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/

Knowledge Discovery Techniques for Bioinformatics, Part II: Machine Learning Methods

Limsoon Wong

Outline

- **Overview of Supervised Learning**
- **Decision Trees Ensembles**
  - Bagging
- **Other Methods**
  - K-Nearest Neighbour
  - Bayesian Approach
  - Hidden Markov Models

Overview of Supervised Learning

Computational 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) with known class labels**
- **Test data is a set of instances whose class labels are to be predicted**

Typical Notations

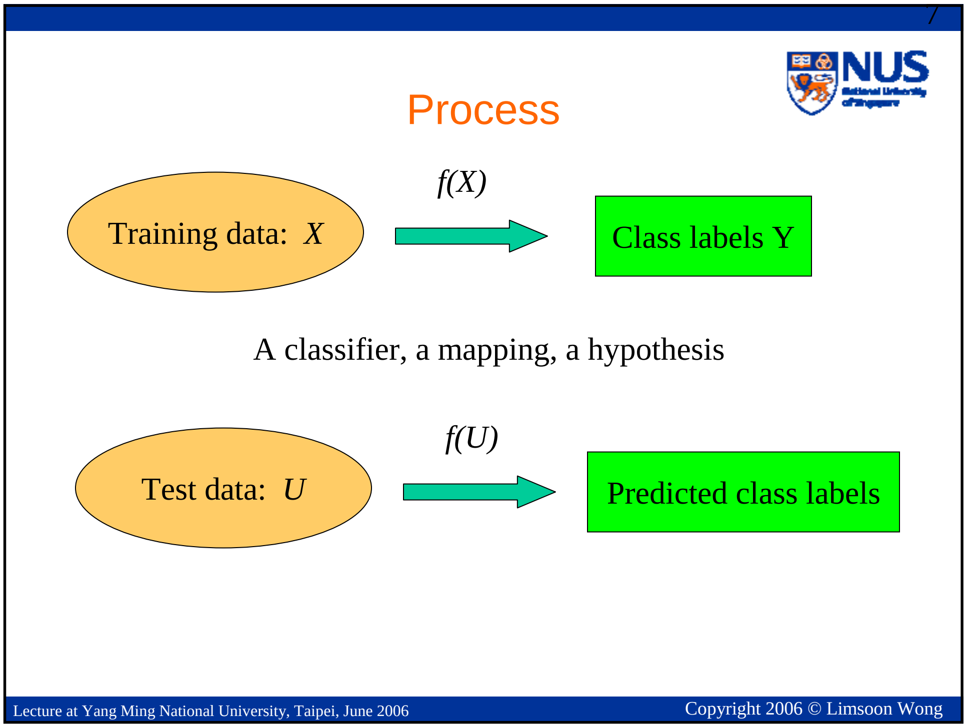
- **Training data**

  $\{\langle x_1, y_1\rangle, \langle x_2, y_2\rangle, \ldots, \langle x_m, y_m\rangle\}$

  where x_j are n-dimensional vectors and y_j are from a discrete space Y. E.g., Y = {normal, disease}

