Data Mining
Classification: Basic Concepts, Decision Trees, and Model Evaluation

Lecture Notes for Chapter 4

Introduction to Data Mining
by
Tan, Steinbach, Kumar

(modified by Predrag Radivojac, 2019)
Classification: Definition

- Given a collection of records (*training set*)
  - Each record contains a set of *attributes*, one of the attributes is the *class*.

- Find a *model* for class attribute as a function of the values of other attributes.

- Goal: *previously unseen* records should be assigned a class as accurately as possible.
  - A *test set* is used to determine the accuracy of the model. Usually, the given data set is divided into training and test sets, with training set used to build the model and test set used to validate it.
Illustrating Classification Task

### Training Set

<table>
<thead>
<tr>
<th>Tid</th>
<th>Attrib1</th>
<th>Attrib2</th>
<th>Attrib3</th>
<th>Class</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Yes</td>
<td>Large</td>
<td>125K</td>
<td>No</td>
</tr>
<tr>
<td>2</td>
<td>No</td>
<td>Medium</td>
<td>100K</td>
<td>No</td>
</tr>
<tr>
<td>3</td>
<td>No</td>
<td>Small</td>
<td>70K</td>
<td>No</td>
</tr>
<tr>
<td>4</td>
<td>Yes</td>
<td>Medium</td>
<td>120K</td>
<td>No</td>
</tr>
<tr>
<td>5</td>
<td>No</td>
<td>Large</td>
<td>95K</td>
<td>Yes</td>
</tr>
<tr>
<td>6</td>
<td>No</td>
<td>Medium</td>
<td>60K</td>
<td>No</td>
</tr>
<tr>
<td>7</td>
<td>Yes</td>
<td>Large</td>
<td>220K</td>
<td>No</td>
</tr>
<tr>
<td>8</td>
<td>No</td>
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<td>Yes</td>
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<td>No</td>
<td>Medium</td>
<td>75K</td>
<td>No</td>
</tr>
<tr>
<td>10</td>
<td>No</td>
<td>Small</td>
<td>90K</td>
<td>Yes</td>
</tr>
</tbody>
</table>

### Test Set

<table>
<thead>
<tr>
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<tbody>
<tr>
<td>11</td>
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<tr>
<td>12</td>
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</tr>
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<tr>
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<td>?</td>
</tr>
<tr>
<td>15</td>
<td>No</td>
<td>Large</td>
<td>67K</td>
<td>?</td>
</tr>
</tbody>
</table>
Examples of Classification Task

- Predicting tumor cells as benign or malignant
- Classifying credit card transactions as legitimate or fraudulent
- Classifying secondary structures of protein as alpha-helix, beta-sheet, or random coil
- Categorizing news stories as finance, weather, entertainment, sports, etc
Classification Techniques

- Decision Tree based Methods
- Rule-based Methods
- Memory based reasoning
- Neural Networks
- Naïve Bayes and Bayesian Belief Networks
- Support Vector Machines
Example of a Decision Tree

### Training Data

<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>
</tr>
<tr>
<td>2</td>
<td>No</td>
<td>Married</td>
<td>100K</td>
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<td>No</td>
<td>Single</td>
<td>90K</td>
<td>Yes</td>
</tr>
</tbody>
</table>

### Model: Decision Tree

- **Refund**: Yes → NO
  - **MarSt**: Single, Divorced → NO
  - **TaxInc**: < 80K → NO
    - **TaxInc**: > 80K → YES
  - **MarSt**: Married → NO
- **Refund**: No → NO
Another Example of Decision Tree

<table>
<thead>
<tr>
<th>Tid</th>
<th>Refund</th>
<th>Marital Status</th>
<th>Taxable Income</th>
<th>Cheat</th>
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<tbody>
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<td>No</td>
</tr>
<tr>
<td>10</td>
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<td>Single</td>
<td>90K</td>
<td>Yes</td>
</tr>
</tbody>
</table>

There could be more than one tree that fits the same data!
Decision Tree Classification Task

**Training Set**

<table>
<thead>
<tr>
<th>Tid</th>
<th>Attrib1</th>
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<td>?</td>
</tr>
</tbody>
</table>
Apply Model to Test Data

Start from the root of tree.

Refund

Yes
NO

No
MarSt
Single, Divorced
Married

TaxInc
< 80K
NO

> 80K
YES

Test Data

<table>
<thead>
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<tr>
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<td>Married</td>
<td>80K</td>
<td>?</td>
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</table>
Apply Model to Test Data

Test Data

Refund | Marital Status | Taxable Income | Cheat
--- | --- | --- | ---
No | Married | 80K | ?

