Introduction to Data Mining

Chapter 8. Classification: Basic Concepts

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Chapter 8. Classification: Basic Concepts

- Classification: Basic Concepts 
- Decision Tree Induction
- Bayes Classification Methods
- Linear Classifier
- Model Evaluation and Selection
- Techniques to Improve Classification Accuracy: Ensemble Methods
- Additional Concepts on Classification
- Summary

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Supervised vs. Unsupervised Learning (1)

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

Training Data with class label:

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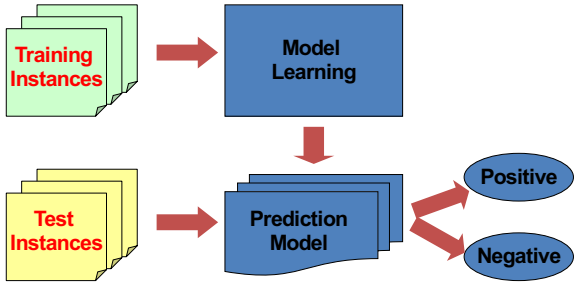

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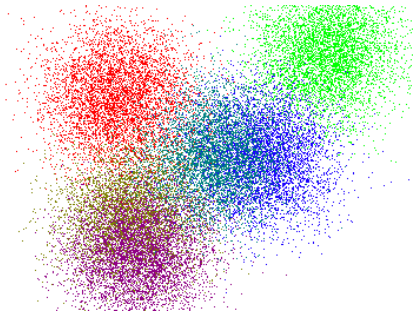
Supervised vs. Unsupervised Learning (2)

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



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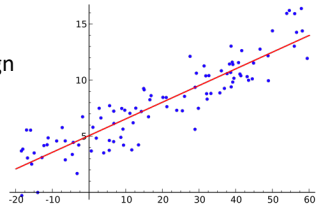
Prediction Problems: Classification vs. Numeric Prediction

- Classification
  - Predict categorical class labels (discrete or nominal)
  - Construct a model based on the training set and the **class labels** (the values in a classifying attribute) and use it in classifying new data
- Numeric prediction
  - Model continuous-valued functions (i.e., predict unknown or missing values)
- Typical applications of classification
  - Credit/loan approval
  - Medical diagnosis: if a tumor is cancerous or benign
  - Fraud detection: if a transaction is fraudulent
  - Web page categorization: which category it is



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Classification—Model Construction, Validation and Testing

- **Model construction**
  - Each sample is assumed to belong to a predefined class (shown by the **class label**)
  - The set of samples used for model construction is **training set**
  - Model: Represented as decision trees, rules, mathematical formulas, or other forms
- **Model Validation and Testing**:
  - **Test:** Estimate accuracy of the model
    - The known label of test sample is compared with the classified result from the model
    - *Accuracy:* % of test set samples that are correctly classified by the model
    - Test set is independent of training set
  - **Validation**: If *the test set* is used to select or refine models, it is called **validation** (or development) **(test) set**
- **Model Deployment:** If the accuracy is acceptable, use the model to classify new data

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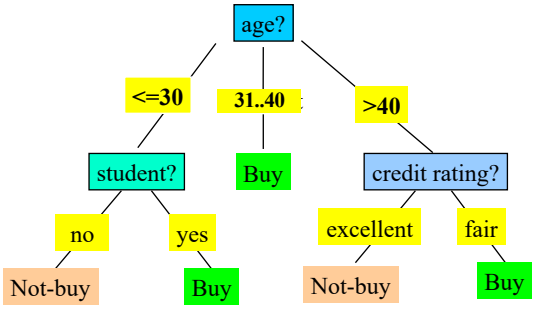
Decision Tree Induction: An Example

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



Training data set: Who buys computer?

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

Note: The data set is adapted from "Playing Tennis" example of R. Quinlan

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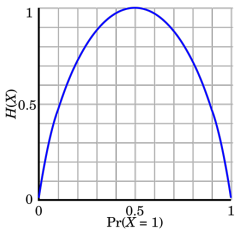
From Entropy to Info Gain: A Review of Entropy

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

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

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

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



m = 2

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Information Gain: An Attribute Selection Measure

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

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

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

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

- Information gained by branching on attribute A

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

I : the expected information needed to classify a given sample
E (entropy) : expected information based on the partitioning into subsets by A

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Example: Attribute Selection with Information Gain

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

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

age	p_i	n_i	$I(p_i, n_i)$
<=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	fair	no
<=30	high	no	excellent	no
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>40	low	yes	fair	yes
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$$Info_{age}(D) = \frac{5}{14}I(2,3) + \frac{4}{14}I(4,0) + \frac{5}{14}I(3,2) = 0.694$$

$\frac{5}{14}I(2,3)$ means "age <=30" has 5 out of 14 samples, with 2 yes'es and 3 no's.

Hence

$$Gain(age) = Info(D) - Info_{age}(D) = 0.246$$

Similarly, we can get

$$Gain(income) = 0.029$$
$$Gain(student) = 0.151$$
$$Gain(credit\_rating) = 0.048$$

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Decision Tree Induction: Algorithm

- Basic algorithm
  - Tree is constructed in a **top-down, recursive, divide-and-conquer manner**
  - At start, all the training examples are at the root
  - Examples are partitioned recursively based on selected attributes
  - On each node, attributes are selected based on the training examples on that node, and a heuristic or statistical measure (e.g., **information gain**)
- Conditions for stopping partitioning
  - All samples for a given node belong to the same class
  - There are no remaining attributes for further partitioning
  - There are no samples left
- Prediction
  - **Majority voting** is employed for classifying the leaf

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How to Handle Continuous-Valued Attributes?

