Data Mining Techniques: Classification and Prediction

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Some slides based on presentations by Han/Kamber, Tan/Steinbach/Kumar, and Andrew Moore

Classification and Prediction Overview

- Introduction
- Decision Trees
- Statistical Decision Theory
- Nearest Neighbor
- Bayesian Classification
- Artificial Neural Networks
- Support Vector Machines (SVMs)
- Prediction
- Accuracy and Error Measures
- Ensemble Methods

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Classification vs. Prediction

- Assumption: after data preparation, have single data set where each record has attributes $X_1,\ldots,X_n$, and Y.
- Goal: learn a function $f:(X_1,\ldots,X_n)\rightarrow Y$, then use this function to predict y for a given input record $(x_1,\ldots,x_n)$.
  - Classification: Y is a discrete attribute, called the class label
    - Usually a categorical attribute with small domain
  - Prediction: Y is a continuous attribute
- Called supervised learning, because true labels (Y-values) are known for the initially provided data
- Typical applications: credit approval, target marketing, medical diagnosis, fraud detection

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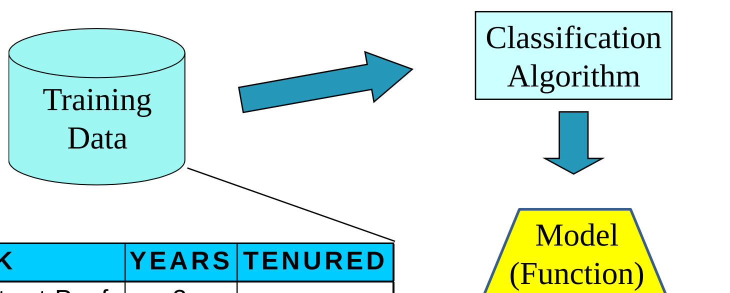
Induction: Model Construction



NAME	RANK	YEARS	TENURED
Mike	Assistant Prof	3	no
Mary	Assistant Prof	7	yes
Bill	Professor	2	yes
Jim	Associate Prof	7	yes
Dave	Assistant Prof	6	no
Anne	Associate Prof	3	no

IF rank = ‘professor’
OR years > 6
THEN tenured = ‘yes’

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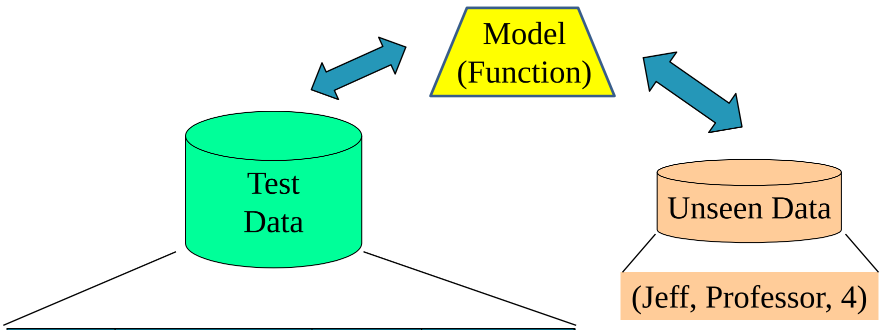
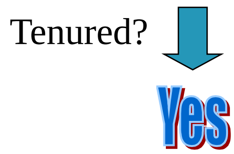
Deduction: Using the Model



NAME	RANK	YEARS	TENURED
Tom	Assistant Prof	2	no
Merlisa	Associate Prof	7	no
George	Professor	5	yes
Joseph	Assistant Prof	7	yes



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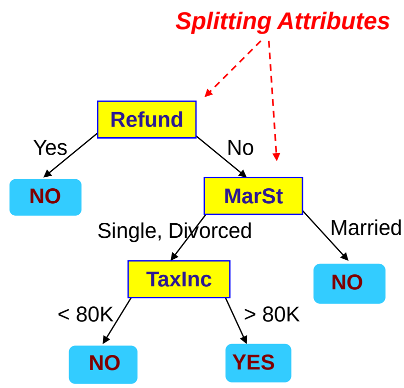
Example of a Decision Tree

categorical categorical continuous class

Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes



Training Data

Model: Decision Tree

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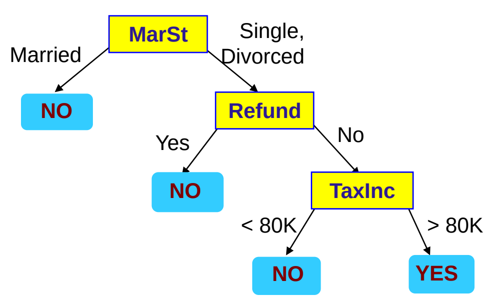
Another Example of Decision Tree

categorical categorical continuous class

Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes



There could be more than one tree that fits the same data!

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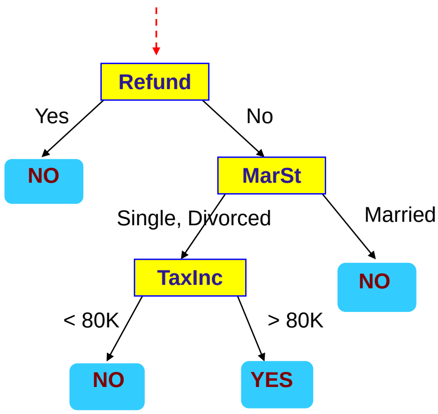
Apply Model to Test Data

Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	**?**

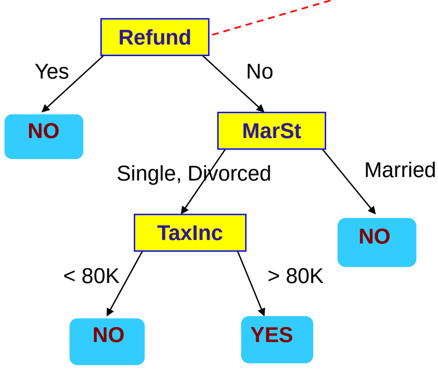
Start from the root of tree.



Apply Model to Test Data

Test Data

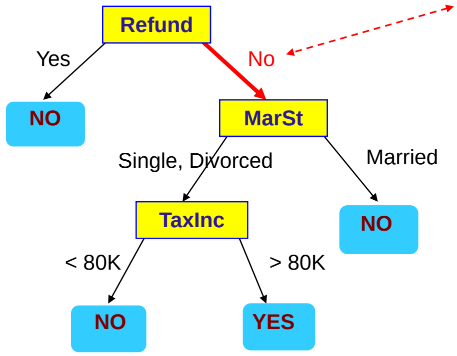
Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	**?**



Apply Model to Test Data

Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



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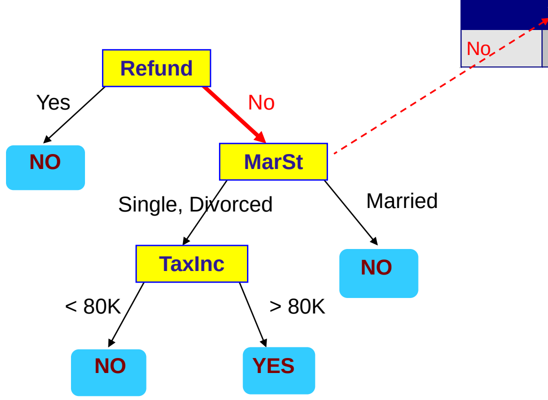
Apply Model to Test Data

Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



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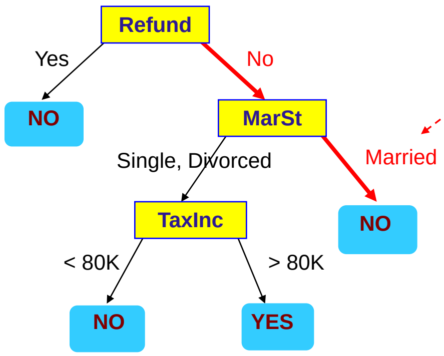
Apply Model to Test Data

Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



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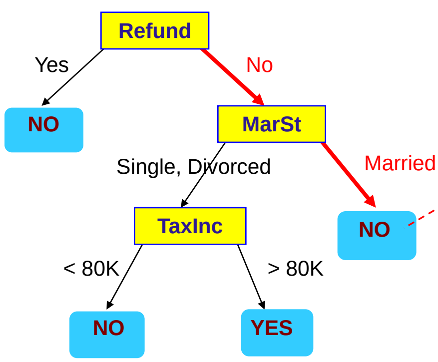
Apply Model to Test Data

Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



Assign Cheat to “No”

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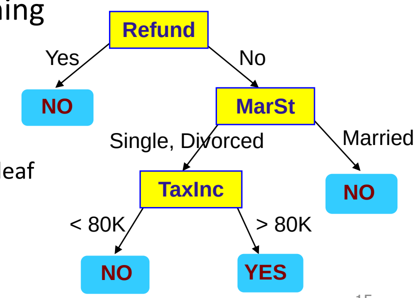
Decision Tree Induction

- Basic greedy algorithm
  - Top-down, recursive divide-and-conquer
  - At start, all the training records are at the root
  - Training records partitioned recursively based on split attributes
  - Split attributes selected based on a heuristic or statistical measure (e.g., information gain)
- Conditions for stopping partitioning
  - Pure node (all records belong to same class)
  - No remaining attributes for further partitioning
    - Majority voting for classifying the leaf
  - No cases left



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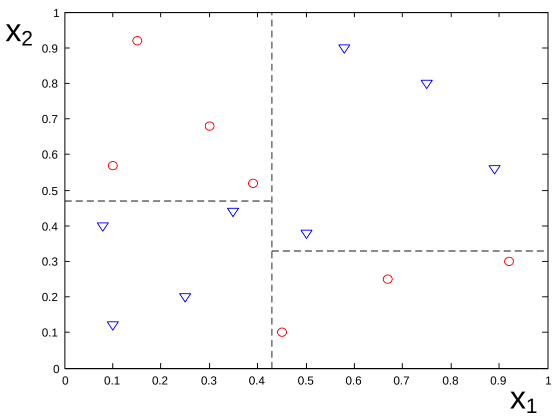
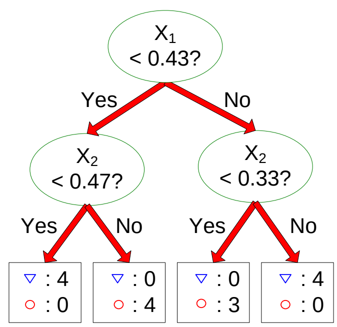
Decision Boundary





Decision boundary = border between two neighboring regions of different classes.

For trees that split on a single attribute at a time, the decision boundary is parallel to the axes.

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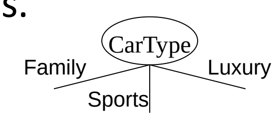
How to Specify Split Condition?

- Depends on attribute types
  - Nominal
  - Ordinal
  - Numeric (continuous)

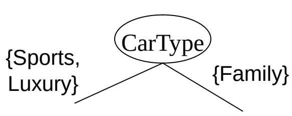
- Depends on number of ways to split
  - 2-way split
  - Multi-way split

Splitting Nominal Attributes

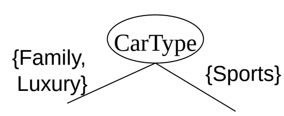
- Multi-way split: use as many partitions as distinct values.



- Binary split: divides values into two subsets; need to find optimal partitioning.

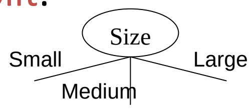


OR

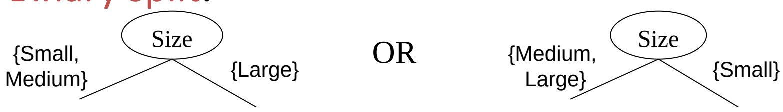


Splitting Ordinal Attributes

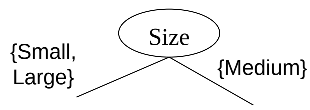
- Multi-way split:



- Binary split:



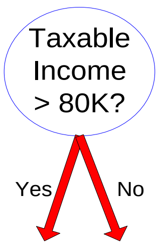
- What about this split?



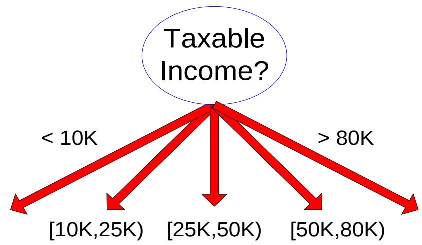
Splitting Continuous Attributes

- Different options
  - Discretization to form an ordinal categorical attribute
    - Static – discretize once at the beginning
    - Dynamic – ranges found by equal interval bucketing, equal frequency bucketing (percentiles), or clustering.
  - Binary Decision: $(A < v)$ or $(A \geq v)$
    - Consider all possible splits, choose best one

Splitting Continuous Attributes



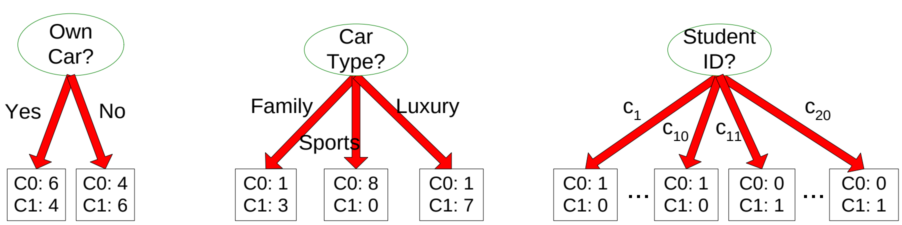
(i) Binary split



(ii) Multi-way split

How to Determine Best Split

Before Splitting: 10 records of class 0,
10 records of class 1



Which test condition is the best?

How to Determine Best Split

- Greedy approach:
  - Nodes with homogeneous class distribution are preferred
- Need a measure of node impurity:

C0: 5 C1: 5	C0: 9 C1: 1
Non-homogeneous, **High degree of impurity**	**Homogeneous,** **Low degree of impurity**

Attribute Selection Measure: Information Gain

- Select attribute with highest information gain
- p_i = probability that an arbitrary record in D belongs to class C_i, i=1,…,m
- Expected information (entropy) needed to classify a record in D:

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

- Information needed after using attribute A to split D into v partitions $D_1, \ldots, D_v$:

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

- Information gained by splitting on attribute A:

$$\text{Gain}_A(D) = \text{Info}(D) - \text{Info}_A(D)$$

Example

- Predict if somebody will buy a computer
- Given data set:

Age	Income	Student	Credit_rating	Buys_computer
≤ 30	High	No	Bad	No
≤ 30	High	No	Good	No
31…40	High	No	Bad	Yes
> 40	Medium	No	Bad	Yes
> 40	Low	Yes	Bad	Yes
> 40	Low	Yes	Good	No
31…40	Low	Yes	Good	Yes
≤ 30	Medium	No	Bad	No
≤ 30	Low	Yes	Bad	Yes
> 40	Medium	Yes	Bad	Yes
≤ 30	Medium	Yes	Good	Yes
31…40	Medium	No	Good	Yes
31…40	High	Yes	Bad	Yes
> 40	Medium	No	Good	No

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Information Gain Example

- Class P: buys_computer = "yes"
- Class N: buys_computer = "no"

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

Age	#yes	#no	I(#yes, #no)
≤ 30	2	3	0.971
31…40	4	0	0
>40	3	2	0.971

Age	Income	Student	Credit_rating	Buys_computer
≤ 30	High	No	Bad	No
≤ 30	High	No	Good	No
31…40	High	No	Bad	Yes
> 40	Medium	No	Bad	Yes
> 40	Low	Yes	Bad	Yes
> 40	Low	Yes	Good	No
31…40	Low	Yes	Good	Yes
≤ 30	Medium	No	Bad	No
≤ 30	Low	Yes	Bad	Yes
> 40	Medium	Yes	Bad	Yes
≤ 30	Medium	Yes	Good	Yes
31…40	Medium	No	Good	Yes
31…40	High	Yes	Bad	Yes
> 40	Medium	No	Good	No

$$\text{Info}_{age}(D) = \frac{5}{14}I(2,3) + \frac{4}{14}I(4,0) + \frac{5}{14}I(3,2) = 0.694$$

- $\frac{5}{14}I(2,3)$ means "age $\leq$ 30" has 5 out of 14 samples, with 2 yes'es and 3 no's.
  - Similar for the other terms
- Hence
  $$\text{Gain}_{age}(D) = \text{Info}(D) - \text{Info}_{age}(D) = 0.246$$
- Similarly,
  $$\text{Gain}_{income}(D) = 0.029$$
  $$\text{Gain}_{student}(D) = 0.151$$
  $$\text{Gain}_{credit\_rating}(D) = 0.048$$
- Therefore we choose age as the splitting attribute

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Gain Ratio for Attribute Selection

- Information gain is biased towards attributes with a large number of values
- Use gain ratio to normalize information gain:
  - $\text{GainRatio}_A(D) = \text{Gain}_A(D) / \text{SplitInfo}_A(D)$

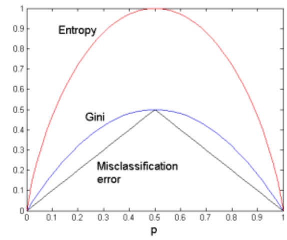
$$\text{SplitInfo}_A(D) = -\sum_{j=1}^{v} \frac{|D_j|}{|D|} \log_2\left(\frac{|D_j|}{|D|}\right)$$

- E.g., $\text{SplitInfo}_{\text{income}}(D) = -\frac{4}{14}\log_2\frac{4}{14} - \frac{6}{14}\log_2\frac{6}{14} - \frac{4}{14}\log_2\frac{4}{14} = 0.926$
- $\text{GainRatio}_{\text{income}}(D) = 0.029/0.926 = 0.031$
- Attribute with maximum gain ratio is selected as splitting attribute

Gini Index

- Gini index, gini(D), is defined as $$\text{gini}(D) = 1 - \sum_{i=1}^{m} p_i^2$$
- If data set D is split on A into v subsets $D_1, \ldots, D_v$, the gini index $\text{gini}_A(D)$ is defined as
$$\text{gini}_A(D) = \sum_{j=1}^{v} \frac{|D_j|}{|D|} \text{gini}(D_j)$$
- Reduction in Impurity:
$$\Delta \text{gini}_A(D) = \text{gini}(D) - \text{gini}_A(D)$$
- Attribute that provides smallest $\text{gini}_{\text{split}}(D)$ (= largest reduction in impurity) is chosen to split the node

Comparing Attribute Selection Measures



- No clear winner
  (and there are many more)
  - Information gain:
    - Biased towards multivalued attributes
  - Gain ratio:
    - Tends to prefer unbalanced splits where one partition is much smaller than the others
  - Gini index:
    - Biased towards multivalued attributes
    - Tends to favor tests that result in equal-sized partitions and purity in both partitions

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Practical Issues of Classification

- Underfitting and overfitting
- Missing values
- Computational cost
- Expressiveness

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How Good is the Model?

- Training set error: compare prediction of training record with true value
  - Not a good measure for the error on unseen data. (Discussed soon.)
- Test set error: for records that were **not** used for training, compare model prediction and true value
  - Use holdout data from available data set

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Training versus Test Set Error

- We'll create a training dataset

Five inputs, all bits, are generated in all 32 possible combinations

Output y = copy of e, except a random 25% of the records have y set to the opposite of e

32 records

a	b	c	d	e	y
0	0	0	0	0	0
0	0	0	0	1	0
0	0	0	1	0	0
0	0	0	1	1	1
0	0	1	0	0	1
:	:	:	:	:	:
1	1	1	1	1	1

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Test Data

- Generate test data using the same method: copy of e, but 25% inverted.
- Some y's that were corrupted in the training set will be uncorrupted in the testing set.
- Some y's that were uncorrupted in the training set will be corrupted in the test set.

a	b	c	d	e	y (training data)	y (test data)
0	0	0	0	0	0	0
0	0	0	0	1	0	1
0	0	0	1	0	0	1
0	0	0	1	1	1	1
0	0	1	0	0	1	1
:	:	:	:	:	:	:
1	1	1	1	1	1	1

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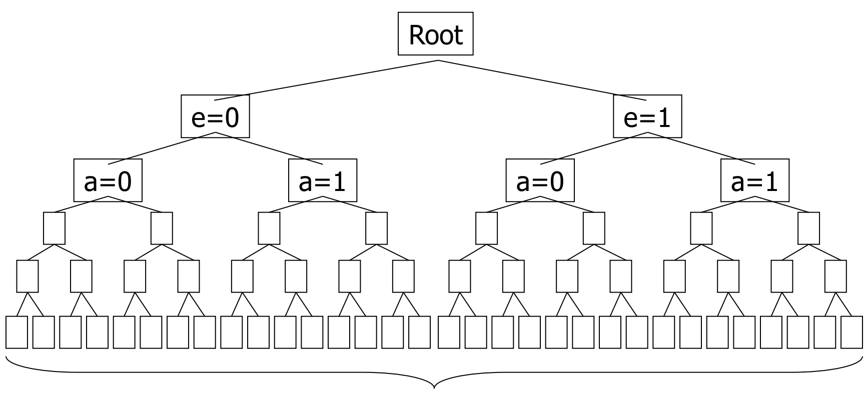
Full Tree for The Training Data



25% of these leaf node labels will be corrupted

Each leaf contains exactly one record, hence no error in predicting the training data!

