For written notes on this lecture, please read chapter 3 of *The Practical Bioinformatician*. Alternatively, please read “Rule-Based Data Mining Methods for Classification Problems in Biomedical Domains”, a tutorial at PKDD04 by Jinyan Li and Limsoon Wong, September 2004. http://www.comp.nus.edu.sg/~wongls/talks/pkdd04/

CS2220: Introduction to Computational Biology
Unit 1b: Essence of Knowledge Discovery

Wong Limsoon
Outline

• Overview of supervised learning
  – Decision trees

• Decision tree ensembles
  – Bagging

• Other methods
  – K-nearest neighbour
  – Support vector machines
  – Naïve Bayes
  – Hidden Markov models
Overview of supervised learning
Supervised learning

• Also called classification

• Learn from past experience, and use the learned knowledge to classify new data

• Knowledge learned by intelligent algorithms

• Examples:
  – Clinical diagnosis for patients
  – Cell type classification
Data

• Classification application involves > 1 class of data. E.g.,
  – Normal vs disease cells for a diagnosis problem

• Training data is a set of instances (samples, points, etc.) with known class labels

• Test data is a set of instances whose class labels are to be predicted
Notations

• Training data

\{ \langle x_1, y_1 \rangle, \langle x_2, y_2 \rangle, \ldots, \langle x_m, y_m \rangle \}\n
where \( x_j \) are \( n \)-dimensional vectors and \( y_j \) are from a discrete space \( Y \).
E.g., \( Y = \{ \text{normal, disease} \} \)

• Test data

\{ \langle u_1, ? \rangle, \langle u_2, ? \rangle, \ldots, \langle u_k, ? \rangle \} \}
Training data: $X$ \hspace{1cm} f(X) \hspace{1cm} Class labels $Y$

Test data: $U$ \hspace{1cm} f(U) \hspace{1cm} Predicted class labels

A classifier, a mapping, a hypothesis
Relational representation

$m$ samples

$n$ features (order of 1000)

<table>
<thead>
<tr>
<th>gene_1</th>
<th>gene_2</th>
<th>gene_3</th>
<th>gene_4</th>
<th>...</th>
<th>gene_n</th>
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<tbody>
<tr>
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<td>x_{12}</td>
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<td>x_{m3}</td>
<td>x_{m4}</td>
<td>...</td>
<td>x_{mn}</td>
</tr>
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</table>

class

P
N
P
N
Features (aka attributes)

• **Categorical features**
  – color = \{red, blue, green\}

• **Continuous or numerical features**
  – gene expression
  – age
  – blood pressure

• **Discretization**
## Example

<table>
<thead>
<tr>
<th>Outlook</th>
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<th>class</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sunny</td>
<td>75</td>
<td>70</td>
<td>true</td>
<td>Play</td>
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<tr>
<td>Sunny</td>
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Recap: Evaluation of a classifier

• Performance on independent blind test data
  – Blind test data properly represent real world

• K-fold cross validation
  – Given a dataset, divide it into k even parts, k-1 of them are used for training, and the rest one part treated as test data

• LOOCV, a special case of K-fold cross validation

• Accuracy, error rate, false positive rate, false negative rate, sensitivity, specificity, precision
Requirements of biomedical classification

• High accuracy, sensitivity, specificity, precision

• High comprehensibility
Importance of rule-based methods

• Systematic selection of a small number of features used for the decision making
  ⇒ Increase comprehensibility of the knowledge patterns

• C4.5 and CART are two commonly used rule induction algorithms---a.k.a. decision tree induction algorithms
Structure of decision trees

• If \( x_1 > a_1 \) & \( x_2 > a_2 \), then it’s A class

• C4.5, CART, two of the most widely used

• Easy interpretation, but accuracy maybe unattractive
Elegance of decision trees

Every path from root to a leaf forms a decision rule
Brief history of decision trees

CLS (Hunt et al. 1966) --- cost driven

CART (Breiman et al. 1984) --- Gini Index

ID3 (Quinlan, 1986) --- Information-driven

C4.5 (Quinlan, 1993) --- Gain ratio + Pruning ideas
A simple dataset

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9 Play samples
5 Don’t
A total of 14.
A decision tree

- Construction of a tree is equivalent to determination of root node of the tree and root nodes of its sub-trees

Exercise: What is the accuracy of this tree?
Food for thought

- What is the accuracy of this decision tree?