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

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Gain Ratio: A Refined Measure for Attribute Selection

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

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

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

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Another Measure: Gini Index

- Gini index: Used in CART, and also in IBM IntelligentMiner
- If a data set D contains examples from n classes, gini index, $gini(D)$ is defined as
  - $gini(D) = 1 - \sum_{j=1}^{n} p_j^2$
    - p_j is the relative frequency of class j in D
- If a data set D is split on A into two subsets D_1 and D_2, the $gini$ index $gini(D)$ is defined as
  - $gini_A(D) = \frac{|D_1|}{|D|} gini(D_1) + \frac{|D_2|}{|D|} gini(D_2)$
- Reduction in Impurity:
  - $\Delta gini(A) = gini(D) - gini_A(D)$
- The attribute provides the smallest $gini_{split}(D)$ (or the largest reduction in impurity) is chosen to split the node (*need to enumerate all the possible splitting points for each attribute*)

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Computation of Gini Index

- Example: D has 9 tuples in buys_computer = "yes" and 5 in "no"

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

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

$$= \frac{10}{14}\left(1 - \left(\frac{7}{10}\right)^2 - \left(\frac{3}{10}\right)^2\right) + \frac{4}{14}\left(1 - \left(\frac{2}{4}\right)^2 - \left(\frac{2}{4}\right)^2\right) = 0.443 = Gini_{income \in \{high\}}(D)$$

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

- All attributes are assumed continuous-valued
- May need other tools, e.g., clustering, to get the possible split values
- Can be modified for categorical attributes

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Other Attribute Selection Measures

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

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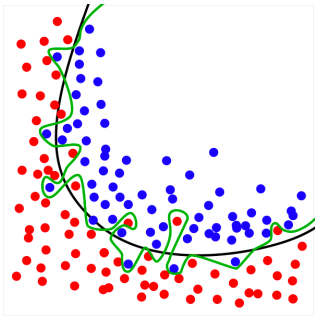
Overfitting and Tree Pruning

- Overfitting: An induced tree may overfit the training data
  - Too many branches, some may reflect anomalies due to noise or outliers
  - Poor accuracy for unseen samples
- Two approaches to avoid overfitting
  - Prepruning: *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
  - Postpruning: *Remove branches* from a "fully grown" tree—get a sequence of progressively pruned trees
    - Use a set of data different from the training data to decide which is the "best pruned tree"



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What Is Bayesian Classification?

- A statistical classifier
  - Perform *probabilistic prediction* (*i.e.,* predict class membership probabilities)
- Foundation—Based on Bayes' Theorem
- Performance
  - A simple Bayesian classifier, *naïve Bayesian classifier*, has comparable performance with decision tree and selected neural network classifiers
- Incremental
  - Each training example can incrementally increase/decrease the probability that a hypothesis is correct—prior knowledge can be combined with observed data
- **Theoretical Standard**
  - Even when Bayesian methods are computationally intractable, they can provide a standard of optimal decision making against which other methods can be measured

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Bayes' Theorem: Basics

- Total probability Theorem: $P(B) = \sum_{i=1}^{M} P(B|A_i)P(A_i)$
- Bayes' Theorem: $P(H|\mathbf{X}) = \frac{P(\mathbf{X}|H)P(H)}{P(\mathbf{X})} = P(\mathbf{X}|H) \times P(H) / P(\mathbf{X})$
  - Let **X** be a data sample ("*evidence*"): class label is unknown
  - Let H be a *hypothesis* that X belongs to class C
  - Classification is to determine P(H|**X**), (i.e., *posteriori probability):* the probability that the hypothesis holds given the observed data sample **X**
  - P(H) (*prior probability*): the initial probability
    - E.g., **X** will buy computer, regardless of age, income, …
  - P(**X**): probability that sample data is observed
  - P(**X**|H) (likelihood): the probability of observing the sample **X**, given that the hypothesis holds
    - E.g., Given that **X** will buy computer, the prob. that X is 31..40, medium income

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Bayes' Theorem: Basics

- Total probability Theorem:

$$p(B) = \sum_{i} p(B|A_i)p(A_i)$$

- Bayes' Theorem:

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

What we should choose — posteriori probability

likelihood — What we just see

prior probability — What we knew previously

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

Prediction can be done based on Bayes' Theorem:

Classification is to derive the maximum posteriori

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Bayes' Theorem Example: Picnic Day

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

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

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

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

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Naïve Bayes Classifier: Making a Naïve Assumption

- Practical difficulty of Naïve Bayes inference: It requires initial knowledge of many probabilities, which may not be available or involving significant computational cost
- A Naïve Special Case
  - Make an additional assumption to simplify the model, but achieve comparable performance.

attributes are conditionally independent (i.e., no dependence relation between attributes)

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

  - Only need to count the class distribution w.r.t. features

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Naïve Bayes Classifier: Training Dataset

Class:
C1:buys_computer = 'yes'
C2:buys_computer = 'no'

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

age	income	student	credit_rating	buys_computer
<=30	high	no	fair	no
<=30	high	no	excellent	no
31…40	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
31…40	low	yes	excellent	yes
<=30	medium	no	fair	no
<=30	low	yes	fair	yes
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<=30	medium	yes	excellent	yes
31…40	medium	no	excellent	yes
31…40	high	yes	fair	yes
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Naïve Bayes Classifier: An Example

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

- $P(C_i)$: P(buys_computer = "yes") = 9/14 = 0.643
  P(buys_computer = "no") = 5/14= 0.357
- Compute $P(X|C_i)$ for each class
  P(age = "<=30"|buys_computer = "yes") = 2/9 = 0.222
  P(age = "<= 30"|buys_computer = "no") = 3/5 = 0.6
  P(income = "medium" | buys_computer = "yes") = 4/9 = 0.444
  P(income = "medium" | buys_computer = "no") = 2/5 = 0.4
  P(student = "yes" | buys_computer = "yes) = 6/9 = 0.667
  P(student = "yes" | buys_computer = "no") = 1/5 = 0.2
  P(credit_rating = "fair" | buys_computer = "yes") = 6/9 = 0.667
  P(credit_rating = "fair" | buys_computer = "no") = 2/5 = 0.4
- **X = (age <= 30 , income = medium, student = yes, credit_rating = fair)**

