
Windy	False	6/9	2/5
	True	3/9	3/5

Naïve Bayes Classifier Example: Likelihood Tables

Outlook	Temp	Humidity	Windy	Play
Rainy	Cool	High	True	?

$$P(Yes \mid X) = P(Rainy \mid Yes) \times P(Cool \mid Yes) \times P(High \mid Yes) \times P(True \mid Yes) \times P(Yes)$$

$$P(Yes \mid X) = 2/9 \times 3/9 \times 3/9 \times 3/9 \times 9/14 = 0.00529 \rightarrow 0.2 = \frac{0.00529}{0.02057 + 0.00529}$$

$$P(No \mid X) = P(Rainy \mid No) \times P(Cool \mid No) \times P(High \mid No) \times P(True \mid No) \times P(No)$$

$$P(No \mid X) = 3/5 \times 1/5 \times 4/5 \times 3/5 \times 5/14 = 0.02057 \rightarrow 0.8 = \frac{0.02057}{0.02057 + 0.00529}$$

Naïve Bayes Classifier: Example 2

Class:
C1:buys_computer = ‘yes’
C2:buys_computer = ‘no’

Data to be classified:
X = (age <=30, Income = medium,
Student = yes, Credit_rating = Fair)

age	income	student	credit_rating	buys_computer
<=30	high	no	fair	no
<=30	high	no	excellent	no
31..40	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
31..40	low	yes	excellent	yes
<=30	medium	no	fair	no
<=30	low	yes	fair	yes
>40	medium	yes	fair	yes
<=30	medium	yes	excellent	yes
31..40	medium	no	excellent	yes
31..40	high	yes	fair	yes
>40	medium	no	excellent	no

Naïve Bayes Classifier: Example 2

Compute $P(X|C_i)$ for each class:

P(age = "<=30" | buys_computer = "yes") = 2/9 = 0.222

P(age = "<= 30" | buys_computer = "no") = 3/5 = 0.6

P(income = "medium" | buys_computer = "yes") = 4/9 = 0.444

P(income = "medium" | buys_computer = "no") = 2/5 = 0.4

P(student = "yes" | buys_computer = "yes") = 6/9 = 0.667

P(student = "yes" | buys_computer = "no") = 1/5 = 0.2

P(credit_rating = "fair" | buys_computer = "yes") = 6/9 = 0.667

P(credit_rating = "fair" | buys_computer = "no") = 2/5 = 0.4

age	income	student	credit_rating	buys_computer
<=30	high	no	fair	no
<=30	high	no	excellent	no
31..40	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
31..40	low	yes	excellent	yes
<=30	medium	no	fair	no
<=30	low	yes	fair	yes
>40	medium	yes	fair	yes
<=30	medium	yes	excellent	yes
31..40	medium	no	excellent	yes
31..40	high	yes	fair	yes
>40	medium	no	excellent	no

Naïve Bayes Classifier: Example 2

X = (age <= 30 , income = medium, student = yes, credit_rating = fair)

$P(X|C_i)$:

P(X|buys_computer = "yes") =

P(age = "<=30"|buys_computer = "yes")

P(income = "medium" | buys_computer = "yes")

P(student = "yes" | buys_computer = "yes)

P(credit_rating = "fair" | buys_computer = "yes")

= 0.222 x 0.444 x 0.667 x 0.667 = 0.044

P(X|buys_computer = "no") =

P(age = "<= 30"|buys_computer = "no")

P(income = "medium" | buys_computer = "no")

P(student = "yes" | buys_computer = "no")

P(credit_rating = "fair" | buys_computer = "no")

= 0.6 x 0.4 x 0.2 x 0.4 = 0.019

$P(X\|C_i)$	C1 = yes	C2 = no
age <= 30	0.222	0.6
Inc. = med.	0.444	0.4
Stu. = yes	0.667	0.2
Credit = fair	0.667	0.4

Conditional probability

$P(X|C_i)*P(C_i)$:

P(X|buys_computer = "yes") * P(buys_computer = "yes") = 0.028

P(X|buys_computer = "no") * P(buys_computer = "no") = 0.007

Therefore, X is classified to class ("buys_computer = yes")

Avoiding the Zero-Probability Problem

- Naïve Bayesian prediction requires each conditional probability be **non-zero**
  - Otherwise, the predicted probability will be zero

$$\mathrm{p}(\mathrm{X}|C_i) = \prod_k p(x_k|C_i) = p(x_1|C_i) \cdot p(x_2|C_i) \cdots\cdots p(x_n|C_i)$$

- Example. Suppose a dataset with 1000 tuples:

  income = low (0), income= medium (990), and income = high (10)

- Use **Laplacian correction** (or Laplacian estimator)
  - *Adding 1 to each case*

    Prob(income = low) = 1/(1000 + 3)

    Prob(income = medium) = (990 + 1)/(1000 + 3)

    Prob(income = high) = (10 + 1)/(1000 + 3)

$$\hat{P}(w_i \mid c) = \frac{count(w_i,c)+1}{\sum_{w \in V}\left(count(w,c)+1\right)}$$

$$= \frac{count(w_i,c)+1}{\left(\sum_{w \in V} count(w,c)\right) + |V|}$$

  - The "corrected" probability estimates are close to their "uncorrected" counterparts

Naïve Bayes Classifier: Strength vs. Weakness

- Strength
  - Performance: A *naïve Bayesian classifier*, has comparable performance with decision tree and selected neural network classifiers
  - Incremental: Each training example can incrementally increase/decrease the probability that a hypothesis is correct—prior knowledge can be combined with observed data

Naïve Bayes Classifier: Strength vs. Weakness

- Weakness
  - Assumption: attributes conditional independence, therefore loss of accuracy
    - E.g., Patient's Profile: (age, family history),
    - Patient's Symptoms: (fever, cough),
    - Patient's Disease: (lung cancer, diabetes).
    - Dependencies among these cannot be modeled by Naïve Bayes Classifier
  - How to deal with these dependencies?

    Use Bayesian Belief Networks (to be covered in the next chapter)

Chapter 8. Classification: Basic Concepts

- Classification: Basic Concepts
- Decision Tree Induction
- Bayes Classification Methods
- Linear Classifier
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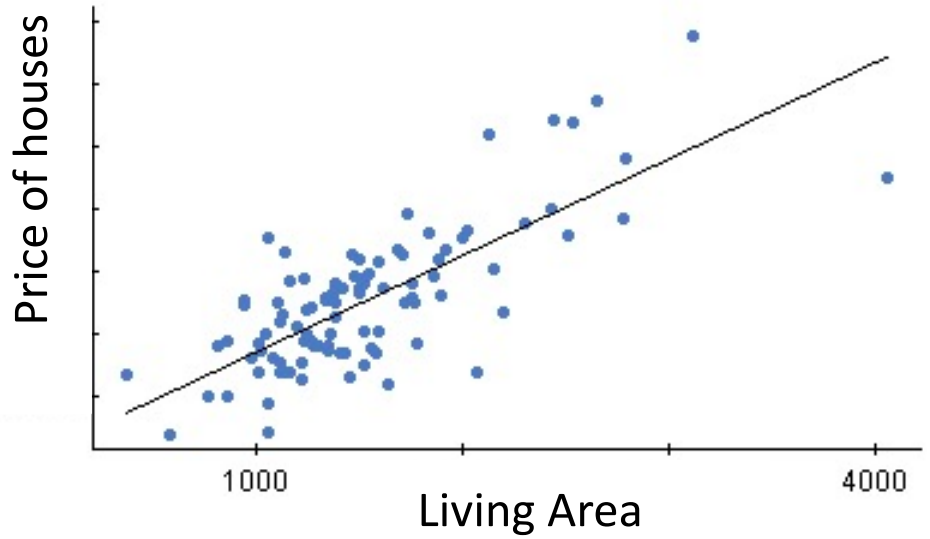
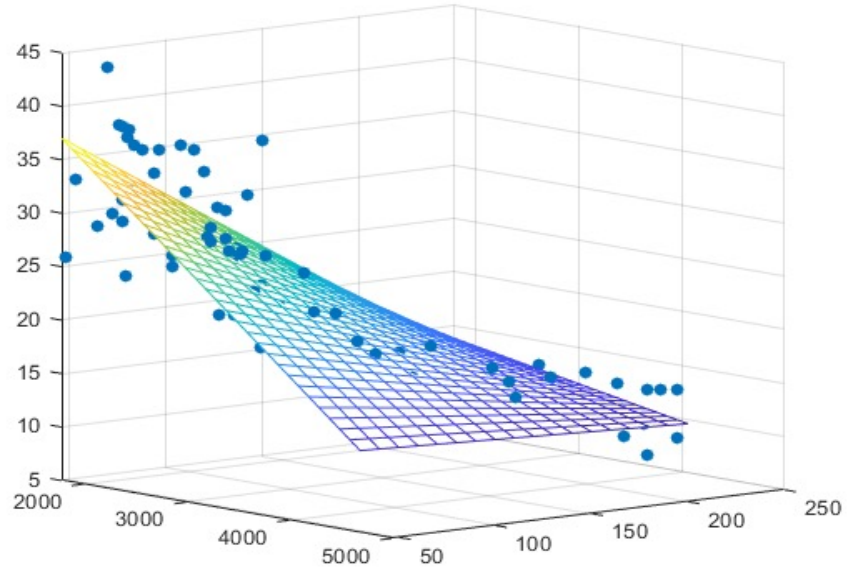
Linear Regression Problem: Example

- Mapping from independent attributes to **continuous value**: x => y
- {living area} => Price of the house
- {college; major; GPA} => Future Income





Linear Regression Problem: Model

- Linear regression
  - Data: n independent objects
    - Observed Value: $y_i, i = 1,2,3, \cdots, n$
    - p-dimensional attributes: $x_i = \left(x_{i1}, x_{i2}, \cdots, x_{ip}\right)^T,\ i = 1,2,3 \cdots, n$
  - Model:
    - Weight vector: $w = \left(w_1, w_2, \cdots, w_p\right)$
    - $y_i = w^T x_i + b$
  - The weight vector w and bias b is the model parameter learnt by data

Linear Regression Model: Solution

- Least Square Method
  - Cost / Loss Function: $\mathrm{L}(w,b) = \Sigma_{i=1}^{m}(y_i - wx_i - b)^2$
  - Optimization Goal: $\underset{(w,b)}{\operatorname{argmin}}\ \mathrm{L}(w,b) = \Sigma_{i=1}^{m}(y_i - wx_i - b)^2$
  - Closed-form solution:
    - $w = \frac{\Sigma_{i=1}^{m} x_i(y_i - \bar{y})}{\Sigma_{i=1}^{m} x_i^2 - 1/m\left(\Sigma_{i=1}^{m} x_i\right)^2}$ $\qquad b = \frac{1}{m}\Sigma_{i=1}^{m}(y_i - wx_i)$

Linear Classification: Perceptron

- Linear classifiers with weight vector $\mathbf{w}$
- Prediction on $\mathbf{x}_i$ is incorrect if $y_i \mathbf{w}^T \mathbf{x}_i < 0$.
- Let $\mathcal{M}(\mathbf{w})$ be the set of points on which prediction is incorrect
- The objective function to be minimized

$$E(\mathbf{w}) = -\sum_{i \in \mathcal{M}(\mathbf{w})} y_i \mathbf{w}^T \mathbf{x}_i$$

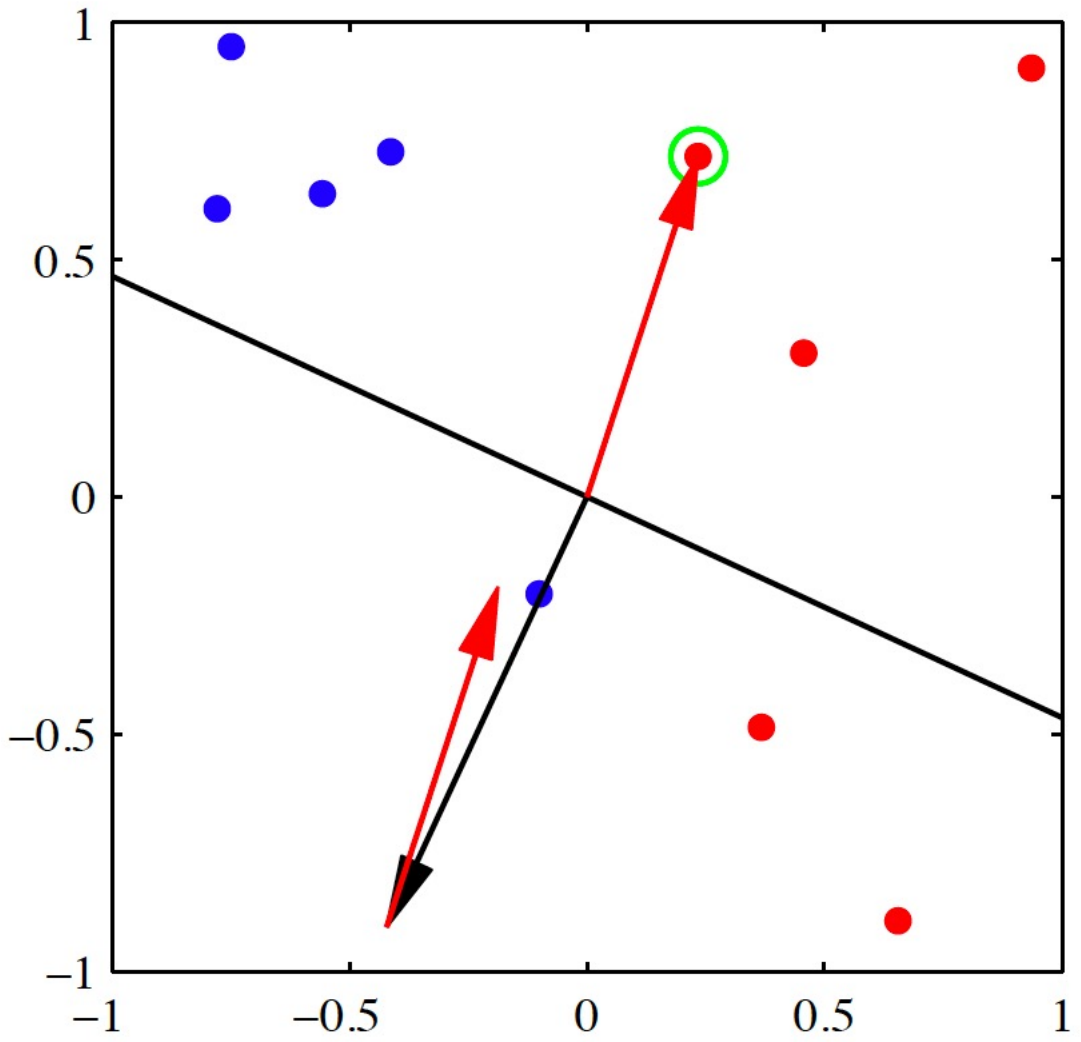
- Algorithm goes through all the points sequentially
  - If prediction is correct, do not change anything
  - If prediction is wrong, and $y_i = +1$ then $\mathbf{w}^{(new)} = \mathbf{w}^{(old)} + \mathbf{x}_i$
  - If prediction is wrong, and $y_i = -1$ then $\mathbf{w}^{(new)} = \mathbf{w}^{(old)} - \mathbf{x}_i$

- For any point $i \in \mathcal{M}(\mathbf{w})$, gradient $\nabla E_i(\mathbf{w}) = -y_i \mathbf{x}_i$
- The gradient based update