Refund
- Yes
  - NO
- No
  - MarSt
    - Single, Divorced
    - TaxInc
      - < 80K
        - NO
      - > 80K
        - YES
  - Married
Apply Model to Test Data

Test Data

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</table>

Refund
- Yes
  - NO

Marital Status
- Single, Divorced
- Married

Taxable Income
- < 80K
  - NO
- > 80K
  - YES
Apply Model to Test Data

Test Data

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Refund

Yes

NO

No

MarSt

Single, Divorced

Married

TaxInc

< 80K

NO

> 80K

YES

NO
Apply Model to Test Data

Test Data

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</tbody>
</table>

Refund

Yes

No

Refund

No

MarSt

Single, Divorced

Married

TaxInc

< 80K

> 80K

NO

NO

YES

NO
Apply Model to Test Data

Test Data

<table>
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<td>80K</td>
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Assign Cheat to “No”
Decision Tree Classification Task

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Decision Tree Induction

- Many Algorithms:
  - Hunt’s Algorithm (one of the earliest)
  - CART
  - ID3, C4.5
  - SLIQ, SPRINT
General Structure of Hunt’s Algorithm

- Let $D_t$ be the set of training records that reach a node $t$
- General Procedure:
  - If $D_t$ contains records that belong to the same class $y_t$, then $t$ is a leaf node labeled as $y_t$
  - If $D_t$ is an empty set, then $t$ is a leaf node labeled by the default class, $y_d$
  - If $D_t$ contains records that belong to more than one class, use an attribute test to split the data into smaller subsets. Recursively apply the procedure to each subset.
Hunt’s Algorithm

Refund

- Don’t Cheat
  - Yes
    - Don’t Cheat
  - No
    - Don’t Cheat

Marital Status

- Refund
  - Yes
    - Don’t Cheat
  - No
    - Single, Divorced
    - Cheat
    - Marital Status
      - Married
        - Refund
          - Yes
            - Don’t Cheat
          - No
            - Taxable Income
              - < 80K
                - Don’t Cheat
              - >= 80K
                - Cheat
        - Don’t Cheat
      - Divorced
        - Refund
          - Yes
            - Single
          - No
            - Married
              - Refund
                - Yes
                  - Married
                  - Taxable Income
                    - 125K
                    - No
                - No
                  - Married
                  - Taxable Income
                    - 100K
                    - No
                - No
                  - Single
                  - Taxable Income
                    - 70K
                    - No
                - Yes
                  - Married
                  - Taxable Income
                    - 120K
                    - No
                - No
                  - Divorced
                  - Taxable Income
                    - 95K
                    - Yes
                - No
                  - Married
                  - Taxable Income
                    - 60K
                    - No
                - Yes
                  - Divorced
                  - Taxable Income
                    - 220K
                    - No
                - No
                  - Single
                  - Taxable Income
                    - 85K
                    - Yes
                - No
                  - Married
                  - Taxable Income
                    - 75K
                    - No
                - No
                  - Single
                  - Taxable Income
                    - 90K
                    - Yes
Tree Induction

- **Greedy strategy.**
  - Split the records based on an attribute test that optimizes certain criterion.

- **Issues**
  - Determine how to split the records
    - How to specify the attribute test condition?
    - How to determine the best split?
  - Determine when to stop splitting
Tree Induction

- Greedy strategy.
  - Split the records based on an attribute test that optimizes certain criterion.

- Issues
  - Determine how to split the records
    - How to specify the attribute test condition?
    - How to determine the best split?
  - Determine when to stop splitting
How to Specify Test Condition?

● 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.
  
  ![Diagram showing multi-way split]

- **Binary split**: Divides values into two subsets. Need to find optimal partitioning.
  
  ![Diagram showing binary split]
Splitting Based on Ordinal 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 Diagram]

- **What about this split?**
Splitting Based on Continuous Attributes

- Different ways of handling
  - **Discretization** to form an ordinal categorical attribute
    - Static – discretize once at the beginning
    - Dynamic – ranges can be found by equal interval bucketing, equal frequency bucketing (percentiles), or clustering.
  - **Binary Decision**: \((A < v)\) or \((A \geq v)\)
    - consider all possible splits and finds the best cut
    - can be more compute intensive
Splitting Based on Continuous Attributes

(i) Binary split

Yes

No

(ii) Multi-way split

< 10K [10K, 25K) [25K, 50K) [50K, 80K) > 80K
Tree Induction

● Greedy strategy.
  – Split the records based on an attribute test that optimizes certain criterion.

● Issues
  – Determine how to split the records
    ◆ How to specify the attribute test condition?
    ◆ How to determine the best split?
  – Determine when to stop splitting
How to determine the Best Split

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

Which test condition is the best?
How to determine the Best Split

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

- Need a measure of node impurity:

<table>
<thead>
<tr>
<th>C0: 5</th>
<th>C0: 9</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1: 5</td>
<td>C1: 1</td>
</tr>
</tbody>
</table>

Non-homogeneous, High degree of impurity

Homogeneous, Low degree of impurity
Measures of Node Impurity

- Gini Index
- Entropy
- Misclassification error
How to Find the Best Split

Before Splitting:

<table>
<thead>
<tr>
<th>C0</th>
<th>N00</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>N01</td>
</tr>
</tbody>
</table>

A?