$P(X|C_i)$: P(X|buys_computer = "yes") = 0.222 x 0.444 x 0.667 x 0.667 = 0.044
P(X|buys_computer = "no") = 0.6 x 0.4 x 0.2 x 0.4 = 0.019

$P(C_i|X) = P(X|C_i)*P(C_i)$: P(X|buys_computer = "yes") * P(buys_computer = "yes") = 0.028
P(X|buys_computer = "no") * P(buys_computer = "no") = 0.007

Therefore, X belongs to class ("buys_computer = yes")

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Avoiding the Zero-Probability Problem

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

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

- Example. Suppose a dataset with 1000 tuples:
  income = low (0), income= medium (990), and income = high (10)
- Use **Laplacian correction** (or Laplacian estimator)
  - *Adding 1 to each case*
    Prob(income = low) = 1/(1000 + 3)
    Prob(income = medium) = (990 + 1)/(1000 + 3)
    Prob(income = high) = (10 + 1)/(1000 + 3)
  - The "corrected" probability estimates are close to their "uncorrected" counterparts

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Naïve Bayes Classifier: Strength vs. Weakness

- Strength
  - Easy to implement
  - Good results obtained in most of the cases
- Weakness
  - Assumption: attributes conditional independence, therefore loss of accuracy
  - Practically, dependencies exist among variables
    - E.g., Patients: Profile: age, family history, etc.
      Symptoms: fever, cough etc.
      Disease: lung cancer, diabetes, etc.
    - Dependencies among these cannot be modeled by Naïve Bayes Classifier
- How to deal with these dependencies?
  - Use Bayesian Belief Networks (to be covered in the next chapter)

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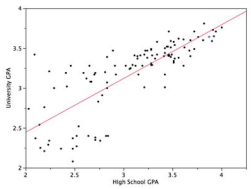
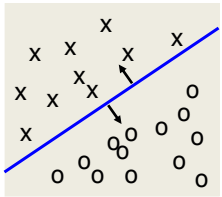
Linear Regression vs. Linear Classifier

- **Linear regression**
  - Data modeled to fit a straight line
    - *Linear equation: Y = w X + b*
  - Often uses the least-square method to fit the line
  - Used to **predict continuous values**



- **Linear Classifier**
  - Built a classification model using a straight line
  - Used for **(categorical data) binary classification**



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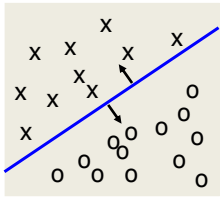
Linear Classifier: General Ideas

- Binary Classification
- $f(x)$ is a linear function based on the example's attribute values
  - The prediction is based on the value of $f(x)$
  - Data above the blue line belongs to class 'x' (i.e., $f(x) > 0$)
  - Data below blue line belongs to class 'o' (i.e., $f(x) < 0$)
- Classical Linear Classifiers
  - Linear Discriminant Analysis (LDA) (not covered)
  - Logistic Regression
  - Perceptron (later)
  - SVM (later)



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Linear Classifier: An Example

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

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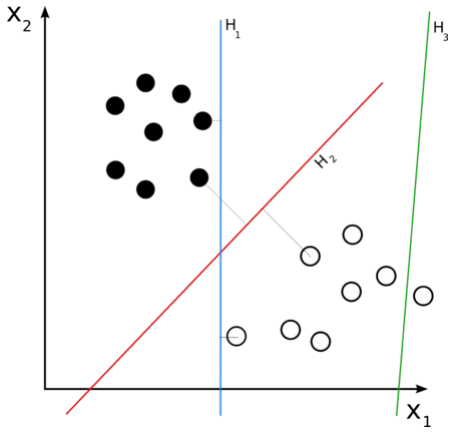
Key Question: Which Line Is Better?

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



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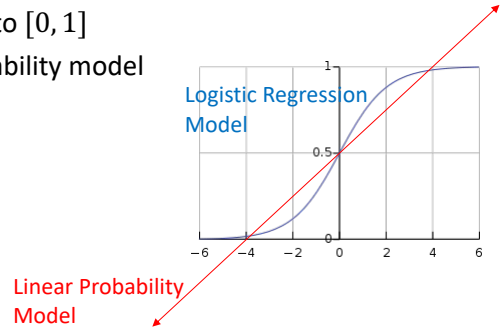
Logistic Regression: General Ideas

- Key Idea: Turns linear predictions into probabilities
- Sigmoid function:
  - $S(x) = \frac{1}{1+e^{-x}} = \frac{e^x}{e^x+1}$
  - Projects $(-\infty, +\infty)$ to $[0, 1]$
- Compare to linear probability model
  - More smooth



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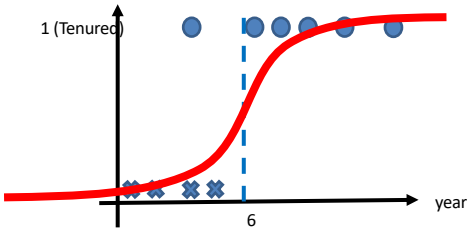
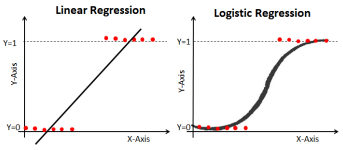
Logistic Regression: An Example

- Suppose we only consider the year as feature





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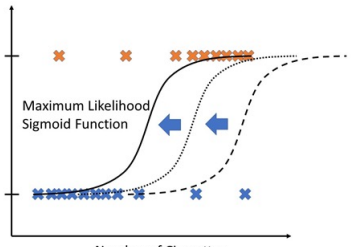
Logistic Regression: Maximum Likelihood

- How to select the correct sigmoid function that best fits the training data?
- The answer is maximum likelihood.
- The prediction function to learn
  - $p(Y = 1 \,|X = x; \boldsymbol{w}) \;= S(w_0 + \sum_{i=1}^{n} w_i \cdot x_i)$
  - $\boldsymbol{w} = (w_0, w_1, w_2, \ldots, w_n)$ are the parameters of the model
- Maximum Likelihood
  - Log likelihood:

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

- There's no close form solution
  - Gradient Descent
  - Update w based on training data.



