Classification (Basic Concepts)

Yu Su, CSE@The Ohio State University
Classification: Basic Concepts

- Classification: Basic Concepts
- Decision Tree Induction
- Model Evaluation and Selection
- Practical Issues of Classification
- Bayes Classification Methods
- Techniques to Improve Classification Accuracy: Ensemble Methods
- Summary

This class

Next class
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Decision Tree Induction: An Example

- Training data set: Buys_computer
- The data set follows an example of Quinlan’s ID3 (Playing Tennis)
- Resulting tree:

```
age?
  <=30  31..40  >40
    student?
      no  yes
        no  yes
    credit rating?
      fair
        no  yes
        no  yes

<table>
<thead>
<tr>
<th>age</th>
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</table>
```
Algorithm for Decision Tree Induction

- Basic algorithm (a greedy algorithm)
  - Tree is constructed in a **top-down recursive divide-and-conquer manner**
  - At start, all the training examples are at the root
  - Attributes are categorical (if continuous-valued, they are discretized in advance)
  - Examples are partitioned recursively based on selected attributes
  - Test attributes are selected on the basis of 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—**majority voting** is employed for classifying the leaf
  - There are no samples left
Algorithm Outline

- Split (node, {data tuples})
  - A <= the best attribute for splitting the {data tuples}
  - Decision attribute for this node <= A
  - For each value of A, create new child node
  - For each child node / subset:
    - If one of the stopping conditions is satisfied: STOP
    - Else: Split (child_node, {subset})

ID3 algorithm: how it works
https://www.youtube.com/watch?v=_XhOdSLIE5c
Algorithm Outline

- Split (node, {data tuples})
  - A <= the **best attribute** for splitting the {data tuples}
  - Decision attribute for this node <= A
  - For each value of A, create new child node
  - For each child node / subset:
    - If one of the stopping conditions is satisfied: STOP
    - Else: Split (child_node, {subset})
Brief 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 $\{y_1, y_2, \ldots, y_m\}$
    \[
    H(Y) = -\sum_{i=1}^{m} p_i \log(p_i) \text{ where } p_i = P(Y = y_i)
    \]
  - Interpretation
    - Higher entropy $\rightarrow$ higher uncertainty
    - Lower entropy $\rightarrow$ lower uncertainty

- **Conditional entropy**
  \[
  H(Y|X) = \sum_{x} p(x)H(Y|X = x)
  \]
Attribute Selection Measure: Information Gain (ID3/C4.5)

- Select the attribute with the highest information gain
- Let $p_i$ be the probability that an arbitrary tuple in $D$ belongs to class $C_i$, estimated by $\frac{|C_{i,D}|}{|D|}$
- 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 $A$
  \[
  Gain(A) = Info(D) - Info_A(D)
  \]
Attribute Selection: Information Gain

- Class P: buys_computer = “yes”
- Class N: buys_computer = “no”

### Attribute Selection

#### Information Gain

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

Look at “age”:

<table>
<thead>
<tr>
<th>age</th>
<th>income</th>
<th>student</th>
<th>credit_rating</th>
<th>buys computer</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt;=30</td>
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<td>fair</td>
<td>no</td>
</tr>
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Attribute Selection: Information Gain

- Class P: buys_computer = “yes”
- Class N: buys_computer = “no”

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

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

\[
\text{Gain}(\text{age}) = \text{Info}(D) - \text{Info}_{\text{age}}(D) = 0.246
\]

Similarly,
\[
\text{Gain}(\text{income}) = 0.029
\]
\[
\text{Gain}(\text{student}) = 0.151
\]
\[
\text{Gain}(\text{credit_rating}) = 0.048
\]
Recursive Procedure

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1. After selecting age at the root node, we will create three child nodes.

2. One child node is associated with red data tuples.

3. How to continue for this child node?

Now, you will make $D = \{\text{red data tuples}\}$ and then select the best attribute to further split $D$. A recursive procedure.
How to Select Test Attribute?

- Depends on attribute types
  - Nominal
  - Ordinal
  - Continuous

- Depends on number of ways to split
  - 2-way split
  - Multi-way split
Splitting Based on Nominal Attributes

- **Multi-way split**: Use as many partitions as distinct values.