Yes

Node N1

<table>
<thead>
<tr>
<th>C0</th>
<th>N10</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>N11</td>
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</tbody>
</table>

No

Node N2

<table>
<thead>
<tr>
<th>C0</th>
<th>N20</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>N21</td>
</tr>
</tbody>
</table>

B?

Yes

Node N3

<table>
<thead>
<tr>
<th>C0</th>
<th>N30</th>
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<tbody>
<tr>
<td>C1</td>
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</tbody>
</table>

No

Node N4

<table>
<thead>
<tr>
<th>C0</th>
<th>N40</th>
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</thead>
<tbody>
<tr>
<td>C1</td>
<td>N41</td>
</tr>
</tbody>
</table>

Gain = M0 – M12 vs M0 – M34
Measure of Impurity: GINI

- Gini Index for a given node $t$:

\[
\text{GINI}(t) = 1 - \sum_j [p(j \mid t)]^2
\]

(Note: $p(j \mid t)$ is the relative frequency of class $j$ at node $t$).

- Maximum $(1 - 1/n_c)$ when records are equally distributed among all classes, implying least interesting information
- Minimum $(0.0)$ when all records belong to one class, implying most interesting information

<table>
<thead>
<tr>
<th></th>
<th>C1</th>
<th>C2</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>0</td>
<td>6</td>
</tr>
<tr>
<td>C2</td>
<td>6</td>
<td>5</td>
</tr>
<tr>
<td>Gini=0.000</td>
<td>Gini=0.278</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>C1</th>
<th>C2</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>1</td>
<td>5</td>
</tr>
<tr>
<td>C2</td>
<td>5</td>
<td>4</td>
</tr>
<tr>
<td>Gini=0.278</td>
<td>Gini=0.444</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>C1</th>
<th>C2</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td>C2</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>Gini=0.444</td>
<td>Gini=0.500</td>
<td></td>
</tr>
</tbody>
</table>
Examples for computing GINI

\[
GINI(t) = 1 - \sum_{j} [p(j \mid t)]^2
\]

<table>
<thead>
<tr>
<th>C1</th>
<th>0</th>
<th>P(C1) = 0/6 = 0</th>
<th>P(C2) = 6/6 = 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>C2</td>
<td>6</td>
<td>( Gini = 1 - P(C1)^2 - P(C2)^2 = 1 - 0 - 1 = 0 )</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>C1</th>
<th>1</th>
<th>P(C1) = 1/6</th>
<th>P(C2) = 5/6</th>
</tr>
</thead>
<tbody>
<tr>
<td>C2</td>
<td>5</td>
<td>( Gini = 1 - (1/6)^2 - (5/6)^2 = 0.278 )</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>C1</th>
<th>2</th>
<th>P(C1) = 2/6</th>
<th>P(C2) = 4/6</th>
</tr>
</thead>
<tbody>
<tr>
<td>C2</td>
<td>4</td>
<td>( Gini = 1 - (2/6)^2 - (4/6)^2 = 0.444 )</td>
<td></td>
</tr>
</tbody>
</table>
Splitting Based on GINI

- Used in CART, SLIQ, SPRINT.
- When a node \( p \) is split into \( k \) partitions (children), the quality of split is computed as,

\[
GINI_{\text{split}} = \sum_{i=1}^{k} \frac{n_i}{n} GINI(i)
\]

where, \( n_i = \) number of records at child \( i \),
\( n = \) number of records at node \( p \).
Binary Attributes: Computing GINI Index

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

Gini(N1) = 1 – (5/6)^2 – (2/6)^2
= 0.194

Gini(N2) = 1 – (1/6)^2 – (4/6)^2
= 0.528

This calculation is not correct! Why?
Categorical Attributes: Computing Gini Index

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

### Multi-way split

<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>
</tr>
</tbody>
</table>

Gini: 0.393

### Two-way split

#### (find best partition of values)

<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>
</tbody>
</table>

Gini: 0.400

<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>
</tbody>
</table>

Gini: 0.419
Continuous Attributes: Computing Gini Index

- Use Binary Decisions based on one value
- Several Choices for the splitting value
  - Number of possible splitting values = Number of distinct values
- 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>
</tr>
<tr>
<td>2</td>
<td>No</td>
<td>Married</td>
<td>100K</td>
<td>No</td>
</tr>
<tr>
<td>3</td>
<td>No</td>
<td>Single</td>
<td>70K</td>
<td>No</td>
</tr>
<tr>
<td>4</td>
<td>Yes</td>
<td>Married</td>
<td>120K</td>
<td>No</td>
</tr>
<tr>
<td>5</td>
<td>No</td>
<td>Divorced</td>
<td>95K</td>
<td>Yes</td>
</tr>
<tr>
<td>6</td>
<td>No</td>
<td>Married</td>
<td>60K</td>
<td>No</td>
</tr>
<tr>
<td>7</td>
<td>Yes</td>
<td>Divorced</td>
<td>220K</td>
<td>No</td>
</tr>
<tr>
<td>8</td>
<td>No</td>
<td>Single</td>
<td>85K</td>
<td>Yes</td>
</tr>
<tr>
<td>9</td>
<td>No</td>
<td>Married</td>
<td>75K</td>
<td>No</td>
</tr>
<tr>
<td>10</td>
<td>No</td>
<td>Single</td>
<td>90K</td>
<td>Yes</td>
</tr>
</tbody>
</table>
Continuous Attributes: Computing Gini Index...