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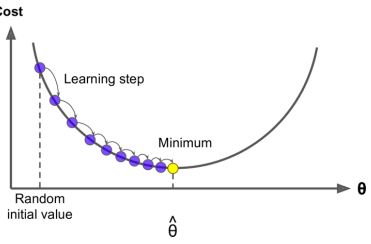
Gradient Descent

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

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

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



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Chapter 8. Classification: Basic Concepts

- Classification: Basic Concepts
- Decision Tree Induction
- Bayes Classification Methods
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Model Evaluation and Selection

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

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Classifier Evaluation Metrics: Confusion Matrix

- **Confusion Matrix:**

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

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

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

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

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

Real-world truth

Predictions

- **Classifier accuracy,** or recognition rate
  - Percentage of test set tuples that are correctly classified
  - **Accuracy = (TP + TN)/All**
- **Error rate:** *1 – accuracy*, or
- **Error rate = (FP + FN)/All**

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

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

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

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

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

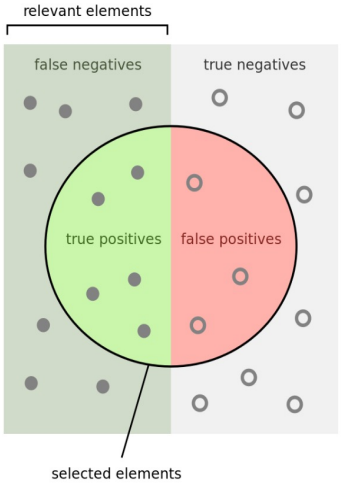
Precision = 

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

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

Recall = 

  - Range: [0, 1]



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

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

- The "inverse" relationship between precision & recall
- ***F* measure (**or ***F*-score):** harmonic mean of precision and recall
  - In general, it is the weighted measure of precision & recall

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

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

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

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

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Classifier Evaluation Metrics: Example

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

Actual Class\Predicted class	cancer = yes	cancer = no	Total	Recognition(%)
cancer = yes	**90**	**210**	300	30.00 (*sensitivity*)
cancer = no	**140**	**9560**	9700	98.56 (*specificity*)
Total	230	9770	10000	96.50 (*accuracy*)

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

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Classifier Evaluation: Holdout

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

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Classifier Evaluation: Cross-Validation

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

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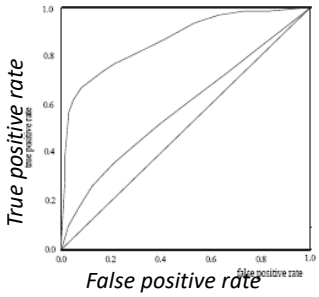
Model Selection: ROC Curves

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



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

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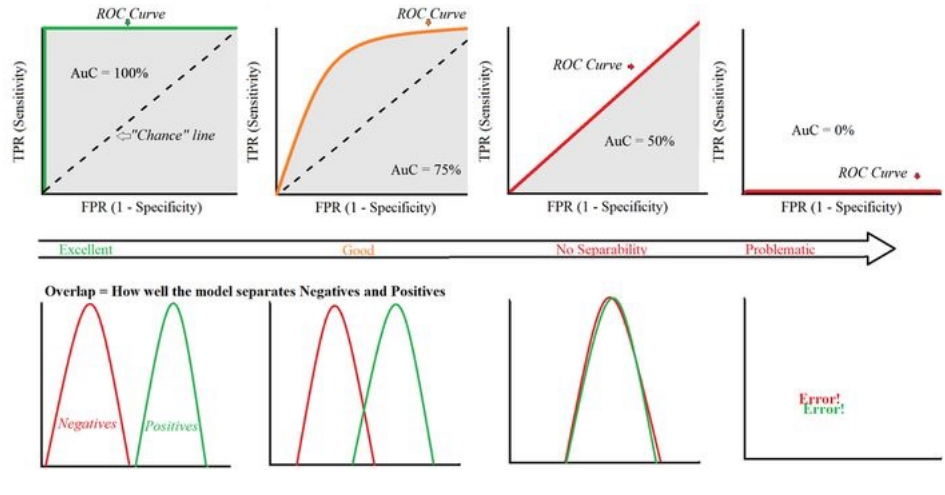

https://www.datasciencecentral.com/roc-curve-explained-in-one-picture/

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Classifier Evaluation: Bootstrap

- **Bootstrap** is a statistical technique used to estimate the accuracy of a classifier (or any model) by resampling the data with replacement. It helps assess the performance of a model without needing a separate test set, and is particularly useful when you have limited data. Here's how it works for estimating a classifier's accuracy:
- **How Bootstrap Works**

1. **Create Resampled Datasets**:
   1. From the original dataset of size NNN, create BBB bootstrap samples by randomly sampling NNN instances **with replacement**.
   2. Each bootstrap sample will have some data points repeated and others omitted.
2. **Train and Test**:
   1. Train the classifier on each bootstrap sample.
   2. Test the classifier on the data points that were **not included** in the sample (called the "out-of-bag" data).
3. **Evaluate Metrics**:
   1. Calculate the performance metric (e.g., accuracy) on the out-of-bag data for each bootstrap iteration.
4. **Aggregate Results**:
   1. Compute the average and standard deviation of the performance metric across all bootstrap samples to estimate accuracy and variability.