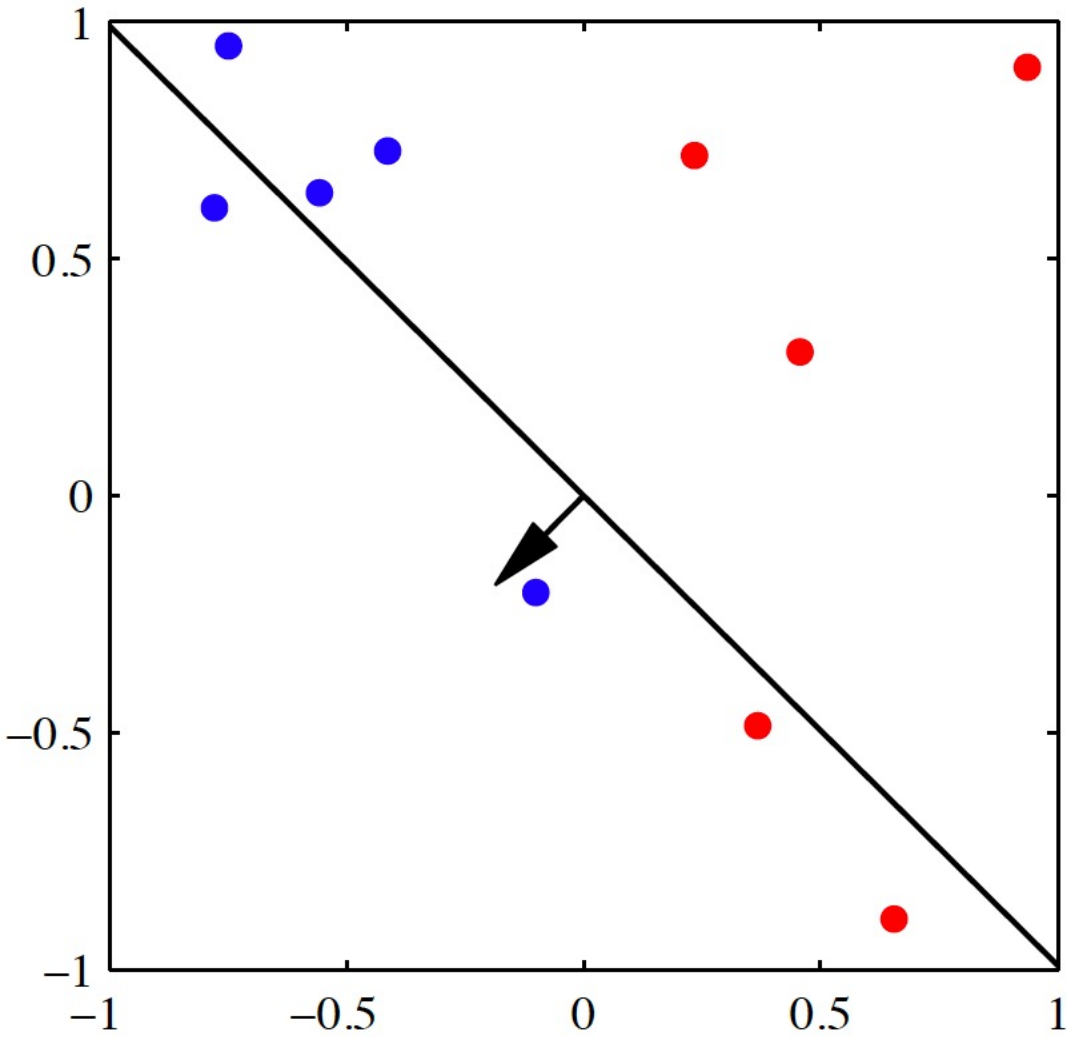
$$\mathbf{w}^{(new)} = \mathbf{w}^{(old)} - \eta \nabla E_i(\mathbf{w}) = \mathbf{w}^{(old)} + \eta y_i \mathbf{x}_i$$

- The learning rate parameter η can be set to 1
- No update corresponding to the correctly predicted points

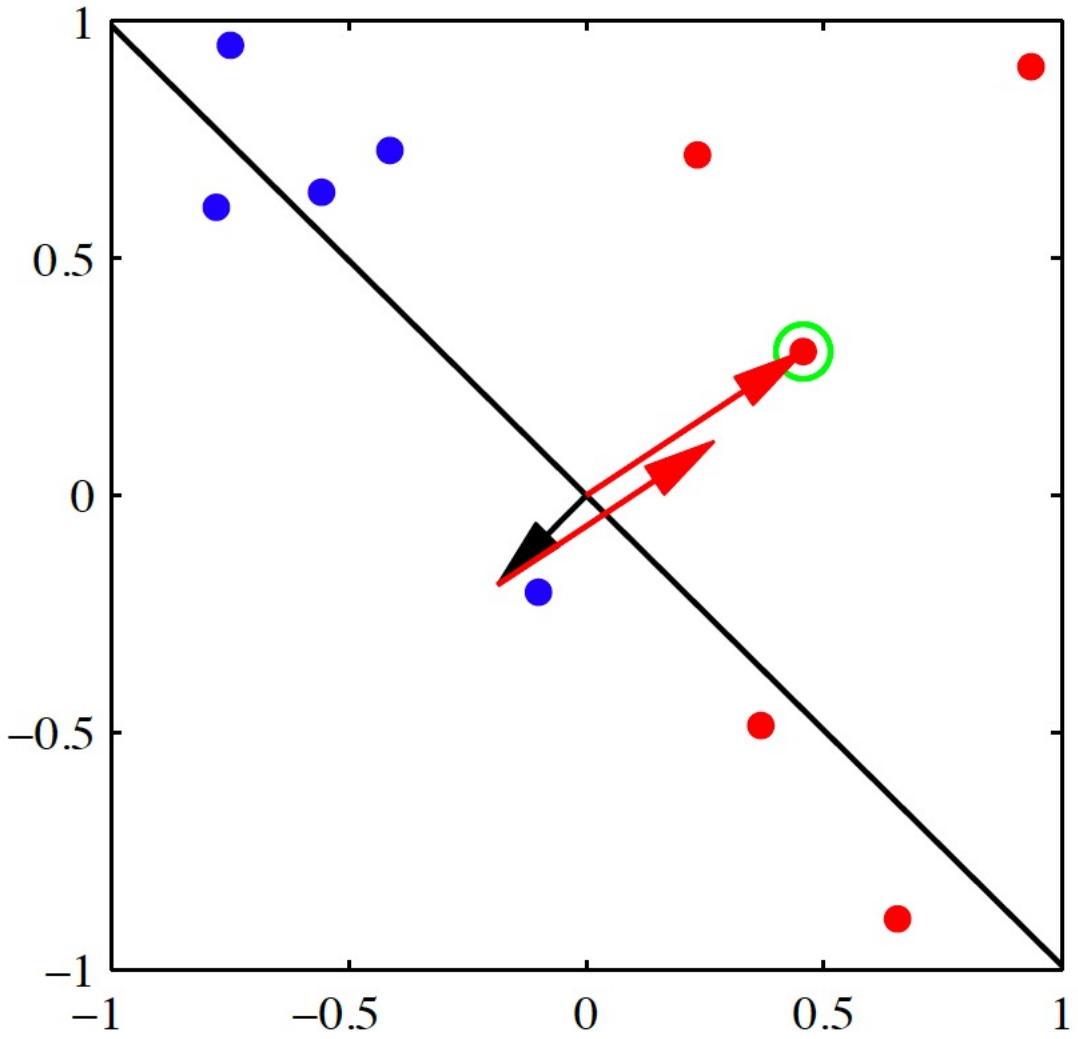
Linear Classification: Example



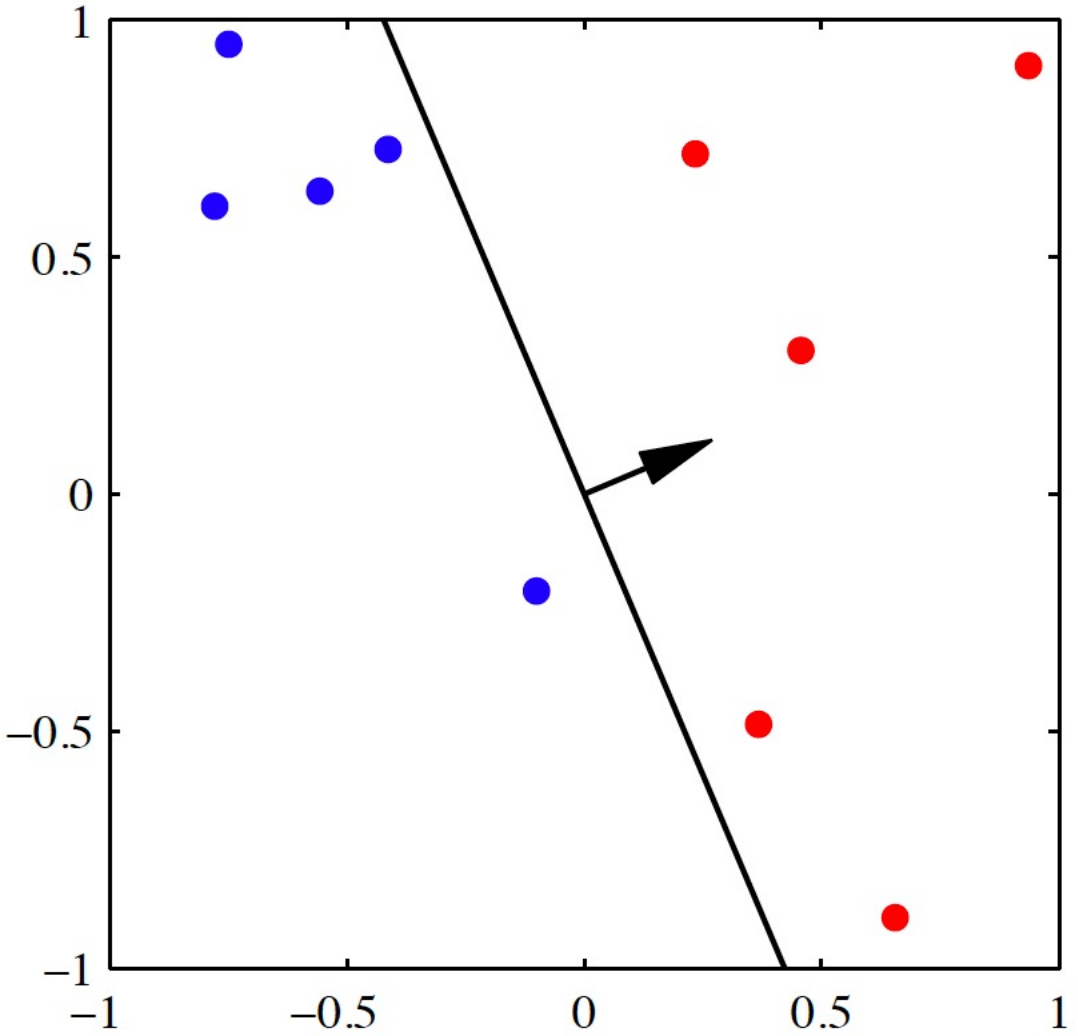
Linear Classification: Example



Linear Classification: Example

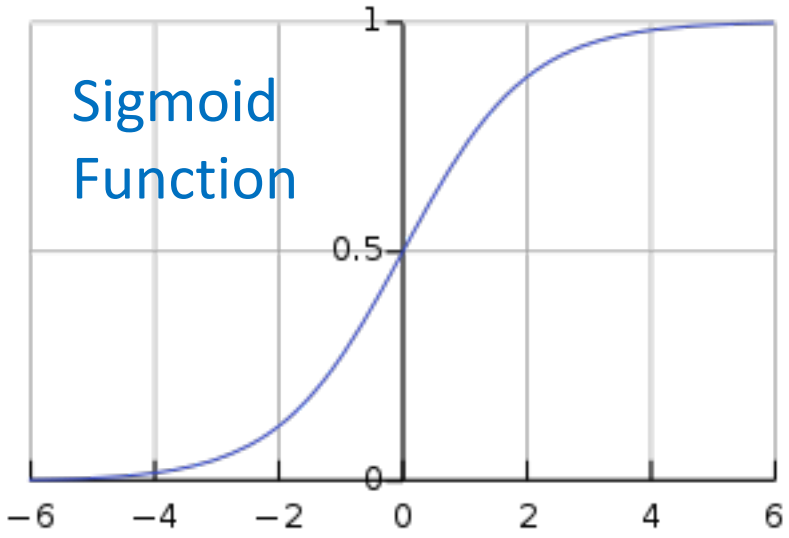


Linear Classification: Example



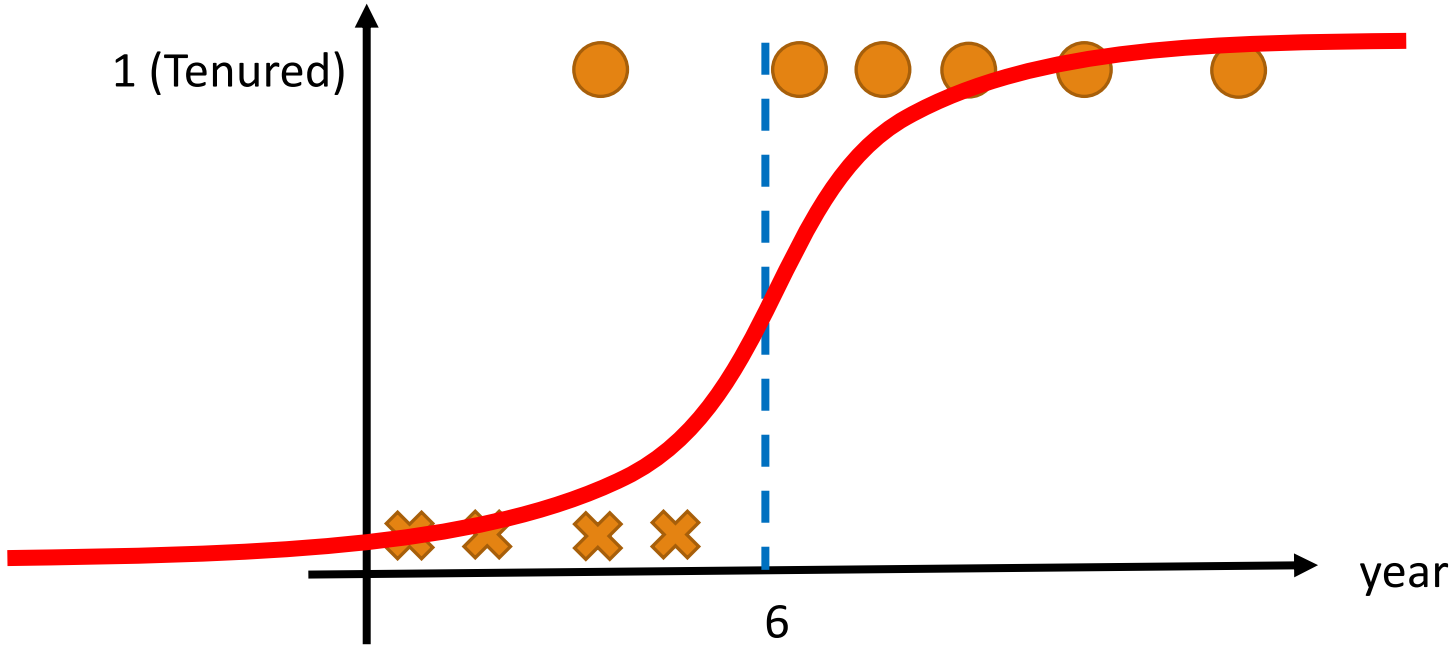
Logistic Regression: General Ideas

- How to solve "classification" problems by regression?
- Key idea of Logistic Regression
  - We need to transform the real value Y into a probability value ∈ [0,1]
- Sigmoid function (differentiable function) :
  - $\sigma(z) = \frac{1}{1+e^{-z}} = \frac{e^z}{e^z+1}$
  - Projects $(-\infty, +\infty)$ to $[0, 1]$
  - Not only LR uses this function, but also neural network, deep learning
- The projected value change sharply around zero point
- Notice that $\ln \frac{y}{1-y} = w^T x + b$