- For efficient computation: for each attribute,
  - Sort the attribute on values
  - Linearly scan these values, each time updating the count matrix and computing gini index
  - Choose the split position that has the least gini index

<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>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>125</td>
<td>220</td>
</tr>
<tr>
<td>&lt;=</td>
<td>&gt;</td>
<td>&lt;=</td>
<td>&gt;</td>
<td>&lt;=</td>
<td>&gt;</td>
<td>&lt;=</td>
<td>&gt;</td>
<td>&lt;=</td>
<td>&gt;</td>
<td>&lt;=</td>
</tr>
<tr>
<td>Yes</td>
<td>0</td>
<td>3</td>
<td>0</td>
<td>3</td>
<td>0</td>
<td>3</td>
<td>1</td>
<td>2</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>No</td>
<td>0</td>
<td>7</td>
<td>1</td>
<td>6</td>
<td>2</td>
<td>5</td>
<td>3</td>
<td>4</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>Gini</td>
<td>0.420</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>
</tr>
</tbody>
</table>
Alternative Splitting Criteria based on INFO

- Entropy at a given node \( t \):

\[
Entropy(t) = -\sum_j p(j | t) \log p(j | t)
\]

(NOTE: \( p(j | t) \) is the relative frequency of class \( j \) at node \( t \)).

- Measures homogeneity of a node.
  - Maximum (\( \log n_c \)) when records are equally distributed among all classes implying least information
  - Minimum (0.0) when all records belong to one class, implying most information

- Entropy based computations are similar to the GINI index computations
Examples for computing Entropy

\[ Entropy(t) = - \sum_j p(j \mid t) \log_2 p(j \mid t) \]

<table>
<thead>
<tr>
<th>C1</th>
<th>0</th>
<th>P(C1) = 0/6 = 0</th>
<th>P(C2) = 6/6 = 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>C2</td>
<td>6</td>
<td>Entropy = (-0 \log 0 - 1 \log 1 = -0 - 0 = 0)</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>C1</th>
<th>1</th>
<th>P(C1) = 1/6</th>
<th>P(C2) = 5/6</th>
</tr>
</thead>
<tbody>
<tr>
<td>C2</td>
<td>5</td>
<td>Entropy = (-\frac{1}{6} \log_2 \frac{1}{6} - \frac{5}{6} \log_2 \frac{1}{6} = 0.65)</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>C1</th>
<th>2</th>
<th>P(C1) = 2/6</th>
<th>P(C2) = 4/6</th>
</tr>
</thead>
<tbody>
<tr>
<td>C2</td>
<td>4</td>
<td>Entropy = (-\frac{2}{6} \log_2 \frac{2}{6} - \frac{4}{6} \log_2 \frac{4}{6} = 0.92)</td>
<td></td>
</tr>
</tbody>
</table>
Splitting Based on INFO...

- Information Gain:

\[ GAIN_{\text{split}} = Entropy(p) - \left( \sum_{i=1}^{k} \frac{n_i}{n} \cdot Entropy(i) \right) \]

Parent Node, p is split into k partitions;

- Measures Reduction in Entropy achieved because of the split. Choose the split that achieves most reduction (maximizes GAIN)

- Used in ID3 and C4.5

- Disadvantage: Tends to prefer splits that result in large number of partitions, each being small but pure.
Splitting Based on INFO...

- **Gain Ratio:**

\[
GainRATIO_{split} = \frac{GAIN_{Split}}{SplitINFO}
\]

\[
SplitINFO = -\sum_{i=1}^{k} \frac{n_i}{n} \log \left(\frac{n_i}{n}\right)
\]

Parent Node, p is split into k partitions

- \(n_i\) is the number of records in partition i

- Adjusts Information Gain by the entropy of the partitioning (SplitINFO). Higher entropy partitioning (large number of small partitions) is penalized!