- **Test data**

  $\{\langle u1, ?\rangle, \langle u2, ?\rangle, \ldots, \langle uk, ?\rangle, \}$

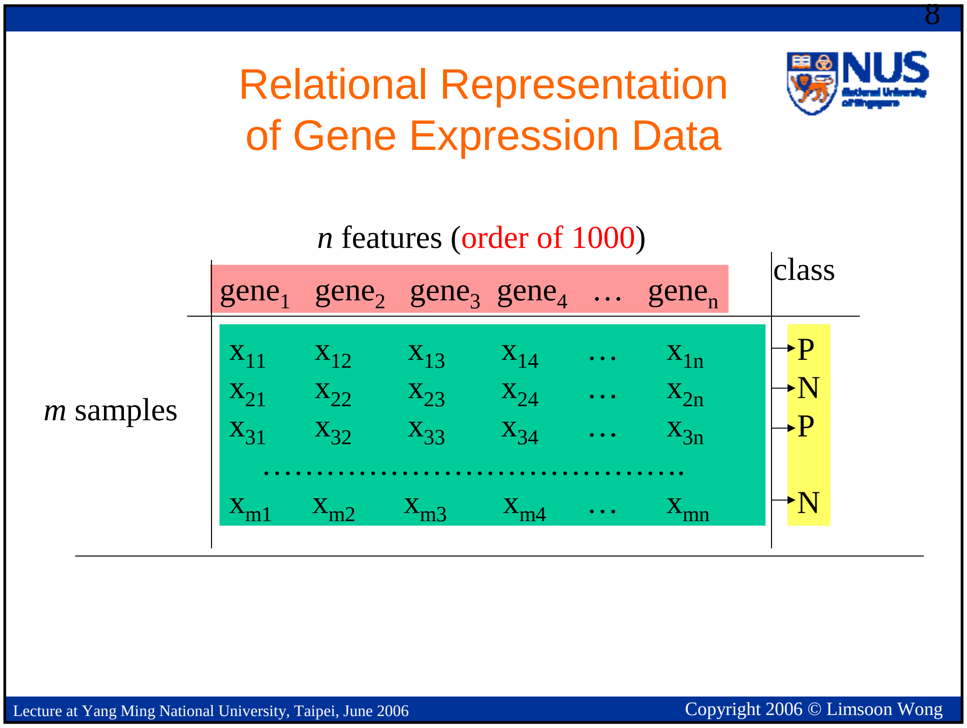


Process

Training data: *X* $\xrightarrow{f(X)}$ Class labels Y

A classifier, a mapping, a hypothesis

Test data: *U* $\xrightarrow{f(U)}$ Predicted class labels



Relational Representation of Gene Expression Data

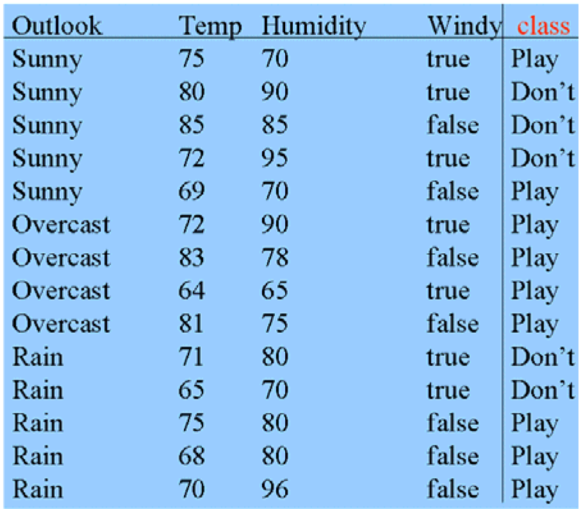
n features (order of 1000)

	$gene_1$	$gene_2$	$gene_3$	$gene_4$	…	$gene_n$	class
m samples	x_{11}	x_{12}	x_{13}	x_{14}	…	x_{1n}	→ P
	x_{21}	x_{22}	x_{23}	x_{24}	…	x_{2n}	→ N
	x_{31}	x_{32}	x_{33}	x_{34}	…	x_{3n}	→ P
	……………………………………						
	x_{m1}	x_{m2}	x_{m3}	x_{m4}	…	x_{mn}	→ N

Features (aka Attributes)

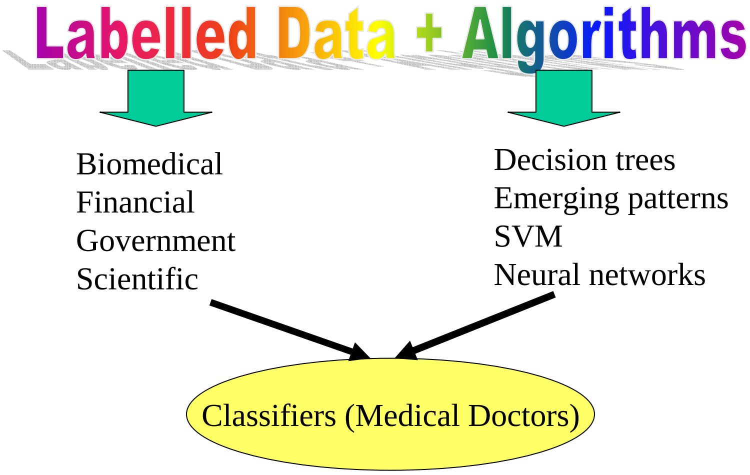
- **Categorical features**
  - color = {red, blue, green}
- **Continuous or numerical features**
  - gene expression
  - age
  - blood pressure
- **Discretization**

An Example



Outlook	Temp	Humidity	Windy	class
Sunny	75	70	true	Play
Sunny	80	90	true	Don’t
Sunny	85	85	false	Don’t
Sunny	72	95	true	Don’t
Sunny	69	70	false	Play
Overcast	72	90	true	Play
Overcast	83	78	false	Play
Overcast	64	65	true	Play
Overcast	81	75	false	Play
Rain	71	80	true	Don’t
Rain	65	70	true	Don’t
Rain	75	80	false	Play
Rain	68	80	false	Play
Rain	70	96	false	Play

Overall Picture of Supervised Learning



Labelled Data + Algorithms

Biomedical
Financial
Government
Scientific

Decision trees
Emerging patterns
SVM
Neural networks

Classifiers (Medical Doctors)

Evaluation of a Classifier

- **Performance on independent blind test data**
- **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 CV**

- **Accuracy, error rate**
- **False positive rate, false negative rate, sensitivity, specificity, precision**

Requirements of Biomedical Classification

- **High accuracy/sensitivity/specificity/precision**
- **High comprehensibility**

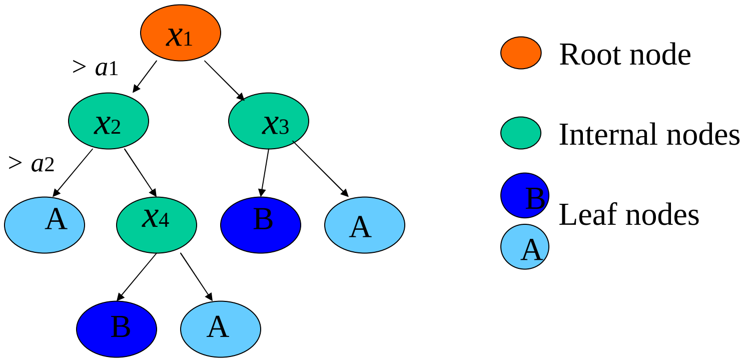
Importance of Rule-Based Methods

- **Systematic selection of a small number of features used for the decision making**

⇒ Increase the 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 generally unattractive**