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Classifier Evaluation: Bootstrap

- **Example of Bootstrap Process**
- For a dataset with 100 instances:

1. Randomly sample 100 instances with replacement to create a bootstrap sample.
   Example: Original dataset = [1,2,3,...,100]; bootstrap sample = [2,5,3,5,97,...].
2. Train the classifier on this sample.
3. Test it on the out-of-bag data (instances not selected in the sample).
4. Repeat the process B times (e.g., B=1000).

- **Limitations of Bootstrap**
  - **Overfitting**: Training on overlapping samples may lead to an optimistic bias if the model overfits.
  - **Computational Cost**: Requires training and testing the model many times, which can be expensive for complex models or large datasets.

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Techniques to Improve Classification Accuracy

- Introducing Ensemble Methods
- Bagging
- Boosting
- Random Forests
- Imbalanced Classification

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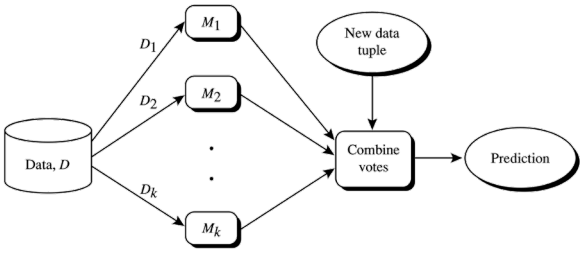
Ensemble Methods: Increasing the Accuracy

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



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Ensemble Methods: Increasing the Accuracy

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

Base model performance

Ensemble performance

	x1	x2	x3
M1	✓	✓	✗
M2	✗	✓	✓
M3	✓	✗	✓
Voting Ensemble	✓	✓	✓

Case 1: Ensemble has positive effect

	x1	x2	x3
M1	✓	✓	✗
M2	✓	✓	✗
M3	✓	✓	✗
Voting Ensemble	✓	✓	✗

Case 2: Ensemble has no effect

	x1	x2	x3
M1	✓	✗	✗
M2	✗	✓	✗
M3	✗	✗	✓
Voting Ensemble	✗	✗	✗

Case 3: Ensemble has negative effect

- Base models should be
  - Accurate
  - Diverse

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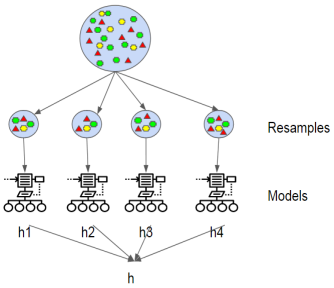
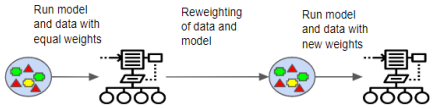
Ensemble Methods: Increasing the Accuracy

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



Bagging



Boosting

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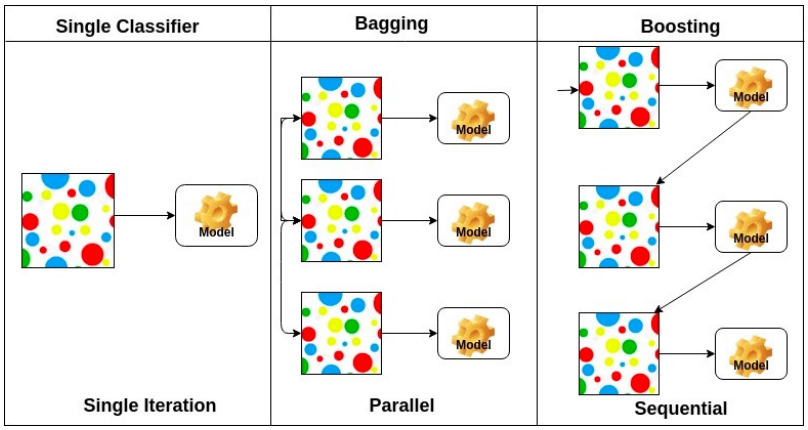

https://www.datacamp.com/community/tutorials/adaboost-classifier-python

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Bagging: Bootstrap Aggregation

- Analogy: Diagnosis based on multiple doctors' majority vote
- **Training**: Given a set D of *d* tuples, at each iteration *i*
  - create bootstrap sample (training set), D_i, by sampling D with replacement
  - learn a classifier model M_i for each training set D_i
- **Classification**: classify an unknown sample **X**
  - Each classifier M_i returns its class prediction
  - The bagged classifier M* counts the votes and assigns the class with the most votes to **X**
- **Prediction**: It can be applied to the prediction of continuous values by taking the average value of each prediction instead of voting
- Accuracy: Improved accuracy in prediction
  - Often significantly better than a single classifier derived from D
  - For noise data: Not considerably worse, more robust

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Boosting

- Analogy: Consult several doctors, based on a combination of weighted diagnoses—weight assigned based on the previous diagnosis accuracy
- How boosting works?
  - **Weights** are assigned to each training tuple
  - A series of k classifiers is iteratively learned
  - After a classifier M_i is learned, the weights are updated to allow the subsequent classifier, M_{i+1}, to **pay more attention to the training tuples that were misclassified** by M_i
  - The final **M* combines the votes** of each individual classifier, where the weight of each classifier's vote is a function of its accuracy
- Boosting algorithm can be extended for numeric prediction
- Comparing with bagging: Boosting tends to have greater accuracy, but it also risks overfitting the model to misclassified data