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Testing The Tree with The Test Set

	1/4 of the tree nodes are corrupted	3/4 are fine
1/4 of the test set records are corrupted	1/16 of the test set will be correctly predicted for the wrong reasons	3/16 of the test set will be wrongly predicted because the test record is corrupted
3/4 are fine	3/16 of the test predictions will be wrong because the tree node is corrupted	9/16 of the test predictions will be fine

In total, we expect to be wrong on 3/8 of the test set predictions

What's This Example Shown Us?

- Discrepancy between training and test set error
- But more importantly
  - …it indicates that there is something we should do about it if we want to predict well on future data.

Suppose We Had Less Data

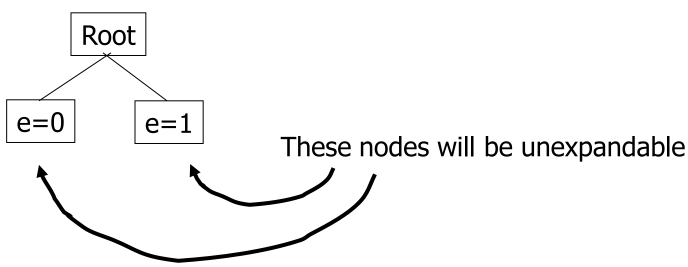
These bits are hidden

Output y = copy of e, except a random 25% of the records have y set to the opposite of e

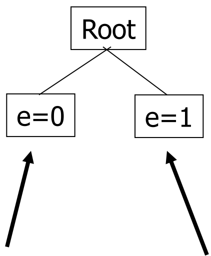
32 records

a	b	c	d	e	y
0	0	0	0	0	0
0	0	0	0	1	0
0	0	0	1	0	0
0	0	0	1	1	1
0	0	1	0	0	1
:	:	:	:	:	:
1	1	1	1	1	1

Tree Learned Without Access to The Irrelevant Bits



Tree Learned Without Access to The Irrelevant Bits



In about 12 of the 16 records in this node the output will be 0

So this will almost certainly predict 0

In about 12 of the 16 records in this node the output will be 1

So this will almost certainly predict 1

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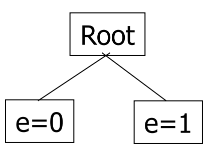
Tree Learned Without Access to The Irrelevant Bits



	almost certainly none of the tree nodes are corrupted	almost certainly all are fine
1/4 of the test set records are corrupted	n/a	1/4 of the test set will be wrongly predicted because the test record is corrupted
3/4 are fine	n/a	3/4 of the test predictions will be fine

In total, we expect to be wrong on only 1/4 of the test set predictions

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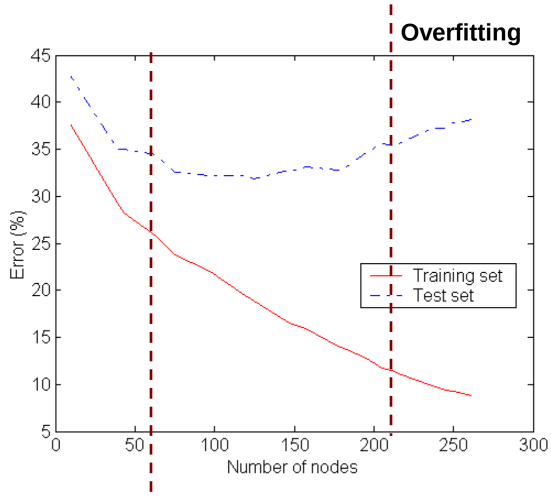
Typical Observation



Model M overfits the training data if another model M′ exists, such that M has smaller error than M′ over the training examples, but M′ has smaller error than M over the entire distribution of instances.

Underfitting: when model is too simple, both training and test errors are large

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Reasons for Overfitting

- Noise
  - Too closely fitting the training data means the model's predictions reflect the noise as well
- Insufficient training data
  - Not enough data to enable the model to generalize beyond idiosyncrasies of the training records
- Data fragmentation (special problem for trees)
  - Number of instances gets smaller as you traverse down the tree
  - Number of instances at a leaf node could be too small to make any confident decision about class

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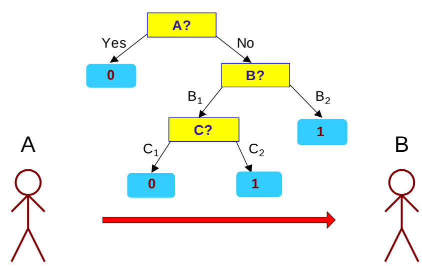
Avoiding Overfitting

- General idea: make the tree smaller
  - Addresses all three reasons for overfitting
- *Pre*pruning: Halt tree construction early
  - Do not split a node if this would result in the goodness measure falling below a threshold
  - Difficult to choose an appropriate threshold, e.g., tree for XOR
- *Post*pruning: Remove branches from a “fully grown” tree
  - Use a set of data different from the training data to decide when to stop pruning
    - Validation data: train tree on training data, prune on validation data, then test on test data

Minimum Description Length (MDL)

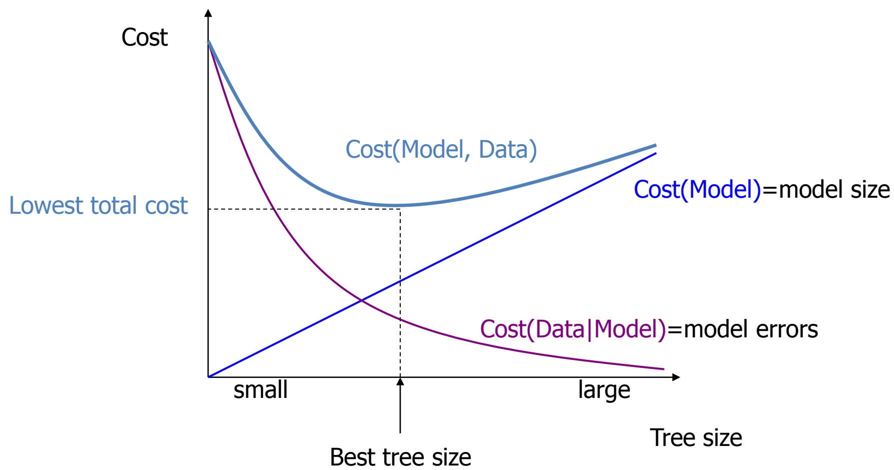
X	y
X_1	1
X_2	0
X_3	0
X_4	1
…	…
X_n	1



X	y
X_1	?
X_2	?
X_3	?
X_4	?
…	…
X_n	?

- Alternative to using validation data
  - Motivation: data mining is about finding regular patterns in data; regularity can be used to compress the data; method that achieves greatest compression found most regularity and hence is best
- Minimize Cost(Model,Data) = Cost(Model) + Cost(Data|Model)
  - Cost is the number of bits needed for encoding.
    - Cost(Data|Model) encodes the misclassification errors.
    - Cost(Model) uses node encoding plus splitting condition encoding.

MDL-Based Pruning Intuition



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Handling Missing Attribute Values

- Missing values affect decision tree construction in three different ways:
  - How impurity measures are computed
  - How to distribute instance with missing value to child nodes
  - How a test instance with missing value is classified

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Distribute Instances

Tid	Refund	Marital Status	Taxable Income	Class
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No

Refund

Yes

Class=Yes	0
Class=No	3

No

Cheat=Yes	2
Cheat=No	4

Tid	Refund	Marital Status	Taxable Income	Class
10	?	Single	90K	Yes

Refund

Yes

Class=Yes	0 + 3/9
Class=No	3

No

Class=Yes	2 + 6/9
Class=No	4

Probability that Refund=Yes is 3/9

Probability that Refund=No is 6/9

Assign record to the left child with weight = 3/9 and to the right child with weight = 6/9

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Computing Impurity Measure

Tid	Refund	Marital Status	Taxable Income	Class
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	?	Single	90K	Yes

Before Splitting: Entropy(Parent)
= -0.3 log(0.3)-(0.7)log(0.7) = 0.881

Split on Refund: assume records with missing values are distributed as discussed before

3/9 of record 10 go to Refund=Yes

6/9 of record 10 go to Refund=No

Entropy(Refund=Yes)

= -(1/3 / 10/3)log(1/3 / 10/3)

– (3 / 10/3)log(3 / 10/3) = 0.469

Entropy(Refund=No)
= -(8/3 / 20/3)log(8/3 / 20/3)

– (4 / 20/3)log(4 / 20/3) = 0.971

Entropy(Children)
= 1/3*0.469 + 2/3*0.971 = 0.804

Gain = 0.881 – 0.804 = 0.077

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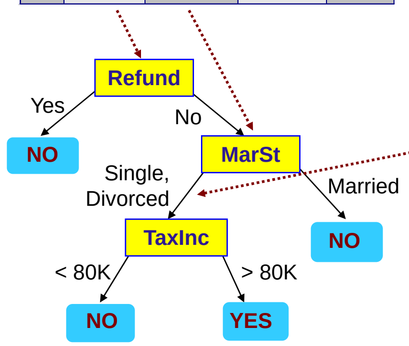
Classify Instances

New record:

Tid	Refund	Marital Status	Taxable Income	Class
11	No	?	85K	?



	Married	Single	Divorced	Total
Class=No	3	1	0	4
Class=Yes	6/9	1	1	2.67
Total	3.67	2	1	6.67

Probability that Marital Status = Married is 3.67/6.67

Probability that Marital Status ={Single,Divorced} is 3/6.67

Tree Cost Analysis

- Finding an optimal decision tree is NP-complete
  - Optimization goal: minimize expected number of binary tests to uniquely identify any record from a given finite set
- Greedy algorithm
  - O(#attributes * #training_instances * log(#training_instances))
    - At each tree depth, all instances considered
    - Assume tree depth is logarithmic (fairly balanced splits)
    - Need to test each attribute at each node
    - What about binary splits?
      - Sort data once on each attribute, use to avoid re-sorting subsets
      - Incrementally maintain counts for class distribution as different split points are explored
- In practice, trees are considered to be fast both for training (when using the greedy algorithm) and making predictions

Tree Expressiveness

- Can represent any finite discrete-valued function
  - But it might not do it very efficiently
    - Example: parity function
      - Class = 1 if there is an even number of Boolean attributes with truth value = True
      - Class = 0 if there is an odd number of Boolean attributes with truth value = True
    - For accurate modeling, must have a complete tree
- Not expressive enough for modeling continuous attributes
  - But we can still use a tree for them in practice; it just cannot accurately represent the true function

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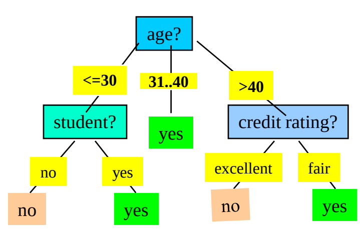
Rule Extraction from a Decision Tree

- One rule is created for each path from the root to a leaf
  - Precondition: conjunction of all split predicates of nodes on path
  - Consequent: class prediction from leaf
- Rules are mutually exclusive and exhaustive
- Example: Rule extraction from buys_computer decision-tree
  - IF age = young AND student = no THEN buys_computer = no
  - IF age = young AND student = yes THEN buys_computer = yes
  - IF age = mid-age THEN buys_computer = yes
  - IF age = old AND credit_rating = excellent THEN buys_computer = yes
  - IF age = young AND credit_rating = fair THEN buys_computer = no



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Classification in Large Databases

- Scalability: Classify data sets with millions of examples and hundreds of attributes with reasonable speed
- Why use decision trees for data mining?
  - Relatively fast learning speed
  - Can handle all attribute types
  - Convertible to simple and easy to understand classification rules
  - Good classification accuracy, but not as good as newer methods (but tree ensembles are top!)

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Scalable Tree Induction

- High cost when the training data at a node does not fit in memory
- Solution 1: special I/O-aware algorithm
  - Keep only class list in memory, access attribute values on disk
  - Maintain separate list for each attribute
  - Use count matrix for each attribute
- Solution 2: Sampling
  - Common solution: train tree on a sample that fits in memory
  - More sophisticated versions of this idea exist, e.g., *Rainforest*
    - Build tree on sample, but do this for many bootstrap samples
    - Combine all into a single new tree that is guaranteed to be almost identical to the one trained from entire data set
    - Can be computed with two data scans

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Tree Conclusions

- Very popular data mining tool
  - Easy to understand
  - Easy to implement
  - Easy to use
    - Little tuning, handles all attribute types and missing values
  - Computationally cheap
- Overfitting problem
- Focused on classification, but easy to extend to prediction (future lecture)

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Classification and Prediction Overview

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- Ensemble Methods

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Theoretical Results

- Trees make sense intuitively, but can we get some hard evidence and deeper understanding about their properties?
- Statistical decision theory can give some answers
- Need some probability concepts first

Random Variables

- Intuitive version of the definition:
  - Can take on one of possibly many values, each with a certain probability (discrete versus continuous)
  - These probabilities define the probability distribution of the random variable
  - E.g., let X be the outcome of a coin toss, then Pr(X='heads')=0.5 and Pr(X='tails')=0.5; distribution is uniform
- Consider a discrete random variable X with numeric values $x_1,\ldots,x_k$
  - Expectation: $E[X] = \Sigma\, x_i * Pr(X=x_i)$
  - Variance: $Var(X) = E[(X – E[X])^2] = E[X^2] – (E[X])^2$

Working with Random Variables

- $E[X + Y] = E[X] + E[Y]$
- $Var(X + Y) = Var(X) + Var(Y) + 2\ Cov(X,Y)$
- For constants a, b
  - $E[aX + b] = a\ E[X] + b$
  - $Var(aX + b) = Var(aX) = a^2\ Var(X)$
- Iterated expectation:
  - $E[X] = E_X[\ E_Y[Y|\ X]\ ]$, where $E_Y[Y|\ X] = \Sigma y_i * Pr(Y=y_i|\ X=x)$ is the expectation of Y for a given value of X, i.e., is a function of X
  - In general for any function f(X,Y): $E_{X,Y}[f(X,Y)] = E_X[\ E_Y[f(X,Y)|\ X]\ ]$

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What is the Optimal Model f(X)?

Let X denote a real - valued random input variable and Y a real - valued random output variable

The squared error of trained model $f(X)$ is $\mathrm{E}_{X,Y}\left[(Y - f(X))^2\right]$

Which function $f(X)$ will minimize the squared error?

Consider the error for a specific value of X and let $\bar{Y} = \mathrm{E}_Y[Y \mid X]$:

$$\mathrm{E}_Y\left[(Y - f(X))^2 \mid X\right] = \mathrm{E}_Y\left[(Y - \bar{Y} + \bar{Y} - f(X))^2 \mid X\right]$$
$$= \mathrm{E}_Y\left[(Y - \bar{Y})^2 \mid X\right] + \mathrm{E}_Y\left[(\bar{Y} - f(X))^2 \mid X\right] + 2\,\mathrm{E}_Y\left[(Y - \bar{Y})(\bar{Y} - f(X)) \mid X\right]$$
$$= \mathrm{E}_Y\left[(Y - \bar{Y})^2 \mid X\right] + \left(\bar{Y} - f(X)\right)^2 + 2(\bar{Y} - f(X))\,\mathrm{E}_Y\left[(Y - \bar{Y}) \mid X\right]$$
$$= \mathrm{E}_Y\left[(Y - \bar{Y})^2 \mid X\right] + \left(\bar{Y} - f(X)\right)^2$$

$$(\text{Notice}: \mathrm{E}_Y\left[(Y - \bar{Y}) \mid X\right] = \mathrm{E}_Y\left[Y \mid X\right] - \mathrm{E}_Y\left[\bar{Y} \mid X\right] = \bar{Y} - \bar{Y} = 0)$$

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Optimal Model f(X) (cont.)

The choice of $f(X)$ does not affect $\mathrm{E}_Y\left[(Y-\bar{Y})^2 \mid X\right]$, but $\left(\bar{Y}-f(X)\right)^2$ is minimized for $f(X)=\bar{Y}=\mathrm{E}_Y[Y \mid X]$.

Note that $\mathrm{E}_{X,Y}\left[(Y-f(X))^2\right]=\mathrm{E}_X\left[\mathrm{E}_Y\left[(Y-f(X))^2 \mid X\right]\right]$. Hence

$$\mathrm{E}_{X,Y}\left[(Y-f(X))^2\right]=\mathrm{E}_X\left[\mathrm{E}_Y\left[(Y-\bar{Y})^2 \mid X\right]+\left(\bar{Y}-f(X)\right)^2\right]$$

Hence the squared error is minimzed by choosing $f(X)=\mathrm{E}_Y[Y \mid X]$ for every X.

(Notice that for minimizing absolute error $\mathrm{E}_{X,Y}\left[|\,Y-f(X)\,|\right]$, one can show that the best model is $f(X)=\mathrm{median}(X \mid Y)$.)

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Implications for Trees

- Best prediction for input X=x is the mean of the Y-values of all records (x(i),y(i)) with x(i)=x
- What about classification?
  - Two classes: encode as 0 and 1, use squared error as before
    - Get f(X) = E[Y| X=x] = 1*Pr(Y=1| X=x) + 0*Pr(Y=0| X=x) = Pr(Y=1| X=x)
  - K classes: can show that for 0-1 loss (error = 0 if correct class, error = 1 if wrong class predicted) the optimal choice is to return the majority class for a given input X=x
    - Called the Bayes classifier
- Problem: How can we estimate E[Y| X=x] or the majority class for X=x from the training data?
  - Often there is just one or no training record for a given X=x
- Solution: approximate it
  - Use Y-values from training records in *neighborhood* around X=x
  - Tree: leaf defines neighborhood in the data space; make sure there are enough records in the leaf to obtain reliable estimate of correct answer

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Bias-Variance Tradeoff

- Let's take this one step further and see if we can understand overfitting through statistical decision theory
- As before, consider two random variables X and Y
- From a training set D with n records, we want to construct a function f(X) that returns good approximations of Y for future inputs X
  - Make dependence of f on D explicit by writing f(X; D)
- Goal: minimize mean squared error over all X, Y, and D, i.e., $E_{X,D,Y}[\ (Y - f(X;D))^2\ ]$

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Bias-Variance Tradeoff Derivation

$E_{X,D,Y}\left[(Y - f(X;D))^2\right] = E_X E_D E_Y\left[(Y - f(X;D))^2 \mid X, D\right]$ Now consider the inner term:

$E_D E_Y\left[(Y - f(X;D))^2 \mid X, D\right] = E_D\left[E_Y\left[(Y - E[Y \mid X])^2 \mid X, D\right] + \left(f(X;D) - E[Y \mid X]\right)^2\right]$

(Same derivation as before for optimal function f(X).)

$= E_Y\left[(Y - E[Y \mid X])^2 \mid X\right] + E_D\left[\left(f(X;D) - E[Y \mid X]\right)^2\right]$

(The first term does not depend on D, hence $E_D\left[E_Y\left[(Y - E[Y \mid X])^2 \mid X, D\right]\right] = E_Y\left[(Y - E[Y \mid X])^2 \mid X\right]$)

Consider the second term:

$E_D\left[\left(f(X;D) - E[Y \mid X]\right)^2\right] = E_D\left[\left(\left(f(X;D) - E_D[f(X;D)\right) + \left(E_D[f(X;D)] - E[Y \mid X]\right)\right)^2\right]$

$= E_D\left[\left(f(X;D) - E_D[f(X;D)]\right)^2\right] + E_D\left[\left(E_D[f(X;D)] - E[Y \mid X]\right)^2\right]$

$\quad + 2E_D\left[\left(\left(f(X;D) - E_D[f(X;D)\right) \cdot \left(E_D[f(X;D)] - E[Y \mid X]\right)\right)\right]$

$= E_D\left[\left(f(X;D) - E_D[f(X;D)]\right)^2\right] + \left(E_D[f(X;D)] - E[Y \mid X]\right)^2$

$\quad + 2E_D\left[f(X;D) - E_D[f(X;D)]\right] \cdot \left(E_D[f(X;D)] - E[Y \mid X]\right)$

$= E_D\left[\left(f(X;D) - E_D[f(X;D)]\right)^2\right] + \left(E_D[f(X;D)] - E[Y \mid X]\right)^2$

(The third term is zero, because $E_D\left[f(X;D) - E_D[f(X;D)]\right] = E_D[f(X;D)] - E_D[f(X;D)] = 0$.)