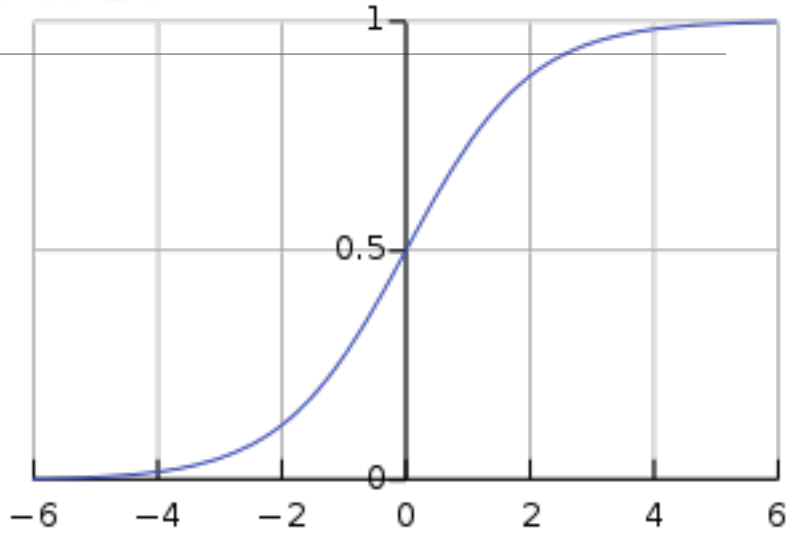


Logistic Regression: An Example

- Suppose we only consider the year as feature
  - Data points are converted by sigmoid function ("activation" function)



Logistic Regression: Model



- The prediction function to learn
- Probability that Y=1:
  - $p(Y = 1 \,|X = x; \boldsymbol{w}) \;= \; Sigmoid(w_0 + \sum_{i=1}^{n} w_i \cdot x_i)$
  - $\boldsymbol{w} = (w_0, w_1, w_2, \ldots, w_n)$ are the parameters
- A single data object with attributes x_i and class label y_i
  - Suppose the probability of $p(\hat{y}_i = 1|x_i, w) = p_i$, then $p(\hat{y}_i = 0|x_i, w) = 1 - p_i$
  - $p(\hat{y}_i = y_i) = p_i^{y_i}(1 - p_i)^{1-y_i}$
- Maximum Likelihood Estimation
  - $L = \Pi_i p_i^{y_i}(1 - p_i)^{1-y_i} = \Pi_i \left(\frac{\exp(w^T x_i)}{1+\exp(w^T x_i)}\right)^{y_i} \left(\frac{1}{1+\exp(w^T x_i)}\right)^{1-y_i}$

Logistic Regression: Optimization

- Maximum Likelihood Estimation
  - $L = \Pi_i p_i^{y_i}(1-p_i)^{1-y_i} = \Pi_i \left(\frac{\exp(w^T x_i)}{1+\exp(w^T x_i)}\right)^{y_i} \left(\frac{1}{1+\exp(w^T x_i)}\right)^{1-y_i}$
- Log likelihood:

$$l(w) = \sum_{i=1}^{N} y_i \log p(Y=1|X=x_i;\boldsymbol{w}) + (1-y_i)\log\big(1-p(Y=1|X=x_i;\boldsymbol{w})\big)$$

$$= \sum_{i=1}^{N} y_i x_i^T \boldsymbol{w} - \log(1+\exp(\boldsymbol{w}^T x_i))$$

- There's no closed form solution
  - Gradient Descent

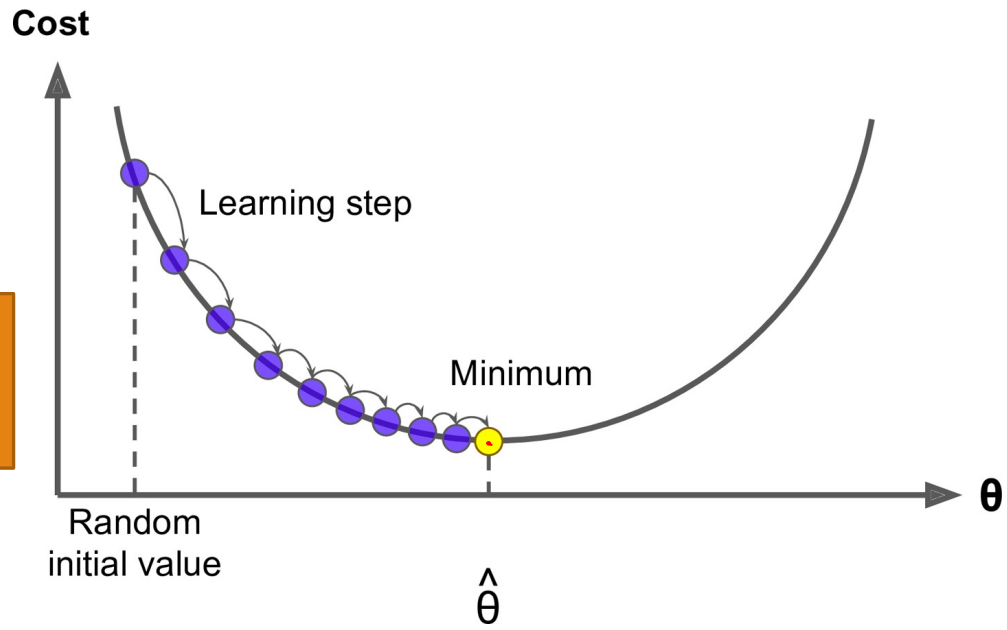
Gradient Descent

- Gradient Descent is an iterative optimization algorithm for finding the minimum of a function (e.g., the negative log likelihood)
- For a function F(x) at a point **a**, F(x) *decreases fastest* if we go in the direction of the negative gradient of **a**

Step size

$$\mathbf{a}_{n+1} = \mathbf{a}_n - \gamma \nabla F(\mathbf{a}_n)$$

When the gradient is zero, we arrive at the local minimum



Convergence Problem

x	y
-5	0
-4	0
-3	0
-2	0
-1	0
1	1
2	1
3	1
4	1
5	1

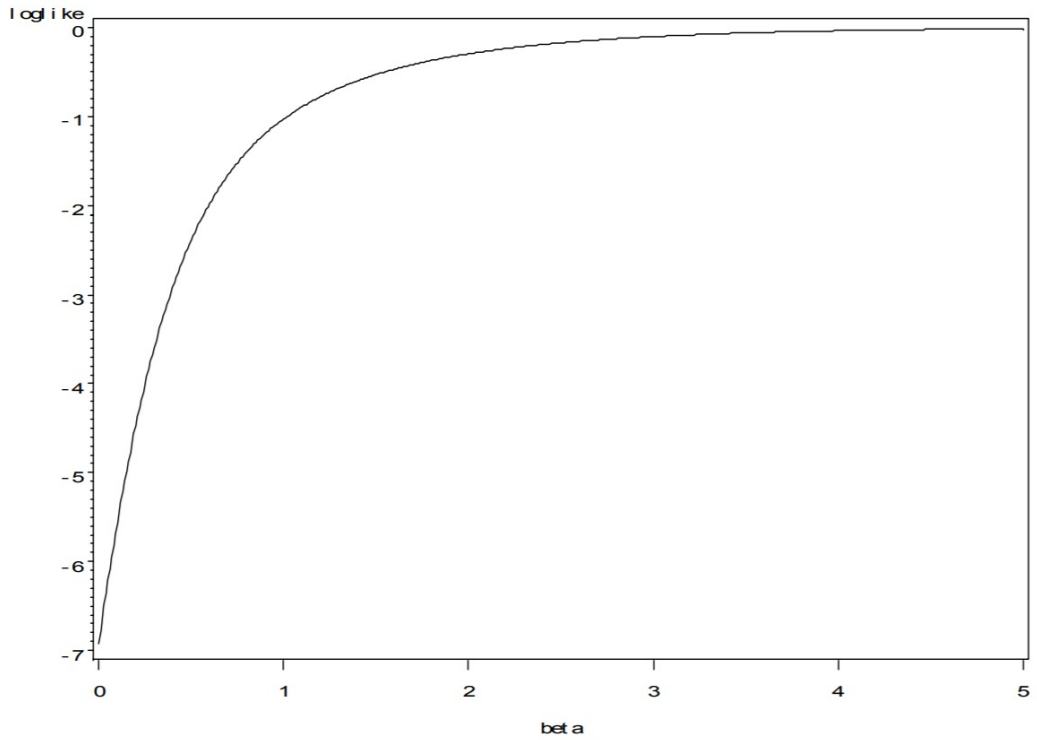


Figure 1. Log-likelihood as a function of the slope under complete separation

		y = 1	y = 0
x	1	5	0
	0	0	10

		y = 1	y = 0
x	1	5	0
	0	15	10

x	y
-5	0
-4	0
-3	0
-2	0
-1	0
0	0
0	1
1	1
2	1
3	1
4	1
5	1

Linear Regression VS. Logistic Regression

- Linear Regression
  - Y: Continuous Value $\in [-\infty, +\infty]$
  - $Y = W^T X + b$
  - Often used in value prediction problems

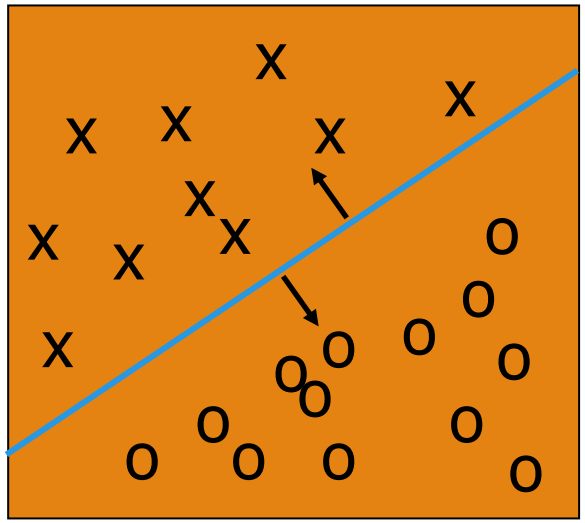
- Logistic Regression
  - Y: A discrete value from m classes
  - $P(Y = C_i) \in [0,1] \ \ and \ \ \Sigma_{i=1}^{m} P(Y = C_i) = 1$
  - Often used in classification problems

Comments on Logistic Regression

- Pros
  - Can handle multiple types of features
  - Fast and easy
  - Generally speaking, more robust and better performance than tree
  - Interpretable: both weights and predicted value
    - Predicted value: probability
    - Weights: effect of the feature. Unit change of log odds
- Cons
  - Linear model: if the decision boundary is not linear, then LR is not good

Linear Classifier: General Ideas

- Binary Classification
- $f(x)$ is a linear function based on the example's attribute values
  - The prediction is based on the value of $f(x)$
  - Data above the blue line belongs to class 'x' (i.e., $f(x) > 0$)
  - Data below blue line belongs to class 'o' (i.e., $f(x) < 0$)
- Classical Linear Classifiers
  - Logistic Regression
  - Linear Discriminant Analysis (LDA)
  - Perceptron
  - SVM

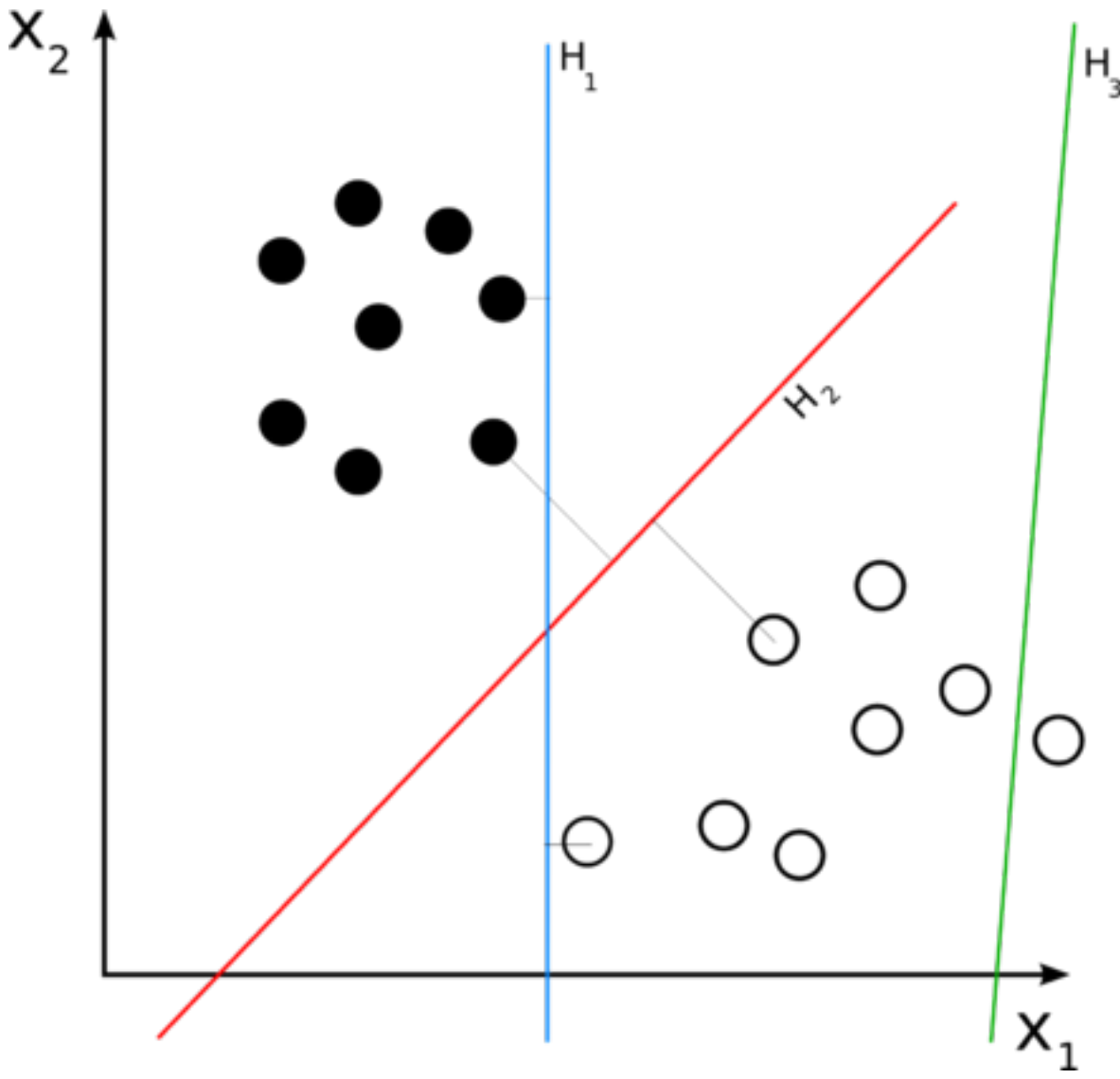


Linear Classifier: An Example

- A toy rule to determine whether a faculty member has tenure
  - Year >= 6 or Title = "Professor" ⇔ Tenure
- How to express the rule as a linear classifier?
- Features
  - $\mathrm{x}_1 (x_1 \geq 0)$ is an integer denoting the year
  - x_2 is a Boolean denoting whether the title is "Professor"
- A feasible linear classifier: $f(x) = (x_1 - 5) + 6 \cdot x_2$
  - When x_2 is True, because $x_1 \geq 0$, $f(x)$ is always greater than 0
  - When x_2 is False, because $f(x) > 0 \Leftrightarrow x_1 \geq 6$
- There are many more feasible classifiers
  - $f(x) = (x_1 - 5.5) + 6 \cdot x_2$
  - $f(x) = 2 \cdot (x_1 - 5) + 11 \cdot x_2$
  - ……

Key Question: Which Line Is Better?