![Multi-way split diagram]

- **Binary split**: Divides values into two subsets. Need to find optimal partitioning.

![Binary split diagrams]
Splitting Based on Continuous Attributes

(i) Binary split

Yes

No

(ii) Multi-way split

< 10K

[10K, 25K)

[25K, 50K)

[50K, 80K)

> 80K
How to Determine the Best Split

- **Greedy approach:**
  - Nodes with **homogeneous** class distribution are preferred

Ideally, data tuples at that node belong to the same class.

<table>
<thead>
<tr>
<th></th>
<th>C0: 5</th>
<th>C1: 5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Non-homogeneous,</td>
<td></td>
<td></td>
</tr>
<tr>
<td>High degree of impurity</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>C0: 9</th>
<th>C1: 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Homogeneous,</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Low degree of impurity</td>
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Rethink about Decision Tree Classification

- Greedy approach:
  - Nodes with *homogeneous* class distribution are preferred

- Need a measure of **node impurity**:
  - Non-homogeneous, High degree of impurity
  - Homogeneous, Low degree of impurity
Measures of Node Impurity

- **Entropy:**
  \[ H(Y) = - \sum_{i=1}^{m} p_i \log(p_i) \quad \text{where} \quad p_i = P(Y = y_i) \]
  - Higher entropy => higher uncertainty, higher node impurity
  - Why entropy is used in information gain

- **Gini Index**

- **Misclassification error**
Gain Ratio for Attribute Selection (C4.5)

- Information gain measure is biased towards attributes with a large number of values
- C4.5 (a successor of ID3) uses gain ratio to overcome the problem (normalization to information gain)

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

- The entropy of the partitioning, or the potential information generated by splitting \( D \) into \( \nu \) partitions.

- \( \text{GainRatio}(A) = \text{Gain}(A) / \text{SplitInfo}(A) \) (normalizing Information Gain)
Gain Ratio for Attribute Selection (C4.5)

- C4.5 (a successor of ID3) uses gain ratio to overcome the problem (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)

- Ex.
  
  \[ Gain(income) = 0.029 \]  
  (from last class, slide 27)

  \[ SplitInfo_{income}(D) = -\frac{4}{14} \times \log_2 \left( \frac{4}{14} \right) - \frac{6}{14} \times \log_2 \left( \frac{6}{14} \right) - \frac{4}{14} \times \log_2 \left( \frac{4}{14} \right) = 1.557 \]

  \[ gain\_ratio(income) = 0.029 / 1.557 = 0.019 \]

- The attribute with the **maximum gain ratio** is selected as the splitting attribute
Gini Index (CART, IBM IntelligentMiner)

- If a data set $D$ contains examples from $n$ classes, gini index, $gini(D)$ is defined as
  \[
gini(D) = 1 - \sum_{j=1}^{n} p_j^2,
\]
  where $p_j$ 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 after the split 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 $gini_A(D)$ (or, the largest reduction in impurity) is chosen to split the node.
Binary Attributes: Computing Gini Index

- Splits into two partitions
- Effect of weighing partitions:
  - Larger and Purer Partitions are sought for.

\[ gini(D) = 1 - \sum_{j=1}^{n} p_j^2 \]

<table>
<thead>
<tr>
<th>Parent</th>
<th>C1</th>
<th>C2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gini</td>
<td>6</td>
<td>6</td>
</tr>
</tbody>
</table>
Binary Attributes: Computing Gini Index

- Splits into two partitions
- Effect of weighing partitions:
  - Larger and Purer Partitions are sought for.