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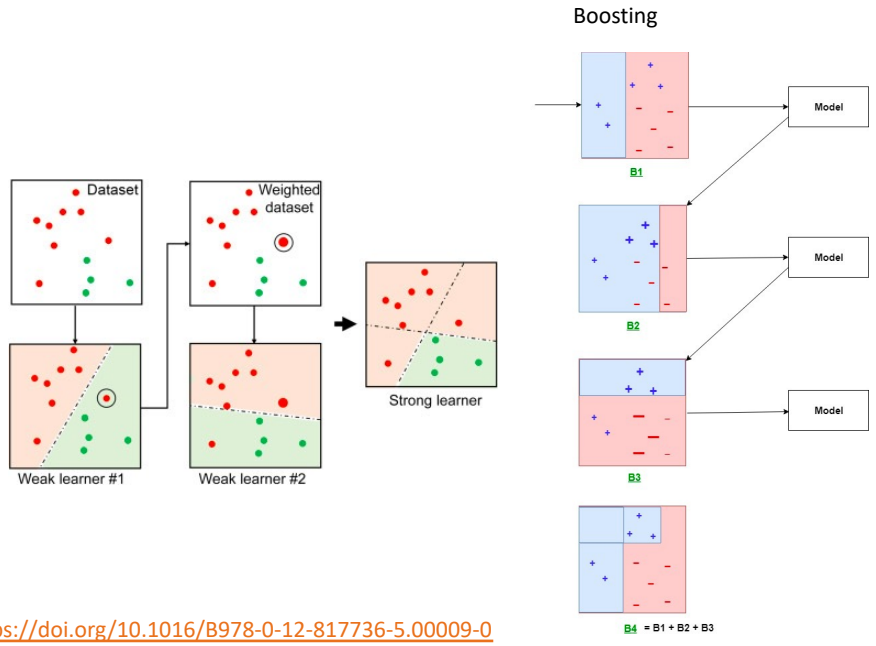

https://doi.org/10.1016/B978-0-12-817736-5.00009-0

https://www.geeksforgeeks.org/boosting-in-machine-learning-boosting-and-adaboost/ 59

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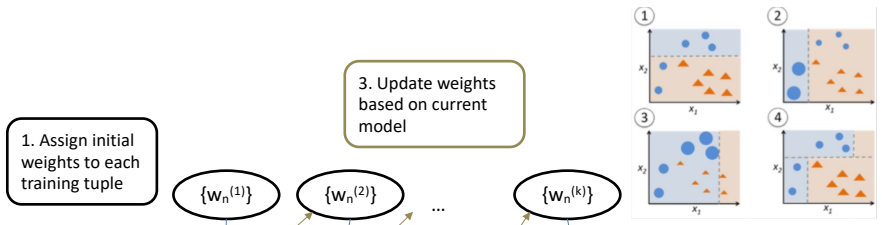
Adaboost (Freund and Schapire, 1997)



Two 'weighting' strategy:

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

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

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

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Adaboost (Freund and Schapire, 1997)

- Given a set of *d* class-labeled tuples, ($\mathbf{X_1}$, y_1), …, ($\mathbf{X_d}$, y_d)
- Initially, all the weights of tuples are set the same (1/d)
- Generate *k* classifiers in *k* rounds. At round i,
  - Tuples from D are sampled (with replacement) to form a training set D_i of the same size
  - Each tuple's chance of being selected is based on its weight
  - A classification model M_i is derived from D_i
  - Its error rate is calculated using D_i as a test set
  - If a tuple is misclassified, its weight is increased; otherwise, it is decreased
- Error rate: err($\mathbf{X_j}$) is the misclassification error of tuple $\mathbf{X_j}$. Classifier M_i error rate is the sum of the weights of the misclassified tuples:

$$error(M_i) = \sum_j^d w_j \times err(\mathbf{X_j})$$

- The weight of classifier M_i's vote is

$$\log \frac{1 - error(M_i)}{error(M_i)}$$

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Gradient Boosting

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

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

Previous model

New weak learner

- Scalable implementation: XGBoost

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Random Forest: Basic Concepts

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

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Random Forest

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

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Ensemble Methods Recap

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

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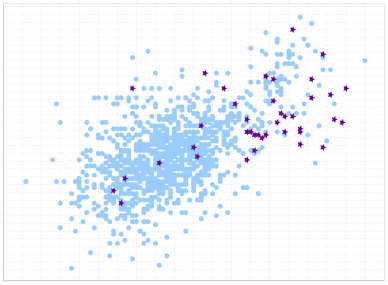
Classification of Class-Imbalanced Data Sets

- Traditional methods assume a balanced distribution of classes and equal error costs. But in real world situations, we may face imbalanced data sets, which has rare positive examples but numerous negative ones.
- Medical diagnosis: Medical screening for a condition is usually performed on a large population of people without the condition, to detect a small minority with it (e.g., HIV prevalence in the USA is ~0.4%)
- Fraud detection: About 2% of credit card accounts are defrauded per year. (Most fraud detection domains are heavily imbalanced.)
- Product defect, accident (oil-spill), disk drive failures, etc.



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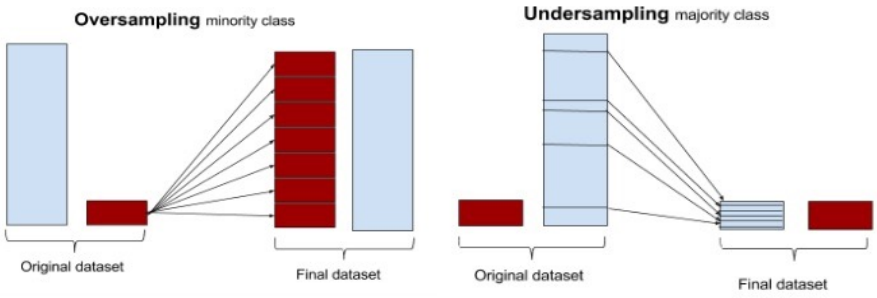
- Typical methods on imbalanced data (Balance the training set)
  - **Oversampling**: Oversample the minority class.
  - **Under-sampling**: Randomly eliminate tuples from majority class
  - **Synthesizing:** Synthesize new minority classes