- Used in C4.5

- Designed to overcome the disadvantage of Information Gain
Splitting Criteria based on Classification Error

- Classification error at a node \( t \):

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

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

**Error**

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

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C2</td>
<td>6</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\[
P(C1) = 0/6 = 0 \quad P(C2) = 6/6 = 1
\]

Error = 1 - \max (0, 1) = 1 - 1 = 0

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C2</td>
<td>5</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\[
P(C1) = 1/6 \quad P(C2) = 5/6
\]

Error = 1 - \max (1/6, 5/6) = 1 - 5/6 = 1/6

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C2</td>
<td>4</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\[
P(C1) = 2/6 \quad P(C2) = 4/6
\]

Error = 1 - \max (2/6, 4/6) = 1 - 4/6 = 1/3
Comparison among Splitting Criteria

For a 2-class problem:
Misclassification Error vs Gini

Gini(N1)
= 1 – (3/3)^2 – (0/3)^2
= 0

Gini(N2)
= 1 – (4/7)^2 – (3/7)^2
= 0.489

Gini(Children)
= 3/10 * 0 + 7/10 * 0.489
= 0.342

Gini improves!!
### Tom Mitchell’s example

<table>
<thead>
<tr>
<th>Day</th>
<th>Outlook</th>
<th>Temperature</th>
<th>Humidity</th>
<th>Wind</th>
<th>Play Tennis?</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Sunny</td>
<td>Hot</td>
<td>High</td>
<td>Weak</td>
<td>No</td>
</tr>
<tr>
<td>2</td>
<td>Sunny</td>
<td>Hot</td>
<td>High</td>
<td>Strong</td>
<td>No</td>
</tr>
<tr>
<td>3</td>
<td>Overcast</td>
<td>Hot</td>
<td>High</td>
<td>Weak</td>
<td>Yes</td>
</tr>
<tr>
<td>4</td>
<td>Rain</td>
<td>Mild</td>
<td>High</td>
<td>Weak</td>
<td>Yes</td>
</tr>
<tr>
<td>5</td>
<td>Rain</td>
<td>Cool</td>
<td>Normal</td>
<td>Weak</td>
<td>Yes</td>
</tr>
<tr>
<td>6</td>
<td>Rain</td>
<td>Cool</td>
<td>Normal</td>
<td>Strong</td>
<td>No</td>
</tr>
<tr>
<td>7</td>
<td>Overcast</td>
<td>Cool</td>
<td>Normal</td>
<td>Strong</td>
<td>Yes</td>
</tr>
<tr>
<td>8</td>
<td>Sunny</td>
<td>Mild</td>
<td>High</td>
<td>Weak</td>
<td>No</td>
</tr>
<tr>
<td>9</td>
<td>Sunny</td>
<td>Cool</td>
<td>Normal</td>
<td>Weak</td>
<td>Yes</td>
</tr>
<tr>
<td>10</td>
<td>Rain</td>
<td>Mild</td>
<td>Normal</td>
<td>Weak</td>
<td>Yes</td>
</tr>
<tr>
<td>11</td>
<td>Sunny</td>
<td>Mild</td>
<td>Normal</td>
<td>Strong</td>
<td>Yes</td>
</tr>
<tr>
<td>12</td>
<td>Overcast</td>
<td>Mild</td>
<td>High</td>
<td>Strong</td>
<td>Yes</td>
</tr>
<tr>
<td>13</td>
<td>Overcast</td>
<td>Hot</td>
<td>Normal</td>
<td>Weak</td>
<td>Yes</td>
</tr>
<tr>
<td>14</td>
<td>Rain</td>
<td>Mild</td>
<td>High</td>
<td>Strong</td>
<td>No</td>
</tr>
</tbody>
</table>
Tree Induction

● Greedy strategy.
  – Split the records based on an attribute test that optimizes certain criterion.

● Issues
  – Determine how to split the records
    ◆ How to specify the attribute test condition?
    ◆ How to determine the best split?
  – Determine when to stop splitting
Stopping Criteria for Tree Induction

- Stop expanding a node when all the records belong to the same class
- Stop expanding a node when all the records have similar attribute values
- Early termination (to be discussed later)
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 from:
http://www.cse.unsw.edu.au/~quinlan/c4.5r8.tar.gz
  - not there any longer, but you can Google it
Practical Issues of Classification

- Underfitting and Overfitting
- Missing Values
- Costs of Classification
500 circular and 500 triangular data points.

Circular points:
\[ 0.5 \leq \sqrt{x_1^2 + x_2^2} \leq 1 \]

Triangular points:
\[ \sqrt{x_1^2 + x_2^2} > 0.5 \text{ or } \sqrt{x_1^2 + x_2^2} < 1 \]
Underfitting and Overfitting

**Underfitting**: when model is too simple, both training and test errors are large
Overfitting due to Noise

Decision boundary is distorted by noise point
Overfitting due to Insufficient Examples

Lack of data points in the lower half of the diagram makes it difficult to predict correctly the class labels of that region.