A Simple Dataset

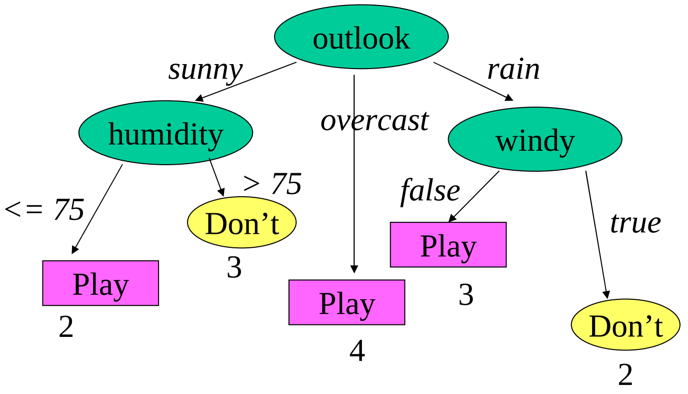
Outlook	Temp	Humidity	Windy	class
Sunny	75	70	true	Play
Sunny	80	90	true	Don't
Sunny	85	85	false	Don't
Sunny	72	95	true	Don't
Sunny	69	70	false	Play
Overcast	72	90	true	Play
Overcast	83	78	false	Play
Overcast	64	65	true	Play
Overcast	81	75	false	Play
Rain	71	80	true	Don't
Rain	65	70	true	Don't
Rain	75	80	false	Play
Rain	68	80	false	Play
Rain	70	96	false	Play

9 Play samples

5 Don't

A total of 14.

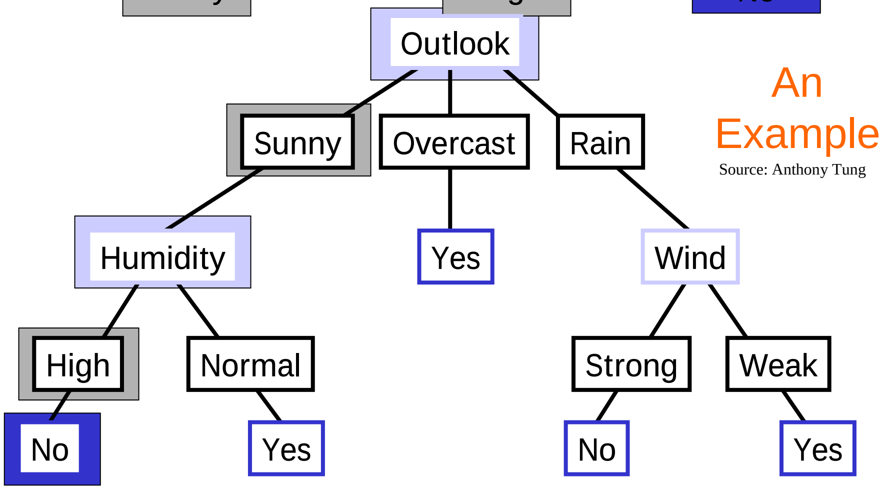
A Decision Tree



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

Exercise: What is the accuracy of this tree?

Outlook	Temperature	Humidity	Wind	PlayTennis
Sunny	Hot	High	Weak	?No



An Example

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

Instance #	Outlook	Temp	Humidity	Windy	class
1	Sunny	75	70	true	Play
2	Sunny	80	90	true	Don’t
3	Sunny	85	85	false	Don’t
4	Sunny	72	95	true	Don’t
5	Sunny	69	70	false	Play
6	Overcast	72	90	true	Play
7	Overcast	83	78	false	Play
8	Overcast	64	65	true	Play
9	Overcast	81	75	false	Play
10	Rain	71	80	true	Don’t
11	Rain	65	70	true	Don’t
12	Rain	75	80	false	Play
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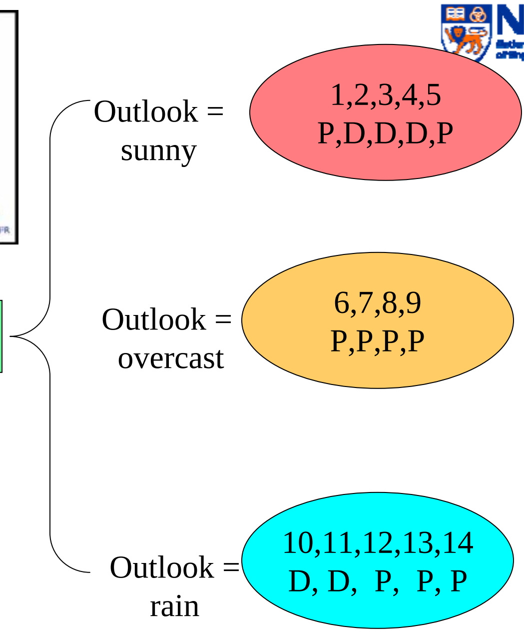
12	Rain	75	80	false	Play
13	Rain	68	80	false	Play
14	Rain	70	96	false	Play

Total 14 training instances



Outlook = sunny

1,2,3,4,5
P,D,D,D,P

Outlook = overcast

6,7,8,9
P,P,P,P

Outlook = rain

10,11,12,13,14
D, D, P, P, P

Instance #	Outlook	Temp	Humidity	Windy	class
1	Sunny	75	70	true	Play
2	Sunny	80	90	true	Don't
3	Sunny	85	85	false	Don't
4	Sunny	72	95	true	Don't
5	Sunny	69	70	false	Play
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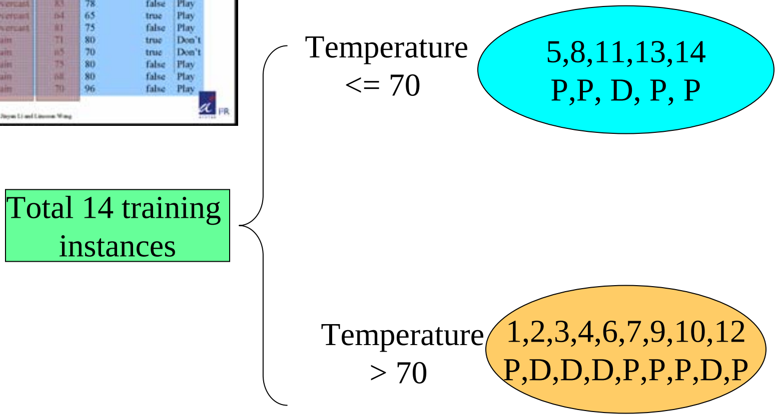