Exercise #1
Outlook | Temperature | Humidity | Wind | PlayTennis
---|---|---|---|---
Sunny | Hot | High | Weak | No

Source: Anthony Tung
Most discriminatory feature

• Every feature can be used to partition the training data

• If the partitions contain a pure class of training instances, then this feature is most discriminatory
Example of partitions

• Categorical feature
  – Number of partitions of the training data is equal to the number of values of this feature

• Numerical feature
  – Two partitions
<table>
<thead>
<tr>
<th>Instance #</th>
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<th>class</th>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>70</td>
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A categorical feature is partitioned based on its number of possible values.
A numerical feature is generally partitioned by choosing a “cutting point”

Total 14 training instances

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</table>

Temperature <= 70

5, 8, 11, 13, 14
P, P, D, P, P

Temperature > 70

1, 2, 3, 4, 6, 7, 9, 10, 12
P, D, D, D, P, P, P, D, P
Decision tree construction

- Select the “best” feature as root node of the whole tree

- Partition dataset into subsets using this feature so that the subsets are as “pure” as possible

- After partition by this feature, select the best feature (wrt the subset of training data) as root node of this sub-tree

- Recursively, until the partitions become pure or almost pure
Let’s construct a decision tree

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Ask the class to pick root node and construct the tree recursively with them…

How good is that tree?

Exercise #2
Three measures to evaluate which feature is best

- Gini index
- Information gain
- Information gain ratio

Look the last two up yourself
Gini index

\[
gini(S) = \frac{\text{diff of two arbitrary specimen in } S}{\text{mean specimen in } S}
\]

\[
= \text{prob(getting two specimen of diff class in } S)\]
\[
= 1 - \text{prob(getting two specimen of same class in } S)\]
\[
= 1 - \sum_i \text{prob( getting specimen of class } i \text{ in } S)^2\]

- Gini index is the expected value of the ratio of the diff of two arbitrary specimens to the mean value of all specimens

- Closer to 1, feature is similar to “background distribution”. Closer to 0, feature is “unexpected”
Gini index

Let $\mathcal{U} = \{C_1, ..., C_k\}$ be all the classes. Suppose we are currently at a node and $D$ is the set of those samples that have been moved to this node. Let $f$ be a feature and $d[f]$ be the value of the feature $f$ in a sample $d$. Let $S$ be a range of values that the feature $f$ can take. Then the Gini index for $f$ in $D$ for the range $S$ is defined as

$$gini_f^D(S) = 1 - \sum_{C_i \in \mathcal{U}} \left( \frac{\{|d \in D | d \in C_i, \ d[f] \in S\}|}{|D|} \right)^2$$

The purity of a split of the value range $S$ of an attribute $f$ by some split-point into subranges $S_1$ and $S_2$ is then defined as

$$gini_f^D(S_1, S_2) = \sum_{S \in \{S_1, S_2\}} \frac{|\{d \in D | d[f] \in S\}|}{|D|} \ast gini_f^D(S)$$

we choose the feature $f$ and the split-point $p$ that minimizes $gini_f^D(S_1, S_2)$ over all possible alternative features and split-points.
### Gini index of “Outlook”

- **gini(Sunny)** = \(1 - (2/5)^2 - (3/5)^2 = 0.48\)
- **gini(Overcast)** = \(1 - (4/4)^2 - (0/5)^2 = 0\)
- **gini(Rain)** = \(1 - (3/5)^2 - (2/5)^2 = 0.48\)
- **gini(Outlook)** = \(\frac{5}{14} \times 0.48 + \frac{4}{14} \times 0 + \frac{5}{14} \times 0.48 = 0.34\)