- There might be many feasible linear functions
  - Both H1 and H2 will work
- Which one is better?
  - H2 looks “better” in the sense that it is also furthest from both groups
  - We will introduce more in the SVM section



Generative vs. Discriminative Classifiers

- X: observed variables (features)
- Y: target variables (class labels)
- A generative classifier models p(Y, X)
  - It models how the data was "generated"? "what is the likelihood this or that class generated this instance?" and pick the one with higher probability
  - Naïve Bayes
  - Bayesian Networks
- A discriminative classifier models p(Y|X)
  - It uses the data to create a decision boundary
  - Logistic Regression
  - Support Vector Machines

Further Comments on Discriminative Classifiers

- Strength
  - Prediction accuracy is generally high
    - As compared to generative models
    - Robust, works when training examples contain errors
  - Fast evaluation of the learned target function
    - Comparing to (covered in future) Bayesian networks (which are normally slow)
- Criticism
  - Long training time
  - Difficult to understand the learned function (weights)
    - Bayesian networks can be used easily for pattern discovery
  - Not easy to incorporate domain knowledge
    - Easy in the form of priors on the data or distributions

Chapter 8. Classification: Basic Concepts

- Classification: Basic Concepts
- Decision Tree Induction
- Bayes Classification Methods
- Linear Classifier
- Model Evaluation and Selection
- Lazy Learning
- Ensemble Methods
- Imbalanced Data Sets
- Summary

Model Evaluation and Selection

- Evaluation metrics
  - How can we measure accuracy?
  - Other metrics to consider?
- Use **validation test set** of class-labeled tuples instead of training set when assessing accuracy
- Methods for estimating a classifier's accuracy
  - Holdout method
  - Cross-validation
  - Bootstrap
- Comparing classifiers:
  - ROC Curves

Classifier Evaluation Metrics: Confusion Matrix

- **Confusion Matrix:**

Actual class\Predicted class	C_1	¬ C_1
C_1	**True Positives (TP)**	**False Negatives (FN)**
¬ C_1	**False Positives (FP)**	**True Negatives (TN)**

- In a confusion matrix w. *m* classes, $CM_{i,j}$ indicates # of tuples in class *i* that were labeled by the classifier as class *j*
  - May have extra rows/columns to provide totals
- **Example of Confusion Matrix:**

Actual class\Predicted class	play_golf = yes	play_golf = no	Total
play_golf = yes	**6954**	**46**	7000
play_golf = no	**412**	**2588**	3000
Total	7366	2634	10000

Classifier Evaluation Metrics: Accuracy, Error Rate, Sensitivity and Specificity

A\P	C	¬C	
C	**TP**	**FN**	**P**
¬C	**FP**	**TN**	**N**
	P'	**N'**	**All**

Real-world truth

Predictions

- **Classifier accuracy,** or recognition rate
  - Percentage of test set tuples that are correctly classified

  Accuracy = (TP + TN)/All
- **Error rate:** *1 – accuracy*, or

  Error rate = (FP + FN)/All

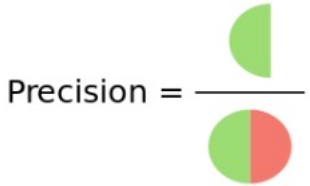
- **Class imbalance problem**
  - One class may be *rare*
    - E.g., fraud, or HIV-positive
  - Significant *majority of the negative class* and minority of the positive class
  - Measures handle the class imbalance problem
    - **Sensitivity** (recall): True positive recognition rate
      - **Sensitivity = TP/P**
    - **Specificity**: True negative recognition rate
      - **Specificity = TN/N**

Classifier Evaluation Metrics: Precision and Recall, and F-measures

A\P	C	¬C	
C	**TP**	**FN**	**P**
¬C	**FP**	**TN**	**N**
	P'	**N'**	**All**

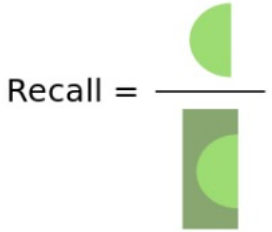
- **Precision**: Exactness: what % of tuples that the classifier labeled as positive are actually positive?

$$\text{P} = \text{Precision} = \frac{\text{TP}}{\text{TP} + \text{FP}}$$

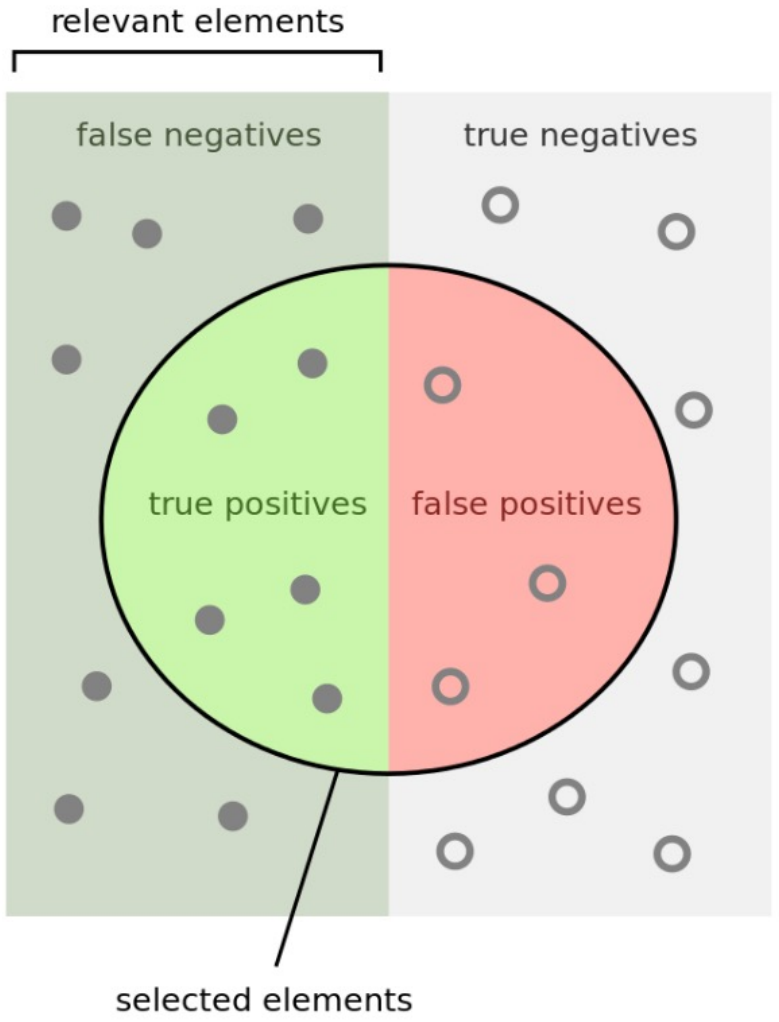


- **Recall:** Completeness: what % of positive tuples did the classifier label as positive?

$$\text{R} = \text{Recall} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$



  - Range: [0, 1]



https://en.wikipedia.org/wiki/Precision_and_recall

Classifier Evaluation Metrics: Precision and Recall, and F-measures

- The "inverse" relationship between precision & recall
- ***We want one number to say if a classifier is good or not***
- ***F* measure (or *F*-score):** harmonic mean of precision and recall
  - In general, it is the weighted measure of precision & recall

$$F_\beta = \frac{1}{\alpha \cdot \frac{1}{P} + (1 - \alpha) \cdot \frac{1}{R}} = \frac{(\beta^2 + 1)P * R}{\beta^2 P + R}$$

Assigning β times as much weight to recall as to precision)

  - ***F1-measure (balanced F-measure)***
    - That is, when β = 1,

$$F_1 = \frac{2P * R}{P + R}$$

Classifier Evaluation Metrics: Example

- Use the same confusion matrix, calculate the measure just introduced

Actual Class\Predicted class	cancer = yes	cancer = no	Total
cancer = yes	**90**	**210**	300
cancer = no	**140**	**9560**	9700
Total	230	9770	10000

  - Sensitivity =
  - Specificity =
  - Accuracy =
  - Error rate =
  - Precision =
  - Recall =
  - F1 =

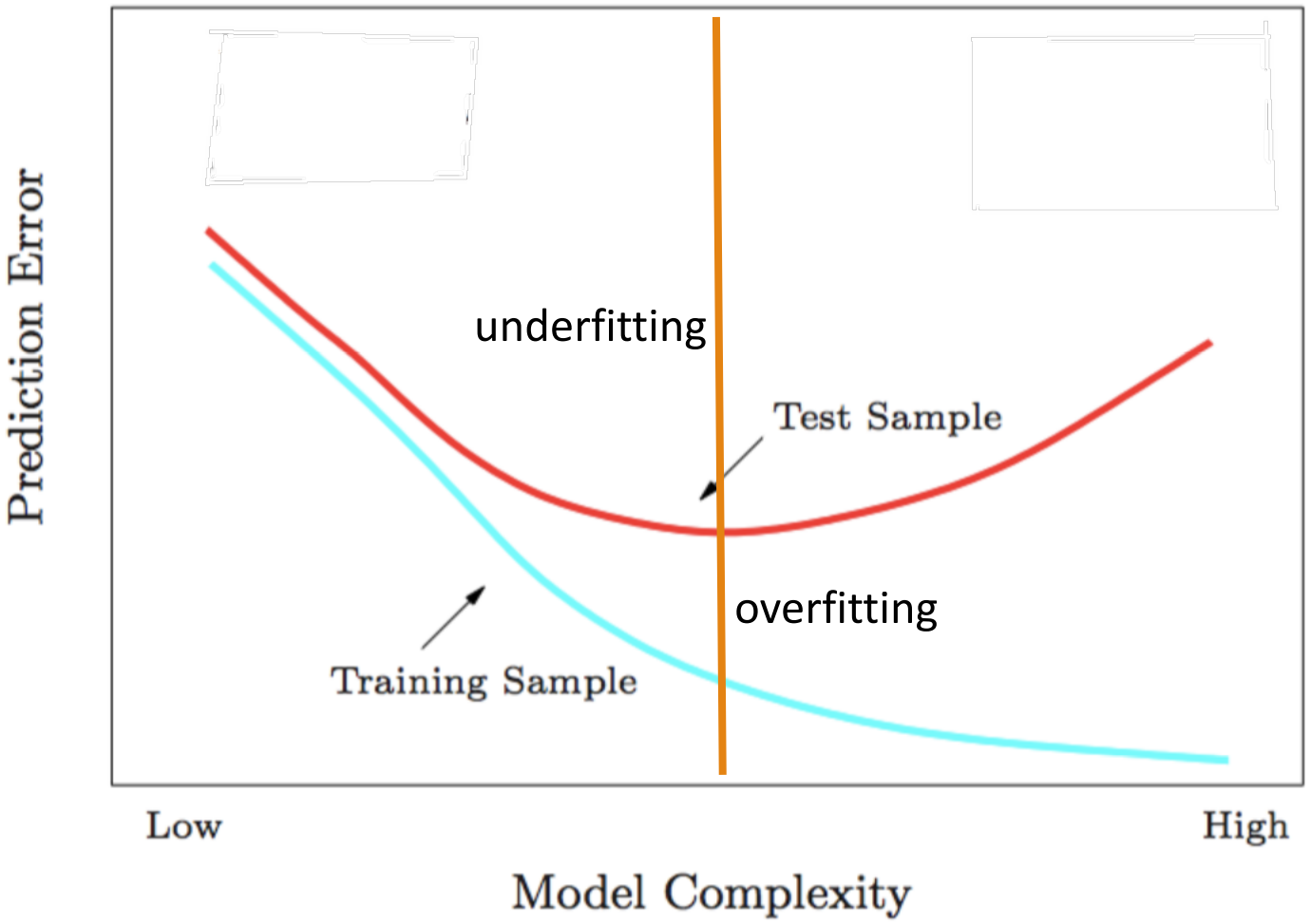
Classifier Evaluation Metrics: Example

- Use the same confusion matrix, calculate the measure just introduced

Actual Class\Predicted class	cancer = yes	cancer = no	Total
cancer = yes	**90**	**210**	300
cancer = no	**140**	**9560**	9700
Total	230	9770	10000

- Sensitivity = TP/P = 90/300 = 30%
- Specificity = TN/N = 9560/9700 = 98.56%
- Accuracy = (TP + TN)/All = (90+9560)/10000 = 96.50%
- Error rate = (FP + FN)/All = (140 + 210)/10000 = 3.50%
- Precision = TP/(TP + FP) = 90/(90 + 140) = 90/230 = 39.13%
- Recall = TP/ (TP + FN) = 90/(90 + 210) = 90/300 = 30.00%
- F1 = 2 P × R /(P + R) = 2 × 39.13% × 30.00%/(39.13% + 30%) = 33.96%

Training Error VS Testing Error



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Classifier Evaluation: Holdout

- **Holdout method**
  - Given data is randomly partitioned into two independent sets
    - Training set (e.g., 2/3) for model construction
    - Test set (e.g., 1/3) for accuracy estimation
  - Repeated random sub-sampling validation: a variation of holdout
    - Repeat holdout k times, accuracy = avg. of the accuracies obtained

Classifier Evaluation: Cross-Validation

- **Cross-validation** (*k*-fold, where k = 10 is most popular)
  - Randomly partition the data into *k mutually exclusive* subsets, each approximately equal size
  - At *i*-th iteration, use D_i as test set and others as training set
  - Leave-one-out: *k* folds where *k* = # of tuples, for small sized data
  - ***Stratified cross-validation***: folds are stratified so that class distribution, in each fold is approximately the same as that in the initial data

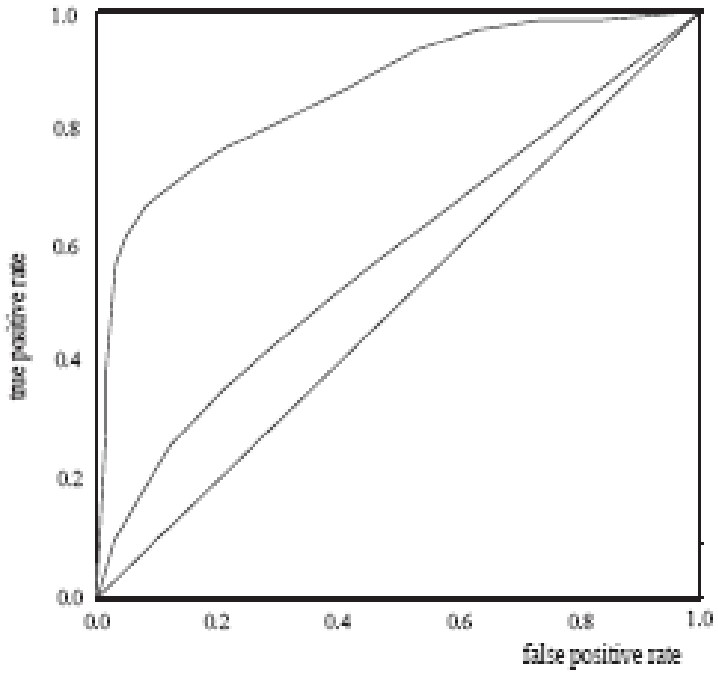
Classifier Evaluation: Bootstrap

- **Bootstrap**
  - Works well with small data sets
  - Samples the given training tuples uniformly *with replacement*
    - Each time a tuple is selected, it is equally likely to be selected again and re-added to the training set
- Several bootstrap methods, and a common one is **.632 bootstrap**
  - A data set with *d* tuples is sampled *d* times, with replacement, resulting in a training set of *d* samples. The data tuples that did not make it into the training set end up forming the test set. About 63.2% of the original data end up in the bootstrap, and the remaining 36.8% form the test set (since $(1 - 1/d)^d \approx e^{-1} = 0.368$)
  - Repeat the sampling procedure *k* times, overall accuracy of the model:

$$Acc(M) = \frac{1}{k}\sum_{i=1}^{k}(0.632 \times Acc(M_i)_{test\_set} + 0.368 \times Acc(M_i)_{train\_set})$$