Total 14 training instances

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

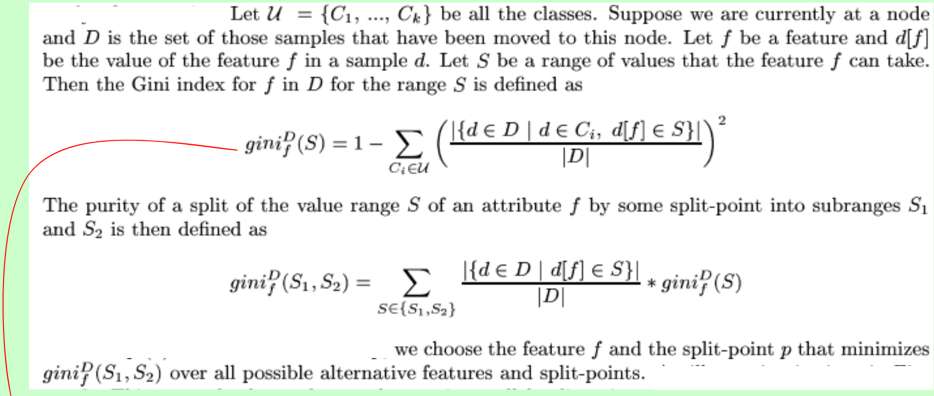
Steps of Decision Tree Construction

- **Select the "best" feature as the root node of the whole tree**
- **After partition by this feature, select the best feature (wrt the subset of training data) as the root node of this sub-tree**
- **Recursively, until the partitions become pure or almost pure**

Three Common Measures to Evaluate Which Feature is Best

- **Gini index**
- **Information gain**
- **Information gain ratio**

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

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

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

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

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.

$$gini_f^D(S) = \sum_{Ci, Cj \in U, i \neq j,} \left(\frac{|\{d \in D \mid d \in Ci, d[f] \in S\}|}{|D|} \right) \left(\frac{|\{d \in D \mid d \in Cj, d[f] \in S\}|}{|D|} \right)$$

i.e., gini measures amt of impurity

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

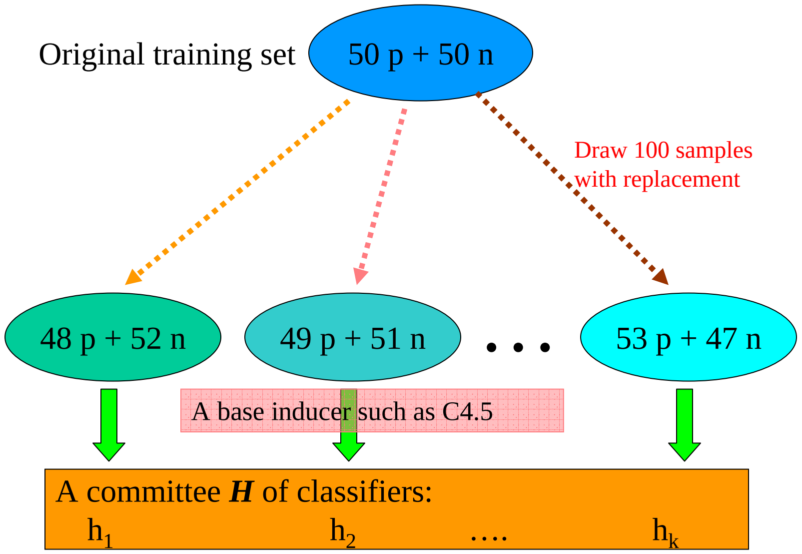
- h_1, h_2, h_3 are indep classifiers w/ accuracy = 60%
- C_1, C_2 are the only classes
- t is a test instance in C_1
- $h(t) = \mathrm{argmax}_{C \in \{C1,C2\}} |\{h_j \in \{h_1, h_2, h_3\} \mid h_j(t) = C\}|$
- Then $\mathrm{prob}(h(t) = C_1)$

$$
\begin{aligned}
&= \mathrm{prob}(h_1(t)=C_1 \;\&\; h_2(t)=C_1 \;\&\; h_3(t)=C_1) + \\
&\quad \mathrm{prob}(h_1(t)=C_1 \;\&\; h_2(t)=C_1 \;\&\; h_3(t)=C_2) + \\
&\quad \mathrm{prob}(h_1(t)=C_1 \;\&\; h_2(t)=C_2 \;\&\; h_3(t)=C_1) + \\
&\quad \mathrm{prob}(h_1(t)=C_2 \;\&\; h_2(t)=C_1 \;\&\; h_3(t)=C_1) \\
&= 60\% * 60\% * 60\% + 60\% * 60\% * 40\% + \\
&\quad 60\% * 40\% * 60\% + 40\% * 60\% * 60\% = 64.8\%
\end{aligned}
$$

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

Draw 100 samples
with replacement

48 p + 52 n

49 p + 51 n

. . .