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Characteristics of C4.5/CART trees:

- Single coverage of training data (elegance)
- Divide-and-conquer splitting strategy
- Fragmentation problem ⇒ Locally reliable but globally insignificant rules
- Miss many globally significant rules; mislead system
Example Use of Decision Tree Methods:

Proteomics Approaches to Biomarker Discovery

- In prostate and bladder cancers (Adam et al. *Proteomics*, 2001)
- In serum samples to detect breast cancer (Zhang et al. *Clinical Chemistry*, 2002)
- In serum samples to detect ovarian cancer (Petricoin et al. *Lancet*; Li & Rao, *PAKDD* 2004)
Decision tree ensembles
Motivating example

- $h_1$, $h_2$, $h_3$ are independent classifiers with accuracy = 60%
- $C_1$, $C_2$ are the only classes
- $t$ is a test instance in $C_1$
- $h(t) = \text{argmax}_{C \in \{C_1, C_2\}} |\{h_j \in \{h_1, h_2, h_3\} | h_j(t) = C\}|$
- Then $\text{prob}(h(t) = C_1)$
  
  \[= \text{prob}(h_1(t) = C_1 \land h_2(t) = C_1 \land h_3(t) = C_1) + \text{prob}(h_1(t) = C_1 \land h_2(t) = C_1 \land h_3(t) = C_2) + \text{prob}(h_1(t) = C_1 \land h_2(t) = C_2 \land h_3(t) = C_1) + \text{prob}(h_1(t) = C_2 \land h_2(t) = C_1 \land h_3(t) = C_1)\]

  \[= 60\% \times 60\% \times 60\% + 60\% \times 60\% \times 40\% + 60\% \times 40\% \times 60\% + 40\% \times 60\% \times 60\% = 64.8\%\]
Bagging

• Proposed by Breiman (1996)

• Also called Bootstrap aggregating

• Make use of randomness injected to training data
Main ideas

Original training set

50 p + 50 n

48 p + 52 n

49 p + 51 n

53 p + 47 n

A base inducer such as C4.5

Draw 100 samples with replacement

A committee $\mathbf{H}$ of classifiers:

$h_1 \quad \quad h_2 \quad \quad \ldots \quad \quad h_k$
Decision making by bagging

Given a new test sample $T$

$$\text{bagged}(T) = \arg\max_{C_j \in \mathcal{U}} |\{h_i \in \mathcal{H} \mid h_i(T) = C_j\}|$$

where $\mathcal{U} = \{C_1, ..., C_r\}$

• What does this formula mean?

Exercise #3
Summary of ensemble classifiers

- Bagging
- Random Forest
- AdaBoost.M1
- Randomization Trees
- CS4

Rules may not be correct when applied to training data

Rules correct

Exercise: Describe the decision tree ensemble classifiers not explained in this ppt
Other machine learning approaches
Outline

• K-nearest neighbor (kNN)
• Support vector machines (SVM)
• Naïve Bayes
• Hidden Markov models (HMM)

Can you present one of these machine learning approaches?

Exercise #4
K-nearest neighbours
How kNN works

• Given a new case

• Find k “nearest” neighbours, i.e., k most similar points in the training data set

• Assign new case to the same class to which most of these neighbours belong

• A common “distance” measure betw samples x and y is

$$\sqrt{\sum_f (x[f] - y[f])^2}$$

where f ranges over features of the samples

Exercise: What does the formula above mean?
Illustration of kNN (k=8)

Neighborhood

5 of class  
3 of class  

Image credit: Zaki
Some issues

- Simple to implement
- Must compare new case against all training cases
  ⇒ May be slow during prediction

- No need to train
- But need to design distance measure properly
  ⇒ May need expert for this