Gini(N1)
= 1 - (5/7)^2 - (2/7)^2
= 0.194

Gini(N2)
= 1 - (1/5)^2 - (4/5)^2
= 0.528

\[ gini(D) = 1 - \sum_{j=1}^{n} p_j^2 \]
Binary Attributes: Computing Gini Index

- Splits into two partitions
- Effect of weighing partitions:
  - Prefer Larger and Purer Partitions.

\[
gini(D) = 1 - \sum_{j=1}^{n} p_j^2
\]

Gini(N1)
\[
= 1 - (5/7)^2 - (2/7)^2 \\
= 0.194
\]

Gini(N2)
\[
= 1 - (1/5)^2 - (4/5)^2 \\
= 0.528
\]

<table>
<thead>
<tr>
<th></th>
<th>N1</th>
<th>N2</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>5</td>
<td>1</td>
</tr>
<tr>
<td>C2</td>
<td>2</td>
<td>4</td>
</tr>
</tbody>
</table>

Gini = 0.333

Gini(Children)
\[
= 7/12 \times 0.194 + 5/12 \times 0.528 \\
= 0.333
\]
Categorical Attributes: Computing Gini Index

- For each distinct value, gather counts for each class in the dataset
- Use the count matrix to make decisions

<table>
<thead>
<tr>
<th>CarType</th>
<th>Family</th>
<th>Sports</th>
<th>Luxury</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>1</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>C2</td>
<td>4</td>
<td>1</td>
<td>1</td>
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<td>0.393</td>
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Multi-way split

<table>
<thead>
<tr>
<th>CarType</th>
<th>{Sports, Luxury}</th>
<th>{Family}</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>3</td>
<td>1</td>
</tr>
<tr>
<td>C2</td>
<td>2</td>
<td>4</td>
</tr>
<tr>
<td>Gini</td>
<td>0.400</td>
<td></td>
</tr>
</tbody>
</table>

Two-way split (find best partition of values)

<table>
<thead>
<tr>
<th>CarType</th>
<th>{Sports}</th>
<th>{Family, Luxury}</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>C2</td>
<td>1</td>
<td>5</td>
</tr>
<tr>
<td>Gini</td>
<td>0.419</td>
<td></td>
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</tbody>
</table>
Continuous Attributes: Computing Gini Index or Information Gain

- To discretize the attribute values
  - Use Binary Decisions based on one splitting value

- Several Choices for the splitting value
  - Number of possible splitting values = Number of distinct values - 1
  - Typically, the midpoint between each pair of adjacent values is considered as a possible split point
    - \((a_i + a_{i+1})/2\) is the midpoint between the values of \(a_i\) and \(a_{i+1}\)

- Each splitting value has a count matrix associated with it
  - Class counts in each of the partitions, \(A < v\) and \(A \geq v\)

- Simple method to choose best \(v\)
  - For each \(v\), scan the database to gather count matrix and compute its Gini index
  - Computationally Inefficient! Repetition of work.

<table>
<thead>
<tr>
<th>Tid</th>
<th>Refund</th>
<th>Marital Status</th>
<th>Taxable Income</th>
<th>Cheat</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Yes</td>
<td>Single</td>
<td>125K</td>
<td>No</td>
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<tr>
<td>2</td>
<td>No</td>
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Continuous Attributes:
Computing Gini Index or expected information requirement

First decide the splitting value to discretize the attribute:

- For efficient computation: for each attribute,
  Step 1: Sort the attribute on values

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Use midpoint
Continuous Attributes:
Computing Gini Index or expected information requirement

First decide the splitting value to discretize the attribute:

- For efficient computation: for each attribute,
  Step 1: Sort the attribute on values
  Step 2: **Linearly scan these values, each time updating the count matrix**

For each splitting value, get its **count matrix**: how many data tuples have:
(a) Taxable income \(\leq 65\) with class label “Yes”,
(b) Taxable income \(\leq 65\) with class label “No”,
(c) Taxable income \(> 65\) with class label “Yes”,
(d) Taxable income \(> 65\) with class label “No”.
Continuous Attributes:
Computing Gini Index or expected information requirement

First decide the splitting value to discretize the attribute:

- For efficient computation: for each attribute,
  - Step 1: Sort the attribute on values
  - Step 2: **Linearly scan these values, each time updating the count matrix**

For each splitting value, get its **count matrix**: how many data tuples have:

(a) Taxable income <=72 with class label “Yes”,
(b) Taxable income <=72 with class label “No”,
(c) Taxable income >72 with class label “Yes”,
(d) Taxable income >72 with class label “No”.