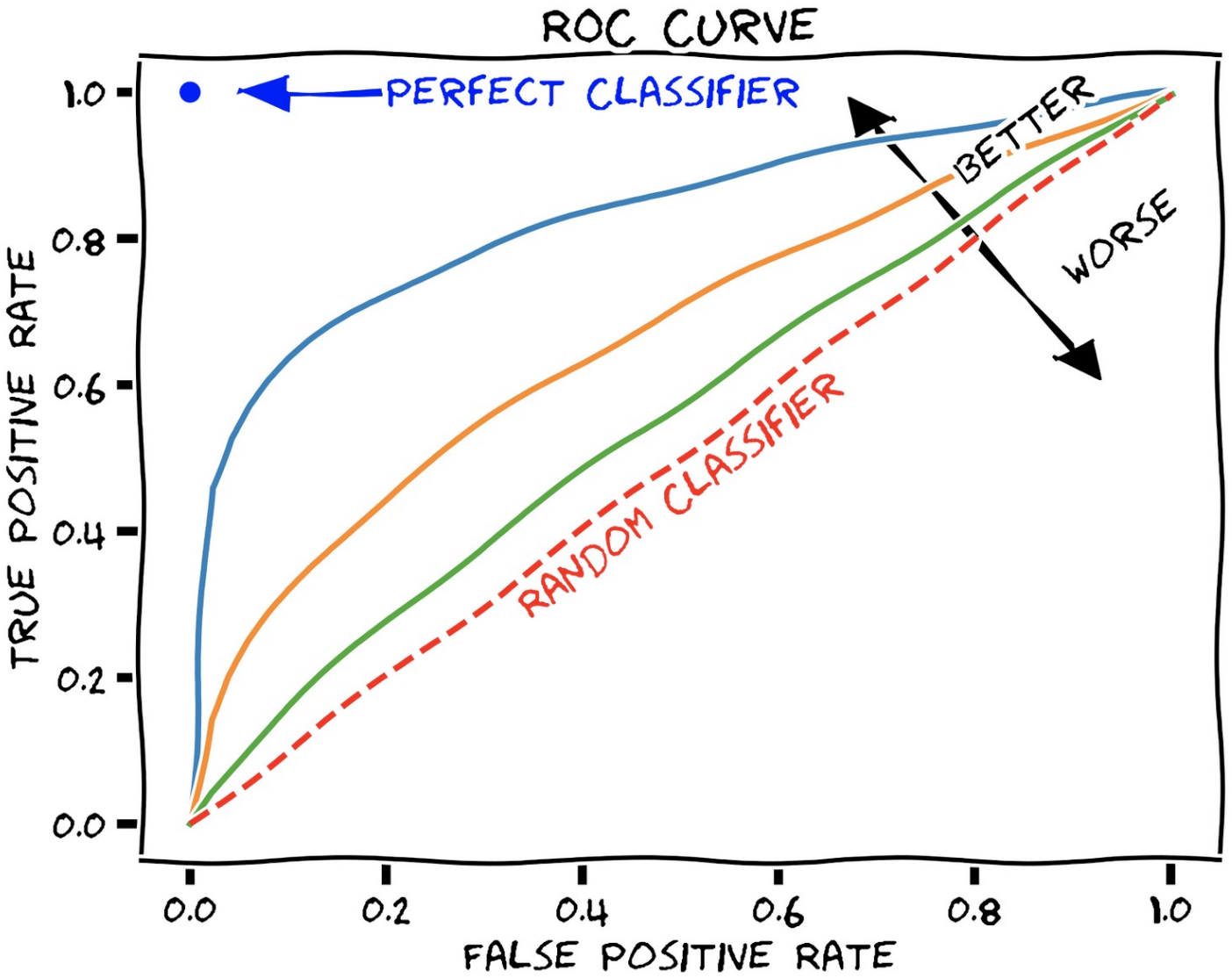
Model Selection: ROC Curves

- **ROC** (Receiver Operating Characteristics) curves: for visual comparison of classification models
- Originated from signal detection theory
- Shows the trade-off between the true positive rate and the false positive rate
- The area under the ROC curve (**AUC**: Area Under Curve) is a measure of the accuracy of the model
- Rank the test tuples in decreasing order: the one that is most likely to belong to the positive class appears at the top of the list
- The closer to the diagonal line (i.e., the closer the area is to 0.5), the less accurate is the model



- Vertical axis represents the true positive rate (TP/P)
- Horizontal axis rep. the false positive rate (FP/N)
- The plot also shows a diagonal line
- A model with perfect accuracy will have an area of 1.0

ROC and AUC


ROC CURVE
PERFECT CLASSIFIER
BETTER
WORSE
RANDOM CLASSIFIER
TRUE POSITIVE RATE
FALSE POSITIVE RATE
0.0
0.2
0.4
0.6
0.8
1.0

Issues Affecting Model Selection

- **Accuracy**
  - classifier accuracy: predicting class label
- **Speed**
  - time to construct the model (training time)
  - time to use the model (classification/prediction time)
- **Robustness**: handling noise and missing values
- **Scalability**: efficiency in disk-resident databases
- **Interpretability**
  - understanding and insight provided by the model
- Other measures, e.g., goodness of rules, such as decision tree size or compactness of classification rules

Model Selection, Statistical Significance

- k-Fold Cross-Validation: Models M1, M2
  - Each classifier gets k error rates $err(M1)_i$, $err(M2)_i$, i=1,…k
  - Comparing average error rate is tricky
  - Need to consider the variance, more generally the distribution of error rates
- Hypothesis testing: Student's t-test
  - Individual error rates follow a t-distribution (under some assumptions)
  - Null hypothesis: the distributions are the same
  - t-statistic for pairwise comparison

$$t = \frac{\overline{err}(M_1) - \overline{err}(M_2)}{\sqrt{var(M_1 - M_2)/k}},$$

where

$$var(M_1 - M_2) = \frac{1}{k} \sum_{i=1}^{k} [err(M_1)_i - err(M_2)_i - (\overline{err}(M_1) - \overline{err}(M_2))]^2$$

Model Selection, Statistical Significance

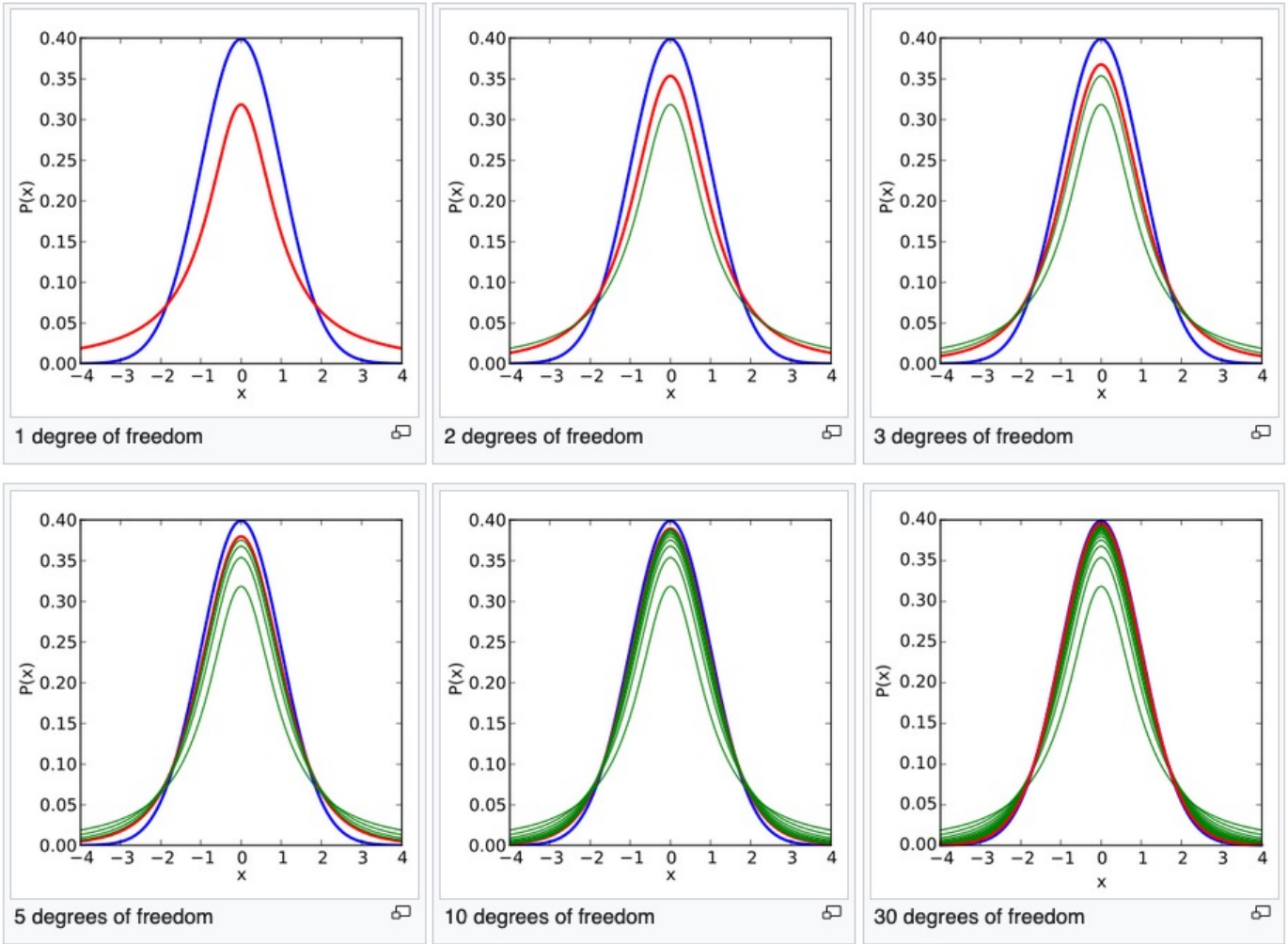
- Compute t-statistic from k-Fold error rates of M1, M2
  - Degrees of freedom is (k-1)
- Consider a significance level, say α=5% (or 1%)
  - Use the fact that t-distribution is symmetric, upper/lower tail at level $\alpha/2$
  - Look up the statistic value t_0 at this level
  - If $t > t_0$ or $t < -t_0$, then the difference is significant, reject null hypothesis

- If there are test sets, two sample t-test based on variance of difference

$$var(M_1 - M_2) = \frac{var(M_1)}{k_1} + \frac{var(M_2)}{k_2},$$

Student's t-distribution

Density of the *t*-distribution (red) for 1, 2, 3, 5, 10, and 30 degrees of freedom compared to the standard normal distribution (blue).
Previous plots shown in green.



Chapter 8. Classification: Basic Concepts

- Classification: Basic Concepts
- Decision Tree Induction
- Bayes Classification Methods
- Linear Classifier
- Model Evaluation and Selection
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- Ensemble Methods
- Imbalanced Data Sets
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Lazy vs. Eager Learning

- Lazy vs. eager learning
  - **Lazy learning** (e.g., instance-based learning): Simply stores training data (or only minor processing) and waits until it is given a test tuple
  - **Eager learning** (the above discussed methods): Given a set of training tuples, constructs a classification model before receiving new (e.g., test) data to classify
- Lazy: less time in training but more time in predicting
- Accuracy
  - Lazy method effectively uses a richer hypothesis space since it uses many local linear functions to form an implicit global approximation to the target function
  - Eager: must commit to a single hypothesis that covers the entire instance space

Lazy Learning

- Nearest neighbor (NN) based
- Prediction is “lazy”
  - Training: keep points around, “lazy”
  - Prediction: find nearest neighbors, make prediction
- Most work happens during prediction
  - Training: proper indexing to help NN search
  - Prediction: find similar points, cases, etc.
- Properties
  - Can be computationally expensive
  - Supports incremental learning

Lazy Learner: Instance-Based Methods

- Instance-based learning:
  - Store training examples and delay the processing ("lazy evaluation") until a new instance must be classified
- Typical approaches
  - *k*-nearest neighbor approach
    - Instances represented as points in a Euclidean space.
  - Locally weighted regression
    - Constructs local approximation
  - Case-based reasoning
    - Uses symbolic representations and knowledge-based inference

k-Nearest Neighbor

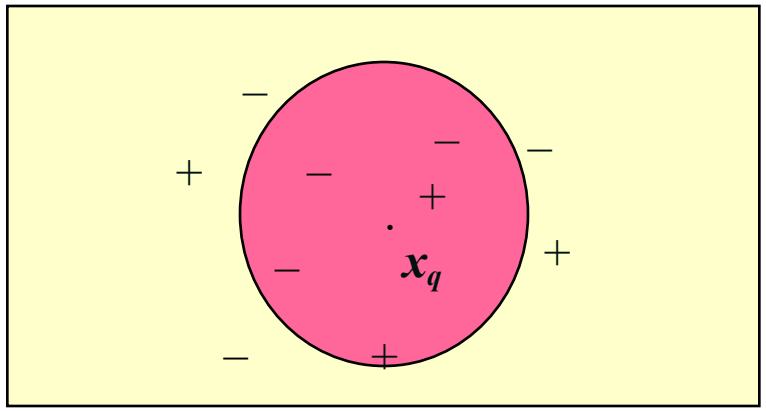
- Nearest neighbor (NN) based
  - Points based on n attributes
  - Have a notion of distance between points
  - Given test point, find k nearest neighbors
  - Prediction: (weighted) majority of k nearest neighbors
- Distance measure
  - Metric, such as Euclidean distance
  - Normalize attributes
  - Generalization to nominal attributes, e.g., same (0) vs different (1)

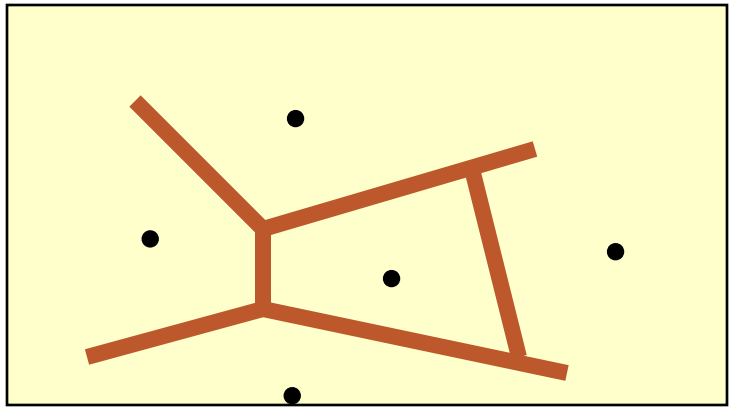
k-Nearest Neighbor

- Nearest neighbor (NN) for numeric prediction
  - Data points (x_i, y_i), i=1,…,n
  - Given test point x_{test}, find k nearest neighbors, from x_i
  - Prediction y_{test}: (weighted) sum of responses (y_i) of k nearest neighbors
  - Weighting based on distance to x_{test}
- Missing values: Worst possible distance, imputation
- Choice of k
  - Should increase with n, choose based on validation set
  - For k=1, gets twice “Bayes error rate” as n --> ∞

The *k*-Nearest Neighbor Algorithm

- All instances correspond to points in the n-D space
- The nearest neighbor are defined in terms of Euclidean distance, dist($\mathbf{X_1}$, $\mathbf{X_2}$)
- Target function could be discrete- or real- valued
- For discrete-valued, *k*-NN returns the most common value among the *k* training examples nearest to x_q
- Vonoroi diagram: the decision surface induced by 1-NN for a typical set of training examples