- Can’t explain prediction outcome
  ⇒ Can’t provide a model of the data
Example Use of kNN

Ovarian cancer diagnosis based on SELDI proteomic data


- Use kNN to diagnose ovarian cancers using proteomic spectra

- Data set is from Petricoin et al., *Lancet* 359:572-577, 2002

**Fig. 1.** Minimum, median and maximum of percentages of correct prediction as a function of the number of top-ranked m/z ratios in 50 independent partitions into learning and validation sets.
Support vector machines
(a) Linear separation not possible w/o errors
(b) Better separation by nonlinear surfaces in input space
(c) Nonlinear surface corr to linear surface in feature space.
Map from input to feature space by “kernel” function \( \Phi \)
\( \Rightarrow \) “Linear learning machine” + kernel function as classifier
Linear learning machines

- Hyperplane separating the x’s and o’s points is given by $(W \cdot X) + b = 0$, with $(W \cdot X) = \sum_j W[j] \cdot X[j]$
- Decision function is $llm(X) = \text{sign}((W \cdot X) + b)$
Linear learning machines

- Solution is a linear combination of training points $X_k$ with labels $Y_k$

$$W = \sum_k \alpha_k Y_k X_k,$$

with $\alpha_k > 0$, and $Y_k = \pm 1$

$\Rightarrow \text{llm}(X) = \text{sign}(\sum_k \alpha_k Y_k (X_k \cdot X) + b)$

“data” appears only in dot product!
Kernel function

- $llm(X) = \text{sign}(\sum_k \alpha_k^* Y_k^* (X_k \cdot X) + b)$

- $svm(X) = \text{sign}(\sum_k \alpha_k^* Y_k^* (\Phi X_k \cdot \Phi X) + b)$

$\Rightarrow svm(X) = \text{sign}(\sum_k \alpha_k^* Y_k^* K(X_k, X) + b)$

where $K(X_k, X) = (\Phi X_k \cdot \Phi X)$
Kernel function

- \( \text{svm}(X) = \text{sign}(\sum_k \alpha_k Y_k K(X_k, X) + b) \)

\( \Rightarrow \) \( K(A, B) \) can be computed w/o computing \( \Phi \)

- In fact replace it w/ lots of more “powerful” kernels besides \((A \cdot B)\). E.g.,
  - \( K(A, B) = (A \cdot B)^d \)
  - \( K(A, B) = \exp(-||A B||^2 / (2*\sigma)), \ldots \)
How SVM works

- \( \text{svm}(X) = \text{sign}(\sum_k \alpha_k Y_k K(X_k, X) + b) \)

- **To find \( \alpha_k \)** is a quadratic programming problem
  
  \[ \begin{align*}
  \text{max: } & \sum_k \alpha_k - 0.5 \sum_k \sum_h \alpha_k \alpha_h Y_k Y_h K(X_k, X_h) \\
  \text{subject to: } & \sum_k \alpha_k Y_k = 0 \\
  & \text{for all } \alpha_k, \ C \geq \alpha_k \geq 0
  \end{align*} \]

- **To find \( b \)**, estimate by averaging
  
  \[ Y_h - \sum_k \alpha_k Y_k K(X_h, X_k) \]
  
  for all \( \alpha_h \geq 0 \)
Example Use of SVM: Recognition of protein translation initiation sites

- Use SVM to recognize protein translation initiation sites from genomic sequences
- Raw data set is same as Liu & Wong, *JBCB* 1:139-168, 2003
Naïve Bayes
Bayes theorem

\[ P(h|d) = \frac{P(d|h) \times P(h)}{P(d)} \]

- \( P(h) \) = prior prob that hypothesis \( h \) holds
- \( P(d|h) \) = prob of observing data \( d \) given \( h \) holds
- \( P(h|d) \) = posterior prob that \( h \) holds given observed data \( d \)
Bayesian approach