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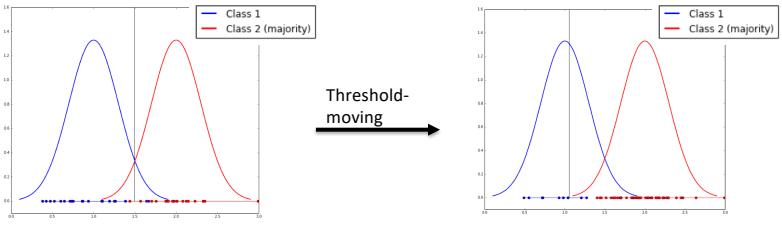
Classification of Class-Imbalanced Data Sets

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



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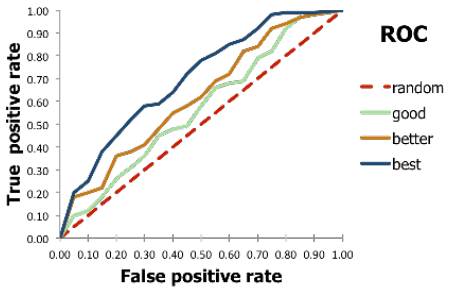
Evaluate imbalanced data classifier

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



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Multiclass Classification

- Classification involving more than two classes (i.e., > 2 Classes)
- Method 1. **One-versus-all**
  - Given *m* classes, train *m* binary classifiers, one for each class
  - Classifier j: treat tuples in class j as *positive* & **all the rest** as *negative*
  - To classify a tuple **X**, the set of classifiers vote as an ensemble
- Method 2. **All-versus-all**: Train a binary classifier for any two classes
  - Given *m* classes, construct $m(m-1)/2$ binary classifiers
  - A classifier is trained using tuples of the two classes
  - To classify a tuple **X**, each classifier votes
    - X is assigned to the class with maximal vote
- Comparison: One-vs.-one tends to perform better than one-vs.-rest
- **A related problem:** multi-label classification (each data tuple could belong to one or more classes)

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Semi-Supervised Learning

- **Definition**: Learning from a mix of labeled and unlabeled data, typically with far more unlabeled data.
- **Goal**: Improve learning performance by leveraging the unlabeled data alongside the labeled data.
- **Example**: Training a model for email spam classification using a small labeled dataset and a large unlabeled dataset.
- **Data**: Combines both labeled and unlabeled data.
- **Similarity**: Shares characteristics with supervised (labeled) and unsupervised (unlabeled) learning.
- **Difference**: Bridges the gap between supervised and unsupervised learning by combining both types of data.

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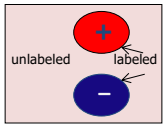
Semi-Supervised Classification

- Semi-supervised: Uses labeled and unlabeled data to build a classifier
- Self-training
  - Build a classifier using the labeled data
  - Use it to label the unlabeled data, and those with the most confident label prediction are added to the set of labeled data
  - Repeat the above process
  - Adv.: easy to understand; Disadv.: may reinforce errors



- Co-training: Use two or more classifiers to teach each other
  - Each learner uses a mutually independent set of features of each tuple to train a good classifier, say f_1 and f_2
  - Then f_1 and f_2 are used to predict the class label for unlabeled data X
  - Teach each other: The tuple having the most confident prediction from f_1 is added to the set of labeled data for f_2 & vice versa
- Other methods include joint probability distribution of features and labels

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Self-Supervised Learning

- **Definition**: A form of unsupervised learning where the model generates its own supervisory signal by creating pseudo-labels from the data.
- **Goal**: Pre-train models by solving tasks derived from data itself, often for use in transfer learning.
- **Example**: Predicting missing words in a sentence (used in training language models like GPT).
- **Data**: Uses unlabeled data but creates internal labels or tasks.
- **Similarity**: Shares use of unlabeled data with unsupervised learning.
- **Difference**: Employs specific pretext tasks to create supervisory signals.

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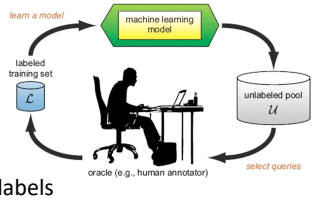
Active Learning



- A special case of semi-supervised learning
  - Unlabeled data: Abundant
  - Class labels are expensive to obtain
- Active learner: Interactively query teachers (oracle) for labels
- Pool-based approach: Uses a pool of unlabeled data
  - L: a small subset of D is labeled, U: a pool of unlabeled data in D
  - Use a query function to carefully select one or more tuples from U and request labels from an oracle (a human annotator)
  - The newly labeled samples are added to L, and learn a model
  - Goal: **Achieve high accuracy using as few labeled data as possible**
- Evaluated using *learning curves*: Accuracy as a function of the number of instances queried (# of tuples to be queried should be small)
- A lot of algorithms have been developed for active learning

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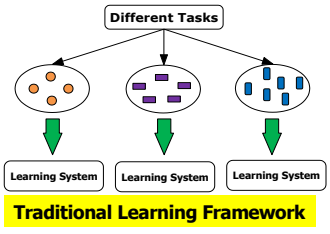
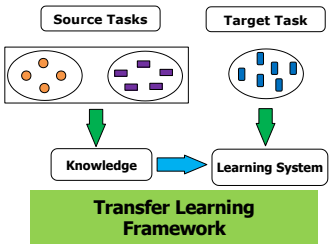
Transfer Learning: Conceptual Framework

- Transfer learning: Extract knowledge from one or more source tasks (e.g., recognizing cars) and apply the knowledge to a target task (e.g., recognizing trucks)
- Traditional learning: Build a new classifier for each new task
- Transfer learning: Build new classifier by applying existing knowledge learned from source tasks
- Many algorithms are developed, applied to text classification, spam filtering, etc.