53 p + 47 n

A base inducer such as C4.5

A committee ***H*** of classifiers:

h_1 h_2 …. h_k

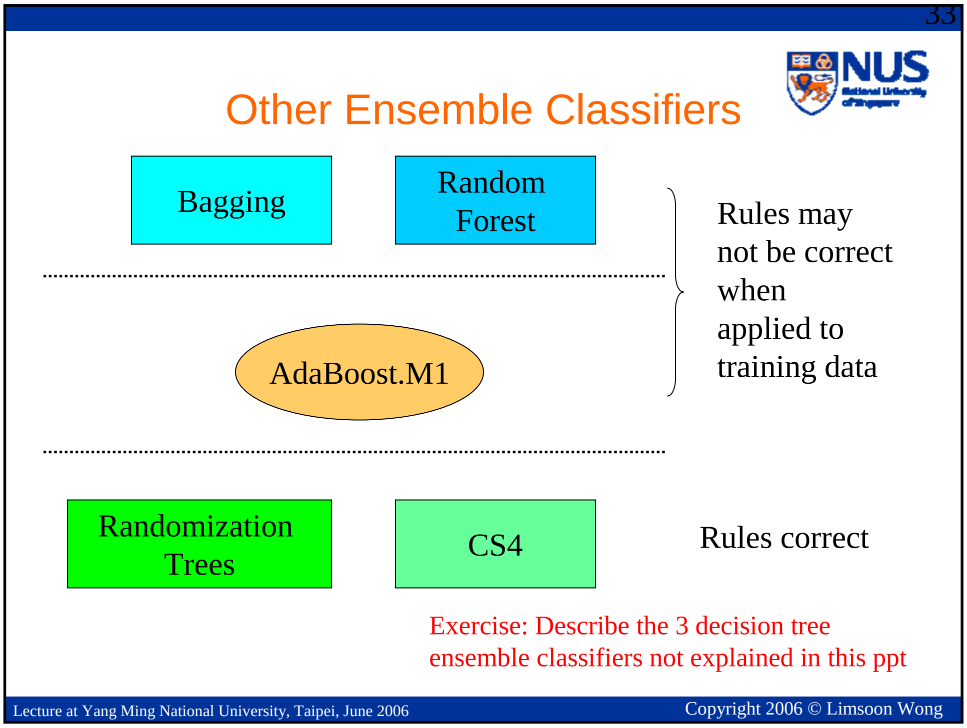
Decision Making by Bagging

Given a new test sample T

$$bagged(T) = \text{argmax}_{C_j \in \mathcal{U}} \left| \{ h_i \in \mathcal{H} \mid h_i(T) = C_j \} \right|$$

$$\text{where } \mathcal{U} = \{C_1, \ldots, C_r\}$$

Exercise: What does the above formula mean?



Other Ensemble Classifiers

Bagging

Random Forest

AdaBoost.M1

Rules may not be correct when applied to training data

Randomization Trees

CS4

Rules correct

Exercise: Describe the 3 decision tree ensemble classifiers not explained in this ppt

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Other Machine Learning Approaches

Outline

- **K-Nearest Neighbour**
- **Bayesian Approach**
- **Hidden Markov Models**

Exercise: Name and describe one other commonly used machine learning method

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

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

where f ranges over features of the samples

Exercise: What does the formula above mean?

Illustration of kNN (k=8)

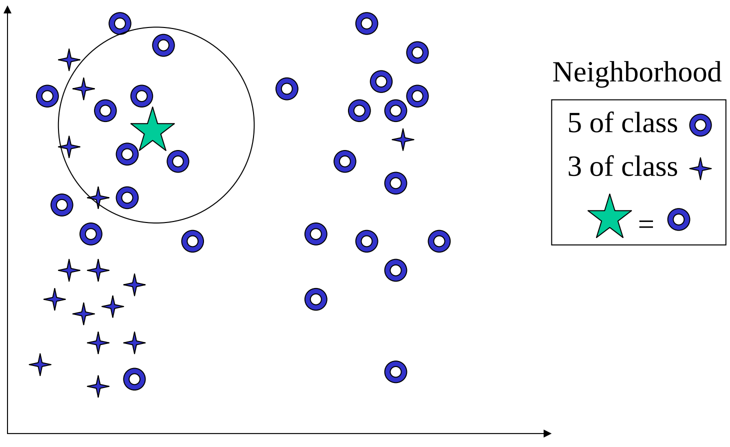


Image credit: Zaki

Some Issues

- **Simple to implement**
- **But need to 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: Segmentation of White Lesion Matter in MRI

- **Anbeek et al, *NeuroImage* 21:1037-1044, 2004**
- **Use kNN to automated segmentation of white matter lesions in cranial MR images**
- **Rely on info from T1-weighted, inversion recovery, proton density-weighted, T2-weighted, & fluid attenuation inversion recovery scans**

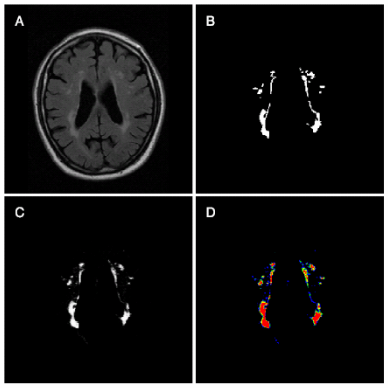


Fig. 3. Classification of a patient with moderate lesion load. (A) FLAIR image, (B) manual segmentation, (C) probability map, (D) segmentations derived from probability map with different thresholds: black: probability (P) = 0, blue: $0 < P \leq 0.3$, green: $0.3 < P \leq 0.5$, yellow: $0.5 < P \leq 0.8$, red: $0.8 < P \leq 1$.