Step 1:

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**Gini**

- 0.420
- 0.400
- 0.375
- 0.343
- 0.417
- 0.400
- 0.300
- 0.343
- 0.375
- 0.400
- 0.420
Continuous Attributes:
Computing Gini Index or expected information requirement

**First decide the splitting value to discretize the attribute:**

- For efficient computation: for each attribute,
  - Step 1: Sort the attribute on values
  - Step 2: **Linearly scan these values, each time updating the count matrix**

For each splitting value, get its **count matrix**: how many data tuples have:

- (a) Taxable income <=80 with class label “Yes”,
- (b) Taxable income <=80 with class label “No”,
- (c) Taxable income >80 with class label “Yes”,
- (d) Taxable income >80 with class label “No”.

**Possible Splitting Values**

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**Sorted Values**

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Continuous Attributes:
Computing Gini Index or expected information requirement

First decide the splitting value to discretize the attribute:

- For efficient computation: for each attribute,
  - Step 1: Sort the attribute on values
  - Step 2: **Linearly scan these values, each time updating the count matrix**

For each splitting value, get its **count matrix**: how many data tuples have:
(a) Taxable income $\leq 172$ with class label “Yes”,
(b) Taxable income $\leq 172$ with class label “No”,
(c) Taxable income $> 172$ with class label “Yes”,
(d) Taxable income $> 172$ with class label “No”.
Continuous Attributes:
Computing Gini Index or expected information requirement

First decide the splitting value to discretize the attribute:

- For efficient computation: for each attribute,
  Step 1: Sort the attribute on values
  Step 2: Linearly scan these values, each time updating the count matrix
  Step 3: Computing Gini index and choose the split position that has the least Gini index

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Step 1: Sorted Values
Possible Splitting Values
Step 2:
Step 3:

For each splitting value v (e.g., 65), compute its Gini index:

\[
gini_{\text{Taxable Income}}(D) = \frac{|D_1|}{|D|} gini(D_1) + \frac{|D_2|}{|D|} gini(D_2)
\]

Here D1 and D2 are two partitions based on v: D1 has taxable income \(\leq v\) and D2 has \(> v\)
Continuous Attributes:
Computing Gini Index or expected information requirement

First decide the splitting value to discretize the attribute:

- For efficient computation: for each attribute,
  - Step 1: Sort the attribute on values
  - Step 2: Linearly scan these values, each time updating the count matrix
  - Step 3: Computing Gini index and choose the split position that has the least Gini index

**Possible Splitting Values**

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**Sorted Values**

- Step 1: Sorted Values
- Step 2: Possible Splitting Values
- Step 3: Gini

- For each splitting value \( v \) (e.g., 72), compute its Gini index:
  \[
gini_{\text{Taxable Income}}(D) = \frac{|D_1|}{|D|} \text{gini}(D_1) + \frac{|D_2|}{|D|} \text{gini}(D_2)
\]

Here \( D_1 \) and \( D_2 \) are two partitions based on \( v \): \( D_1 \) has taxable income \(<=v \) and \( D_2 \) has \( >v \)
Continuous Attributes:
Computing Gini Index or expected information requirement

First decide the splitting value to discretize the attribute:

- For efficient computation: for each attribute,
  - Step 1: Sort the attribute on values
  - Step 2: Linearly scan these values, each time updating the count matrix
  - Step 3: Computing Gini index and choose the split position that has the least Gini index

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Possible Splitting Values

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Step 3:

Choose this splitting value (=97) with the least Gini index to discretize Taxable Income.
**Continuous Attributes:**

**Computing Gini Index or expected information requirement**

First decide the splitting value to discretize the attribute:

- For efficient computation: for each attribute,
  - Step 1: Sort the attribute on values
  - Step 2: Linearly scan these values, each time updating the count matrix
  - Step 3: **Computing expected information requirement and choose the split position that has the least value**

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If Information Gain is used for attribute selection,

Similarly to calculating Gini index, for each splitting value, compute \( \text{Info}_{\text{Taxable Income}}(D) \):

\[
\text{Info}_{\text{Taxable Income}}(D) = \sum_{j=1}^{2} \frac{|D_j|}{|D|} \times \text{Info}(D_j)
\]
Continuous Attributes:
Computing Gini Index or expected information requirement

First decide the splitting value to discretize the attribute:

- For efficient computation: for each attribute,
  - Step 1: Sort the attribute on values
  - Step 2: Linearly scan these values, each time updating the count matrix
  - Step 3: Computing Gini index and choose the split position that has the least Gini index

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Step 1: Sort the attribute on values
Step 2: Linearly scan these values, each time updating the count matrix
Step 3: Computing Gini index and choose the split position that has the least Gini index

Choose this splitting value (=97 here) with the least Gini index or expected information requirement to discretize Taxable Income.
Continuous Attributes: Computing Gini Index or expected information requirement

First decide the splitting value to discretize the attribute:

- For efficient computation: for each attribute,
  - **Step 1:** Sort the attribute on values
  - **Step 2:** Linearly scan these values, each time updating the count matrix
  - **Step 3:** Computing Gini index and choose the split position that has the least Gini index

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<td>&lt;=</td>
<td>&gt;</td>
<td>&lt;=</td>
<td>&gt;</td>
<td>&lt;=</td>
<td>&gt;</td>
</tr>
<tr>
<td>Gini</td>
<td>0.400</td>
<td>0.375</td>
<td>0.343</td>
<td>0.417</td>
<td>0.400</td>
<td>0.300</td>
<td>0.343</td>
<td>0.375</td>
<td>0.400</td>
<td></td>
</tr>
</tbody>
</table>

At each level of the decision tree, for attribute selection, (1) First, discretize a continuous attribute by deciding the splitting value; (2) Then, compare the discretized attribute with other attributes in terms of Gini Index reduction or Information Gain.
Continuous Attributes:
Computing Gini Index or expected information requirement

First decide the splitting value to discretize the attribute:

- For efficient computation: for each attribute,
  - Step 1: Sort the attribute on values
  - Step 2: Linearly scan these values, each time updating the count matrix
  - Step 3: **Computing Gini index and choose the split position that has the least Gini index**

For each attribute, only scan the data tuples once

<table>
<thead>
<tr>
<th>Cheat</th>
<th>No</th>
<th>No</th>
<th>No</th>
<th>Yes</th>
<th>Yes</th>
<th>Yes</th>
<th>No</th>
<th>No</th>
<th>No</th>
<th>No</th>
</tr>
</thead>
<tbody>
<tr>
<td>Taxable Income</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sorted Values</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>60</td>
<td>70</td>
<td>75</td>
<td>85</td>
<td>90</td>
<td>95</td>
<td>100</td>
<td>120</td>
<td>125</td>
<td>220</td>
<td></td>
</tr>
</tbody>
</table>

**Step 1:**
Possible Splitting Values

<table>
<thead>
<tr>
<th>&lt;= &gt;</th>
<th>&lt;= &gt;</th>
<th>&lt;= &gt;</th>
<th>&lt;= &gt;</th>
<th>&lt;= &gt;</th>
<th>&lt;= &gt;</th>
<th>&lt;= &gt;</th>
<th>&lt;= &gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>65</td>
<td>72</td>
<td>80</td>
<td>87</td>
<td>92</td>
<td>97</td>
<td>110</td>
<td>122</td>
</tr>
</tbody>
</table>

**Step 2:**

<table>
<thead>
<tr>
<th>Yes</th>
<th>No</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 3 0 3 0 3 1 2 2 1 3 0 3 0 3 0 3 0 3 0</td>
<td></td>
</tr>
<tr>
<td>1 6 2 5 3 4 3 4 3 4 3 4 3 5 2 6 1</td>
<td></td>
</tr>
</tbody>
</table>

**Step 3:**

<table>
<thead>
<tr>
<th>Gini</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.400 0.375 0.343 0.417 0.400</td>
</tr>
</tbody>
</table>

At each level of the decision tree, for attribute selection, (1) First, discretize a continuous attribute by deciding the splitting value; (2) Then, compare the discretized attribute with other attributes in terms of Gini Index reduction or Information Gain.
Another Impurity Measure: Misclassification Error

- Classification error at a node $t$:

  $$\text{Error}(t) = 1 - \max_i P(i \mid t)$$

  - $P(i \mid t)$ means the relative frequency of class $i$ at node $t$.