Discussion on the *k*-NN Algorithm

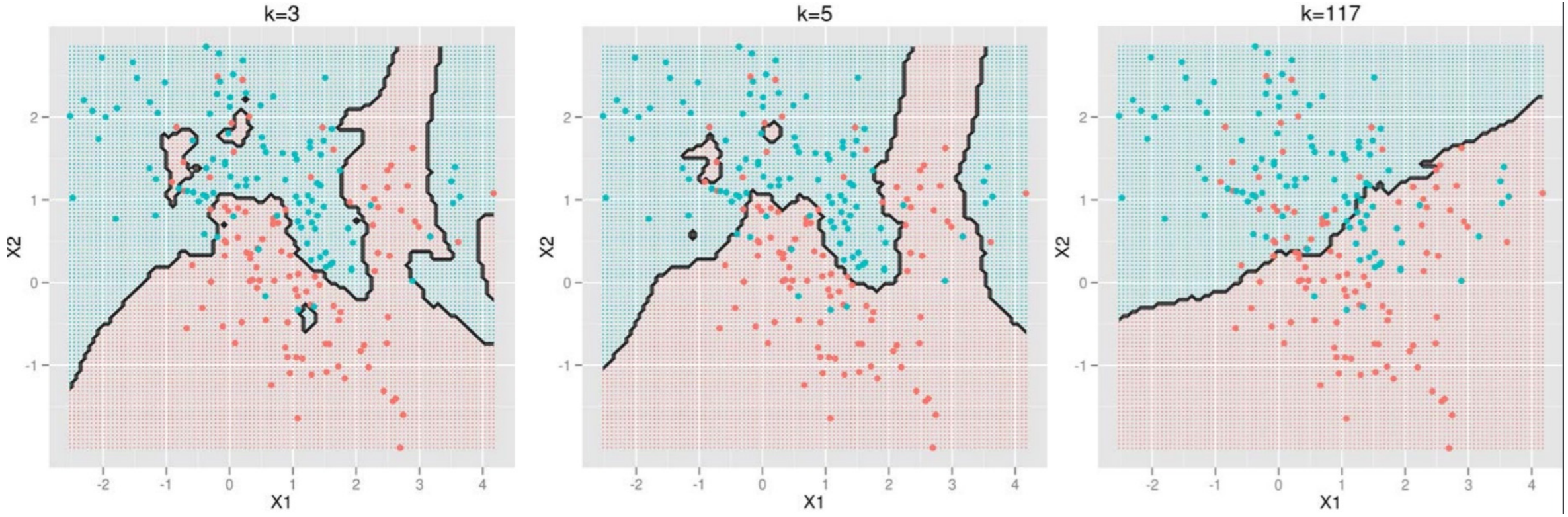
- *k*-NN for real-valued prediction for a given unknown tuple
  - Returns the mean values of the *k* nearest neighbors
- Distance-weighted nearest neighbor algorithm
  - Weight the contribution of each of the *k* neighbors according to their distance to the query x_q
    - Give greater weight to closer neighbors

$$w = \frac{1}{d(x_q, x_i)^2}$$

- Robust to noisy data by averaging *k*-nearest neighbors
- Curse of dimensionality: distance between neighbors could be dominated by irrelevant attributes
  - To overcome it, axes stretch or elimination of the least relevant attributes

Selection of k for kNN

- The number of neighbors k
  - Small k: overfitting (high var., low bias)
  - Big k: bringing too many irrelevant points (high bias, low var.)



http://scott.fortmann-roe.com/docs/BiasVariance.html

k-Nearest Neighbor

- Importance of distance in Nearest neighbor (NN)
  - Can suffer based on bad distances, learn (parametric) distances
  - Can suffer due to noisy attributes; weighting, pruning of noisy attributes
- Can be extremely slow
  - O(|D|) comparisons are needed to classify
  - Using search trees, can be reduced to O(log|D|)
  - Parallel implementations
- Speeding up computations
  - Partial distance calculations
  - Editing, compressing to reduce number of points
  - Locality sensitive hashing, approximate NN, with high probability

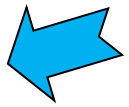
Case-Based Reasoning

- Store “cases” with symbolic representation
- Prediction based on NN type idea
  - Find if an identical case exists
  - If not, find cases which have similar components
  - E.g., cases are graphs, find similarity on subgraphs
  - Combine solution from such related cases to solve the new case
- Challenges
  - Good similarity metric among cases
  - Salient features for indexing training cases
- Trade-offs: Accuracy vs. Efficiency
  - Prune, compress, index, etc., for efficiency

Case-Based Reasoning (CBR)

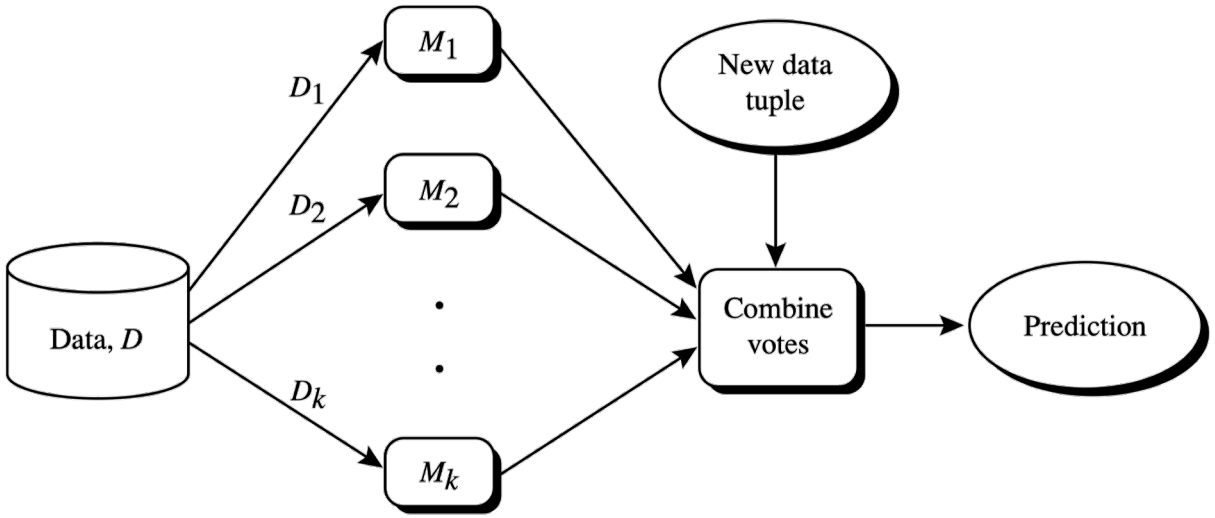
- **CBR**: Uses a database of problem solutions to solve new problems
- Store symbolic description (tuples or cases)—not points in a Euclidean space
- Applications: Customer-service (product-related diagnosis), legal ruling
- Methodology
  - Instances represented by rich symbolic descriptions (e.g., function graphs)
  - Search for similar cases, multiple retrieved cases may be combined
  - Tight coupling between case retrieval, knowledge-based reasoning, and problem solving
- Challenges
  - Find a good similarity metric
  - Indexing based on syntactic similarity measure, and when failure, backtracking, and adapting to additional cases

Chapter 8. Classification: Basic Concepts

- Classification: Basic Concepts
- Decision Tree Induction
- Bayes Classification Methods
- Linear Classifier
- Model Evaluation and Selection
- Lazy Learning
- Ensemble Methods 
- Imbalanced Data Sets
- Summary

Ensemble Methods: Increasing the Accuracy

- Ensemble methods
  - Use a combination of models to increase accuracy
  - Combine a series of *k* learned models, M_1, M_2, …, M_k, with the aim of creating an **improved** model M*



Ensemble Methods: Increasing the Accuracy

- What are the requirements to generate an improved model?
  - Example: majority voting

Base model performance →

Ensemble performance →

	x_1	x_2	x_3
M_1	✓	✓	✗
M_2	✗	✓	✓
M_3	✓	✗	✓
Voting Ensemble	✓	✓	✓

Case 1:
Ensemble has positive effect

	x_1	x_2	x_3
M_1	✓	✓	✗
M_2	✓	✓	✗
M_3	✓	✓	✗
Voting Ensemble	✓	✓	✗

Case 2:
Ensemble has no effect

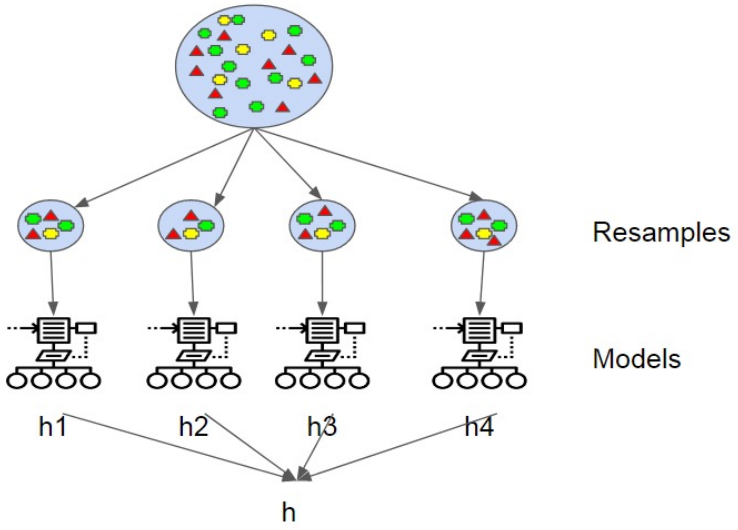
	x_1	x_2	x_3
M_1	✓	✗	✗
M_2	✗	✓	✗
M_3	✗	✗	✓
Voting Ensemble	✗	✗	✗

Case 3:
Ensemble has negative effect

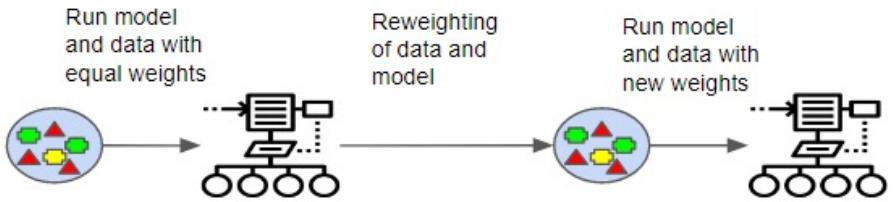
- Base models should be
  - Accurate
  - Diverse

Ensemble Methods: Increasing the Accuracy

- Popular ensemble methods
  - Bagging: Trains each model using a subset of the training set, and models learned in parallel
  - Boosting: Trains each new model instance to emphasize the training instances that previous models mis-classified, and models learned in order



Bagging



Boosting

Bagging: Bootstrap Aggregation

- Analogy: Diagnosis based on multiple doctors' majority vote

- Training
  - For i = 1 to k
    - create bootstrap sample, D_i, by sampling D with replacement;
    - use D_i and the learning scheme to derive a model, M_i ;

- Classification: classify an unknown sample **X**
  - let each of the k models classify X and return the majority vote

- Prediction:
  - To predict continuous variables, use average prediction instead of vote

Bagging: Bootstrap Aggregation

Algorithm: Bagging. The bagging algorithm—create an ensemble of classification models for a learning scheme where each model gives an equally weighted prediction.

Input:

- D, a set of d training tuples;
- k, the number of models in the ensemble;
- a classification learning scheme (e.g., decision tree algorithm, naïve Bayes, etc.).

Output: The ensemble—a composite model, M^*.

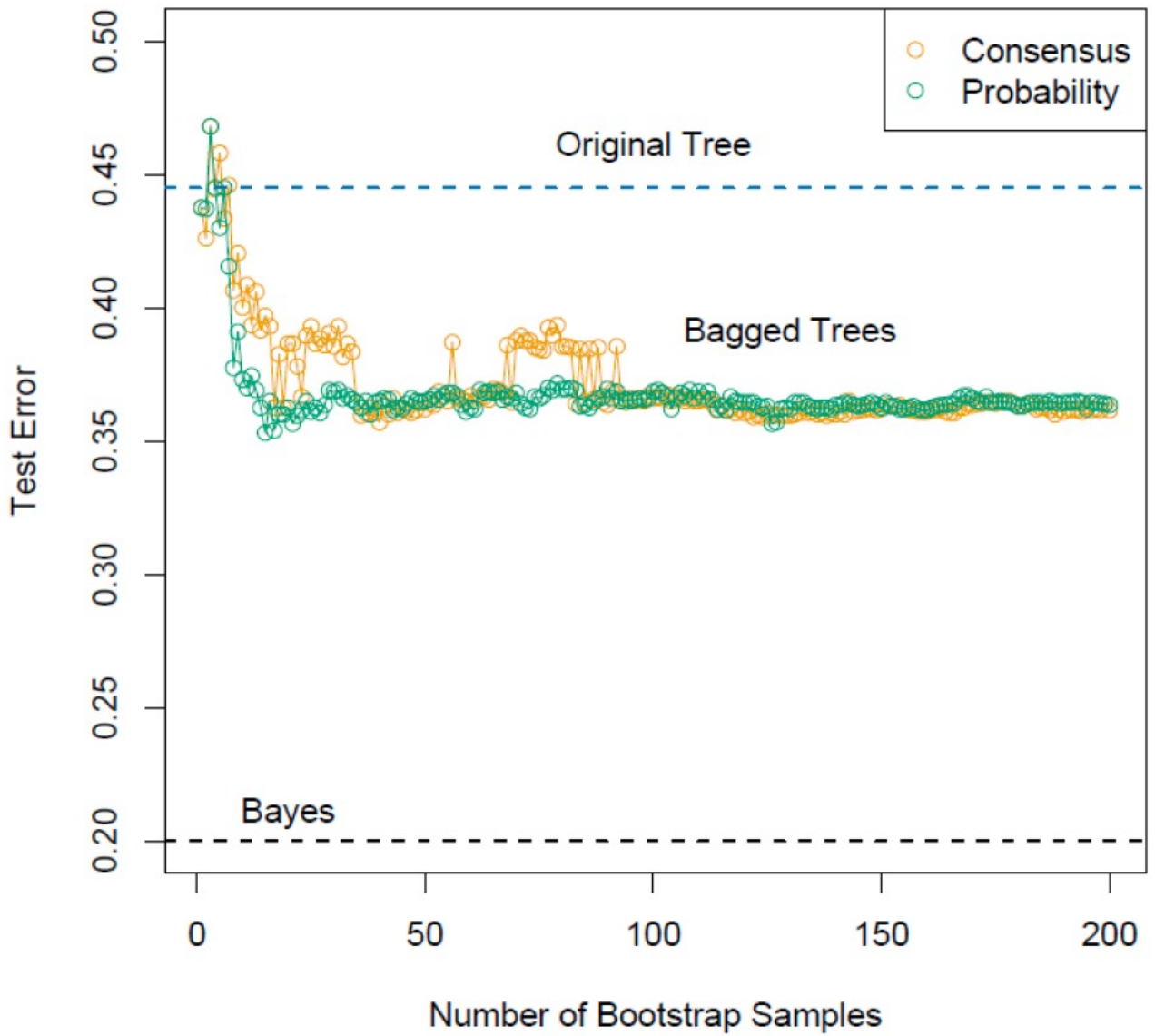
Method:

(1) **for** $i = 1$ to k **do** // create k models:
(2) create bootstrap sample, D_i, by sampling D with replacement;
(3) use D_i and the learning scheme to derive a model, M_i.
(4) **endfor**

To use the ensemble to classify a tuple, X:

(1) let each of the k models classify X and return the majority vote;