Overall we therefore obtain:

$E_{X,D,Y}\left[(Y - f(X;D))^2\right] = E_X\left[\left(E_D[f(X;D)] - E[Y \mid X]\right)^2 + E_D\left[\left(f(X;D) - E_D[f(X;D)]\right)^2\right] + E_Y\left[(Y - E[Y \mid X])^2 \mid X\right]\right]$

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Bias-Variance Tradeoff and Overfitting

$(E_D[f(X;D)] - E[Y \mid X])^2$: **bias**

$E_D\left[(f(X;D) - E_D[f(X;D)])^2\right]$: **variance**

$E_Y\left[(Y - E[Y \mid X])^2 \mid X\right]$: **irreducible error** (does not depend on f and is simply the variance of Y given X.)

- Option 1: $f(X;D) = E[Y| X,D]$
  - Bias: since $E_D[E[Y| X,D]] = E[Y| X]$, bias is zero
  - Variance: $(E[Y| X,D]-E_D[E[Y| X,D]])^2 = (E[Y| X,D]-E[Y| X])^2$ can be very large since $E[Y| X,D]$ depends heavily on D
  - Might overfit!
- Option 2: $f(X;D)=X$ (or other function independent of D)
  - Variance: $(X-E_D[X])^2=(X-X)^2=0$
  - Bias: $(E_D[X]-E[Y| X])^2=(X-E[Y| X])^2$ can be large, because $E[Y| X]$ might be completely different from X
  - Might underfit!
- Find best compromise between fitting training data too closely (option 1) and completely ignoring it (option 2)

Implications for Trees

- Bias decreases as tree becomes larger
  - Larger tree can fit training data better
- Variance increases as tree becomes larger
  - Sample variance affects predictions of larger tree more
- Find right tradeoff as discussed earlier
  - Validation data to find best pruned tree
  - MDL principle

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Lazy vs. Eager Learning

- Lazy learning: Simply stores training data (or only minor processing) and waits until it is given a test record
- Eager learning: Given a training set, constructs a classification model before receiving new (test) data to classify
- General trend: Lazy = faster training, slower predictions
- Accuracy: not clear which one is better!
  - Lazy method: typically driven by local decisions
  - Eager method: driven by global and local decisions

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Nearest-Neighbor

- Recall our statistical decision theory analysis: Best prediction for input X=x is the mean of the Y-values of all records (x(i),y(i)) with x(i)=x (majority class for classification)
- Problem was to estimate E[Y| X=x] or majority class for X=x from the training data
- Solution was to approximate it
  - Use Y-values from training records in neighborhood around X=x

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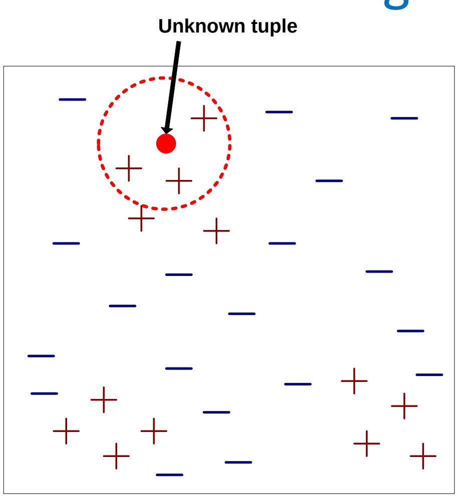
Nearest-Neighbor Classifiers



- Requires:
  - Set of stored records
  - Distance metric for pairs of records
    - Common choice: Euclidean

$$d(\mathbf{p},\mathbf{q}) = \sqrt{\sum_i (p_i - q_i)^2}$$

  - Parameter k
    - Number of nearest neighbors to retrieve
- To classify a record:
  - Find its k nearest neighbors
  - Determine output based on (distance-weighted) average of neighbors' output

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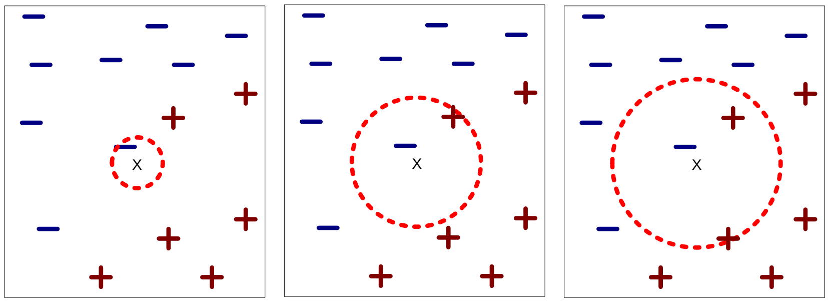
Definition of Nearest Neighbor



(a) 1-nearest neighbor (b) 2-nearest neighbor (c) 3-nearest neighbor

K-nearest neighbors of a record x are data points that have the k smallest distance to x

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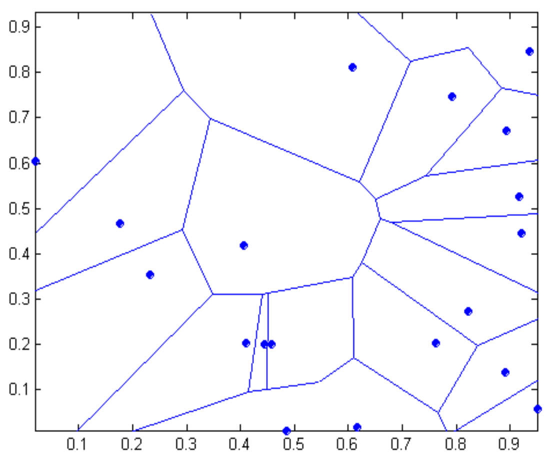
1-Nearest Neighbor

Voronoi Diagram



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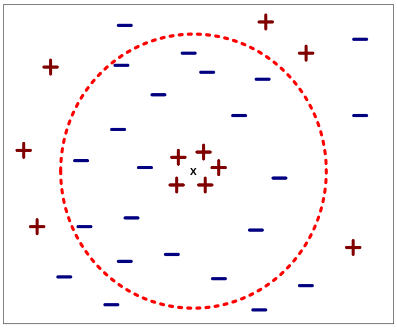
Nearest Neighbor Classification

- Choosing the value of k:
  - k too small: sensitive to noise points
  - k too large: neighborhood may include points from other classes



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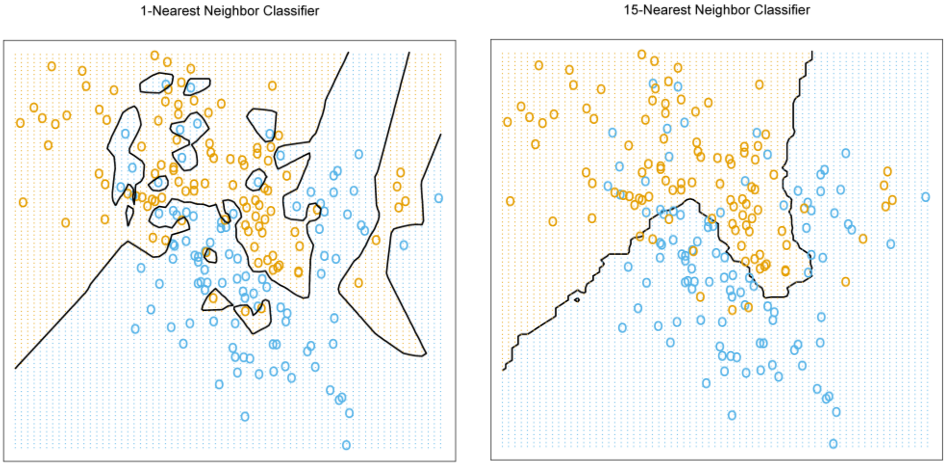
Effect of Changing k



Source: Hastie, Tibshirani, and Friedman. The Elements of Statistical Learning

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Explaining the Effect of k

- Recall the bias-variance tradeoff
- Small k, i.e., predictions based on few neighbors
  - High variance, low bias
- Large k, e.g., average over entire data set
  - Low variance, but high bias
- Need to find k that achieves best tradeoff
- Can do that using validation data

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Scaling Issues

- Attributes may have to be scaled to prevent distance measures from being dominated by one of the attributes
- Example:
  - Height of a person may vary from 1.5m to 1.8m
  - Weight of a person may vary from 90lb to 300lb
  - Income of a person may vary from $10K to $1M
  - Income difference would dominate record distance

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Other Problems

- Problem with Euclidean measure:
  - High dimensional data: curse of dimensionality
  - Can produce counter-intuitive results

1 1 1 1 1 1 1 1 1 1 1 0	vs	1 0 0 0 0 0 0 0 0 0 0 0
0 1 1 1 1 1 1 1 1 1 1 1		0 0 0 0 0 0 0 0 0 0 0 1
d = 1.4142		**d = 1.4142**

  - Solution: Normalize the vectors to unit length
- Irrelevant attributes might dominate distance
  - Solution: eliminate them

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Computational Cost

- Brute force: O(#trainingRecords)
  - For each training record, compute distance to test record, keep if among top-k
- Pre-compute Voronoi diagram (expensive), then search spatial index of Voronoi cells: if lucky O(log(#trainingRecords))
- Store training records in multi-dimensional search tree, e.g., R-tree: if lucky O(log(#trainingRecords))
- Bulk-compute predictions for many test records using spatial join between training and test set
  - Same worst-case cost as one-by-one predictions, but usually much faster in practice

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Bayesian Classification

- Performs probabilistic prediction, i.e., predicts class membership probabilities
- Based on Bayes' Theorem
- Incremental training
  - Update probabilities as new training records arrive
  - Can combine prior knowledge with observed data
- Even when Bayesian methods are computationally intractable, they can provide a standard of optimal decision making against which other methods can be measured

Bayesian Theorem: Basics

- **X** = random variable for data records ("evidence")
- H = hypothesis that specific record **X**=**x** belongs to class C
- Goal: determine P(H| **X**=**x**)
  - Probability that hypothesis holds given a record **x**
- P(H) = prior probability
  - The initial probability of the hypothesis
  - E.g., person **x** will buy computer, regardless of age, income etc.
- P(**X**=**x**) = probability that data record **x** is observed
- P(**X**=**x**| H) = probability of observing record **x**, given that the hypothesis holds
  - E.g., given that **x** will buy a computer, what is the probability that **x** is in age group 31...40, has medium income, etc.?

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Bayes' Theorem

- Given data record **x**, the posterior probability of a hypothesis H, P(H| **X**=**x**), follows from Bayes theorem:

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

- Informally: posterior = likelihood * prior / evidence
- Among all candidate hypotheses H, find the maximally probably one, called maximum a posteriori (MAP) hypothesis
- Note: P(**X**=**x**) is the same for all hypotheses
- If all hypotheses are equally probable a priori, we only need to compare P(**X**=**x**| H)
  - Winning hypothesis is called the maximum likelihood (ML) hypothesis
- Practical difficulties: requires initial knowledge of many probabilities and has high computational cost

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Towards Naïve Bayes Classifier

- Suppose there are m classes $C_1, C_2, \ldots, C_m$
- Classification goal: for record **x**, find class C_i that has the maximum posterior probability $P(C_i | \mathbf{X}=\mathbf{x})$
- Bayes' theorem:

$$P(C_i | \mathbf{X}=\mathbf{x}) = \frac{P(\mathbf{X}=x | C_i) P(C_i)}{P(\mathbf{X}=\mathbf{x})}$$

- Since $P(\mathbf{X}=\mathbf{x})$ is the same for all classes, only need to find maximum of $P(\mathbf{X}=\mathbf{x} | C_i) P(C_i)$

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Computing $P(\mathbf{X}=\mathbf{x}|C_i)$ and $P(C_i)$

- Estimate $P(C_i)$ by counting the frequency of class C_i in the training data
- Can we do the same for $P(\mathbf{X}=\mathbf{x}|C_i)$?
  - Need very large set of training data
  - Have $|X_1|*|X_2|*\ldots*|X_d|*m$ different combinations of possible values for X and C_i
  - Need to see every instance **x** many times to obtain reliable estimates
- Solution: decompose into lower-dimensional problems

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Example: Computing P(**X**=**x**|C_i) and P(C_i)

- P(buys_computer = yes) = 9/14
- P(buys_computer = no) = 5/14
- P(age>40, income=low, student=no, credit_rating=bad| buys_computer=yes) = 0 ?

Age	Income	Student	Credit_rating	Buys_computer
≤ 30	High	No	Bad	No
≤ 30	High	No	Good	No
31...40	High	No	Bad	Yes
> 40	Medium	No	Bad	Yes
> 40	Low	Yes	Bad	Yes
> 40	Low	Yes	Good	No
31...40	Low	Yes	Good	Yes
≤ 30	Medium	No	Bad	No
≤ 30	Low	Yes	Bad	Yes
> 40	Medium	Yes	Bad	Yes
≤ 30	Medium	Yes	Good	Yes
31...40	Medium	No	Good	Yes
31...40	High	Yes	Bad	Yes
> 40	Medium	No	Good	No

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Conditional Independence

- X, Y, Z random variables
- X is conditionally independent of Y, given Z, if P(X| Y,Z) = P(X| Z)
  – Equivalent to: P(X,Y| Z) = P(X| Z) * P(Y| Z)
- Example: people with longer arms read better
  – Confounding factor: age
    - Young child has shorter arms and lacks reading skills of adult
  – If age is fixed, observed relationship between arm length and reading skills disappears

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Derivation of Naïve Bayes Classifier

- Simplifying assumption: all input attributes conditionally independent, given class

$$P(\mathbf{X}=(x_1,\ldots,x_d)\,|\,C_i)=\prod_{k=1}^{d}P(X_k=x_k\,|\,C_i)=P(X_1=x_1\,|\,C_i)\cdot P(X_2=x_2\,|\,C_i)\cdots P(X_d=x_d\,|\,C_i)$$

- Each $P(X_k=x_k|\ C_i)$ can be estimated robustly
  - If X_k is categorical attribute
    - $P(X_k=x_k|\ C_i)$ = #records in C_i that have value x_k for X_k, divided by #records of class C_i in training data set
  - If X_k is continuous, we could discretize it
    - Problem: interval selection
      - Too many intervals: too few training cases per interval
      - Too few intervals: limited choices for decision boundary

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Estimating $P(X_k=x_k|\ C_i)$ for Continuous Attributes without Discretization

- $P(X_k=x_k|\ C_i)$ computed based on Gaussian distribution with mean μ and standard deviation σ:

$$g(x,\mu,\sigma)=\frac{1}{\sqrt{2\pi}\sigma}e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

as

$$\mathrm{P}(X_k=x_k\,|\,C_i)=g(x_k,\mu_{k,C_i},\sigma_{k,C_i})$$

- Estimate $\mu_{k,Ci}$ from sample mean of attribute X_k for all training records of class C_i
- Estimate $\sigma_{k,Ci}$ similarly from sample

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Naïve Bayes Example

- Classes:
  - C_1:buys_computer = yes
  - C_2:buys_computer = no
- Data sample **x**
  - age ≤ 30,
  - income = medium,
  - student = yes, and
  - credit_rating = fair

Age	Income	Student	Credit_rating	Buys_computer
≤ 30	High	No	Bad	No
≤ 30	High	No	Good	No
31…40	High	No	Bad	Yes
> 40	Medium	No	Bad	Yes
> 40	Low	Yes	Bad	Yes
> 40	Low	Yes	Good	No
31…40	Low	Yes	Good	Yes
≤ 30	Medium	No	Bad	No
≤ 30	Low	Yes	Bad	Yes
> 40	Medium	Yes	Bad	Yes
≤ 30	Medium	Yes	Good	Yes
31…40	Medium	No	Good	Yes
31…40	High	Yes	Bad	Yes
> 40	Medium	No	Good	No

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Naïve Bayesian Computation

- Compute $P(C_i)$ for each class:
  - P(buys_computer = “yes”) = 9/14 = 0.643
  - P(buys_computer = “no”) = 5/14= 0.357
- Compute $P(X_k=x_k| C_i)$ 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
- Compute P(**X**=**x**| C_i) using the Naive Bayes assumption
  - P(≤30, medium, yes, fair |buys_computer = “yes”) = 0.222 * 0.444 * 0.667 * 0.667 = 0.044
  - P(≤30, medium, yes, fair | buys_computer = “no”) = 0.6 * 0.4 * 0.2 * 0.4 = 0.019
- Compute final result P(**X**=**x**| C_i) * P(C_i)
  - P(**X**=**x** | buys_computer = “yes”) * P(buys_computer = “yes”) = 0.028
  - P(**X**=**x** | buys_computer = “no”) * P(buys_computer = “no”) = 0.007
- Therefore we predict buys_computer = “yes” for
  input **x** = (age = “≤30”, income = “medium”, student = “yes”, credit_rating = “fair”)

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Zero-Probability Problem

- Naïve Bayesian prediction requires each conditional probability to be non-zero (why?)

$$P(\mathbf{X}=(x_1,\ldots,x_d)\,|\,C_i)=\prod_{k=1}^{d}P(X_k=x_k\,|\,C_i)=P(X_1=x_1\,|\,C_i)\cdot P(X_2=x_2\,|\,C_i)\cdots P(X_d=x_d\,|\,C_i)$$

- Example: 1000 records for buys_computer=yes with income=low (0), income= medium (990), and income = high (10)
  - For input with income=low, conditional probability is zero
- Use Laplacian correction (or Laplace estimator) by adding 1 dummy record to each income level
    - Prob(income = low) = 1/1003
    - Prob(income = medium) = 991/1003
    - Prob(income = high) = 11/1003
  - "Corrected" probability estimates close to their "uncorrected" counterparts, but none is zero

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Naïve Bayesian Classifier: Comments

- Easy to implement
- Good results obtained in many cases
  - Robust to isolated noise points
  - Handles missing values by ignoring the instance during probability estimate calculations
  - Robust to irrelevant attributes
- Disadvantages
  - Assumption: class conditional independence, therefore loss of accuracy
  - Practically, dependencies exist among variables
- How to deal with these dependencies?

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Probabilities

- Summary of elementary probability facts we have used already and/or will need soon
- Let X be a random variable as usual
- Let A be some predicate over its possible values
  - A is true for some values of X, false for others
  - E.g., X is outcome of throw of a die, A could be "value is greater than 4"
- P(A) is the fraction of possible worlds in which A is true
  - P(die value is greater than 4) = 2 / 6 = 1/3

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Axioms

- $0 \leq P(A) \leq 1$
- P(True) = 1
- P(False) = 0
- $P(A \vee B) = P(A) + P(B) - P(A \wedge B)$

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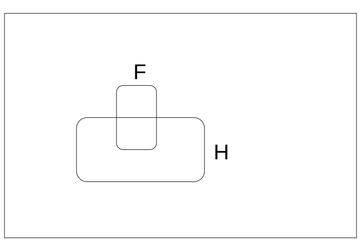
Theorems from the Axioms

- $0 \leq P(A) \leq 1$, $P(True) = 1$, $P(False) = 0$
- $P(A \vee B) = P(A) + P(B) - P(A \wedge B)$

- From these we can prove:
  - $P(\text{not } A) = P(\sim A) = 1 - P(A)$
  - $P(A) = P(A \wedge B) + P(A \wedge \sim B)$

Conditional Probability

- $P(A|B)$ = Fraction of worlds in which B is true that also have A true



H = "Have a headache"
F = "Coming down with Flu"

P(H) = 1/10
P(F) = 1/40
P(H|F) = 1/2

"Headaches are rare and flu is rarer, but if you're coming down with flu there's a 50-50 chance you'll have a headache."