- Insufficient number of training records in the region causes the decision tree to predict the test examples using other training records that are irrelevant to the classification task.
Notes on Overfitting

- Overfitting results in decision trees that are more complex than necessary

- Training error no longer provides a good estimate of how well the tree will perform on previously unseen records

- Need new ways for estimating errors
Estimating Generalization Errors

- **Re-substitution errors**: error on training ($\sum e(t)$)
- **Generalization errors**: error on testing ($\sum e'(t)$)

**Methods for estimating generalization errors**:
- **Optimistic approach**: $e'(t) = e(t)$
- **Pessimistic approach**:
  - For each leaf node: $e'(t) = (e(t)+0.5)$
  - Total errors: $e'(T) = e(T) + N \times 0.5$ (N: number of leaf nodes)
  - For a tree with 30 leaf nodes and 10 errors on training (out of 1000 instances):
    - Training error $= \frac{10}{1000} = 1\%$
    - Generalization error $= \frac{10 + 30\times0.5}{1000} = 2.5\%$
- **Reduced error pruning (REP)**:
  - uses validation data set to estimate generalization error
Occam’s Razor

- Given two models of similar generalization errors, one should prefer the simpler model over the more complex model.

- For complex models, there is a greater chance that it was fitted accidentally by errors in data.

- Therefore, one should include model complexity when evaluating a model.
Minimum Description Length (MDL)

- **Cost(Model,Data)** = **Cost(Data|Model)** + **Cost(Model)**
  - **Cost** is the number of bits needed for encoding.
  - Search for the least costly model.

- **Cost(Data|Model)** encodes the misclassification errors.

- **Cost(Model)** uses node encoding (number of children) plus splitting condition encoding.

<table>
<thead>
<tr>
<th>X</th>
<th>y</th>
</tr>
</thead>
<tbody>
<tr>
<td>X_1</td>
<td>1</td>
</tr>
<tr>
<td>X_2</td>
<td>0</td>
</tr>
<tr>
<td>X_3</td>
<td>0</td>
</tr>
<tr>
<td>X_4</td>
<td>1</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>X_n</td>
<td>1</td>
</tr>
</tbody>
</table>

A → B

<table>
<thead>
<tr>
<th>X</th>
<th>y</th>
</tr>
</thead>
<tbody>
<tr>
<td>X_1</td>
<td>?</td>
</tr>
<tr>
<td>X_2</td>
<td>?</td>
</tr>
<tr>
<td>X_3</td>
<td>?</td>
</tr>
<tr>
<td>X_4</td>
<td>?</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>X_n</td>
<td>?</td>
</tr>
</tbody>
</table>
How to Address Overfitting

- **Pre-Pruning (Early Stopping Rule)**
  - Stop the algorithm before it becomes a fully-grown tree
  - Typical stopping conditions for a node:
    - Stop if all instances belong to the same class
    - Stop if all the attribute values are the same
  - More restrictive conditions:
    - Stop if number of instances is less than some user-specified threshold
    - Stop if class distribution of instances are independent of the available features (e.g., using $\chi^2$ test)
    - Stop if expanding the current node does not improve impurity measures (e.g., Gini or information gain).
How to Address Overfitting...

- Post-pruning
  - Grow decision tree to its entirety
  - Trim the nodes of the decision tree in a bottom-up fashion
  - If generalization error improves after trimming, replace sub-tree by a leaf node.
  - Class label of leaf node is determined from majority class of instances in the sub-tree
  - Can use MDL for post-pruning
Example of Post-Pruning

<table>
<thead>
<tr>
<th>Class = Yes</th>
<th>20</th>
</tr>
</thead>
<tbody>
<tr>
<td>Class = No</td>
<td>10</td>
</tr>
<tr>
<td>Error</td>
<td>10/30</td>
</tr>
</tbody>
</table>

Training Error (Before splitting) = 10/30
Pessimistic error = (10 + 0.5)/30 = 10.5/30
Training Error (After splitting) = 9/30
Pessimistic error (After splitting)
	= (9 + 4 \times 0.5)/30 = 11/30
PRUNE!
Examples of Post-pruning

- Optimistic error?
  
  Don’t prune for both cases

- Pessimistic error?
  
  Don’t prune case 1, prune case 2

- Reduced error pruning?
  
  Depends on validation set
Handling Missing Attribute Values

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

<table>
<thead>
<tr>
<th>Tid</th>
<th>Refund</th>
<th>Marital Status</th>
<th>Taxable Income</th>
<th>Class</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Yes</td>
<td>Single</td>
<td>125K</td>
<td>No</td>
</tr>
<tr>
<td>2</td>
<td>No</td>
<td>Married</td>
<td>100K</td>
<td>No</td>
</tr>
<tr>
<td>3</td>
<td>No</td>
<td>Single</td>
<td>70K</td>
<td>No</td>
</tr>
<tr>
<td>4</td>
<td>Yes</td>
<td>Married</td>
<td>120K</td>
<td>No</td>
</tr>
<tr>
<td>5</td>
<td>No</td>
<td>Divorced</td>
<td>95K</td>
<td>Yes</td>
</tr>
<tr>
<td>6</td>
<td>No</td>
<td>Married</td>
<td>60K</td>
<td>No</td>
</tr>
<tr>
<td>7</td>
<td>Yes</td>
<td>Divorced</td>
<td>220K</td>
<td>No</td>
</tr>
<tr>
<td>8</td>
<td>No</td>
<td>Single</td>
<td>85K</td>
<td>Yes</td>
</tr>
<tr>
<td>9</td>
<td>No</td>
<td>Married</td>
<td>75K</td>
<td>No</td>
</tr>
<tr>
<td>10</td>
<td>?</td>
<td>Single</td>
<td>90K</td>
<td>Yes</td>
</tr>
</tbody>
</table>