Bagging: Bootstrap Aggregation



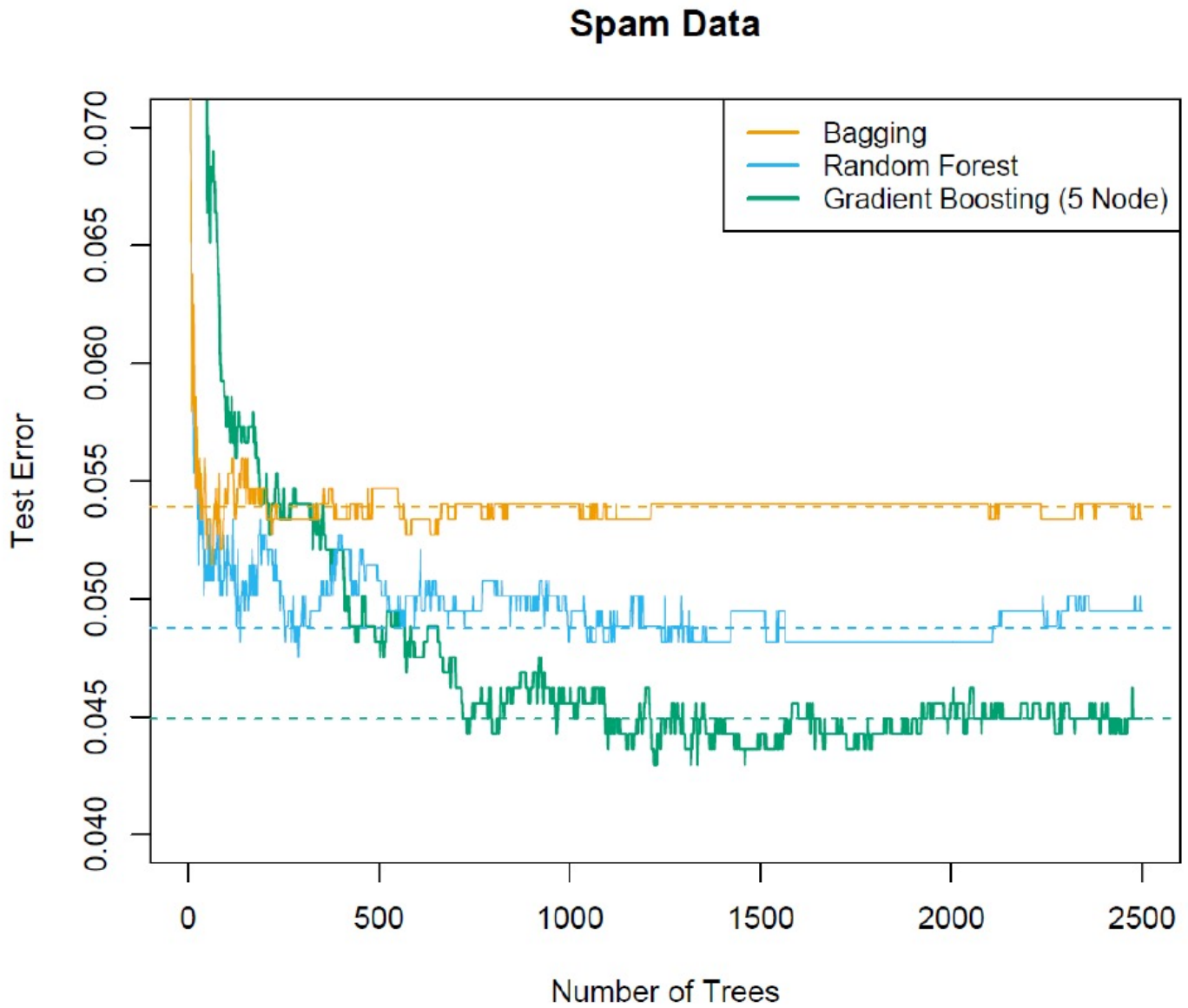
Random Forest: Basic Concepts

- Random Forest (first proposed by L. Breiman in 2001)
  - Bagging with **decision trees** as base models
  - *Data bagging*
    - Use a **subset of training data** by sampling with replacement for each tree
  - *Feature bagging* ⟵ Advantage of decision trees – more diversity
    - At each node use a **random selection of attributes** as candidates and split by the best attribute among them
  - During classification, each tree votes and the most popular class is returned

Random Forest

- Two Methods to construct Random Forest:
  - Forest-RI (*random input selection*): Randomly select, at each node, F attributes as candidates for the split at the node. The CART methodology is used to grow the trees to maximum size
  - Forest-RC (*random linear combinations*): Creates new attributes (or features) that are a linear combination of the existing attributes (reduces the correlation between individual classifiers)
- Comparable in accuracy to Adaboost, but more robust to errors and outliers
- Insensitive to the number of attributes selected for consideration at each split, and faster than typical bagging or boosting

Ensemble Methods: Comparison



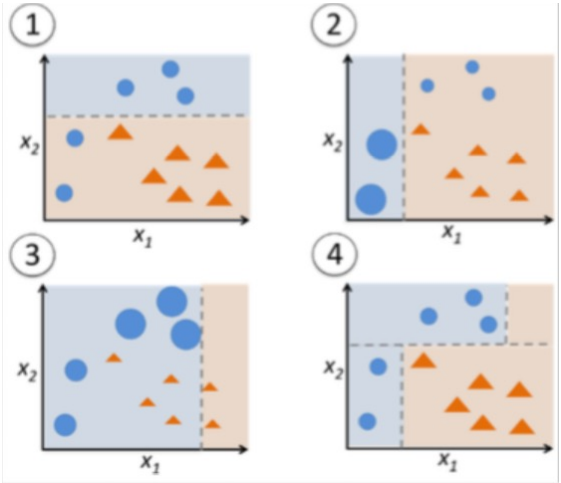
Boosting

- Analogy: Consult several doctors, based on a combination of weighted diagnoses—weight assigned based on the previous diagnosis accuracy
- How boosting works?
  - A series of k classifiers are iteratively learned
  - After a classifier M_i is learned, set the subsequent classifier, M_{i+1}, to **pay more attention to the training tuples that were misclassified** by M_i
  - The final **M* combines the votes** of each individual classifier, where the weight of each classifier's vote is a function of its accuracy
- Boosting algorithm can be extended for numeric prediction

Adaboost (Freund and Schapire, 1997)

1. Assign initial weights to each training tuple

3. Update weights based on current model



$\{w_n^{(1)}\}$ $\{w_n^{(2)}\}$ ... $\{w_n^{(k)}\}$

M_1 M_2 ... M_k

2. Train base classifier on weighted dataset

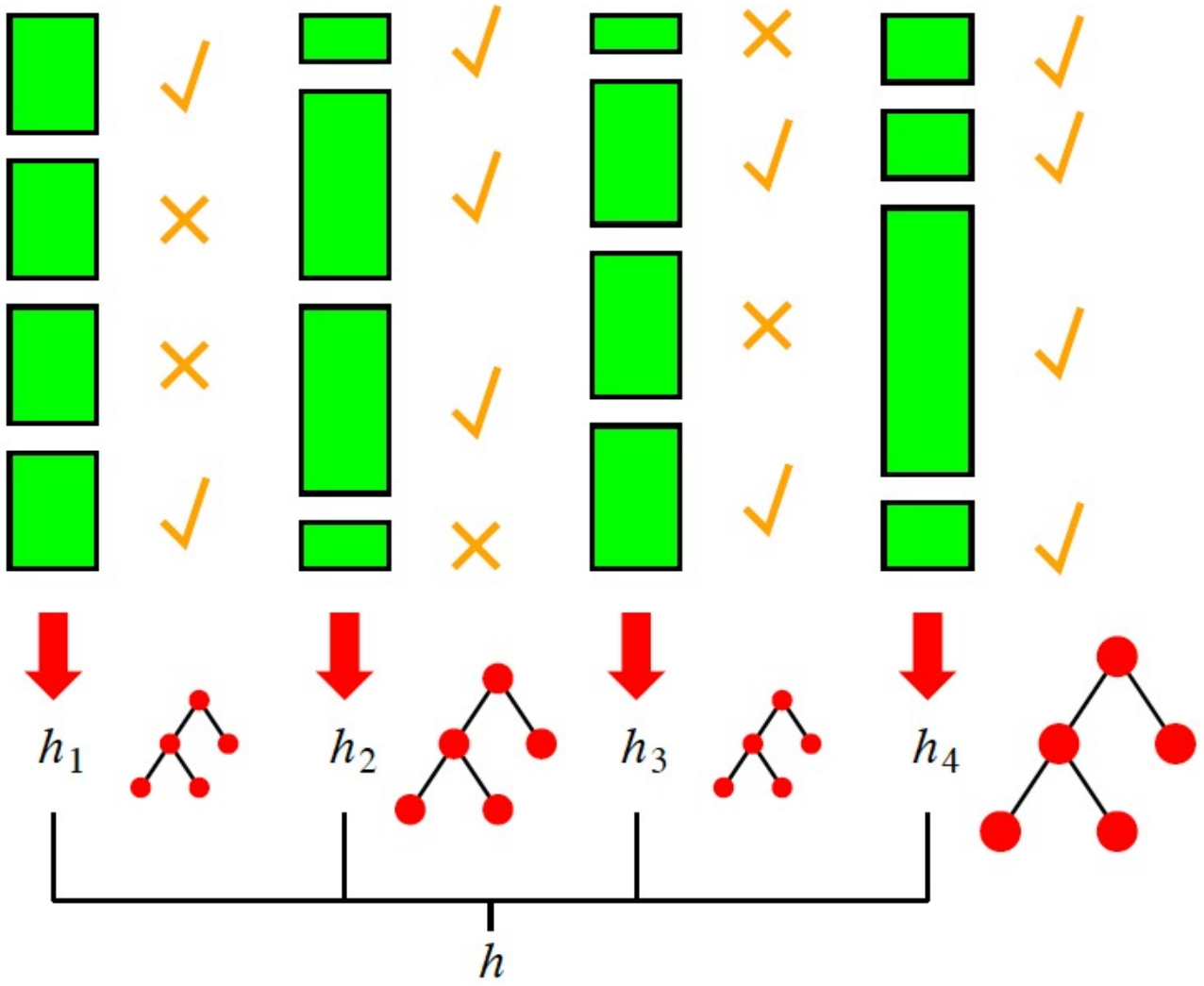
Two 'weighting' strategy:

1. Assign weights to each training example
2. Sample dataset based on weight distribution

$$M^*(x) = \text{sign}\left(\sum_{i=1}^{k} \alpha_i M_i(x)\right)$$

4. After base classifiers are trained, they are combined to give the final classifier

Adaboost



Adaboost (Freund and Schapire, 1997)

- **Input**: Training set $D = \{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\}$
- Initialize all weights $\{w_n^{(1)}\}$ to 1/N
- For round i = 1 to k,
  - Fit a classifier M_i based on weighted error function

$$J_m = \sum_{n=1}^{N} w_n^{(i)} I(M_i(x_n) \neq y_n)$$

  - Evaluate error rate $\epsilon_i = J_m / \sum w_n^{(i)}$ (stop iteration if ϵ_i < threshold)

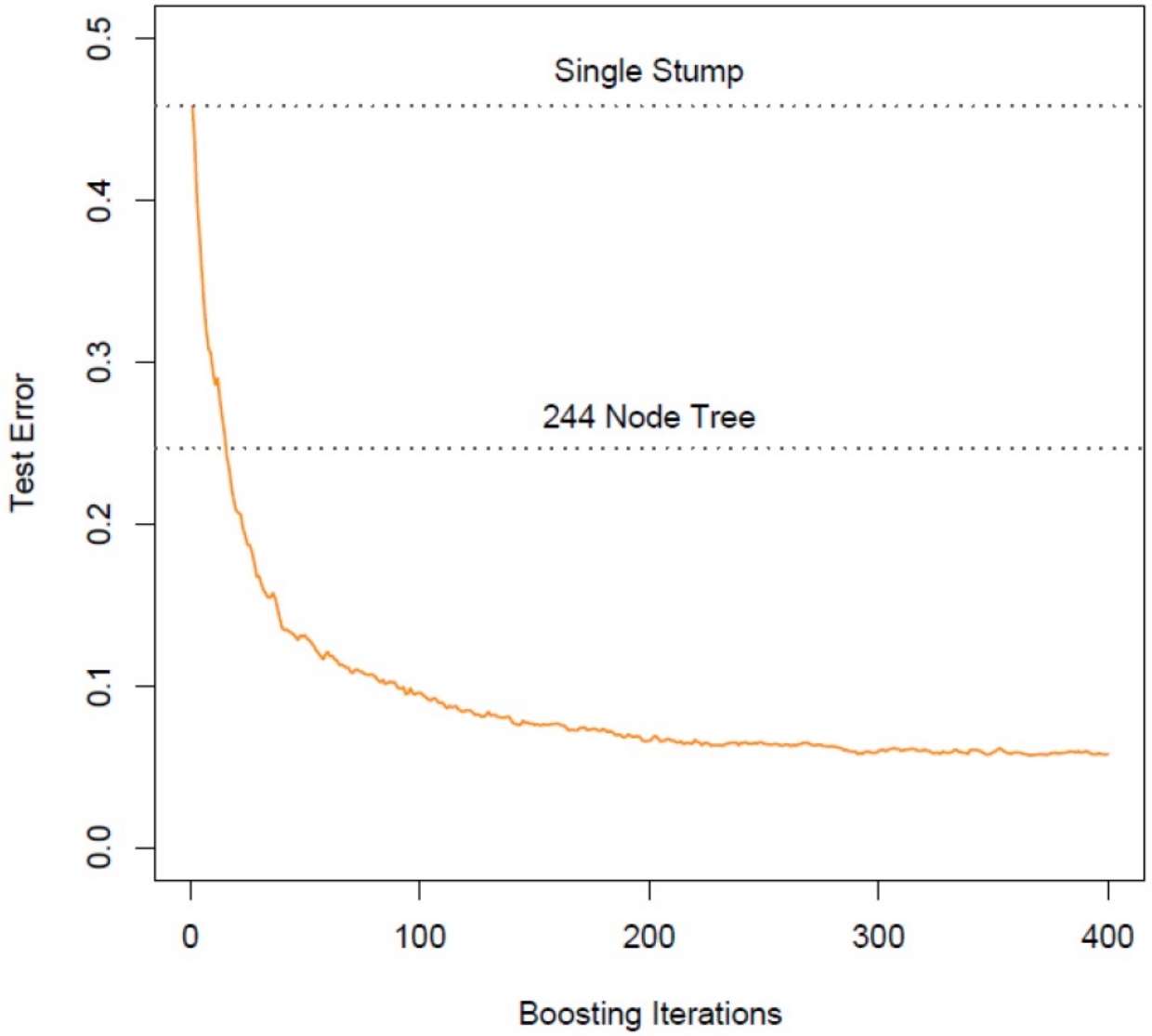
    and the base model M_i's vote $\alpha_i = \frac{1}{2} \ln\left(\frac{1-\epsilon_i}{\epsilon_i}\right)$

  - Update weights

$$w_n^{(i+1)} = w_n^{(i)} \exp\{\alpha_i \cdot I(M_i(x_n) \neq y_n)\}$$

- The final model is given by voting based on $\{\alpha_n\}$

Adaboost, with Decision Stumps



Gradient Boosting

- Operates on:
  - A differentiable loss function
  - A weak learner to make predictions (usually trees)
  - An additive model to add weak learners to minimize the loss function
- Each time adds an additional weak learner

$$
\begin{aligned}
\hat{y}_i^{(0)} &= 0 \\
\hat{y}_i^{(1)} &= f_1(x_i) = \hat{y}_i^{(0)} + f_1(x_i) \\
\hat{y}_i^{(2)} &= f_1(x_i) + f_2(x_i) = \hat{y}_i^{(1)} + f_2(x_i) \\
&\dots \\
\hat{y}_i^{(t)} &= \sum_{k=1}^{t} f_k(x_i) = \hat{y}_i^{(t-1)} + f_t(x_i)
\end{aligned}
$$

Previous model

New weak learner

- Scalable implementation: XGBoost

Gradient Boosting

Algorithm: Gradient Tree Boosting for Regression.