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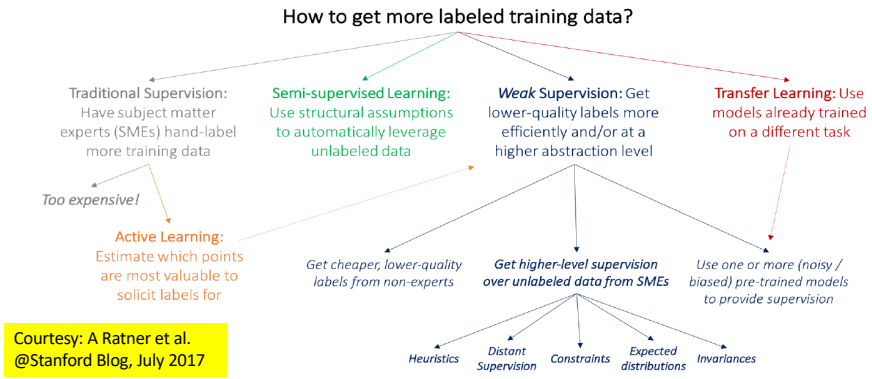
Relationships Among Different Kinds of Supervisions



Courtesy: A Ratner et al. @Stanford Blog, July 2017

Many areas of machine learning are motivated by the bottleneck of labeled training data, but are divided at a high-level by what information they leverage instead.

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Chapter 8. Classification: Basic Concepts

- Classification: Basic Concepts
- Decision Tree Induction
- Bayes Classification Methods
- Linear Classifier
- Model Evaluation and Selection
- Techniques to Improve Classification Accuracy: Ensemble Methods
- Additional Concepts on Classification
- Summary

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Summary

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

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Classification Is to Derive the Maximum Posteriori

- Let D be a training set of tuples and their associated class labels, and each tuple is represented by an n-D attribute vector **X** = (x_1, x_2, …, x_n)
- Suppose there are *m* classes C_1, C_2, …, C_m.
- Classification is to derive the maximum posteriori, i.e., the maximal $P(C_i|\mathbf{X})$
- This can be derived from Bayes' theorem

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

- Since P(X) is constant for all classes, only

needs to be maximized $P(C_i|\mathbf{X}) \propto P(\mathbf{X}|C_i)P(C_i)$

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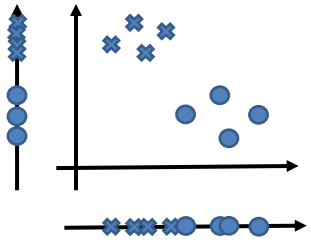
Linear Discriminant Analysis (LDA)

- Linear Discriminant Analysis **(**LDA) works when the attributes are all continuous
  - For the categorical attributes, discriminant correspondence analysis is the equivalent technique
- Basic Ideas: Project all samples on a line such that different classes are well separated
- Example: Suppose we have 2 classes and 2-dimensional samples $x_1, \ldots, x_n$
  - n_1 samples come from class 1
  - n_2 samples come from class 2
- Let the line direction be given by unit vector $\boldsymbol{v}$
- There are two candidates of projections
  - Vertical: $\boldsymbol{v} = (0,1)$
  - Horizontal: $\boldsymbol{v} = (1,0)$
- Which one looks better?
- How to mathematically measure it?



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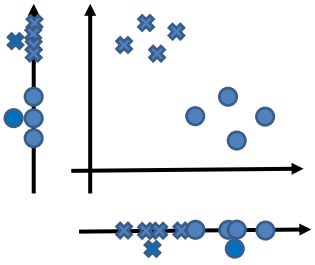
Fisher's LDA (**Linear Discriminant Analysis)**

- $\boldsymbol{v^T x_i}$ is the distance of projection of $\boldsymbol{x_i}$ from the origin
- Let $\boldsymbol{\mu_1}$ and $\boldsymbol{\mu_2}$ be the means of class 1 and class 2 in the original space
  - $\boldsymbol{\mu_1} = \frac{1}{n_1}\sum_{i\in\text{class }1} \boldsymbol{x_i}$
  - $\boldsymbol{\mu_2} = \frac{1}{n_2}\sum_{i\in\text{class }2} \boldsymbol{x_i}$
- The distance between the means of the projected points
  - $|\boldsymbol{v^T\mu_1} - \boldsymbol{v^T\mu_2}|$
  - Good? No. Horizontal one may have larger distance



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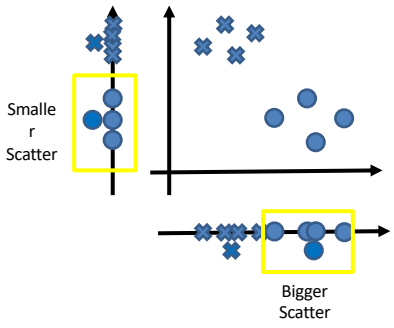
Fisher's LDA (con't)

- Normalization needed
- Scatter: Sample variance multiplied by n
  - $s_1 = \sum_{i\in\text{class }1}(\boldsymbol{v^T x_i} - \boldsymbol{v^T\mu_1})^2$
  - $s_2 = \sum_{i\in\text{class }2}(\boldsymbol{v^T x_i} - \boldsymbol{v^T\mu_2})^2$
- Fisher's LDA
  - Maximize $J(\boldsymbol{v}) = \frac{(\boldsymbol{v^T\mu_1} - \boldsymbol{v^T\mu_2})^2}{s_1+s_2}$
  - Closed-form optimal solution



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Fisher's LDA: Summary

- Advantages
  - Useful for dimension reduction
  - Easy to extend to multi-classes
- Fisher's LDA will fail
  - When $\boldsymbol{\mu_1} = \boldsymbol{\mu_2}$, $J(\boldsymbol{v})$ is always 0.
  - When classes have large overlap when projected to any line

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