- Measures misclassification error made by a node.
  - Maximum ($1 - 1/n_c$) when records are equally distributed among all classes, implying most impurity
  - Minimum (0.0) when all records belong to one class, implying least impurity
### Examples for Misclassification Error

**Error formula:**

\[
\text{Error}(t) = 1 - \max_i P(i \mid t)
\]

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>0</td>
<td>P(C1) = 0/6 = 0 \hspace{1em} P(C2) = 6/6 = 1</td>
</tr>
<tr>
<td>C2</td>
<td>6</td>
<td>Error = 1 - \max (0, 1) = 1 - 1 = 0</td>
</tr>
</tbody>
</table>

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>1</td>
<td>P(C1) = 1/6 \hspace{1em} P(C2) = 5/6</td>
</tr>
<tr>
<td>C2</td>
<td>5</td>
<td>Error = 1 - \max (1/6, 5/6) = 1 - 5/6 = 1/6</td>
</tr>
</tbody>
</table>

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>2</td>
<td>P(C1) = 2/6 \hspace{1em} P(C2) = 4/6</td>
</tr>
<tr>
<td>C2</td>
<td>4</td>
<td>Error = 1 - \max (2/6, 4/6) = 1 - 4/6 = 1/3</td>
</tr>
</tbody>
</table>
Comparison among Impurity Measure

For a 2-class problem:

Entropy = $-p \log(p) - (1-p) \log(1-p)$

Gini = $1 - p^2 - (1-p)^2$

Error = $1 - \max(p, 1-p)$
Other Attribute Selection Measures

- **CHAID**: a popular decision tree algorithm, measure based on $\chi^2$ test for independence
- **C-SEP**: performs better than info. gain and gini index in certain cases
- **G-statistic**: has a close approximation to $\chi^2$ distribution
- **MDL (Minimal Description Length) principle** (i.e., 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
- **Multivariate splits (partition based on multiple variable combinations)**
  - **CART**: finds multivariate splits based on a linear comb. of attrs.
- **Which attribute selection measure is the best?**
  - Most give good results, none is significantly superior than others
Decision Tree Based Classification

- Advantages:
  - Inexpensive to construct
  - Extremely fast at classifying unknown records
  - Easy to interpret for small-sized trees
  - Accuracy is comparable to other classification techniques for many simple data sets
Example: C4.5

- Simple depth-first construction.
- Uses Information Gain
- Sorts Continuous Attributes at each node.
- Needs entire data to fit in memory.
- Unsuitable for Large Datasets.
  - Needs out-of-core sorting.

- You can download the software online, e.g.,
Classification: Basic Concepts

- Classification: Basic Concepts
- Decision Tree Induction
- Model Evaluation and Selection
- Practical Issues of Classification
- Bayes Classification Methods
- Techniques to Improve Classification Accuracy: Ensemble Methods
- Summary
Model Evaluation

- **Metrics for Performance Evaluation**
  - How to evaluate the performance of a model?

- **Methods for Performance Evaluation**
  - How to obtain reliable estimates?

- **Methods for Model Comparison**
  - How to compare the relative performance among competing models?
Metrics for Performance Evaluation

- Focus on the predictive capability of a model
  - Rather than how fast it takes to classify or build models, scalability, etc.
- Confusion Matrix:

<table>
<thead>
<tr>
<th>ACTUAL CLASS</th>
<th>PREDICTED CLASS</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Class=Yes</td>
</tr>
<tr>
<td>Class=Yes</td>
<td>a</td>
</tr>
<tr>
<td>Class=No</td>
<td>c</td>
</tr>
</tbody>
</table>

- a: TP (true positive)
- b: FN (false negative)
- c: FP (false positive)
- d: TN (true negative)
Classifier Evaluation Metrics: Confusion Matrix

Confusion Matrix:

<table>
<thead>
<tr>
<th>Actual class</th>
<th>Predicted class</th>
<th>$C_1$</th>
<th>$\neg C_1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_1$</td>
<td>True Positives (TP)</td>
<td></td>
<td>False Negatives (FN)</td>
</tr>
<tr>
<td>$\neg C_1$</td>
<td>False Positives (FP)</td>
<td></td>
<td>True Negatives (TN)</td>
</tr>
</tbody>
</table>