Example Use of kNN: Ovarian Cancer Diagnosis Based on SELDI Proteomic Data

- **Li et al, *Bioinformatics* 20:1638-1640, 2004**
- **Use kNN to diagnose ovarian cancers using proteomic spectra**
- **Data set is from Petricoin et al., *Lancet* 359:572-577, 2002**

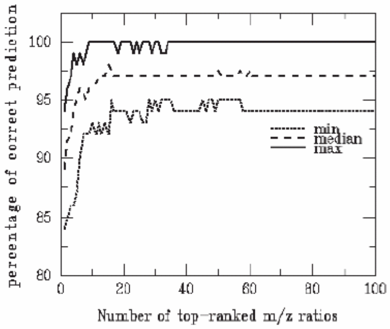


Fig. 1. Minimum, median and maximum of percentages of correct prediction as a function of the number of top-ranked m/z ratios in 50 independent partitions into learning and validation sets.

Bayesian Approach

Bayes Theorem

$$P(h|d) = \frac{P(d|h) * P(h)}{P(d)}$$

- *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 w/ feature vector $\{f_1 = v_1, \ldots, f_n = v_n\}$, the most probable classification is given by

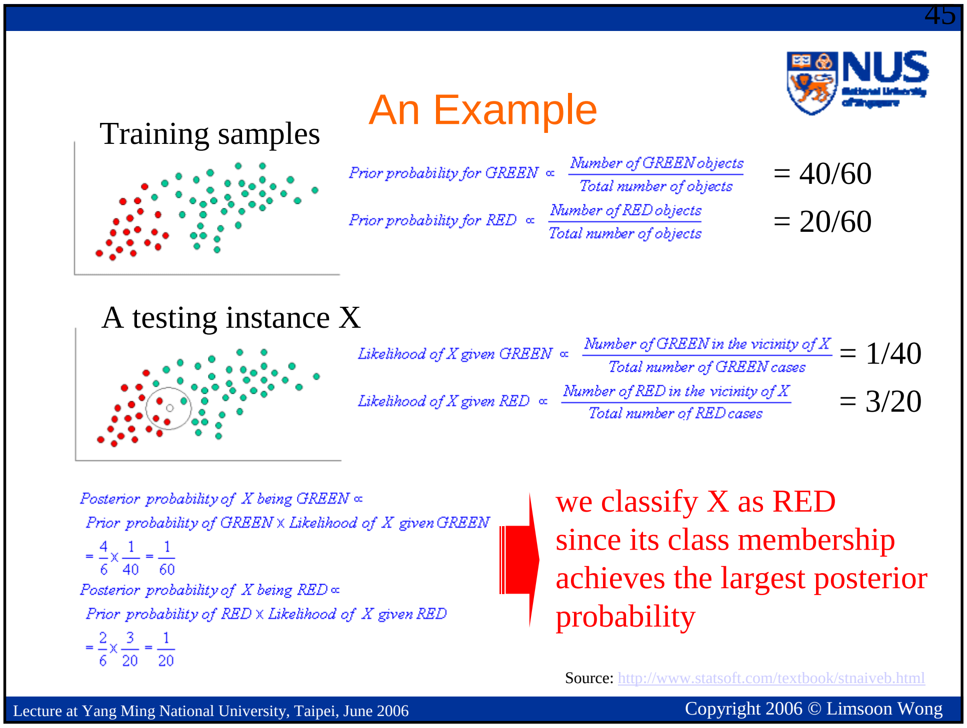
$$\text{argmax}_{h_j \in H} P(h_j | f_1 = v_1, \ldots, f_n = v_n)$$

- Using Bayes Theorem, rewrites to

$$\text{argmax}_{h_j \in H} \frac{P(f_1 = v_1, \ldots, f_n = v_n | h_j) * P(h_j)}{P(f_1 = v_1, \ldots, f_n = v_n)}$$

- Since denominator is independent of h_j, this simplifies to

$$\text{argmax}_{h_j \in H} P(f_1 = v_1, \ldots, f_n = v_n | h_j) * P(h_j)$$



An Example

Training samples

$$\text{Prior probability for GREEN} \propto \frac{\text{Number of GREEN objects}}{\text{Total number of objects}} = 40/60$$

$$\text{Prior probability for RED} \propto \frac{\text{Number of RED objects}}{\text{Total number of objects}} = 20/60$$

A testing instance X

$$\text{Likelihood of X given GREEN} \propto \frac{\text{Number of GREEN in the vicinity of X}}{\text{Total number of GREEN cases}} = 1/40$$

$$\text{Likelihood of X given RED} \propto \frac{\text{Number of RED in the vicinity of X}}{\text{Total number of RED cases}} = 3/20$$

Posterior probability of X being GREEN ∝
Prior probability of GREEN × Likelihood of X given GREEN