Definition of Conditional Probability

$$P(A|B) = \frac{P(A \wedge B)}{P(B)}$$

Corollary: the Chain Rule

$$P(A \wedge B) = P(A|B)\, P(B)$$

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Multivalued Random Variables

- Suppose X can take on more than 2 values
- X is a random variable with arity k if it can take on exactly one value out of $\{v_1, v_2, \ldots, v_k\}$
- Thus

$$P(X = v_i \wedge X = v_j) = 0 \text{ if } i \neq j$$

$$P(X = v_1 \vee X = v_2 \vee \ldots \vee X = v_k) = 1$$

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Easy Fact about Multivalued Random Variables

- Using the axioms of probability
  - $0 \le P(A) \le 1$, P(True) = 1, P(False) = 0
  - $P(A \vee B) = P(A) + P(B) - P(A \wedge B)$
- And assuming that X obeys

$$P(X = v_i \wedge X = v_j) = 0 \text{ if } i \neq j$$

$$P(X = v_1 \vee X = v_2 \vee \ldots \vee X = v_k) = 1$$

- We can prove that

$$P(X = v_1 \vee X = v_2 \vee \ldots \vee X = v_i) = \sum_{j=1}^{i} P(X = v_j)$$

- And therefore: $\sum_{j=1}^{k} P(X = v_j) = 1$

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Useful Easy-to-Prove Facts

$$P(A \mid B) + P(\sim A \mid B) = 1$$

$$\sum_{j=1}^{k} P(X = v_j \mid B) = 1$$

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The Joint Distribution

Example: Boolean variables A, B, C

Recipe for making a joint distribution of d variables:

The Joint Distribution

Example: Boolean variables A, B, C

Recipe for making a joint distribution of d variables:

1. Make a truth table listing all combinations of values of your variables (has 2^d rows for d Boolean variables).

A	B	C
0	0	0
0	0	1
0	1	0
0	1	1
1	0	0
1	0	1
1	1	0
1	1	1

The Joint Distribution

Example: Boolean variables A, B, C

Recipe for making a joint distribution of d variables:

1. Make a truth table listing all combinations of values of your variables (has 2^d rows for d Boolean variables).
2. For each combination of values, say how probable it is.

A	B	C	Prob
0	0	0	0.30
0	0	1	0.05
0	1	0	0.10
0	1	1	0.05
1	0	0	0.05
1	0	1	0.10
1	1	0	0.25
1	1	1	0.10

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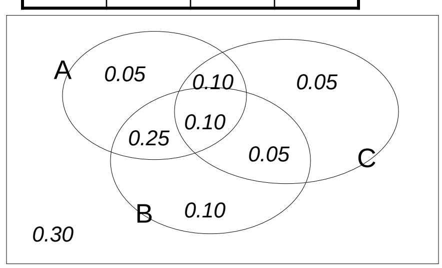
The Joint Distribution

Example: Boolean variables A, B, C

Recipe for making a joint distribution of d variables:

1. Make a truth table listing all combinations of values of your variables (has 2^d rows for d Boolean variables).
2. For each combination of values, say how probable it is.
3. If you subscribe to the axioms of probability, those numbers must sum to 1.

A	B	C	Prob
0	0	0	0.30
0	0	1	0.05
0	1	0	0.10
0	1	1	0.05
1	0	0	0.05
1	0	1	0.10
1	1	0	0.25
1	1	1	0.10



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Using the Joint Dist.

gender	hours_worked	wealth	
Female	v0:40.5-	poor	0.253122
		rich	0.0245895
	v1:40.5+	poor	0.0421768
		rich	0.0116293
Male	v0:40.5-	poor	0.331313
		rich	0.0971295
	v1:40.5+	poor	0.134106
		rich	0.105933

Once you have the JD you can ask for the probability of any logical expression involving your attribute

$$P(E) = \sum_{\text{rows matching } E} P(\text{row})$$

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Using the Joint Dist.

gender	hours_worked	wealth	
Female	v0:40.5-	poor	0.253122
		rich	0.0245895
	v1:40.5+	poor	0.0421768
		rich	0.0116293
Male	v0:40.5-	poor	0.331313
		rich	0.0971295
	v1:40.5+	poor	0.134106
		rich	0.105933

P(Poor $\wedge$ Male) = 0.4654

$$P(E) = \sum_{\text{rows matching } E} P(\text{row})$$

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Using the Joint Dist.

gender	hours_worked	wealth	
Female	v0:40.5-	poor	0.253122
		rich	0.0245895
	v1:40.5+	poor	0.0421768
		rich	0.0116293
Male	v0:40.5-	poor	0.331313
		rich	0.0971295
	v1:40.5+	poor	0.134106
		rich	0.105933

P(Poor) = 0.7604

$$P(E) = \sum_{\text{rows matching } E} P(\text{row})$$

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Inference with the Joint Dist.

gender	hours_worked	wealth	
Female	v0:40.5-	poor	0.253122
		rich	0.0245895
	v1:40.5+	poor	0.0421768
		rich	0.0116293
Male	v0:40.5-	poor	0.331313
		rich	0.0971295
	v1:40.5+	poor	0.134106
		rich	0.105933

$$P(E_1 \mid E_2) = \frac{P(E_1 \wedge E_2)}{P(E_2)} = \frac{\sum_{\text{rows matching } E_1 \text{ and } E_2} P(\text{row})}{\sum_{\text{rows matching } E_2} P(\text{row})}$$

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Inference with the Joint Dist.

gender	hours_worked	wealth	
Female	v0:40.5-	poor	0.253122
		rich	0.0245895
	v1:40.5+	poor	0.0421768
		rich	0.0116293
Male	v0:40.5-	poor	0.331313
		rich	0.0971295
	v1:40.5+	poor	0.134106
		rich	0.105933

$$P(E_1 \mid E_2) = \frac{P(E_1 \wedge E_2)}{P(E_2)} = \frac{\sum_{\text{rows matching } E_1 \text{ and } E_2} P(\text{row})}{\sum_{\text{rows matching } E_2} P(\text{row})}$$

P(Male | Poor) = 0.4654 / 0.7604 = 0.612

Joint Distributions

- Good news: Once you have a joint distribution, you can answer important questions that involve uncertainty.
- Bad news: Impossible to create joint distribution for more than about ten attributes because there are so many numbers needed when you build it.

What Would Help?

- Full independence
  - P(gender=g ∧ hours_worked=h ∧ wealth=w) = P(gender=g) * P(hours_worked=h) * P(wealth=w)
  - Can reconstruct full joint distribution from a few marginals
- Full conditional independence given class value
  - Naïve Bayes
- What about something between Naïve Bayes and general joint distribution?

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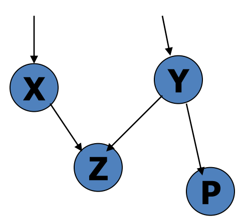
Bayesian Belief Networks

- Subset of the variables conditionally independent
- Graphical model of causal relationships
  - Represents dependency among the variables
  - Gives a specification of joint probability distribution



- ❑ Nodes: random variables
- ❑ Links: dependency
- ❑ X and Y are the parents of Z, and Y is the parent of P
- ❑ Given Y, Z and P are independent
- ❑ Has no loops or cycles

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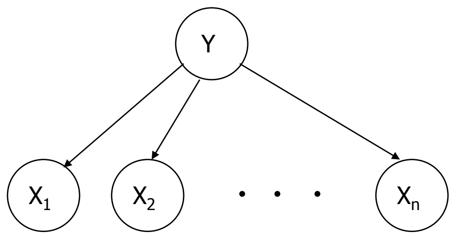
Bayesian Network Properties

- Each variable is conditionally independent of its non-descendents in the graph, given its parents
- Naïve Bayes as a Bayesian network:



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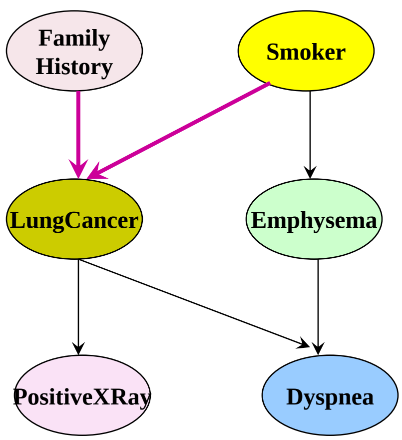
Bayesian Belief Network Example



Bayesian Belief Networks

Conditional probability table (**CPT**) for variable LungCancer:

	(FH, S)	(FH, ~S)	(~FH, S)	(~FH, ~S)
LC	0.8	0.5	0.7	0.1
~LC	0.2	0.5	0.3	0.9

CPT shows the conditional probability for each possible combination of its parents

Easy to compute joint distribution for all attributes $X_1, \ldots, X_d$, from CPT:

$$P(\mathbf{X} = (x_1, \ldots, x_d)) = \prod_{i=1}^{d} P(X_i = x_i \mid \text{parents}(X_i))$$

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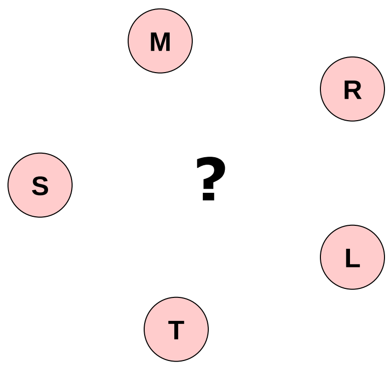
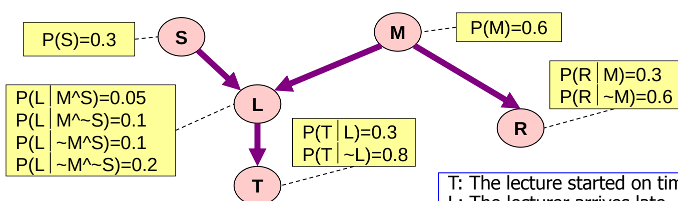
Creating a Bayes Network

T: The lecture started on time
L: The lecturer arrives late
R: The lecture concerns data mining
M: The lecturer is Mike
S: It is snowing



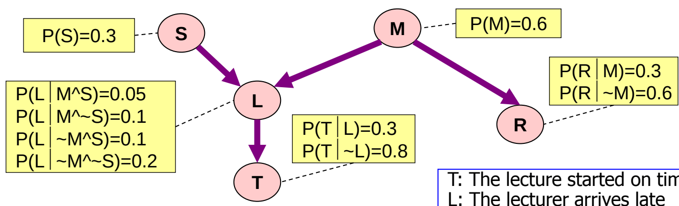
Computing with Bayes Net



T: The lecture started on time
L: The lecturer arrives late
R: The lecture concerns data mining
M: The lecturer is Mike
S: It is snowing

$$P(T \wedge {\sim}R \wedge L \wedge {\sim}M \wedge S)$$
$$= P(T \mid {\sim}R \wedge L \wedge {\sim}M \wedge S) * P({\sim}R \wedge L \wedge {\sim}M \wedge S)$$
$$= P(T \mid L) * P({\sim}R \wedge L \wedge {\sim}M \wedge S)$$
$$= P(T \mid L) * P({\sim}R \mid L \wedge {\sim}M \wedge S) * P(L \wedge {\sim}M \wedge S)$$
$$= P(T \mid L) * P({\sim}R \mid {\sim}M) * P(L \wedge {\sim}M \wedge S)$$
$$= P(T \mid L) * P({\sim}R \mid {\sim}M) * P(L \mid {\sim}M \wedge S) * P({\sim}M \wedge S)$$
$$= P(T \mid L) * P({\sim}R \mid {\sim}M) * P(L \mid {\sim}M \wedge S) * P({\sim}M \mid S) * P(S)$$
$$= P(T \mid L) * P({\sim}R \mid {\sim}M) * P(L \mid {\sim}M \wedge S) * P({\sim}M) * P(S)$$

Computing with Bayes Net



T: The lecture started on time
L: The lecturer arrives late
R: The lecture concerns data mining
M: The lecturer is Mike
S: It is snowing

P(R | T ^ ~S)
= P(R ^ T ^ ~S) / P(T ^ ~S)
= P(R ^ T ^ ~S) / (P(R ^ T ^ ~S) + P(~R ^ T ^ ~S))

P(R ^ T ^ ~S): Compute as P(L ^ M ^ R ^ T ^ ~S) + P(~L ^ M ^ R ^ T ^ ~S)
+ P(L ^ ~M ^ R ^ T ^ ~S) + P(~L ^ ~M ^ R ^ T ^ ~S)
Compute P(~R ^ T ^ ~S) similarly

Any problem here? Yes, possibly many terms to be computed…

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Inference with Bayesian Networks

- Want to compute P(C_i| **X**=**x**)
  - Assume the output attribute Y node's parents are all input attribute nodes and all these input values are given
  - Then we have P(C_i| **X**=**x**) = P(C_i| parents(Y)), i.e., we can read it directly from CPT
- What if values are given only for a subset of attributes?
  - Can still compute it from the Bayesian network
  - But: exact inference of probabilities in general for an arbitrary Bayesian network is NP-hard
  - Solutions: probabilistic inference, trade precision for efficiency

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Training Bayesian Networks

- Several scenarios:
  - Given both the network structure and all variables are observable: learn only the CPTs
  - Network structure known, some hidden variables: gradient descent (greedy hill-climbing) method, analogous to neural network learning
  - Network structure unknown, all variables observable: search through the model space to reconstruct network topology
  - Unknown structure, all hidden variables: No good algorithms known for this purpose
- Ref.: D. Heckerman: Bayesian networks for data mining

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Classification and Prediction Overview

- Introduction
- Decision Trees
- Statistical Decision Theory
- Nearest Neighbor
- Bayesian Classification
- Artificial Neural Networks
- Support Vector Machines (SVMs)
- Prediction
- Accuracy and Error Measures
- Ensemble Methods

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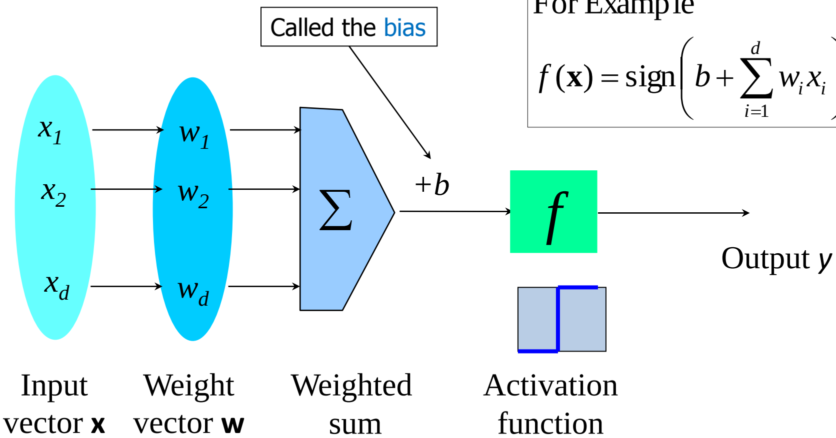
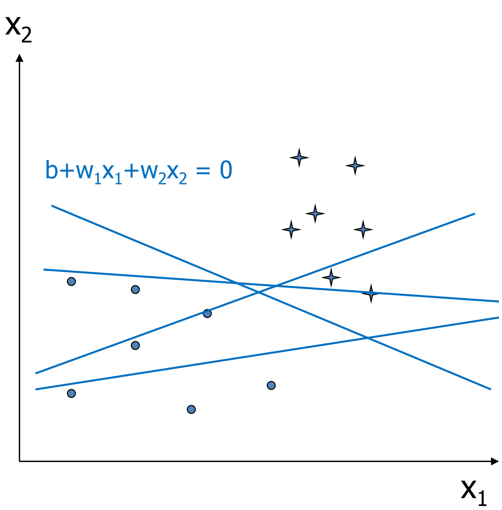
Basic Building Block: Perceptron

For Example

$$f(\mathbf{x}) = \text{sign}\left(b + \sum_{i=1}^{d} w_i x_i\right)$$



Perceptron Decision Hyperplane



Input: $\{(x_1, x_2, y), \ldots\}$

Output: classification function f(**x**)

f(**x**) > 0: return +1

f(**x**) ≤ 0: return = -1

Decision hyperplane: b+**w**·**x** = 0

Note: b+**w**·**x** > 0, if and only if

$$\sum_{i=1}^{d} w_i x_i > -b$$

b represents a threshold for when the perceptron "fires".

Representing Boolean Functions

- AND with two-input perceptron
  - $b=-0.8$, $w_1=w_2=0.5$
- OR with two-input perceptron
  - $b=-0.3$, $w_1=w_2=0.5$
- m-of-n function: true if at least m out of n inputs are true
  - All input weights 0.5, threshold weight b is set according to m, n
- Can also represent NAND, NOR
- What about XOR?

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Perceptron Training Rule

- Goal: correct +1/-1 output for each training record
- Start with random weights, select constant η (learning rate)
- For each training record ($\mathbf{x}$, y)
  - Let $f_{old}(\mathbf{x})$ be the output of the current perceptron for $\mathbf{x}$
  - Set $b := b + \Delta b$, where $\Delta b = \eta(y - f_{old}(\mathbf{x}))$
  - For all i, set $w_i := w_i + \Delta w_i$, where $\Delta w_i = \eta(y - f_{old}(\mathbf{x}))x_i$
- Keep iterating over training records until all are correctly classified
- Converges to correct decision boundary, if the classes are linearly separable and a small enough η is used
  - Why?

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Gradient Descent

- If training records are not linearly separable, find best fit approximation.
  - Gradient descent to search the space of possible weight vectors
  - Basis for Backpropagation algorithm
- Consider un-thresholded perceptron (no sign function applied), i.e., u(**x**) = b + **w**·**x**
- Measure training error by squared error

$$E(b,\mathbf{w}) = \frac{1}{2}\sum_{(\mathbf{x},y)\in D}\left(y-\mathrm{u}(\mathbf{x})\right)^2$$

  - D = training data

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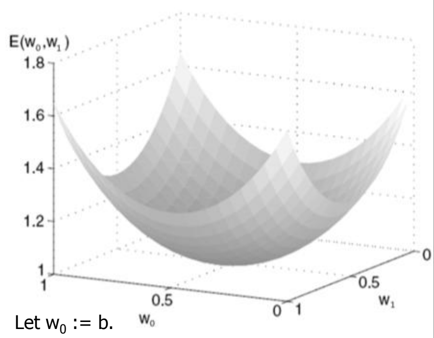
Gradient Descent Rule

- Find weight vector that minimizes E(b,**w**) by altering it in direction of steepest descent
  - Set (b,**w**) := (b,**w**) + Δ(b,**w**), where Δ(b,**w**) = -η ∇E(b,**w**)
    - -∇E(b,**w**)=[$\partial E/\partial b$, $\partial E/\partial w_1$,…, $\partial E/\partial w_n$] is the gradient, hence

$$b := b - \eta\frac{\partial \mathrm{E}}{\partial b} = b - \eta\left(-\sum_{(\mathbf{x},y)\in D}\left(y-\mathrm{u}(\mathbf{x})\right)\right)$$

$$w_i := w_i - \eta\frac{\partial \mathrm{E}}{\partial w_i} = w_i - \eta\sum_{(\mathbf{x},y)\in D}\left(y-\mathrm{u}(\mathbf{x})\right)(-x_i)$$

- Start with random weights, iterate until convergence
  - Will converge to global minimum if η is small enough



Let w_0 := b.