Example of Confusion Matrix:

<table>
<thead>
<tr>
<th>Actual class</th>
<th>buy_computer = yes</th>
<th>buy_computer = no</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>buy_computer = yes</td>
<td>6954</td>
<td>46</td>
<td>7000</td>
</tr>
<tr>
<td>buy_computer = no</td>
<td>412</td>
<td>2588</td>
<td>3000</td>
</tr>
<tr>
<td>Total</td>
<td>7366</td>
<td>2634</td>
<td>10000</td>
</tr>
</tbody>
</table>

- Given $m$ classes, an entry, $CM_{ij}$ in a confusion matrix indicates # of tuples in class $i$ that were labeled by the classifier as class $j$
- May have extra rows/columns to provide totals
## Classifier Evaluation Metrics: Accuracy, Error Rate

<table>
<thead>
<tr>
<th>A \ P</th>
<th>C</th>
<th>¬C</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>TP</td>
<td>FN</td>
</tr>
<tr>
<td>¬C</td>
<td>FP</td>
<td>TN</td>
</tr>
<tr>
<td>P'</td>
<td>N'</td>
<td>All</td>
</tr>
</tbody>
</table>

- **Classifier Accuracy**, or recognition rate:
  - percentage of test set tuples that are correctly classified
  - \[ \text{Accuracy} = \frac{(TP + TN)}{\text{All}} \]

- **Error rate**: \(1 - \text{accuracy}\), or
  - \[ \text{Error rate} = \frac{(FP + FN)}{\text{All}} \]
Limitation of Accuracy

- Consider a 2-class problem
  - Number of Class 0 examples = 9990
  - Number of Class 1 examples = 10

- If a model predicts everything to be class 0,
  Accuracy is $\frac{9990}{10000} = 99.9\%$

- Accuracy is misleading because model does not detect any class 1 example
**Cost Matrix**

<table>
<thead>
<tr>
<th>ACTUAL CLASS</th>
<th>PREDICTED CLASS</th>
<th>Class=Yes</th>
<th>Class=No</th>
</tr>
</thead>
<tbody>
<tr>
<td>Class=Yes</td>
<td>C(Yes</td>
<td>Yes)</td>
<td>C(No</td>
</tr>
<tr>
<td>Class=No</td>
<td>C(Yes</td>
<td>No)</td>
<td>C(No</td>
</tr>
</tbody>
</table>

$C(i|j)$: Cost of misclassifying one class $j$ example as class $i$
### Computing Cost of Classification

#### Cost Matrix

<table>
<thead>
<tr>
<th>ACTUAL CLASS</th>
<th>PREDICTED CLASS</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>+</td>
</tr>
<tr>
<td>+</td>
<td>-1</td>
</tr>
<tr>
<td>-</td>
<td>1</td>
</tr>
</tbody>
</table>

#### Model $M_1$

<table>
<thead>
<tr>
<th>ACTUAL CLASS</th>
<th>PREDICTED CLASS</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>+</td>
</tr>
<tr>
<td>+</td>
<td>150</td>
</tr>
<tr>
<td>-</td>
<td>60</td>
</tr>
</tbody>
</table>

Accuracy = 80%
Cost = 3910

#### Model $M_2$

<table>
<thead>
<tr>
<th>ACTUAL CLASS</th>
<th>PREDICTED CLASS</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>+</td>
</tr>
<tr>
<td>+</td>
<td>250</td>
</tr>
<tr>
<td>-</td>
<td>5</td>
</tr>
</tbody>
</table>

Accuracy = 90%
Cost = 4255
Cost-Sensitive Measures

Precision (p) = \frac{a}{a + c}

Recall (r) = \frac{a}{a + b}

F - measure (F) = \frac{2rp}{r + p} = \frac{2a}{2a + b + c}

- Precision is biased towards C(Yes|Yes) & C(Yes|No)
- Recall is biased towards C(Yes|Yes) & C(No|Yes)
- F-measure is biased towards all except C(No|No)