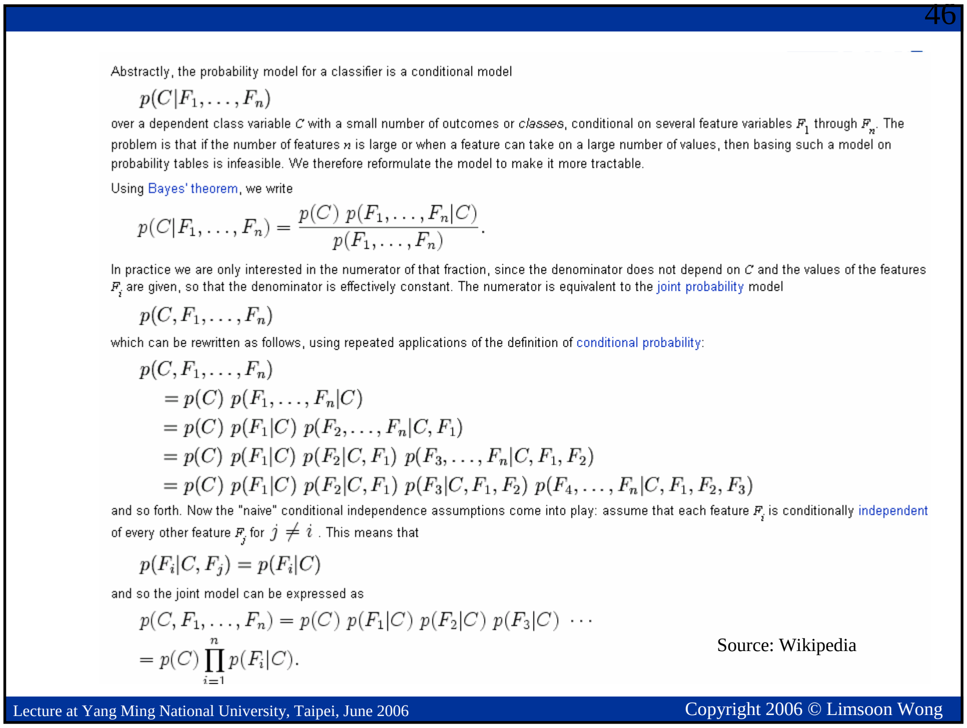
$$= \frac{4}{6} \times \frac{1}{40} = \frac{1}{60}$$

Posterior probability of X being RED ∝
Prior probability of RED × Likelihood of X given RED

$$= \frac{2}{6} \times \frac{3}{20} = \frac{1}{20}$$

we classify X as RED since its class membership achieves the largest posterior probability

Source: http://www.statsoft.com/textbook/stnaiveb.html



Abstractly, the probability model for a classifier is a conditional model

$$p(C|F_1,\dots,F_n)$$

over a dependent class variable C with a small number of outcomes or *classes*, conditional on several feature variables F_1 through F_n. The problem is that if the number of features n is large or when a feature can take on a large number of values, then basing such a model on probability tables is infeasible. We therefore reformulate the model to make it more tractable.

Using Bayes' theorem, we write

$$p(C|F_1,\dots,F_n) = \frac{p(C)\ p(F_1,\dots,F_n|C)}{p(F_1,\dots,F_n)}.$$

In practice we are only interested in the numerator of that fraction, since the denominator does not depend on C and the values of the features F_i are given, so that the denominator is effectively constant. The numerator is equivalent to the joint probability model

$$p(C,F_1,\dots,F_n)$$

which can be rewritten as follows, using repeated applications of the definition of conditional probability:

$$\begin{aligned}
&p(C,F_1,\dots,F_n)\\
&\quad= p(C)\ p(F_1,\dots,F_n|C)\\
&\quad= p(C)\ p(F_1|C)\ p(F_2,\dots,F_n|C,F_1)\\
&\quad= p(C)\ p(F_1|C)\ p(F_2|C,F_1)\ p(F_3,\dots,F_n|C,F_1,F_2)\\
&\quad= p(C)\ p(F_1|C)\ p(F_2|C,F_1)\ p(F_3|C,F_1,F_2)\ p(F_4,\dots,F_n|C,F_1,F_2,F_3)
\end{aligned}$$

and so forth. Now the "naive" conditional independence assumptions come into play: assume that each feature F_i is conditionally independent of every other feature F_j for $j \neq i$. This means that

$$p(F_i|C,F_j) = p(F_i|C)$$

and so the joint model can be expressed as

$$\begin{aligned}
p(C,F_1,\dots,F_n) &= p(C)\ p(F_1|C)\ p(F_2|C)\ p(F_3|C)\ \cdots\\
&= p(C)\prod_{i=1}^{n} p(F_i|C).
\end{aligned}$$

Source: Wikipedia

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 sufficiently large**
- **"Solved" by assuming $f_1, \ldots, f_n$ are conditionally independent of each other**
- **Then** $\text{argmax}_{h_j \in H} P(f_1 = v_1, \ldots, f_n = v_n | h_j) * P(h_j)$

$$= \text{argmax}_{h_j \in H} \prod_i P(f_i = v_i | h_j) * P(h_j)$$

- **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 $P(f_j=v_j|h_j)$?

Example Use of Bayesian: Design of Screens for Macromolecular Crystallization

- **Hennessy et al., *Acta Cryst* D56:817-827, 2000**
- **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**

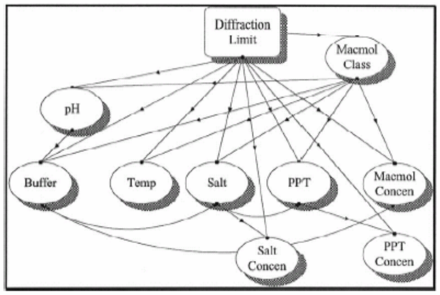
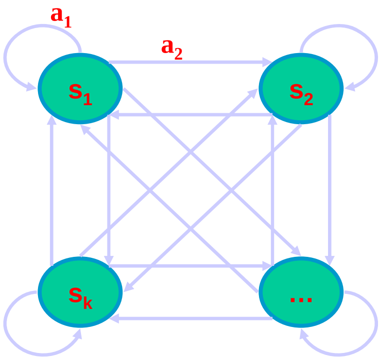


Figure 1
Crystallization parameter dependency graph. The graph represents the parameters included in the calculation of the estimated probability of success and their dependencies. A connecting arc from pH to buffer indicates that the probability distribution for the buffer may depend on the value of the pH. The lack of a connecting arc between two parameters reflects conditional independence (the probability distribution for a parameter is independent of the value of the other parameter).