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Gradient Descent Summary

- Epoch updating (aka batch mode)
  - Do until satisfied with model
    - Compute gradient over entire training set
    - Update all weights based on gradient
- Case updating (aka incremental mode, stochastic gradient descent)
  - Do until satisfied with model
    - For each training record
      - Compute gradient for this single training record
      - Update all weights based on gradient
- Case updating can approximate epoch updating arbitrarily close if η is small enough
- Perceptron training rule and case updating might seem identical
  - Difference: error computation on thresholded vs. unthresholded output

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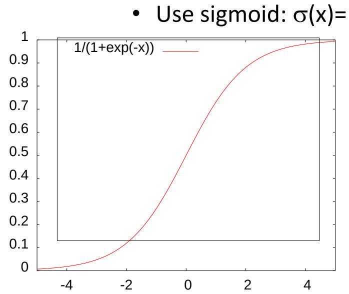
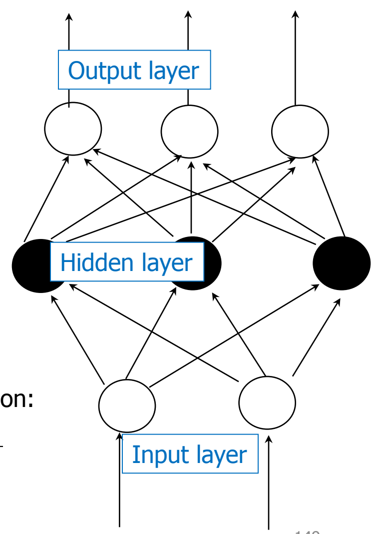
Multilayer Feedforward Networks

- Use another perceptron to combine output of lower layer
  - What about linear units only? Can only construct linear functions!
  - Need nonlinear component
    - sign function: not differentiable (gradient descent!)
    - Use sigmoid: $\sigma(x)=1/(1+e^{-x})$



Perceptron function:

$$y = \frac{1}{1+e^{-b-\mathbf{w}\cdot\mathbf{x}}}$$



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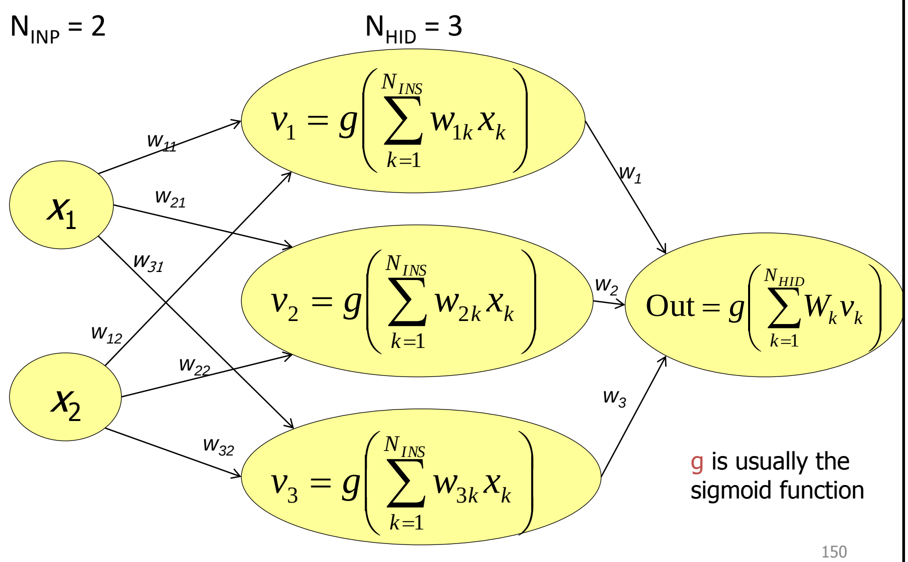
1-Hidden Layer Net Example



g is usually the sigmoid function

Making Predictions

- Inputs: all input data attributes
  - Record fed simultaneously into the units of the input layer
  - Then weighted and fed simultaneously to a hidden layer
    - Number of hidden layers is arbitrary, although usually only one
- Weighted outputs of the last hidden layer are the input to the units in the output layer, which emits the network's prediction
- The network is feed-forward
  - None of the weights cycles back to an input unit or to an output unit of a previous layer
- Statistical point of view: neural networks perform nonlinear regression

Backpropagation Algorithm

- We discussed gradient descent to find the best weights for a *single* perceptron using simple un-thresholded function
  - If sigmoid (or other differentiable) function is applied to weighted sum, use *complete function* for gradient descent
- Multiple perceptrons: optimize over all weights of all perceptrons
  - Problems: huge search space, local minima
- Backpropagation
  - Initialize all weights with small random values
  - Iterate many times
    - Compute gradient, starting at output and working back
      - Error of hidden unit h: how do we get the true output value? Use weighted sum of errors of each unit influenced by h.
    - Update all weights in the network

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Overfitting

- When do we stop updating the weights?
  - Might overfit to training data
- Overfitting tends to happen in later iterations
  - Weights initially small random values
  - Weights all similar => smooth decision surface
  - Surface complexity increases as weights diverge
- Preventing overfitting
  - Weight decay: decrease each weight by small factor during each iteration, or
  - Use validation data to decide when to stop iterating

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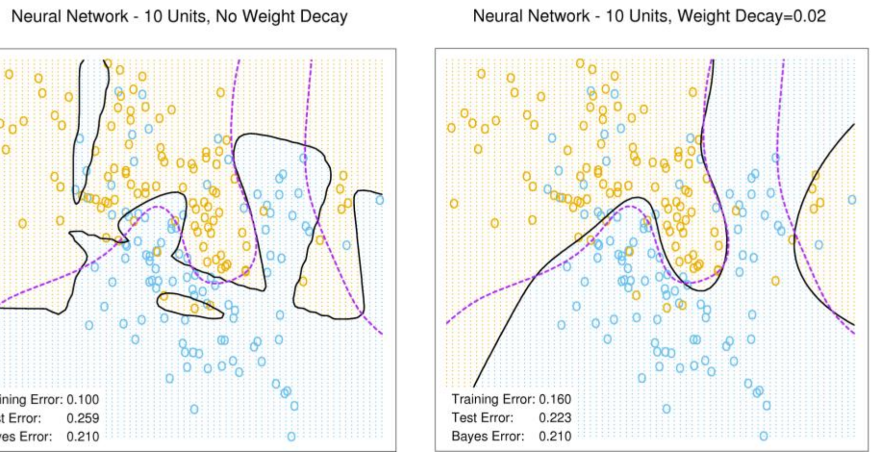
Neural Network Decision Boundary



Source: Hastie, Tibshirani, and Friedman. The Elements of Statistical Learning

Backpropagation Remarks

- Computational cost
  - Each interation costs O(|D|*|**w**|), with |D| training records and |**w**| weights
  - Number of iterations can be exponential in n, the number of inputs (in practice often tens of thousands)
- Local minima can trap the gradient descent algorithm
  - Convergence guaranteed to *local* minimum, not *global*
- Backpropagation highly effective in practice
  - Many variants to deal with local minima issue
  - E.g., case updating might avoid local minimum

Defining a Network

1. Decide network topology
   - # input units, # hidden layers, # units in each hidden layer, # output units
2. Normalize input values for each attribute to [0.0, 1.0]
   - Transform nominal and ordinal attributes: one input unit *per domain value*, each initialized to 0
   - Why not map the attribute to a single input with domain [0.0, 1.0]?
3. Output for classification task with >2 classes: one output unit per class
4. Choose learning rate η
   - Too small: can take days instead of minutes to converge
   - Too large: diverges (MSE gets larger while the weights increase and usually oscillate)
   - Heuristic: set it to 1 / (#training iterations)
5. If model accuracy is unacceptable, re-train with different network topology, different set of initial weights, or different learning rate
   - Might need a lot of trial-and-error

Representational Power

- Boolean functions
  - Each can be represented by a 2-layer network
  - Number of hidden units can grow exponentially with number of inputs
    - Create hidden unit for each input record
    - Set its weights to activate only for that input
    - Implement output unit as OR gate that only activates for desired output patterns
- Continuous functions
  - Every bounded continuous function can be approximated arbitrarily close by a 2-layer network
- Any function can be approximated arbitrarily close by a 3-layer network

Neural Network as a Classifier

- Weaknesses
  - Long training time
  - Many non-trivial parameters, e.g., network topology
  - Poor interpretability: What is the meaning behind learned weights and hidden units?
    - Note: hidden units are alternative representation of input values, capturing their relevant features
- Strengths
  - High tolerance to noisy data
  - Well-suited for continuous-valued inputs and outputs
  - Successful on a wide array of real-world data
  - Techniques exist for extraction of rules from neural networks

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Classification and Prediction Overview

- Introduction
- Decision Trees
- Statistical Decision Theory
- Nearest Neighbor
- Bayesian Classification
- Artificial Neural Networks
- Support Vector Machines (SVMs)
- Prediction
- Accuracy and Error Measures
- Ensemble Methods

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SVM—Support Vector Machines

- Newer and very popular classification method
- Uses a nonlinear mapping to transform the original training data into a higher dimension
- Searches for the optimal separating hyperplane (i.e., "decision boundary") in the new dimension
- SVM finds this hyperplane using support vectors ("essential" training records) and margins (defined by the support vectors)

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SVM—History and Applications

- Vapnik and colleagues (1992)
  - Groundwork from Vapnik & Chervonenkis' statistical learning theory in 1960s
- Training can be slow but accuracy is high
  - Ability to model complex nonlinear decision boundaries (margin maximization)
- Used both for classification and prediction
- Applications: handwritten digit recognition, object recognition, speaker identification, benchmarking time-series prediction tests

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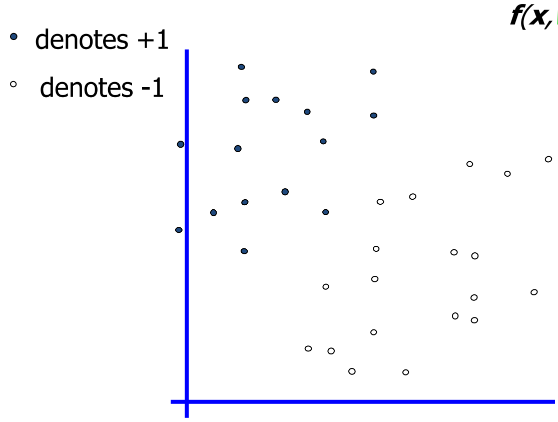
Linear Classifiers

$f(\mathbf{x},\mathbf{w},b) = sign(\mathbf{w}\cdot\mathbf{x} + b)$

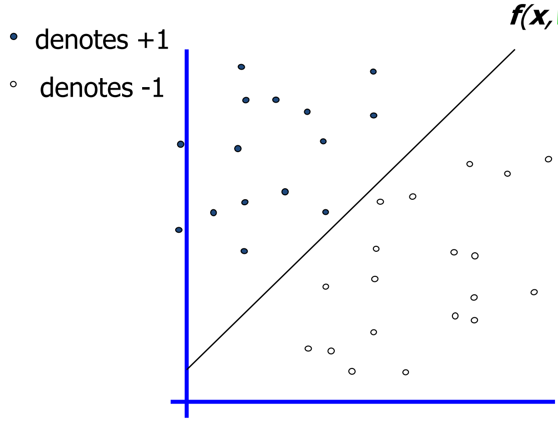


How would you classify this data?

163

Linear Classifiers

$f(\mathbf{x},\mathbf{w},b) = sign(\mathbf{w}\cdot\mathbf{x} + b)$

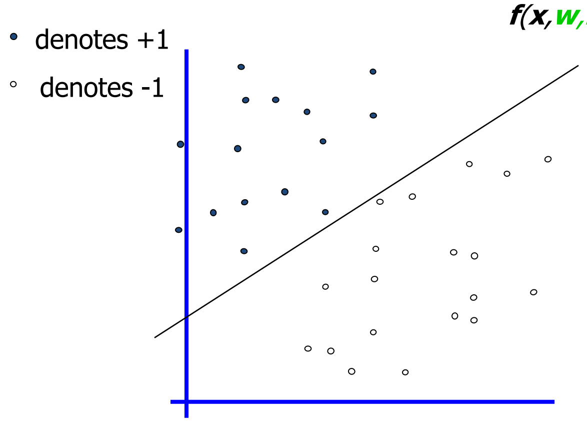


How would you classify this data?

164

Linear Classifiers

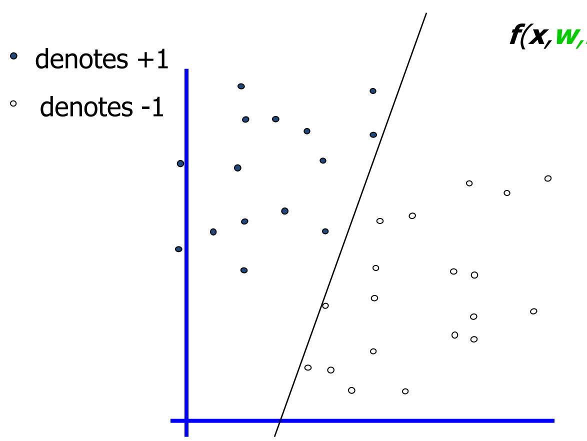
$f(\mathbf{x},\mathbf{w},b) = sign(\mathbf{w}\cdot\mathbf{x} + b)$



How would you classify this data?

Linear Classifiers

$f(\mathbf{x},\mathbf{w},b) = sign(\mathbf{w}\cdot\mathbf{x} + b)$

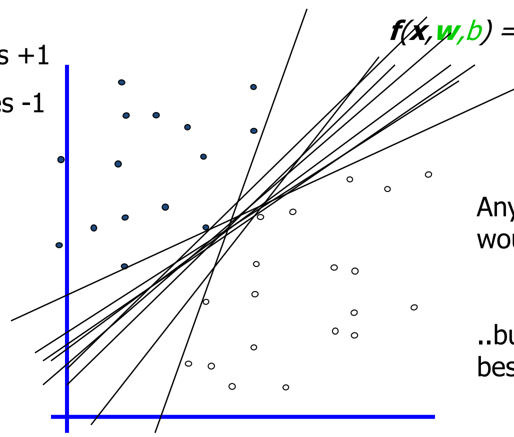


How would you classify this data?

Linear Classifiers

- denotes +1
- denotes -1

$f(\mathbf{x},\mathbf{w},b) = sign(\mathbf{w}\cdot\mathbf{x} + b)$



Any of these would be fine..

..but which is best?

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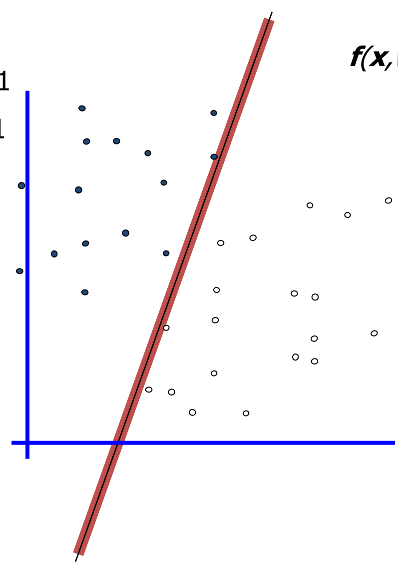
Classifier Margin

- denotes +1
- denotes -1

$f(\mathbf{x},\mathbf{w},b) = sign(\mathbf{w}\cdot\mathbf{x} + b)$



Define the margin of a linear classifier as the width that the boundary could be increased by before hitting a data record.

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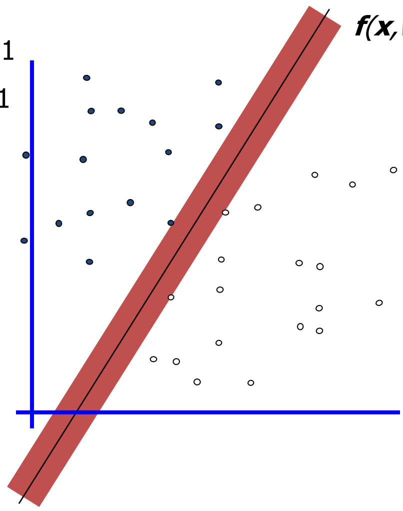
Maximum Margin

- denotes +1
- ◦ denotes -1



$f(\mathbf{x},\mathbf{w},b) = sign(\mathbf{w}\cdot\mathbf{x} + b)$

Find the maximum margin linear classifier.

This is the simplest kind of SVM, called linear SVM or LSVM.

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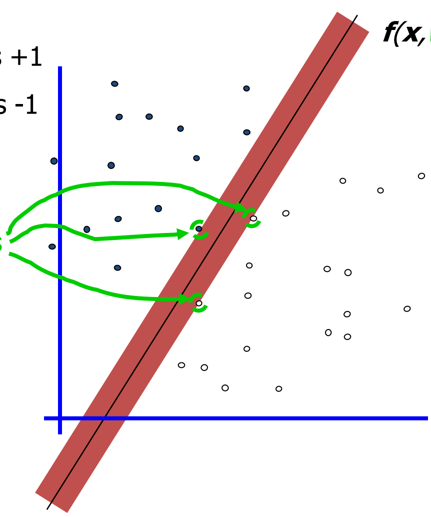
Maximum Margin

- denotes +1
- ◦ denotes -1

$f(\mathbf{x},\mathbf{w},b) = sign(\mathbf{w}\cdot\mathbf{x} + b)$

Support Vectors are those datapoints that the margin pushes up against



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Why Maximum Margin?

- If we made a small error in the location of the boundary, this gives us the least chance of causing a misclassification.
- Model is immune to removal of any non-support-vector data records.
- There is some theory (using VC dimension) that is related to (but not the same as) the proposition that this is a good thing.
- Empirically it works very well.

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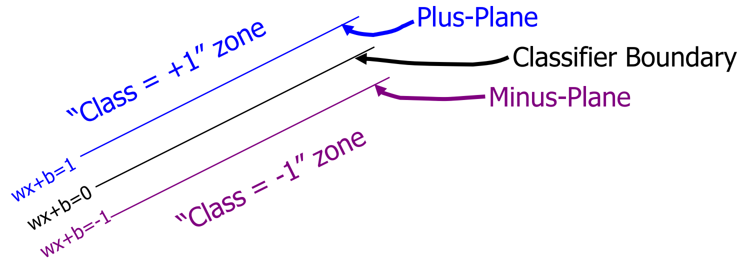
Specifying a Line and Margin



- Plus-plane = $\{ \mathbf{x} : \mathbf{w} \cdot \mathbf{x} + b = +1 \}$
- Minus-plane = $\{ \mathbf{x} : \mathbf{w} \cdot \mathbf{x} + b = -1 \}$

Classify as	+1	if	$\mathbf{w} \cdot \mathbf{x} + b \geq 1$
	-1	if	$\mathbf{w} \cdot \mathbf{x} + b \leq -1$
	what	if	$-1 < \mathbf{w} \cdot \mathbf{x} + b < 1$?

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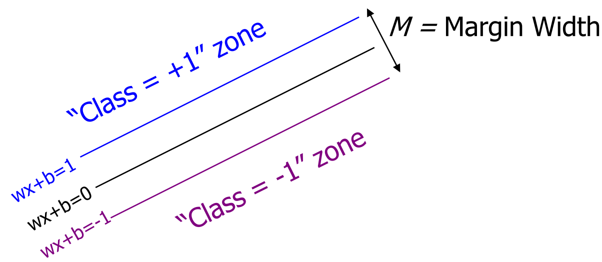
Computing Margin Width



- Plus-plane = { **x** : **w**·**x** + b = +1 }
- Minus-plane = { **x** : **w**·**x** + b = -1 }
- Goal: compute M in terms of **w** and b
  - Note: vector **w** is perpendicular to plus-plane
    - Consider two vectors **u** and **v** on plus-plane and show that **w**·(**u**-**v**)=0
    - Hence it is also perpendicular to the minus-plane

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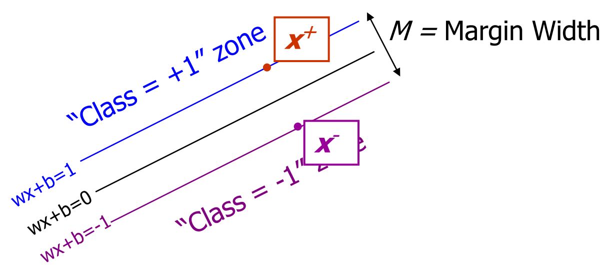
Computing Margin Width



- Choose arbitrary point $\mathbf{x}^-$ on minus-plane
- Let $\mathbf{x}^+$ be the point in plus-plane closest to $\mathbf{x}^-$
- Since vector **w** is perpendicular to these planes, it holds that $\mathbf{x}^+ = \mathbf{x}^- + \lambda\mathbf{w}$, for some value of λ

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Putting It All Together

- We have so far:
  - $\mathbf{w} \cdot \mathbf{x}^+ + b = +1$ and $\mathbf{w} \cdot \mathbf{x}^- + b = -1$
  - $\mathbf{x}^+ = \mathbf{x}^- + \lambda \mathbf{w}$
  - $|\mathbf{x}^+ - \mathbf{x}^-| = M$
- Derivation:
  - $\mathbf{w} \cdot (\mathbf{x}^- + \lambda \mathbf{w}) + b = +1$, hence $\mathbf{w} \cdot \mathbf{x}^- + b + \mathbf{w} \lambda \mathbf{w} = 1$
  - This implies $\lambda \mathbf{w} \cdot \mathbf{w} = 2$, i.e., $\lambda = 2 / \mathbf{w} \cdot \mathbf{w}$
  - Since $M = |\mathbf{x}^+ - \mathbf{x}^-| = |\lambda \mathbf{w}| = \lambda\ |\mathbf{w}| = \lambda(\mathbf{w} \cdot \mathbf{w})^{0.5}$
  - We obtain $M = 2\ (\mathbf{w} \cdot \mathbf{w})^{0.5} / \mathbf{w} \cdot \mathbf{w} = 2 / (\mathbf{w} \cdot \mathbf{w})^{0.5}$

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Finding the Maximum Margin

- How do we find **w** and b such that the margin is maximized and *all training records are in the correct zone for their class*?
- Solution: Quadratic Programming (QP)
- QP is a well-studied class of optimization algorithms to maximize a quadratic function of some real-valued variables subject to linear constraints.
  - There exist algorithms for finding such constrained quadratic optima efficiently and reliably.