Missing value

Before Splitting:
Entropy(Parent) = -0.3 \log(0.3) - (0.7)\log(0.7) = 0.8813

\[
\begin{array}{|c|c|c|}
\hline
\text{Refund} & \text{Class} = \text{Yes} & \text{Class} = \text{No} \\
\hline
\text{Yes} & 0 & 3 \\
\text{No} & 2 & 4 \\
\text{?} & 1 & 0 \\
\hline
\end{array}
\]

Split on Refund:
Entropy(Refund=Yes) = 0

Entropy(Refund=No)
= \(-\frac{2}{6}\log(\frac{2}{6}) - \frac{4}{6}\log(\frac{4}{6}) = 0.9183

Entropy(Children)
= 0.3 (0) + 0.6 (0.9183) = 0.551

Gain = 0.9 \times (0.8813 - 0.551) = 0.3303
Distribute Instances

<table>
<thead>
<tr>
<th>Tid</th>
<th>Refund</th>
<th>Marital Status</th>
<th>Taxable Income</th>
<th>Class</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Yes</td>
<td>Single</td>
<td>125K</td>
<td>No</td>
</tr>
<tr>
<td>2</td>
<td>No</td>
<td>Married</td>
<td>100K</td>
<td>No</td>
</tr>
<tr>
<td>3</td>
<td>No</td>
<td>Single</td>
<td>70K</td>
<td>No</td>
</tr>
<tr>
<td>4</td>
<td>Yes</td>
<td>Married</td>
<td>120K</td>
<td>No</td>
</tr>
<tr>
<td>5</td>
<td>No</td>
<td>Divorced</td>
<td>95K</td>
<td>Yes</td>
</tr>
<tr>
<td>6</td>
<td>No</td>
<td>Married</td>
<td>60K</td>
<td>No</td>
</tr>
<tr>
<td>7</td>
<td>Yes</td>
<td>Divorced</td>
<td>220K</td>
<td>No</td>
</tr>
<tr>
<td>8</td>
<td>No</td>
<td>Single</td>
<td>85K</td>
<td>Yes</td>
</tr>
<tr>
<td>9</td>
<td>No</td>
<td>Married</td>
<td>75K</td>
<td>No</td>
</tr>
</tbody>
</table>

Probability that Refund=Yes is \(3/9\)
Probability that Refund=No is \(6/9\)
Assign record to the left child with weight \(= 3/9\) and to the right child with weight \(= 6/9\)
Classify Instances

New record:

<table>
<thead>
<tr>
<th>Tid</th>
<th>Refund</th>
<th>Marital Status</th>
<th>Taxable Income</th>
<th>Class</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>No</td>
<td>?</td>
<td>85K</td>
<td>?</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>Married</th>
<th>Single</th>
<th>Divorced</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Class=No</td>
<td>3</td>
<td>1</td>
<td>0</td>
<td>4</td>
</tr>
<tr>
<td>Class=Yes</td>
<td>6/9</td>
<td>1</td>
<td>1</td>
<td>2.67</td>
</tr>
<tr>
<td>Total</td>
<td>3.67</td>
<td>2</td>
<td>1</td>
<td>6.67</td>
</tr>
</tbody>
</table>

Probability that Marital Status = Married is 3.67/6.67

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

New record:

<table>
<thead>
<tr>
<th>Tid</th>
<th>Refund</th>
<th>Marital Status</th>
<th>Taxable Income</th>
<th>Class</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>No</td>
<td>?</td>
<td>85K</td>
<td>?</td>
</tr>
</tbody>
</table>

Table:

<table>
<thead>
<tr>
<th>Class</th>
<th>Married</th>
<th>Single</th>
<th>Divorced</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Class=No</td>
<td>3</td>
<td>1</td>
<td>0</td>
<td>4</td>
</tr>
<tr>
<td>Class=Yes</td>
<td>0</td>
<td>15/9</td>
<td>1</td>
<td>2.67</td>
</tr>
<tr>
<td>Total</td>
<td>3</td>
<td>24/9</td>
<td>1</td>
<td>6.67</td>
</tr>
</tbody>
</table>

Probability that Marital Status = Married is 3/6.67
Probability that Marital Status = {Single, Divorced} is 3.67/6.67

Corrected table!
Other Issues

- Data Fragmentation
- Search Strategy
- Expressiveness
- Tree Replication
Data Fragmentation

- Number of instances gets smaller as you traverse down the tree
- Number of instances at the leaf nodes could be too small to make any statistically significant decision
Search Strategy

- Finding an optimal decision tree is NP-hard

- The algorithm presented so far uses a greedy, top-down, recursive partitioning strategy to induce a reasonable solution