Hidden Markov Models

What is a HMM

- **HMM is a stochastic generative model for sequences**
- **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 according to *T* while emitting symbols according to *E***



The 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, …, & states *S* = s_1, s_2, …, 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

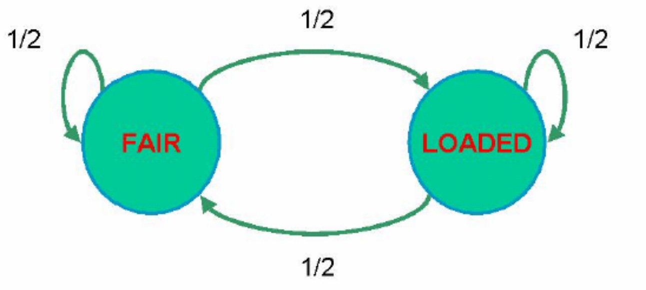
- Given the model parameters, compute the probability of a particular output sequence. Solved by the **forward algorithm**
- Given the model parameters, find the most likely sequence of (hidden) states which could have generated a given output sequence. Solved by the **Viterbi algorithm**
- Given an 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) = 1/6, i = 1..6**
  - Loaded dice
    - **P(i) = 1/10, i = 1..5**
    - **P(i) = 1/2, i = 6**
- **Casino switches betw fair & loaded die with prob 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



Emission Matrix

E(1|Fair) = 1/6
E(2|Fair) = 1/6
E(3|Fair) = 1/6
E(4|Fair) = 1/6
E(5|Fair) = 1/6
E(6|Fair) = 1/6

E(1|Loaded) = 1/10
E(2|Loaded) = 1/10
E(3|Loaded) = 1/10
E(4|Loaded) = 1/10
E(5|Loaded) = 1/10
E(6|Loaded) = 1/2

Transition Matrix

T(Loaded,Loaded) = 1/2
T(Loaded,Fair) = 1/2
T(Fair,Fair) = 1/2
T(Fair,Loaded) = 1/2
T(?,Fair) = 1.0
T(?,Loaded) = 0.0

1, 6, 2, 6?
We were probably cheated...

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

$$\begin{aligned}
Prob(X, S = Fair, Loaded, Fair, Loaded) &= E(1|Fair) * T(?, Fair) * \\
&\quad E(6|Loaded) * T(Fair, Loaded) * \\
&\quad E(2|Loaded) * T(Loaded, Fair) * \\
&\quad E(6|Loaded) * T(Fair, Loaded) \\
&= \frac{1}{6} * 1 * \frac{1}{2} * \frac{1}{2} * \frac{1}{6} * \frac{1}{2} * \frac{1}{2} * \frac{1}{2} \\
&= 8.6806 * 10^{-4}
\end{aligned}$$

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**

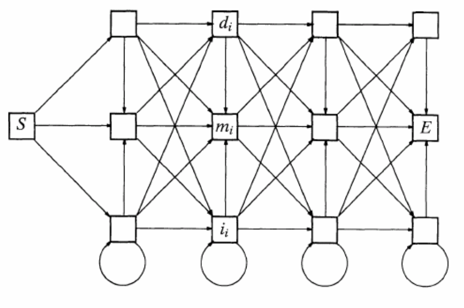


FIG. 1. HMM architecture. S and E are the start and end states. Sequence of main states m_i is the backbone. Side states d_i (resp. i_i) correspond to deletions (resp. insertions).

Example Use of HMM: Gene Finding in Bacterial Genomes

- **Borodovsky et al., *NAR* 23:3554-3562, 1995**
- **Investigated statistical features of 3 classes (wrt level of codon usage bias) of E. coli genes**
- **HMM for nucleotide sequences of each class was developed**

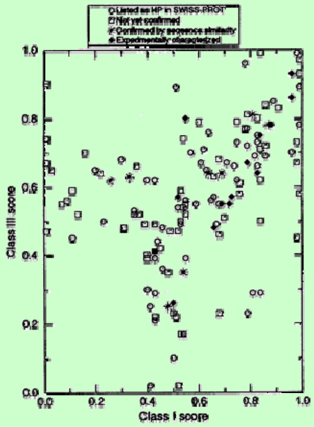


Figure 4. Distribution of GeneMark scores for 126 new genes. The x axis represents the score computed by GM5_ECO1 program, y axis represents the score computed by GM4_ECO3 program. The quadrant $x < 0.4$, $y < 0.4$ is empty since a threshold of 0.4 was applied.

Any Question?

WEKA
The University of Waikato

- 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?

Acknowledgements

- **Most of the slides used in this ppt came from a tutorial that I gave with JinyanLi at the *8th European Conference on Principles and Practice of Knowledge Discovery in Databases*, Pisa, Italy, 20-24 September 2004**
- **This dishonest casino example came from slides I inherited from Ken Sung**

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