Input:

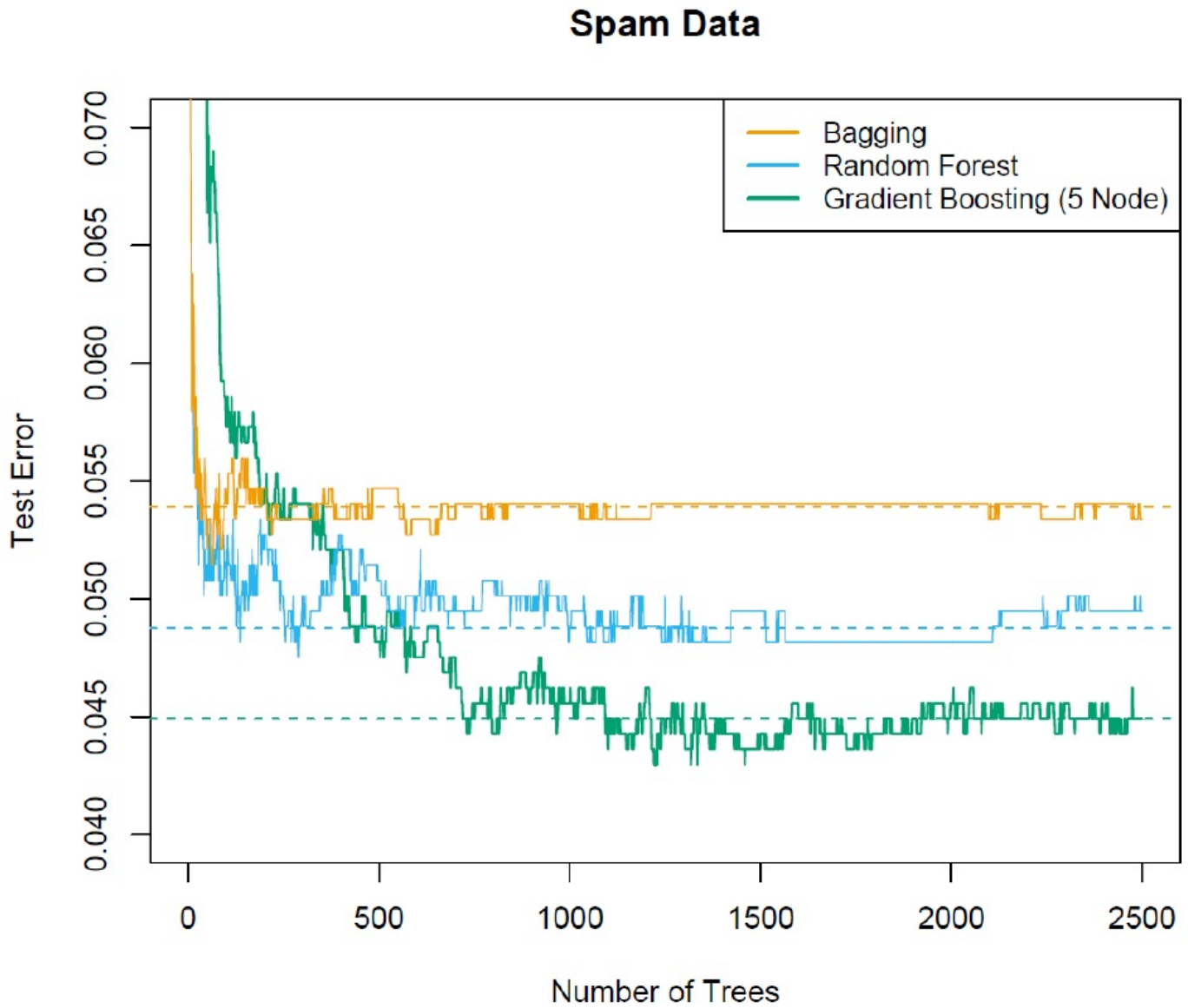
- D, a set of n training tuples $\{(x_1, y_1), ..., (x_n, y_n)\}$, where x_i is the attribute vector of the i^{th} training tuple and y_i is its true target output value;
- k, the number of rounds (one base regression model is generated per round);
- a differential loss function Loss $= \sum_{i=1}^{n} L(y_i, F(x_i))$.

Output: A composite regression model $F(x)$.

Method:

(1) initialize the regression model $F(x) = \frac{\sum_{i=1}^{n} y_i}{n}$;
(2) **for** $t = 1$ to k **do** // construct a new weak learner $M_t(x)$ for each round:
(3) **for** $i = 1$ to n //each training tuple:
(4) calculate $\hat{y}_i = F(x_i)$; //predicted value by the current model $F(x)$
(5) calculate the negative gradient $r_i = -\frac{\partial L(y_i, \hat{y}_i)}{\partial \hat{y}_i}$;
(6) **endfor**
(7) fit a regression tree model $M_t(x)$ for the training set $\{(x_1, r_1), ..., (x_n, r_n)\}$;
(8) update the composite regression model $F(x) \leftarrow F(x) + M_t(x)$.
(9) **endfor**

Ensemble Methods: Comparison



Ensemble Methods Recap

- Random forest and XGBoost are the most commonly used algorithms for tabular data
- Pros
  - Good performance for tabular data, requires no data scaling
  - Can scale to large datasets
  - Can handle missing data to some extent
- Cons
  - Can overfit to training data if not tuned properly
  - Lack of interpretability (compared to decision trees)

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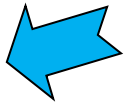
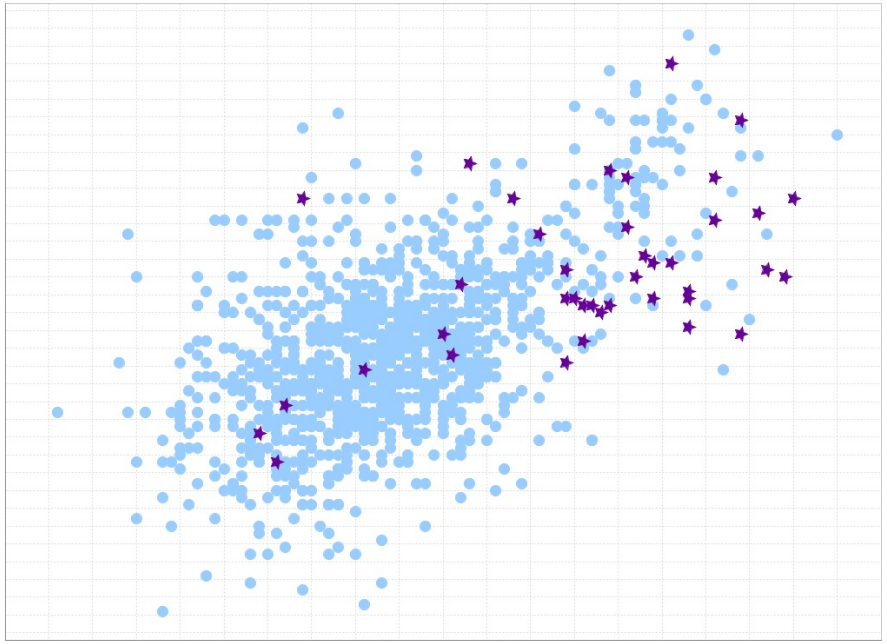


Classification of Class-Imbalanced Data Sets

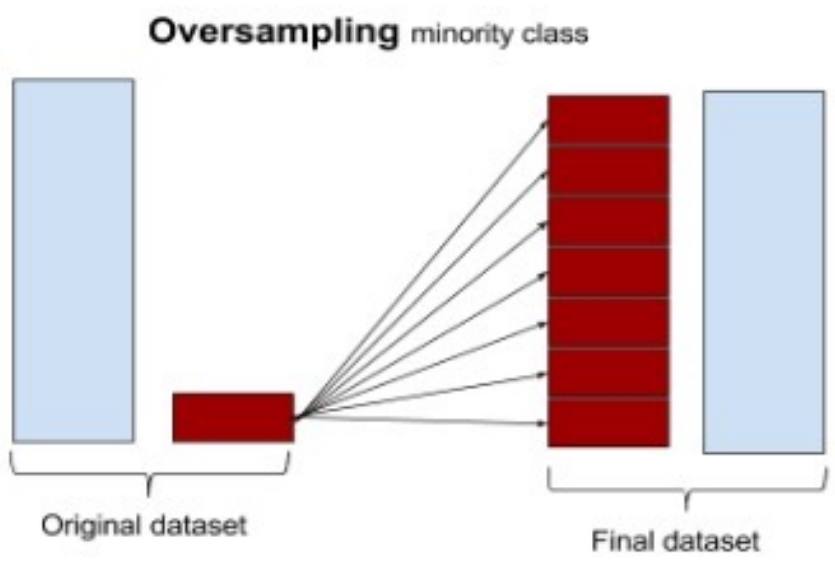
- Traditional methods assume a balanced distribution of classes and equal error costs. But in real world situations, we may face imbalanced data sets, which has rare positive examples but numerous negative ones.

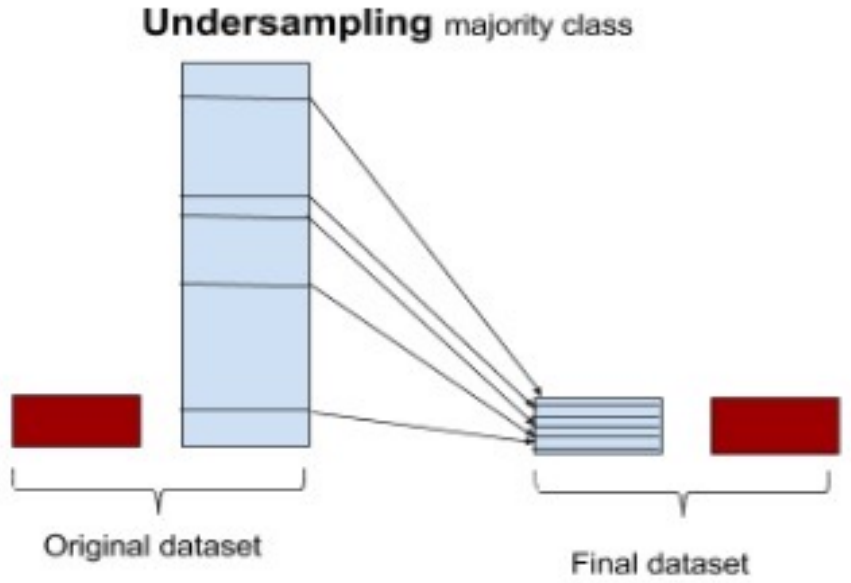


  - Medical diagnosis: Medical screening for a condition is usually performed on a large population of people without the condition, to detect a small minority with it (e.g., HIV prevalence in the USA is ~0.4%)
  - Fraud detection: About 2% of credit card accounts are defrauded per year. (Most fraud detection domains are heavily imbalanced.)
  - Product defect, accident (oil-spill), disk drive failures, etc.

Classification of Class-Imbalanced Data Sets

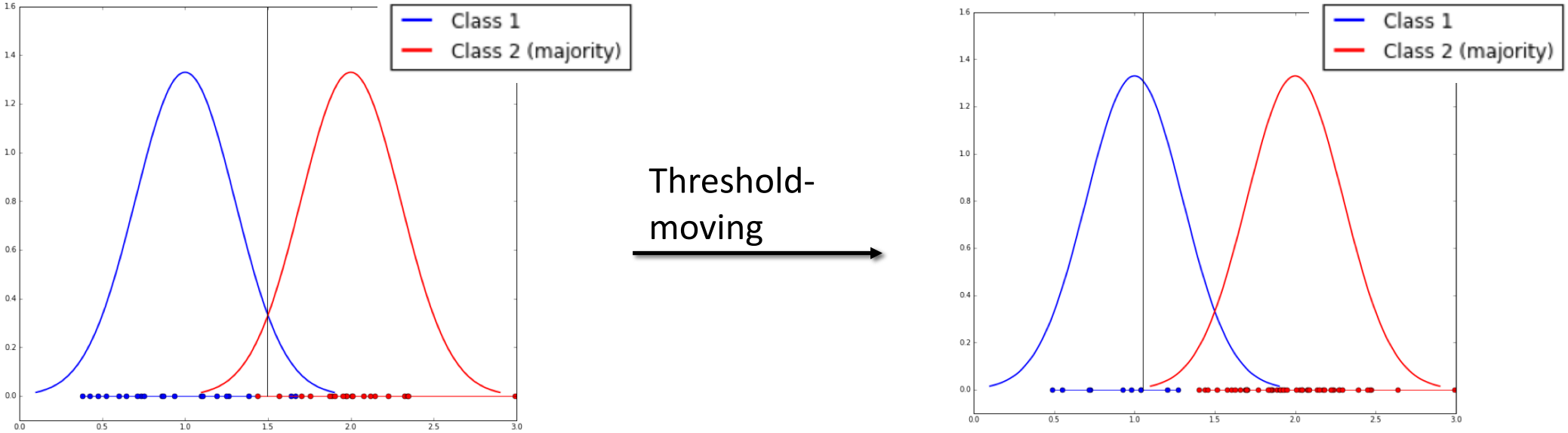
- Typical methods on imbalanced data (Balance the training set)
  - **Oversampling**: Oversample the minority class.
  - **Under-sampling**: Randomly eliminate tuples from majority class
  - **Synthesizing:** Synthesize new minority classes





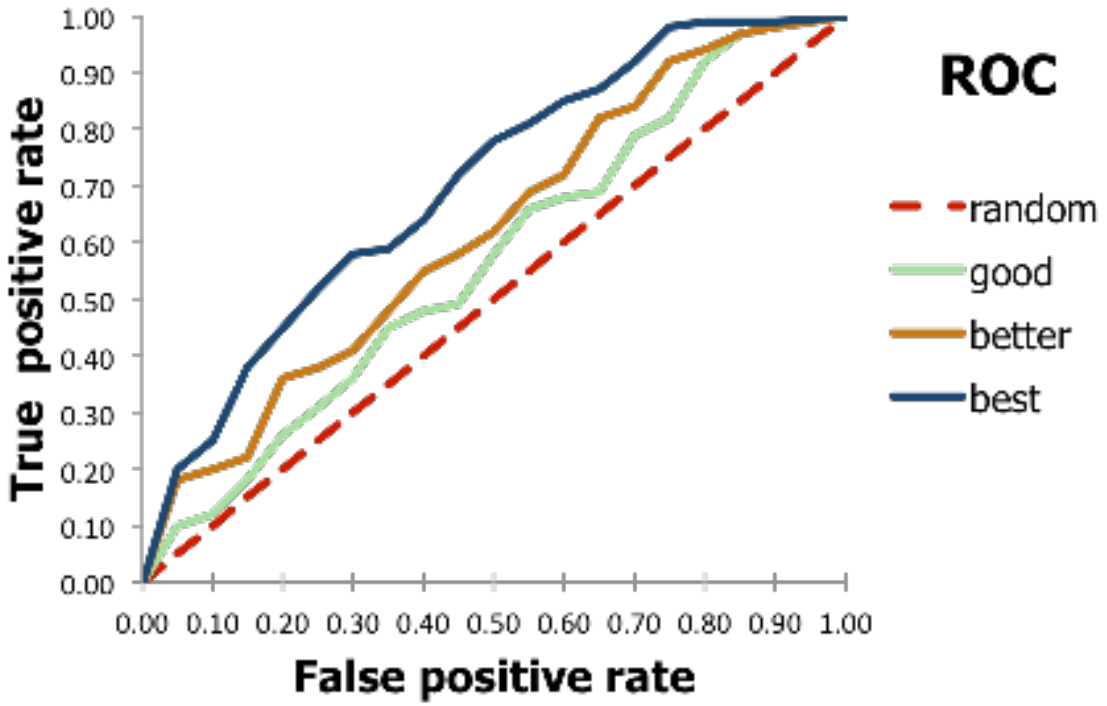
Classification of Class-Imbalanced Data Sets

- Typical methods on imbalanced data (At the algorithm level)
  - **Threshold-moving**: Move the decision threshold, t, so that the rare class tuples are easier to classify, and hence, less chance of costly false negative errors
  - **Class weight adjusting**: Since false negative costs more than false positive, we can give larger weight to false negative
- **Ensemble techniques**: Ensemble multiple classifiers introduced in the following chapter



Evaluate imbalanced data classifier

- Can we use Accuracy to evaluate imbalanced data classifier?
- Accuracy simply counts the number of errors. If a data set has 2% positive labels and 98% negative labels, a classifier that map all inputs to negative class will get an accuracy of 98%!
- ROC Curve



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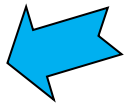
- Summary 

Summary

- Classification: Model construction from a set of training data
- Effective and scalable methods
  - Decision tree induction, Bayes classification methods, linear classifier, …
  - No single method has been found to be superior over all others for all data sets
- Evaluation metrics: Accuracy, sensitivity, specificity, precision, recall, *F* measure
- Model evaluation: Holdout, cross-validation, bootstrapping, ROC curves (AUC)
- Improve Classification Accuracy: Bagging, boosting
- Additional concepts on classification: Multiclass classification, semi-supervised classification, active learning, transfer learning, weak supervision

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