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Quadratic Programming

Find $\underset{\mathbf{u}}{\arg\max} \quad c + \mathbf{d}^T\mathbf{u} + \frac{\mathbf{u}^T R \mathbf{u}}{2}$ ← Quadratic criterion

Subject to

$$\left.\begin{aligned} a_{11}u_1 + a_{12}u_2 + \ldots + a_{1m}u_m &\le b_1 \\ a_{21}u_1 + a_{22}u_2 + \ldots + a_{2m}u_m &\le b_2 \\ &\vdots \\ a_{n1}u_1 + a_{n2}u_2 + \ldots + a_{nm}u_m &\le b_n \end{aligned}\right\}$$

n additional linear inequality constraints

And subject to

$$\left.\begin{aligned} a_{(n+1)1}u_1 + a_{(n+1)2}u_2 + \ldots + a_{(n+1)m}u_m &= b_{(n+1)} \\ a_{(n+2)1}u_1 + a_{(n+2)2}u_2 + \ldots + a_{(n+2)m}u_m &= b_{(n+2)} \\ &\vdots \\ a_{(n+e)1}u_1 + a_{(n+e)2}u_2 + \ldots + a_{(n+e)m}u_m &= b_{(n+e)} \end{aligned}\right\}$$

e additional linear equality constraints

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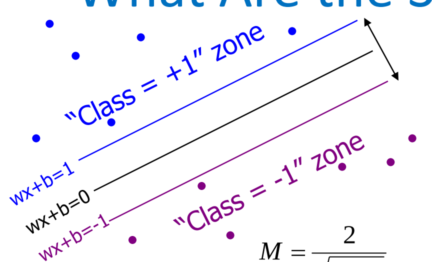
What Are the SVM Constraints?



$M = \frac{2}{\sqrt{\mathbf{w} \cdot \mathbf{w}}}$

- What is the quadratic optimization criterion?
- Consider n training records ($\mathbf{x}$(k), y(k)), where y(k) = +/- 1
- How many constraints will we have?
- What should they be?

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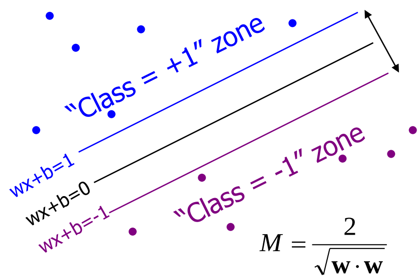
What Are the SVM Constraints?



- What is the quadratic optimization criterion?
  - Minimize **w**·**w**
- Consider n training records (**x**(k), y(k)), where y(k) = +/- 1
- How many constraints will we have? n.
- What should they be?

For each $1 \le k \le n$:

$\mathbf{w} \cdot \mathbf{x}(k) + b \ge 1$, if y(k)=1

$\mathbf{w} \cdot \mathbf{x}(k) + b \le -1$, if y(k)=-1

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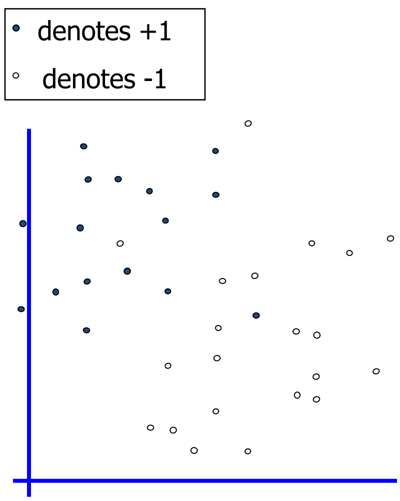
Problem: Classes Not Linearly Separable



- Inequalities for training records are not satisfiable by any **w** and b

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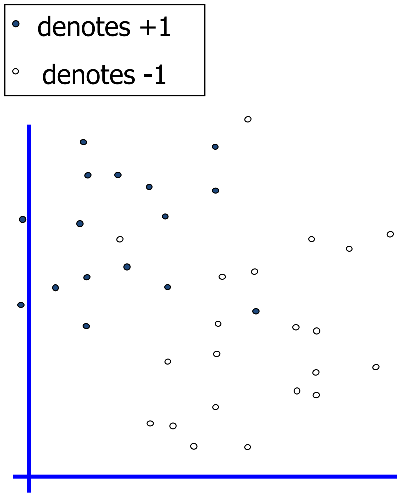
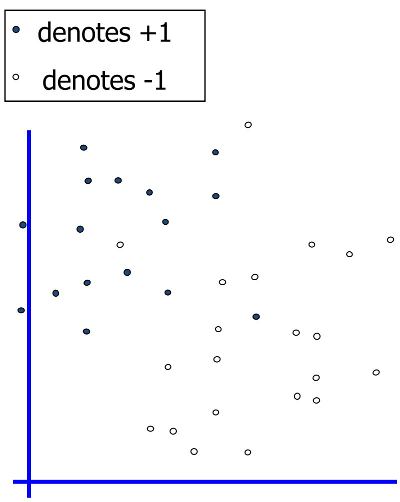
Solution 1?



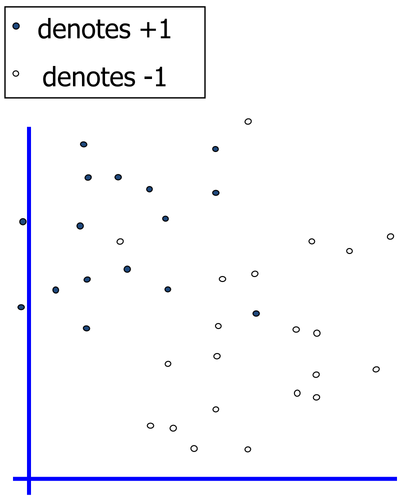
- Find minimum **w**·**w**, while also minimizing number of training set errors
  - Not a well-defined optimization problem (cannot optimize two things at the same time)

Solution 2?



- Minimize **w**·**w** + C·(#trainSetErrors)
  - C is a tradeoff parameter
- Problems:
  - Cannot be expressed as QP, hence finding solution might be slow
  - Does not distinguish between disastrous errors and near misses

Solution 3



- Minimize **w**·**w** + C·(distance of error records to their correct place)
- This works!
- But still need to do something about the unsatisfiable set of inequalities

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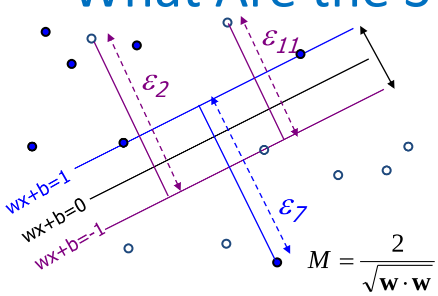
What Are the SVM Constraints?



- What is the quadratic optimization criterion?
  - Minimize

$$\frac{1}{2}\mathbf{w} \cdot \mathbf{w} + C\sum_{k=1}^{n} \varepsilon_k$$

- Consider n training records ($\mathbf{x}$(k), y(k)), where y(k) = +/- 1
- How many constraints will we have? n.
- What should they be?

For each $1 \leq k \leq n$:

$\mathbf{w} \cdot \mathbf{x}(k) + b \geq 1 - \varepsilon_k$, if y(k)=1

$\mathbf{w} \cdot \mathbf{x}(k) + b \leq -1 + \varepsilon_k$, if y(k)=-1

$\varepsilon_k \geq 0$

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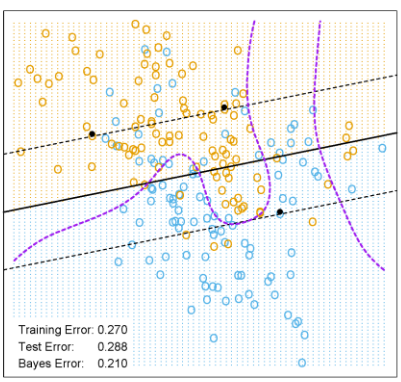
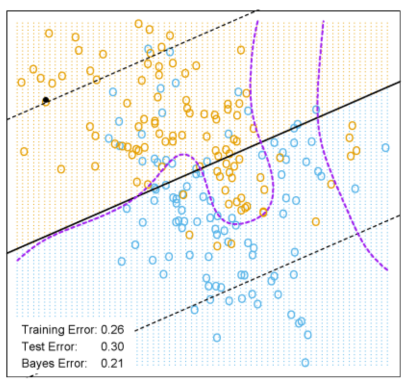
Facts About the New Problem Formulation

- Original QP formulation had d+1 variables
  - w_1, w_2,…, w_d and b
- New QP formulation has d+1+n variables
  - w_1, w_2,…, w_d and b
  - ε_1, ε_2,…, ε_n
- C is a new parameter that needs to be set for the SVM
  - Controls tradeoff between paying attention to margin size versus misclassifications

Effect of Parameter C



$C = 10000$



$C = 0.01$

Source: Hastie, Tibshirani, and Friedman. The Elements of Statistical Learning

An Equivalent QP (The "Dual")

Maximize $$\sum_{k=1}^{n} \alpha_k - \frac{1}{2}\sum_{k=1}^{n}\sum_{l=1}^{n} \alpha_k \alpha_l \cdot y(k) \cdot y(l) \cdot \mathbf{x}(k) \cdot \mathbf{x}(l)$$

Subject to these constraints: $$\forall k : 0 \le \alpha_k \le C \qquad \sum_{k=1}^{n} \alpha_k y(k) = 0$$

Then define:

$$\mathbf{w} = \sum_{k=1}^{n} \alpha_k \cdot y(k) \cdot \mathbf{x}(k)$$

$$b = \underset{k:0<\alpha_k<C}{\mathrm{AVG}} \left\{ \frac{1}{y(k)} - \mathbf{x}(k) \cdot \mathbf{w} \right\}$$

Then classify with:

***f*(*x*,*w*,*b*) = *sign*(*w*·*x* + *b*)**

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Important Facts

- Dual formulation of QP can be optimized more quickly, but result is equivalent
- Data records with $\alpha_k > 0$ are the support vectors
  - Those with $0 < \alpha_k < C$ lie on the plus- or minus-plane
  - Those with $\alpha_k = C$ are on the wrong side of the classifier boundary (have $\varepsilon_k > 0$)
- Computation for **w** and b only depends on those records with $\alpha_k > 0$, i.e., the support vectors
- Alternative QP has another major advantage, as we will see now...

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Easy To Separate

What would SVMs do with this data?

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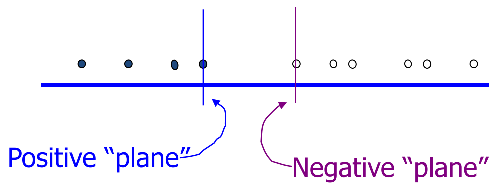
Easy To Separate

Not a big surprise



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Harder To Separate

What can be done about this?

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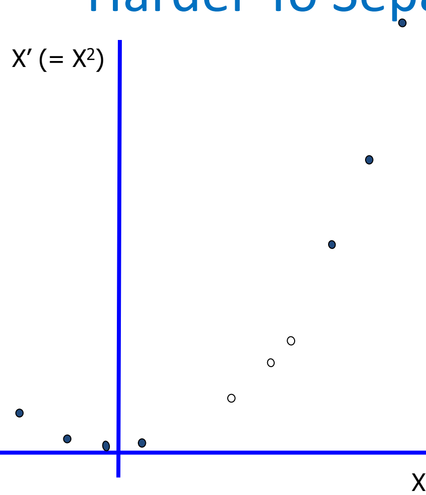
Harder To Separate



Non-linear basis functions:

Original data: (X, Y)

Transformed: (X, X^2, Y)

Think of X^2 as a new attribute, e.g., X′

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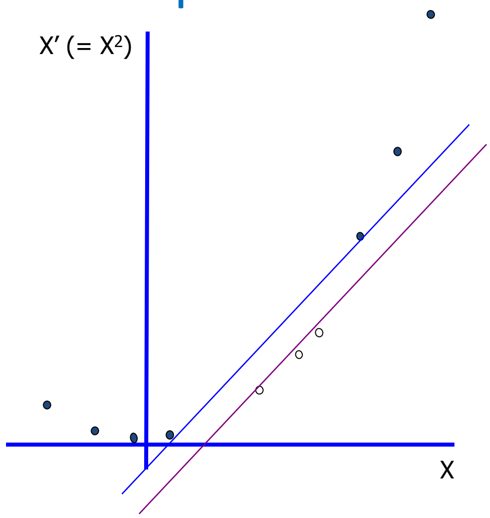
Now Separation Is Easy Again



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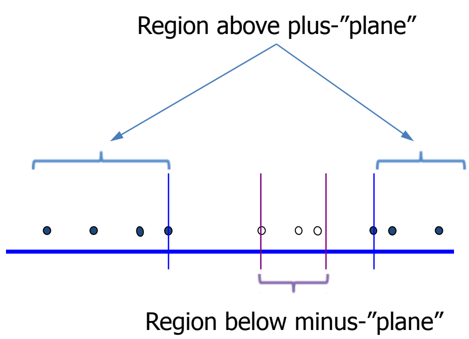
Corresponding "Planes" in Original Space



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Common SVM Basis Functions

- Polynomial of attributes $X_1, \ldots, X_d$ of certain max degree, e.g., $X_2 + X_1X_3 + X_4^2$
- Radial basis function
  - Symmetric around center, i.e., KernelFunction($|\mathbf{X} - \mathbf{c}|$ / kernelWidth)
- Sigmoid function of **X**, e.g., hyperbolic tangent
- Let $\Phi(\mathbf{x})$ be the transformed input record
  - Previous example: $\Phi(\ (x)\ ) = (x, x^2)$

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Quadratic Basis Functions

$$\Phi(\mathbf{x}) = \begin{pmatrix} 1 \\ \sqrt{2}x_1 \\ \sqrt{2}x_2 \\ : \\ \sqrt{2}x_d \\ x_1^2 \\ x_2^2 \\ : \\ x_d^2 \\ \sqrt{2}x_1x_2 \\ \sqrt{2}x_1x_3 \\ : \\ \sqrt{2}x_1x_d \\ \sqrt{2}x_2x_3 \\ : \\ \sqrt{2}x_1x_d \\ : \\ \sqrt{2}x_{d-1}x_d \end{pmatrix}
\begin{array}{l} \left.\right\} \text{Constant Term} \\ \left.\begin{matrix} \\ \\ \\ \\ \end{matrix}\right\} \text{Linear Terms} \\ \left.\begin{matrix} \\ \\ \\ \\ \end{matrix}\right\} \text{Pure Quadratic Terms} \\ \left.\begin{matrix} \\ \\ \\ \\ \\ \\ \\ \\ \end{matrix}\right\} \text{Quadratic Cross-Terms} \end{array}$$

Number of terms
(assuming d input attributes):

(d+2)-choose-2

= (d+2)(d+1)/2

$\approx d^2/2$

Why did we choose this specific transformation?

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Dual QP With Basis Functions

Maximize $\sum_{k=1}^{n} \alpha_k - \frac{1}{2}\sum_{k=1}^{n}\sum_{l=1}^{n} \alpha_k \alpha_l \cdot y(k) \cdot y(l) \cdot \mathbf{\Phi}(\mathbf{x}(k)) \cdot \mathbf{\Phi}(\mathbf{x}(l))$

Subject to these constraints: $\forall k : 0 \leq \alpha_k \leq C$ $\quad \sum_{k=1}^{n} \alpha_k y(k) = 0$

Then define:

$$\mathbf{w} = \sum_{k=1}^{n} \alpha_k \cdot y(k) \cdot \mathbf{\Phi}(\mathbf{x}(k))$$

$$b = \underset{k:0<\alpha_k<C}{\mathrm{AVG}} \left\{ \frac{1}{y(k)} - \mathbf{\Phi}(\mathbf{x}(k)) \cdot \mathbf{w} \right\}$$

Then classify with:

f(**x**,**w**,b) = sign(**w**·Φ(**x**) + b)

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Computation Challenge

- Input vector **x** has d components (its d attribute values)
- The transformed input vector **Φ**(**x**) has $d^2/2$ components
- Hence computing **Φ**(**x**(k))·**Φ**(**x**(l)) now costs order $d^2/2$ instead of order d operations (additions, multiplications)
- ...or is there a better way to do this?
  - Take advantage of properties of certain transformations

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Quadratic Dot Products

$$
\mathbf{\Phi}(\mathbf{a})\cdot\mathbf{\Phi}(\mathbf{b}) =
\begin{pmatrix} 1 \\ \sqrt{2}a_1 \\ \sqrt{2}a_2 \\ : \\ \sqrt{2}a_d \\ a_1^2 \\ a_2^2 \\ : \\ a_d^2 \\ \sqrt{2}a_1a_2 \\ \sqrt{2}a_1a_3 \\ : \\ \sqrt{2}a_1a_d \\ \sqrt{2}a_2a_3 \\ : \\ \sqrt{2}a_1a_d \\ : \\ \sqrt{2}a_{d-1}a_d \end{pmatrix}
\bullet
\begin{pmatrix} 1 \\ \sqrt{2}b_1 \\ \sqrt{2}b_2 \\ : \\ \sqrt{2}b_d \\ b_1^2 \\ b_2^2 \\ : \\ b_d^2 \\ \sqrt{2}b_1b_2 \\ \sqrt{2}b_1b_3 \\ : \\ \sqrt{2}b_1b_d \\ \sqrt{2}b_2b_3 \\ : \\ \sqrt{2}b_1b_d \\ : \\ \sqrt{2}b_{d-1}b_d \end{pmatrix}
$$

$$1$$
$$+$$
$$\sum_{i=1}^{m} 2a_ib_i$$
$$+$$
$$\sum_{i=1}^{m} a_i^2b_i^2$$
$$+$$
$$\sum_{i=1}^{m}\sum_{j=i+1}^{m} 2a_ia_jb_ib_j$$

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Quadratic Dot Products

$$\mathbf{\Phi}(\mathbf{a})\cdot\mathbf{\Phi}(\mathbf{b}) =$$
$$1+2\sum_{i=1}^{d} a_ib_i + \sum_{i=1}^{d} a_i^2b_i^2 + \sum_{i=1}^{d}\sum_{j=i+1}^{d} 2a_ia_jb_ib_j$$

Now consider another function of **a** and **b**:

$$(\mathbf{a}\cdot\mathbf{b}+1)^2$$
$$=(\mathbf{a}\cdot\mathbf{b})^2+2\mathbf{a}\cdot\mathbf{b}+1$$
$$=\left(\sum_{i=1}^{d} a_ib_i\right)^2 + 2\sum_{i=1}^{d} a_ib_i + 1$$
$$=\sum_{i=1}^{d}\sum_{j=1}^{d} a_ib_ia_jb_j + 2\sum_{i=1}^{d} a_ib_i + 1$$
$$=\sum_{i=1}^{d}(a_ib_i)^2 + 2\sum_{i=1}^{d}\sum_{j=i+1}^{d} a_ib_ia_jb_j + 2\sum_{i=1}^{d} a_ib_i + 1$$

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Quadratic Dot Products

- The results of $\mathbf{\Phi}(\mathbf{a})\cdot\mathbf{\Phi}(\mathbf{b})$ and of $(\mathbf{a}\cdot\mathbf{b}+1)^2$ are identical
- Computing $\mathbf{\Phi}(\mathbf{a})\cdot\mathbf{\Phi}(\mathbf{b})$ costs about $d^2/2$, while computing $(\mathbf{a}\cdot\mathbf{b}+1)^2$ costs only about d+2 operations
- This means that we can work in the high-dimensional space ($d^2/2$ dimensions) where the training records are more easily separable, but pay about the same cost as working in the original space (d dimensions)
- Savings are even greater when dealing with higher-degree polynomials, i.e., degree q>2, that can be computed as $(\mathbf{a}\cdot\mathbf{b}+1)^q$