- Let $H$ be all possible classes. Given a test instance with feature vector $\{f_1 = v_1, \ldots, f_n = v_n\}$, the most probable classification is given by

$$\arg\max_{h_j \in H} P(h_j | f_1 = v_1, \ldots, f_n = v_n)$$

- Using Bayes' Theorem, rewrites to

$$\arg\max_{h_j \in H} \frac{P(f_1 = v_1, \ldots, f_n = v_n | h_j) \ast P(h_j)}{P(f_1 = v_1, \ldots, f_n = v_n)}$$

- Since denominator is independent of $h_j$, this simplifies to

$$\arg\max_{h_j \in H} P(f_1 = v_1, \ldots, f_n = v_n | h_j) \ast P(h_j)$$
Naïve Bayes

- But estimating $P(f_1=v_1, \ldots, f_n=v_n|h_j)$ accurately may not be feasible unless training data set is large

- “Solved” by assuming $f_1, \ldots, f_n$ are conditionally independent of each other

- Then

  $$\arg\max_{h_j \in H} P(f_1 = v_1, \ldots, f_n = v_n|h_j) \times P(h_j)$$

  $$= \arg\max_{h_j \in H} \prod_i P(f_i = v_i|h_j) \times P(h_j)$$

  where $P(h_j)$ and $P(f_i=v_i|h_j)$ can often be estimated reliably from typical training data set

Exercise: How do you estimate $P(h_j)$ and $P(f_i=v_i|h_j)$?
Independence vs Conditional independence

- Independence: $P(A,B) = P(A) \times P(B)$
- Conditional Independence: $P(A,B|C) = P(A|C) \times P(B|C)$
- Indep does not imply conditional indep
  - Consider tossing a fair coin twice
    - A is event of getting head in 1st toss
    - B is event of getting head in 2nd toss
    - C is event of getting exactly one head
  - Then $A=\{HT, HH\}$, $B=\{HH, TH\}$ and $C=\{HT, TH\}$
  - $P(A,B|C) = P(\{HH\}|C)=0$
  - $P(A|C) = P(A,C)/P(C) = P(\{HT\})/P(C)=(1/4)/(1/2) =1/2$
  - Similarly, $P(B|C) =1/2$

Source: Choi Kwok Pui
Example Use of Bayesian: Design of screens for macromolecular crystallization


- Xtallization of proteins requires search of expt settings to find right conditions for diffraction-quality xtals

- BMCD is a db of known xtallization conditions

- Use Bayes to determine prob of success of a set of expt conditions based on BMCD
Hidden Markov models
What is a HMM

- HMM is a stochastic generative model for seqs
- Defined by model parameters
  - finite set of states $S$
  - finite alphabet $A$
  - transition prob matrix $T$
  - emission prob matrix $E$
- Move from state to state as per $T$ while emitting symbols as per $E$
Order of a HMM

• In $n$th order HMM, $T$ & $E$ depend on all $n$ previous states

• E.g., for 1st order HMM, given emissions $X = x_1, x_2, \ldots$, & states $S = s_1, s_2, \ldots$, the prob of this seq is

$$Prob(X, S) = \prod_i Prob(x_i|s_i) = \prod_i E(x_i|s_i) * T(s_{i-1}, s_i)$$
Using HMM

• Given the model parameters, compute the probability of a particular output sequence. Solved by the forward algorithm

• Given the model parameters, find the most likely sequence of (hidden) states which could have generated a given output sequence. Solved by the Viterbi algorithm

• Given an output sequence, find the most likely set of state transition and output probabilities. Solved by the Baum-Welch algorithm

Exercise: Describe these algorithms
Example: Dishonest casino

• Casino has two dices:
  – Fair dice
    • \( P(i) = \frac{1}{6}, \ i = 1..6 \)
  – Loaded dice
    • \( P(i) = \frac{1}{10}, \ i = 1..5 \)
    • \( P(i) = \frac{1}{2}, \ i = 6 \)

• Casino switches betw fair & loaded die with prob \( \frac{1}{2} \). Initially, dice is always fair

• Game:
  – You bet $1
  – You roll
  – Casino rolls
  – Highest number wins $2

• Question: Suppose we played 2 games, and the sequence of rolls was 1, 6, 2, 6. Were we likely to have been cheated?
"Visualization" of dishonest casino

![Diagram of state transition between Fair and Loaded states.]