Weighted Accuracy = \frac{w_1a + w_4d}{w_1a + w_2b + w_3c + w_4d}

<table>
<thead>
<tr>
<th>ACTUAL CLASS</th>
<th>PREDICTED CLASS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Class=Yes</td>
<td>Class=No</td>
</tr>
<tr>
<td>Class=Yes</td>
<td>a (TP)</td>
</tr>
<tr>
<td>Class=No</td>
<td>c (FP)</td>
</tr>
<tr>
<td>Class=No</td>
<td>b (FN)</td>
</tr>
<tr>
<td>Class=No</td>
<td>d (TN)</td>
</tr>
</tbody>
</table>
Classifier Evaluation Metrics: Sensitivity and Specificity

- **Classifier Accuracy**, or recognition rate: percentage of test set tuples that are correctly classified
  
  \[
  \text{Accuracy} = \frac{\text{TP} + \text{TN}}{\text{All}}
  \]

- **Error rate**: \(1 - \text{accuracy}\), or
  
  \[
  \text{Error rate} = \frac{\text{FP} + \text{FN}}{\text{All}}
  \]

- **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

- **Sensitivity**: True Positive recognition rate
  - \(\text{Sensitivity} = \frac{\text{TP}}{\text{P}}\)

- **Specificity**: True Negative recognition rate
  - \(\text{Specificity} = \frac{\text{TN}}{\text{N}}\)
Methods for Performance Evaluation

- How to obtain a reliable estimate of performance?

- Performance of a model may depend on other factors besides the learning algorithm:
  - Class distribution
  - Cost of misclassification
  - Size of training and test sets
Learning Curve

- Learning curve shows how accuracy changes with varying sample size

- Requires a sampling schedule for creating learning curve:
  - Arithmetic sampling (Langley, et al)
  - Geometric sampling (Provost et al)

Effect of small sample size:
- Bias in the estimate
- Variance of estimate
Methods of Estimation

- **Holdout**
  - E.g., reserve 2/3 for training and 1/3 for testing

- Random subsampling
  - Repeated holdout

- Cross validation
  - Partition data into k disjoint subsets
  - k-fold: train on k-1 partitions, test on the remaining one
  - Leave-one-out: k=n

- Stratified sampling
  - oversampling vs undersampling

- **Bootstrap**
  - Sampling with replacement
Evaluating Classifier Accuracy: Holdout & Cross-Validation Methods

- **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
  - Random sampling: a variation of holdout
    - Repeat holdout k times, accuracy = avg. of the accuracies obtained

- **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 dist. in each fold is approx. the same as that in the initial data
Evaluating Classifier Accuracy: Bootstrap

- **Bootstrap**
  - Works well with small data sets
  - Samples the given training tuples uniformly with replacement
    - Each time a tuple is selected, it is equally likely to be selected again and re-added to the training set

- Several bootstrap methods, and a common one is .632 bootstrap
  - A data set with \(d\) tuples is sampled \(d\) times, with replacement, resulting in a training set of \(d\) samples. The data tuples that did not make it into the training set end up forming the test set. About 63.2% of the original data end up in the bootstrap, and the remaining 36.8% form the test set (since \((1 - 1/d)^d \approx e^{-1} = 0.368\))
  - Repeat the sampling procedure \(k\) times, overall accuracy of the model:

\[
Acc(M) = \frac{1}{k} \sum_{i=1}^{k} (0.632 \times Acc(M_i)_{\text{test-set}} + 0.368 \times Acc(M_i)_{\text{train-set}})
\]
Model Evaluation

- **Metrics for Performance Evaluation**
  - How to evaluate the performance of a model?

- **Methods for Performance Evaluation**
  - How to obtain reliable estimates?

- **Methods for Model Comparison**
  - How to compare the relative performance among competing models?
ROC (Receiver Operating Characteristic) Curve

(True Positive Rate, True Positive Rate):

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

- Diagonal line:
  - Random guessing
  - Below diagonal line:
    - prediction is opposite of the true class
Using ROC for Model Comparison

- No model consistently outperform the other
  - $M_1$ is better for small FPR
  - $M_2$ is better for large FPR

- Area Under the ROC curve
  - Ideal: Area = 1
  - Random guess (diagonal line): Area = 0.5
Classification: Basic Concepts

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