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Any Other Computation Problems?

$$\mathbf{w} = \sum_{k=1}^{n} \alpha_k \cdot y(k) \cdot \mathbf{\Phi}(\mathbf{x}(k)) \qquad b = \underset{k:0<\alpha_k<C}{\mathrm{AVG}} \left\{ \frac{1}{y(k)} - \mathbf{\Phi}(\mathbf{x}(k)) \cdot \mathbf{w} \right\}$$

- What about computing w?
  - Finally need $\mathbf{f}(\mathbf{x},\mathbf{w},b) = \mathrm{sign}(\mathbf{w}\cdot\mathbf{\Phi}(\mathbf{x}) + b)$:

$$\mathbf{w} \cdot \mathbf{\Phi}(\mathbf{x}) = \sum_{k=1}^{n} \alpha_k \cdot y(k) \cdot \mathbf{\Phi}(\mathbf{x}(k)) \cdot \mathbf{\Phi}(\mathbf{x})$$

  - Can be computed using the same trick as before
- Can apply the same trick again to b, because

$$\mathbf{\Phi}(\mathbf{x}(k)) \cdot \mathbf{w} = \sum_{j=1}^{n} \alpha_j \cdot y(j) \cdot \mathbf{\Phi}(\mathbf{x}(k)) \cdot \mathbf{\Phi}(\mathbf{x}(j))$$

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SVM Kernel Functions

- For which transformations, called kernels, does the same trick work?
- Polynomial: K(**a**,**b**)=(**a** · **b** +1)^q
- Radial-Basis-style (RBF):

$$K(\mathbf{a},\mathbf{b}) = \exp\left(-\frac{(\mathbf{a}-\mathbf{b})^2}{2\sigma^2}\right)$$

  – Neural-net-style sigmoidal:

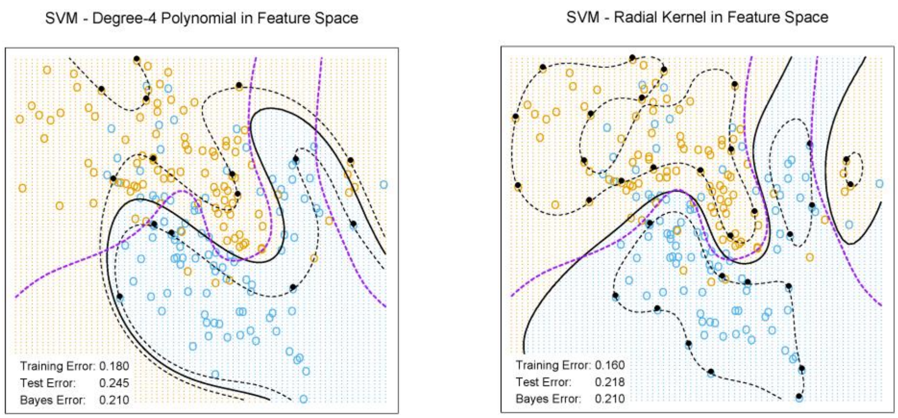
$$K(\mathbf{a},\mathbf{b}) = \tanh(\kappa \cdot \mathbf{a} \cdot \mathbf{b} - \delta)$$

σ, κ and δ are magic parameters that must be chosen by a model selection method.

Overfitting

- With the right kernel function, computation in high dimensional transformed space is no problem
- But what about overfitting? There are so many parameters...
- Usually not a problem, due to maximum margin approach
  - Only the support vectors determine the model, hence SVM complexity depends on number of support vectors, not dimensions (still, in higher dimensions there might be more support vectors)
  - Minimizing **w**·**w** discourages extremely large weights, which smoothes the function (recall weight decay for neural networks!)

Different Kernels



Source: Hastie, Tibshirani, and Friedman. The Elements of Statistical Learning

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Multi-Class Classification

- SVMs can only handle two-class outputs (i.e. a categorical output variable with arity 2).
- What can be done?
- Answer: with output arity N, learn N SVM's
  - SVM 1 learns "Output==1" vs "Output != 1"
  - SVM 2 learns "Output==2" vs "Output != 2"
  - :
  - SVM N learns "Output==N" vs "Output != N"
- To predict the output for a new input, just predict with each SVM and find out which one puts the prediction the furthest into the positive region.

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Why Is SVM Effective on High Dimensional Data?

- Complexity of trained classifier is characterized by the number of support vectors, not dimensionality of the data
- If all other training records are removed and training is repeated, the same separating hyperplane would be found
- The number of support vectors can be used to compute an upper bound on the expected error rate of the SVM, which is independent of data dimensionality
- Thus, an SVM with a small number of support vectors can have good generalization, even when the dimensionality of the data is high

SVM vs. Neural Network

- SVM
  - Relatively new concept
  - Deterministic algorithm
  - Nice Generalization properties
  - Hard to train – learned in batch mode using quadratic programming techniques
  - Using kernels can learn very complex functions
- Neural Network
  - Relatively old
  - Nondeterministic algorithm
  - Generalizes well but doesn't have strong mathematical foundation
  - Can easily be learned in incremental fashion
  - To learn complex functions—use multilayer perceptron (not that trivial)

Classification and Prediction Overview

- Introduction
- Decision Trees
- Statistical Decision Theory
- Nearest Neighbor
- Bayesian Classification
- Artificial Neural Networks
- Support Vector Machines (SVMs)
- Prediction
- Accuracy and Error Measures
- Ensemble Methods

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What Is Prediction?

- Essentially the same as classification, but output is continuous, not discrete
  - Construct a model
  - Use model to predict continuous output value for a given input
- Major method for prediction: regression
  - Many variants of regression analysis in statistics literature; not covered in this class
- Neural network and k-NN can do regression “out-of-the-box”
- SVMs for regression exist
- What about trees?

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Regression Trees and Model Trees

- Regression tree: proposed in CART system (Breiman et al. 1984)
  - CART: Classification And Regression Trees
  - Each leaf stores a continuous-valued prediction
    - Average output value for the training records that reach the leaf
- Model tree: proposed by Quinlan (1992)
  - Each leaf holds a regression model—a multivariate linear equation

- Training: like for classification trees, but uses *variance* instead of purity measure for selecting split predicates

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Classifier Accuracy Measures

		Predicted class		total
		buy_computer = yes	buy_computer = no	
True class	buy_computer = yes	6954	46	7000
	buy_computer = no	412	2588	3000
total		7366	2634	10000

- Accuracy of a classifier M, acc(M): percentage of test records that are correctly classified by M
  - Error rate (misclassification rate) of M = 1 – acc(M)
  - Given m classes, CM[i,j], an entry in a confusion matrix, indicates # of records in class i that are labeled by the classifier as class j

	C_1	C_2
C_1	True positive	False negative
C_2	False positive	True negative

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Precision and Recall

- Precision: measure of exactness
  - t-pos / (t-pos + f-pos)
- Recall: measure of completeness
  - t-pos / (t-pos + f-neg)
- F-measure: combination of precision and recall
  - 2 * precision * recall / (precision + recall)

- Note: Accuracy = (t-pos + t-neg) / (t-pos + t-neg + f-pos + f-neg)

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Limitation of Accuracy

- Consider a 2-class problem
  - Number of Class 0 examples = 9990
  - Number of Class 1 examples = 10
- If model predicts everything to be class 0, accuracy is 9990/10000 = 99.9 %
  - Accuracy is misleading because model does not detect any class 1 example
- Always predicting the majority class defines the baseline
  - A good classifier should do better than baseline

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Cost-Sensitive Measures: Cost Matrix

	PREDICTED CLASS		
ACTUAL CLASS	C(i|j)	**Class=Yes**	**Class=No**
	Class=Yes	C(Yes|Yes)	C(No|Yes)
	Class=No	C(Yes|No)	C(No|No)

C(i\| j): Cost of misclassifying class j example as class i

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Computing Cost of Classification

Cost Matrix	PREDICTED CLASS		
ACTUAL CLASS	C(i|j)	+	-
	+	-1	100
	-	1	0

Model M_1	PREDICTED CLASS		
ACTUAL CLASS		+	-
	+	150	40
	-	60	250

Accuracy = 80%

Cost = 3910

Model M_2	PREDICTED CLASS		
ACTUAL CLASS		+	-
	+	250	45
	-	5	200

Accuracy = 90%

Cost = 4255

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Prediction Error Measures

- Continuous output: it matters how far off the prediction is from the true value
- Loss function: distance between y and predicted value y'
  - Absolute error: | y – y' |
  - Squared error: $(y - y')^2$
- Test error (generalization error): average loss over the test set
- Mean absolute error: $$\frac{1}{n}\sum_{i=1}^{n}|y(i)-y'(i)|$$ Mean squared error: $$\frac{1}{n}\sum_{i=1}^{n}(y(i)-y'(i))^2$$
- Relative absolute error: $$\frac{\sum_{i=1}^{n}|y(i)-y'(i)|}{\sum_{i=1}^{n}|y(i)-\bar{y}|}$$ Relative squared error: $$\frac{\sum_{i=1}^{n}(y(i)-y'(i))^2}{\sum_{i=1}^{n}(y(i)-\bar{y})^2}$$
- Squared-error exaggerates the presence of outliers

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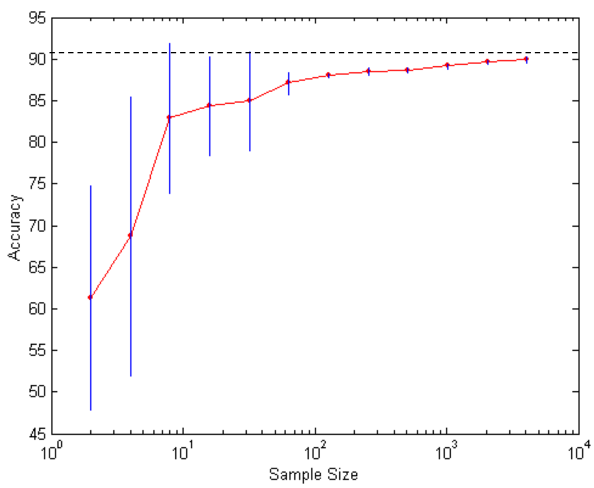
Evaluating a Classifier or Predictor

- Holdout method
  - The given data set is randomly partitioned into two sets
    - Training set (e.g., 2/3) for model construction
    - Test set (e.g., 1/3) for accuracy estimation
  - Can repeat holdout multiple times
    - Accuracy = avg. of the accuracies obtained
- Cross-validation (k-fold, where k = 10 is most popular)
  - Randomly partition data into k mutually exclusive subsets, each approximately equal size
  - In i-th iteration, use D_i as test set and others as training set
  - Leave-one-out: k folds where k = # of records
    - Expensive, often results in high variance of performance metric

Learning Curve



- Accuracy versus sample size
- Effect of small sample size:
  - Bias in estimate
  - Variance of estimate
- Helps determine how much training data is needed
  - Still need to have enough test and validation data to be representative of distribution

ROC (Receiver Operating Characteristic)

- Developed in 1950s for signal detection theory to analyze noisy signals
  – Characterizes trade-off between positive hits and false alarms
- ROC curve plots T-Pos rate (y-axis) against F-Pos rate (x-axis)
- Performance of each classifier is represented as a point on the ROC curve
  – Changing the threshold of the algorithm, sample distribution or cost matrix changes the location of the point

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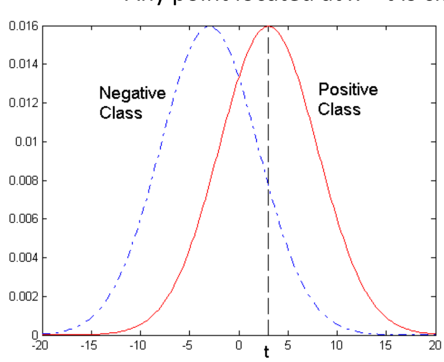
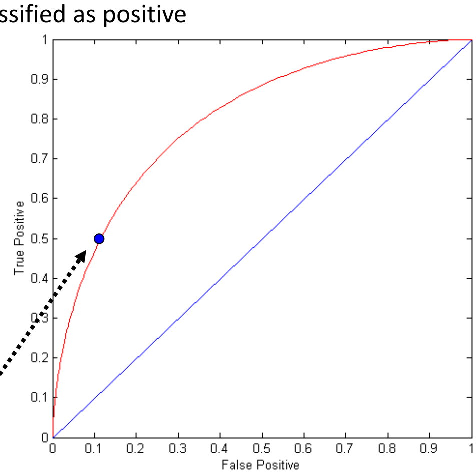
ROC Curve

- 1-dimensional data set containing 2 classes (positive and negative)
  – Any point located at x > t is classified as positive



At threshold t:

TPR=0.5, FPR=0.12



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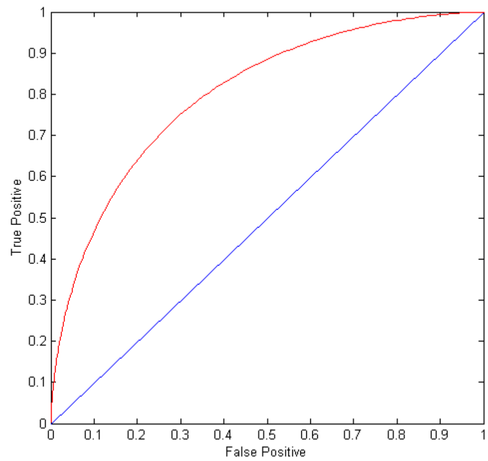
ROC Curve

(TPR, FPR):

- (0,0): declare everything to be negative class
- (1,1): declare everything to be positive class
- (1,0): ideal

- Diagonal line:
  - Random guessing



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Diagonal Line for Random Guessing

- Classify a record as positive with fixed probability p, irrespective of attribute values
- Consider test set with *a* positive and *b* negative records
- True positives: p*a, hence true positive rate = (p*a)/a = p
- False positives: p*b, hence false positive rate = (p*b)/b = p
- For every value 0≤p≤1, we get point (p,p) on ROC curve

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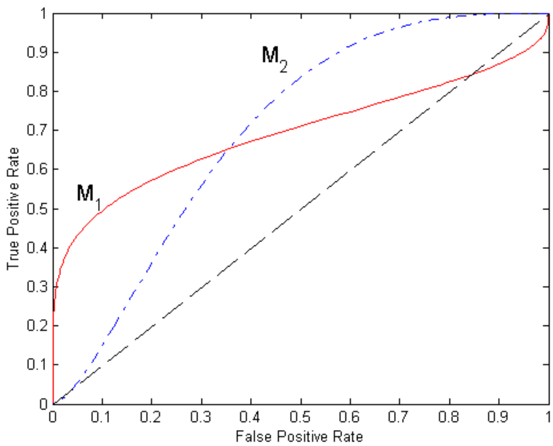
Using ROC for Model Comparison



- Neither model consistently outperforms the other
  - M1 better for small FPR
  - M2 better for large FPR
- Area under the ROC curve
  - Ideal: area = 1
  - Random guess: area = 0.5

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How to Construct an ROC curve

record	P(+|**x**)	True Class
1	0.95	+
2	0.93	+
3	0.87	-
4	0.85	-
5	0.85	-
6	0.85	+
7	0.76	-
8	0.53	+
9	0.43	-
10	0.25	+

- Use classifier that produces posterior probability P(+|**x**) for each test record **x**
- Sort records according to P(+|**x**) in decreasing order
- Apply threshold at each unique value of P(+|**x**)
  - Count number of TP, FP, TN, FN at each threshold
  - TP rate, TPR = TP/(TP+FN)
  - FP rate, FPR = FP/(FP+TN)

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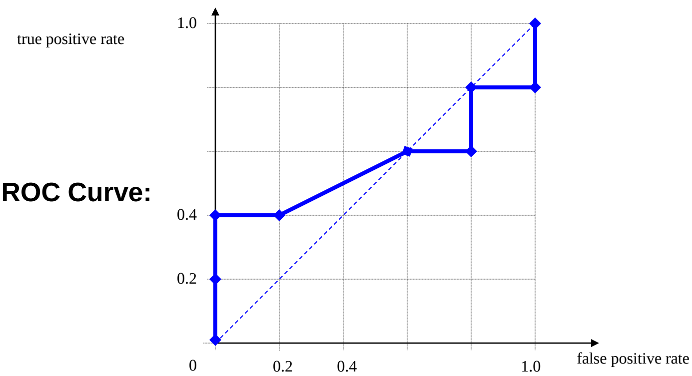
How To Construct An ROC Curve

Class	+	-	+	-	+	-	-	-	+	+	
Threshold >=	0.25	0.43	0.53	0.76	0.85	0.85	0.85	0.87	0.93	0.95	1.00
TP	5	4	4	3	3			2	2	1	0
FP	5	5	4	4	3			1	0	0	0
TN	0	0	1	1	2			4	5	5	5
FN	0	1	1	2	2			3	3	4	5
TPR	1	0.8	0.8	0.6	0.6			0.4	0.4	0.2	0
FPR	1	1	0.8	0.8	0.6			0.2	0	0	0

ROC Curve:



Test of Significance

- Given two models:
  - Model M1: accuracy = 85%, tested on 30 instances
  - Model M2: accuracy = 75%, tested on 5000 instances
- Can we say M1 is better than M2?
  - How much confidence can we place on accuracy of M1 and M2?
  - Can the difference in accuracy be explained as a result of random fluctuations in the test set?

Confidence Interval for Accuracy

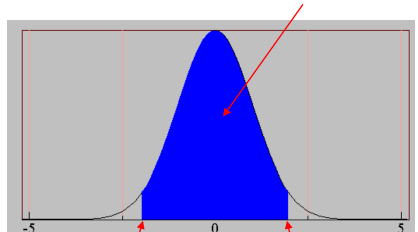
- Classification can be regarded as a Bernoulli trial
  - A Bernoulli trial has 2 possible outcomes, "correct" or "wrong" for classification
  - Collection of Bernoulli trials has a Binomial distribution
    - Probability of getting c correct predictions if model accuracy is p (=probability to get a single prediction right):

$$\binom{n}{c} p^c (1-p)^{n-c}$$

- Given c, or equivalently, ACC = c / n and n (#test records), can we predict p, the true accuracy of the model?