<table>
<thead>
<tr>
<th>Emission Matrix</th>
<th>Transition Matrix</th>
</tr>
</thead>
<tbody>
<tr>
<td>E(1</td>
<td>Fair) = 1/6</td>
</tr>
<tr>
<td>E(2</td>
<td>Fair) = 1/6</td>
</tr>
<tr>
<td>E(3</td>
<td>Fair) = 1/6</td>
</tr>
<tr>
<td>E(4</td>
<td>Fair) = 1/6</td>
</tr>
<tr>
<td>E(5</td>
<td>Fair) = 1/6</td>
</tr>
<tr>
<td>E(6</td>
<td>Fair) = 1/6</td>
</tr>
</tbody>
</table>
1, 6, 2, 6?
We were probably cheated...

\[
\begin{align*}
Prob(X, S = \text{Fair}, \text{Fair}, \text{Fair}, \text{Fair}) &= E(1|\text{Fair}) \times T(?, \text{Fair}) \times \\
& \quad E(6|\text{Fair}) \times T(\text{Fair}, \text{Fair}) \times \\
& \quad E(2|\text{Fair}) \times T(\text{Fair}, \text{Fair}) \times \\
& \quad E(6|\text{Fair}) \times T(\text{Fair}, \text{Fair}) \\
& = \frac{1}{6} \times \frac{1}{6} \times \frac{1}{2} \times \frac{1}{6} \times \frac{1}{2} \times \frac{1}{6} \times \frac{1}{2} \times \frac{1}{6} \times \frac{1}{2} \\
& = 9.6451 \times 10^{-5}
\end{align*}
\]

\[
\begin{align*}
Prob(X, S = \text{Fair}, \text{Loaded}, \text{Fair}, \text{Loaded}) &= E(1|\text{Fair}) \times T(?, \text{Fair}) \times \\
& \quad E(6|\text{Loaded}) \times T(\text{Fair}, \text{Loaded}) \times \\
& \quad E(2|\text{Fair}) \times T(\text{Loaded}, \text{Fair}) \times \\
& \quad E(6|\text{Loaded}) \times T(\text{Fair}, \text{Loaded}) \\
& = \frac{1}{6} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{6} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \\
& = 8.6806 \times 10^{-4}
\end{align*}
\]
Example Use of HMM: Protein families modelling

- Baldi et al., *PNAS* 91:1059-1063, 1994
- HMM is used to model families of biological sequences, such as kinases, globins, & immunoglobulins
- Bateman et al., *NAR* 32:D138-D141, 2004
- HMM is used to model 6190 families of protein domains in Pfam

Fig. 1. HMM architecture. $S$ and $E$ are the start and end states. Sequence of main states $m_i$ is the backbone. Side states $d_i$ (resp. $i_i$) correspond to deletions (resp. insertions).
Concluding remarks...
What have we learned?

• Decision trees

• Decision trees ensembles
  – Bagging

• Other methods
  – K-nearest neighbour
  – Support vector machines
  – Naïve Bayes
  – Hidden Markov models
Any question?
• http://www.cs.waikato.ac.nz/ml/weka

• Weka is a collection of machine learning algorithms for data mining tasks. The algorithms can either be applied directly to a dataset or called from your own Java code. Weka contains tools for data pre-processing, classification, regression, clustering, association rules, and visualization.

Exercise: Download a copy of WEKA. What are the names of classifiers in WEKA that correspond to C4.5 and SVM?
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• The “indep vs conditional indep” example came from Choi Kwok Pui
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