Confidence Interval for Accuracy

Area = 1 - α



$Z_{\alpha/2}$ $Z_{1-\alpha/2}$

- Binomial distribution for X="number of correctly classified test records out of n"
  - E(X)=pn, Var(X)=p(1-p)n
- Accuracy = X / n
  - E(ACC) = p, Var(ACC) = p(1-p) / n
- For large test sets (n>30), Binomial distribution is closely approximated by normal distribution with same mean and variance
  - ACC has a normal distribution with mean=p, variance=p(1-p)/n

$$\mathrm{P}\left(Z_{\alpha/2} < \frac{\mathrm{ACC} - p}{\sqrt{p(1-p)/n}} < Z_{1-\alpha/2} \right) = 1 - \alpha$$

- Confidence Interval for p:

$$p = \frac{2n \cdot \mathrm{ACC} + Z_{\alpha/2}^2 \pm \sqrt{Z_{\alpha/2}^2 + 4n \cdot \mathrm{ACC} - 4n \cdot \mathrm{ACC}^2}}{2(n + Z_{\alpha/2}^2)}$$

Confidence Interval for Accuracy

- Consider a model that produces an accuracy of 80% when evaluated on 100 test instances
  - n = 100, ACC = 0.8
  - Let 1-α = 0.95 (95% confidence)
  - From probability table, $Z_{\alpha/2} = 1.96$

N	50	100	500	1000	5000
p(lower)	0.670	0.711	0.763	0.774	0.789
p(upper)	0.888	0.866	0.833	0.824	0.811

1-α	Z
0.99	2.58
0.98	2.33
0.95	1.96
0.90	1.65

$$p = \frac{2n \cdot \mathrm{ACC} + Z^2_{\alpha/2} \pm \sqrt{Z^2_{\alpha/2} + 4n \cdot \mathrm{ACC} - 4n \cdot \mathrm{ACC}^2}}{2(n + Z^2_{\alpha/2})}$$

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Comparing Performance of Two Models

- Given two models M1 and M2, which is better?
  - M1 is tested on D_1 (size=n_1), found error rate = e_1
  - M2 is tested on D_2 (size=n_2), found error rate = e_2
  - Assume D_1 and D_2 are independent
  - If n_1 and n_2 are sufficiently large, then

$$\mathrm{err}_1 \sim N(\mu_1, \sigma_1)$$
$$\mathrm{err}_2 \sim N(\mu_2, \sigma_2)$$

  - Estimate: $\hat{\mu}_i = e_i$ and $\hat{\sigma}_i^2 = \dfrac{e_i(1-e_i)}{n_i}$

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Testing Significance of Accuracy Difference

- Consider random variable d = $err_1 - err_2$
  - Since err_1, err_2 are normally distributed, so is their difference
  - Hence d ~ N (d_t, σ_t) where d_t is the true difference
- Estimator for d_t:
  - $E[d] = E[err_1 - err_2] = E[err_1] - E[err_2] \approx e_1 - e_2$
  - Since D_1 and D_2 are independent, variance adds up:

$$\hat{\sigma}_t^2 = \hat{\sigma}_1^2 + \hat{\sigma}_2^2 = \frac{e_1(1-e_1)}{n_1} + \frac{e_2(1-e_2)}{n_2}$$

  - At (1-α) confidence level, $d_t = \mathrm{E}[d] \pm Z_{\alpha/2}\hat{\sigma}_t$

An Illustrative Example

- Given: M1: $n_1 = 30$, $e_1 = 0.15$
  M2: $n_2 = 5000$, $e_2 = 0.25$
- $E[d] = |e_1 - e_2| = 0.1$
- 2-sided test: $d_t = 0$ versus $d_t \neq 0$

$$\hat{\sigma}_t^2 = \frac{0.15(1-0.15)}{30} + \frac{0.25(1-0.25)}{5000} = 0.0043$$

- At 95% confidence level, $Z_{\alpha/2} = 1.96$

$$d_t = 0.100 \pm 1.96\sqrt{0.0043} = 0.100 \pm 0.128$$

- Interval contains zero, hence difference may not be statistically significant
- But: may reject null hypothesis ($d_t \neq 0$) at lower confidence level

Significance Test for K-Fold Cross-Validation

- Each learning algorithm produces k models:
  - L1 produces M11 , M12, …, M1k
  - L2 produces M21 , M22, …, M2k
- Both models are tested on the same test sets D_1, D_2,…, D_k
  - For each test set, compute $d_j = e_{1,j} - e_{2,j}$
  - For large enough k, d_j is normally distributed with mean d_t and variance σ_t
  - Estimate:

$$\hat{\sigma}_t^2 = \frac{\sum_{j=1}^{k}(d_j - \bar{d})^2}{k(k-1)}$$

$$d_t = \bar{d} \pm t_{1-\alpha,k-1}\hat{\sigma}_t$$

t-distribution: get t coefficient $t_{1-\alpha,k-1}$ from table by looking up confidence level ($1-\alpha$) and degrees of freedom (k-1)

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- Nearest Neighbor
- Bayesian Classification
- Artificial Neural Networks
- Support Vector Machines (SVMs)
- Prediction
- Accuracy and Error Measures
- Ensemble Methods

Ensemble Methods

- Construct a set of classifiers from the training data
- Predict class label of previously unseen records by aggregating predictions made by multiple classifiers

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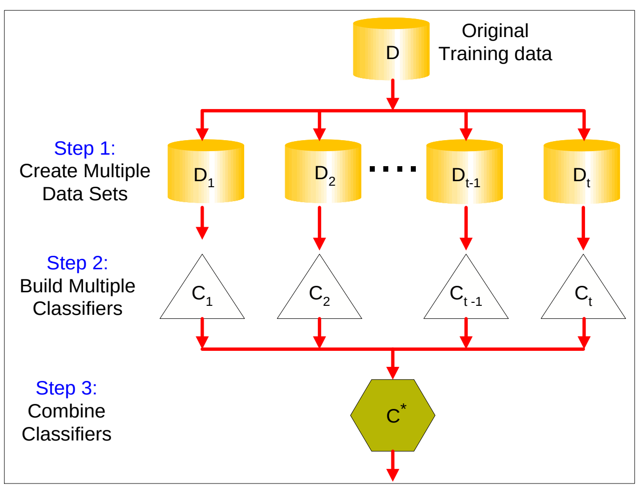
General Idea



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Why Does It Work?

- Consider 2-class problem
- Suppose there are 25 base classifiers
  - Each classifier has error rate ε = 0.35
  - Assume the classifiers are independent
- Return majority vote of the 25 classifiers
  - Probability that the ensemble classifier makes a wrong prediction:

$$\sum_{i=13}^{25} \binom{25}{i} \varepsilon^i (1-\varepsilon)^{25-i} = 0.06$$

Base Classifier vs. Ensemble Error

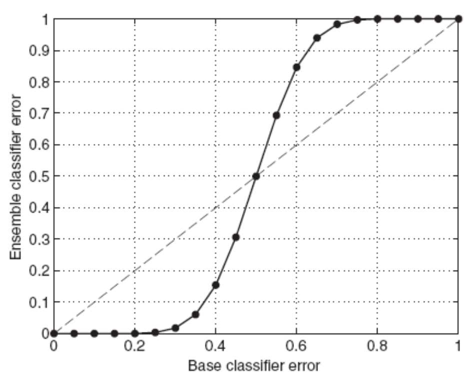

Figure 5.30. Comparison between errors of base classifiers and errors of the ensemble classifier.

Model Averaging and Bias-Variance Tradeoff

- Single model: lowering bias will usually increase variance
  - "Smoother" model has lower variance but might not model function well enough
- Ensembles can overcome this problem
  1. Let models overfit
     - Low bias, high variance
  2. Take care of the variance problem by averaging many of these models
- This is the basic idea behind bagging

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Bagging: Bootstrap Aggregation

- Given training set with n records, sample n records randomly with replacement

Original Data	1	2	3	4	5	6	7	8	9	10
Bagging (Round 1)	7	8	10	8	2	5	10	10	5	9
Bagging (Round 2)	1	4	9	1	2	3	2	7	3	2
Bagging (Round 3)	1	8	5	10	5	5	9	6	3	7

- Train classifier for each bootstrap sample
- Note: each training record has probability $1 – (1 – 1/n)^n$ of being selected at least once in a sample of size n

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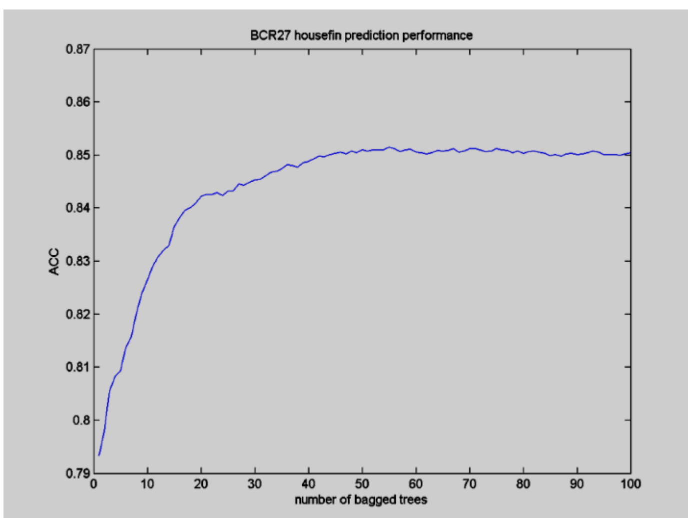
Bagged Trees

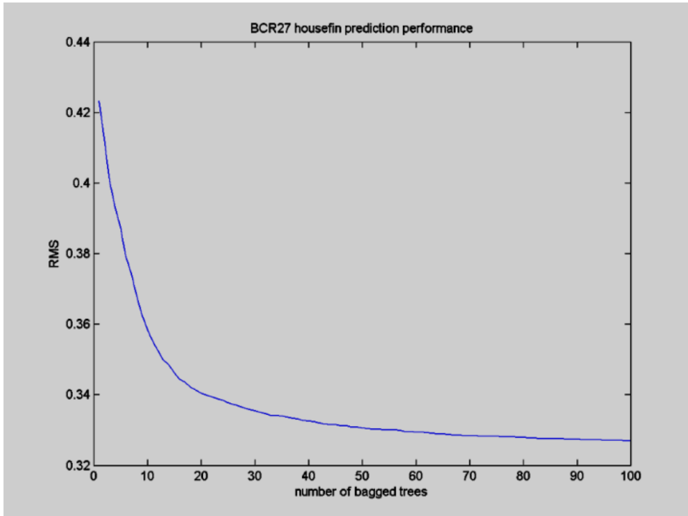
- Create k trees from training data
  - Bootstrap sample, grow large trees
- Design goal: independent models, high variability between models
- Ensemble prediction = average of individual tree predictions (or majority vote)
- Works the same way for other classifiers

(1/k)·  + (1/k)·  +…+ (1/k)· 

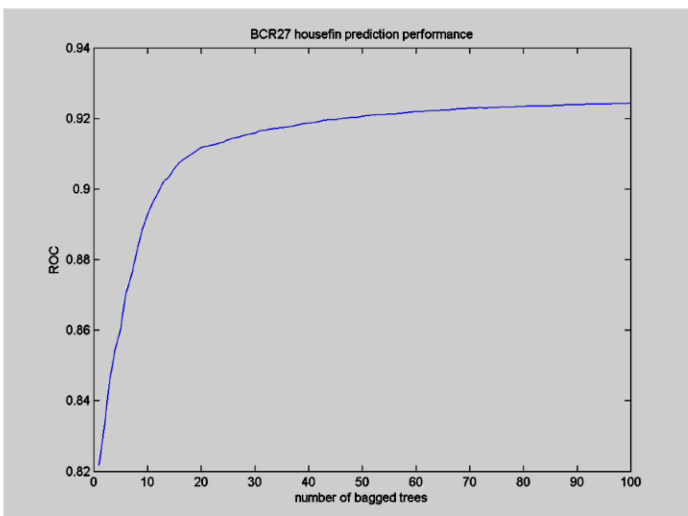
Typical Result



Typical Result



Typical Result

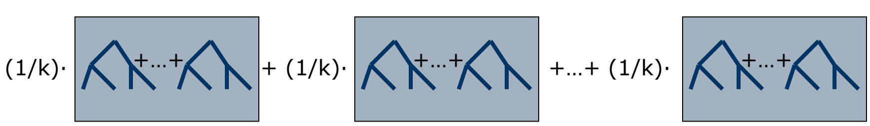


Bagging Challenges

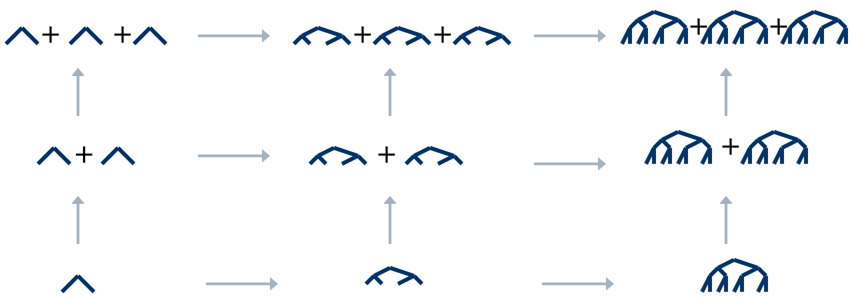
- Ideal case: all models independent of each other
- Train on independent data samples
  - Problem: limited amount of training data
    - Training set needs to be representative of data distribution
  - Bootstrap sampling allows creation of many “almost” independent training sets
- Diversify models, because similar sample might result in similar tree
  - Random Forest: limit choice of split attributes to small random subset of attributes (new selection of subset for each node) when training tree
  - Use different model types in same ensemble: tree, ANN, SVM, regression models

Additive Grove

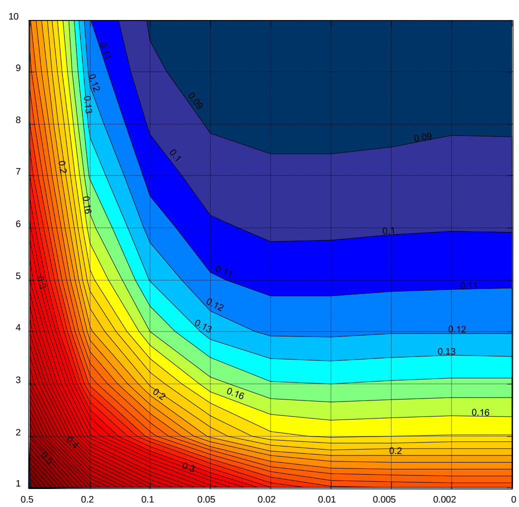
- Ensemble technique for predicting continuous output
- Instead of individual trees, train additive models
  - Prediction of single Grove model = sum of tree predictions
- Prediction of ensemble = average of individual Grove predictions
- Combines large trees and additive models
  - Challenge: how to train the additive models without having the first trees fit the training data too well
    - Next tree is trained on residuals of previously trained trees in same Grove model
    - If previously trained trees capture training data too well, next tree is mostly trained on noise



Training Groves



Typical Grove Performance

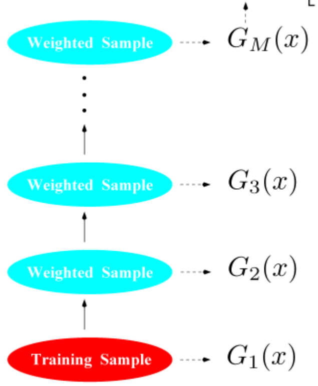


- Root mean squared error
  - Lower is better
- Horizontal axis: tree size
  - Fraction of training data when to stop splitting
- Vertical axis: number of trees in each single Grove model
- 100 bagging iterations

Boosting

FINAL CLASSIFIER

$$G(x) = \text{sign}\left[\sum_{m=1}^{M} \alpha_m G_m(x)\right]$$



- Iterative procedure to adaptively change distribution of training data by focusing more on previously misclassified records
  - Initially, all n records are assigned equal weights
  - Record weights may change at the end of each boosting round

Boosting

- Records that are wrongly classified will have their weights increased
- Records that are classified correctly will have their weights decreased

Original Data	1	2	3	4	5	6	7	8	9	10
Boosting (Round 1)	7	3	2	8	7	9	4	10	6	3
Boosting (Round 2)	5	4	9	4	2	5	1	7	4	2
Boosting (Round 3)	4	4	8	10	4	5	4	6	3	4

- Assume record 4 is hard to classify
- Its weight is increased, therefore it is more likely to be chosen again in subsequent rounds

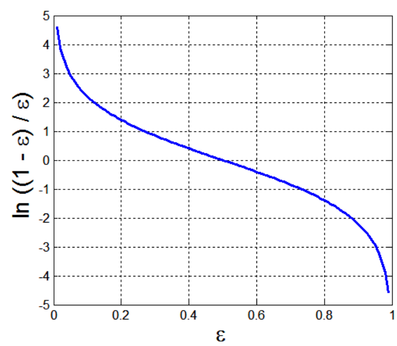
Example: AdaBoost

- Base classifiers: $C_1, C_2, \ldots, C_T$
- Error rate (n training records, w_j are weights that sum to 1):

$$\varepsilon_i = \sum_{j=1}^{n} w_j \delta\left(C_i(x_j) \neq y_j\right)$$

- Importance of a classifier:

$$\alpha_i = \ln\left(\frac{1-\varepsilon_i}{\varepsilon_i}\right)$$



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AdaBoost Details

- Weight update:

$$w_j^{(i+1)} = \frac{w_j^{(i)}}{Z_i} \cdot \begin{cases} \dfrac{\varepsilon_i}{1-\varepsilon_i} & \text{if } C_i(x_j) = y_j \\ 1 & \text{if } C_i(x_j) \neq y_j \end{cases}$$

where Z_i is the normalization factor

- Weights initialized to 1/n
- Z_i ensures that weights add to 1
- If any intermediate rounds produce error rate higher than 50%, the weights are reverted back to 1/n and the resampling procedure is repeated
- Final classification:

$$C^*(x) = \arg\max_y \sum_{i=1}^{T} \alpha_i \delta\left(C_i(x) = y\right)$$

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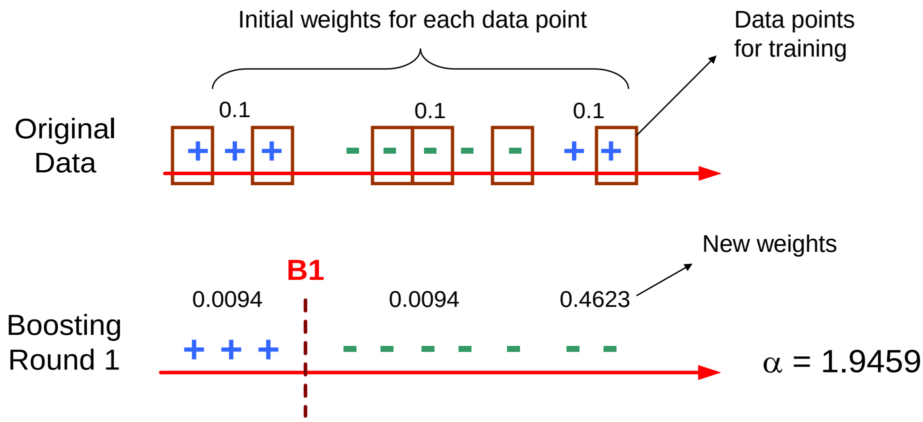
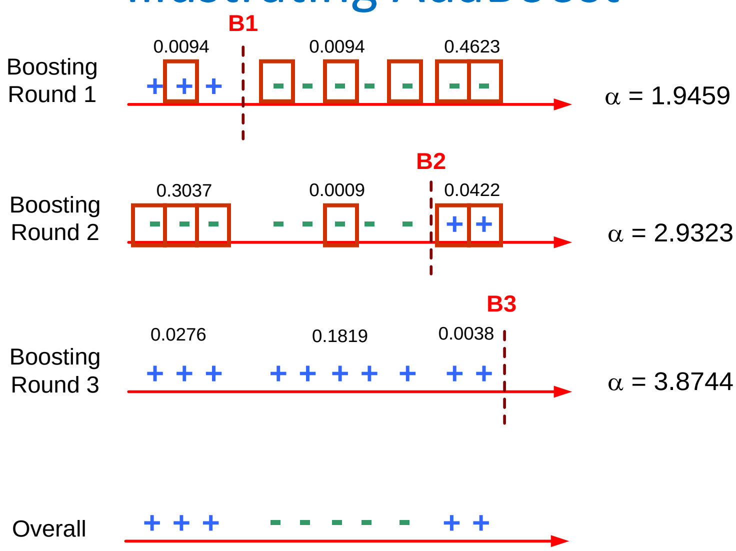
Illustrating AdaBoost



Note: The numbers appear to be wrong, but they convey the right idea…

Illustrating AdaBoost



Note: The numbers appear to be wrong, but they convey the right idea…

Bagging vs. Boosting

- Analogy
  - Bagging: diagnosis based on multiple doctors' majority vote
  - Boosting: weighted vote, based on doctors' previous diagnosis accuracy
- Sampling procedure
  - Bagging: records have same weight; easy to train in parallel
  - Boosting: weights record higher if model predicts it wrong; inherently sequential process
- Overfitting
  - Bagging robust against overfitting
  - Boosting susceptible to overfitting: make sure individual models do not overfit
- Accuracy usually significantly better than a single classifier
  - Best boosted model often better than best bagged model
- Additive Grove
  - Combines strengths of bagging and boosting (additive models)
  - Shown empirically to make better predictions on many data sets
  - Training more tricky, especially when data is very noisy

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Classification/Prediction Summary

- Forms of data analysis that can be used to train models from data and then make predictions for new records
- Effective and scalable methods have been developed for decision tree induction, Naive Bayesian classification, Bayesian networks, rule-based classifiers, Backpropagation, Support Vector Machines (SVM), nearest neighbor classifiers, and many other classification methods
- Regression models are popular for prediction. Regression trees, model trees, and ANNs are also used for prediction.

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Classification/Prediction Summary

- K-fold cross-validation is a popular method for accuracy estimation, but determining accuracy on large test set is equally accepted
  - If test sets are large enough, a significance test for finding the best model is not necessary
- Area under ROC curve and many other common performance measures exist
- Ensemble methods like bagging and boosting can be used to increase overall accuracy by learning and combining a series of individual models
  - Often state-of-the-art in prediction quality, but expensive to train, store, use
- No single method is superior over all others for all data sets
  - Issues such as accuracy, training and prediction time, robustness, interpretability, and scalability must be considered and can involve trade-offs

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