- Other strategies?
  - Bottom-up
  - Bi-directional
Expressiveness

- Decision tree provides expressive representation for learning discrete-valued function
  - But they do not generalize well to certain types of Boolean functions
    - Example: parity function:
      - Class = 1 if there is an even number of Boolean attributes with truth value = True
      - Class = 0 if there is an odd number of Boolean attributes with truth value = True
    - For accurate modeling, must have a complete tree

- Not expressive enough for modeling continuous variables
  - Particularly when test condition involves only a single attribute at a time
• Border line between two neighboring regions of different classes is known as decision boundary

• Decision boundary is parallel to axes because test condition involves a single attribute at a time
Oblique Decision Trees

- Test condition may involve multiple attributes
- More expressive representation
- Finding optimal test condition is computationally expensive
Tree Replication

- Same subtree appears in multiple branches
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?
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>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Class=Yes</td>
<td>Class=No</td>
</tr>
<tr>
<td>Class=Yes</td>
<td>a</td>
<td>b</td>
</tr>
<tr>
<td>Class=No</td>
<td>c</td>
<td>d</td>
</tr>
</tbody>
</table>

- a: TP (true positive)
- b: FN (false negative)
- c: FP (false positive)
- d: TN (true negative)
### Metrics for Performance Evaluation...

<table>
<thead>
<tr>
<th>ACTUAL CLASS</th>
<th>PREDICTED CLASS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Class=Yes</td>
<td>Class=Yes</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>d (TN)</td>
</tr>
</tbody>
</table>

- **Most widely-used metric:**

\[
\text{Accuracy} = \frac{a + d}{a + b + c + d} = \frac{TP + TN}{TP + TN + FP + FN}
\]
Limitation of Accuracy

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

- If model predicts everything to be class 0, accuracy is 9990/10000 = 99.9%
  - Accuracy is misleading because model does not detect any class 1 example
**Cost Matrix**

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

\[C(i|j)\]: Cost of misclassifying class \(j\) example as class \(i\)
Computing Cost of Classification

<table>
<thead>
<tr>
<th>Cost Matrix</th>
<th>PREDICTED CLASS</th>
</tr>
</thead>
<tbody>
<tr>
<td>ACTUAL CLASS</td>
<td>C(i</td>
</tr>
<tr>
<td>+</td>
<td>-1</td>
</tr>
<tr>
<td>-</td>
<td>1</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Model M₁</th>
<th>PREDICTED CLASS</th>
</tr>
</thead>
<tbody>
<tr>
<td>ACTUAL CLASS</td>
<td>+</td>
</tr>
<tr>
<td>+</td>
<td>150</td>
</tr>
<tr>
<td>-</td>
<td>60</td>
</tr>
</tbody>
</table>

Accuracy = 80%
Cost = 3910

<table>
<thead>
<tr>
<th>Model M₂</th>
<th>PREDICTED CLASS</th>
</tr>
</thead>
<tbody>
<tr>
<td>ACTUAL CLASS</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 vs Accuracy

<table>
<thead>
<tr>
<th>Count</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>

\[
N = a + b + c + d
\]

Accuracy is proportional to cost if
1. \(C(\text{Yes}|\text{No})=C(\text{No}|\text{Yes}) = q\)
2. \(C(\text{Yes}|\text{Yes})=C(\text{No}|\text{No}) = p\)

\[
\text{Accuracy} = \frac{a + d}{N}
\]

\[
\text{Cost} = p \times (a + d) + q \times (b + c)
\]

\[
\begin{aligned}
&= p \times (a + d) + q \times (N - a - d) \\
&= q \times N - (q - p) \times (a + d) \\
&= N \times [q - (q - p) \times \text{Accuracy}]
\end{aligned}
\]
Cost-Sensitive Measures

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

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

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

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

\[ \text{Weighted Accuracy} = \frac{w_1 a + w_4 d}{w_1 a + w_2 b + w_3 c + w_4 d} \]
ROC (Receiver Operating Characteristic)

- Developed in 1950s for signal detection theory to analyze noisy signals
  - Characterize the trade-off between positive hits and false alarms
- ROC curve plots TP (on the y-axis) against FP (on the x-axis)
- Performance of each classifier represented as a point on the ROC curve
  - changing the threshold of algorithm, sample distribution or cost matrix changes the location of the point
ROC Curve

- 1-dimensional data set containing 2 classes (positive and negative)
- any points located at $x > t$ is classified as positive
At threshold \( t \):

- TP = 0.5, FN = 0.5, FP = 0.12, FN = 0.88

- 1-dimensional data set containing 2 classes (positive and negative)
- any points located at \( x > t \) is classified as positive
ROC Curve

(TP,FP):
- (0,0): declare everything to be negative class
- (1,1): declare everything to be positive class
- (1,0): 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: $\text{Area} = 1$
  - Random guess: $\text{Area} = 0.5$
How to Construct an ROC curve

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

- Use classifier that produces posterior probability for each test instance P(+|A)

- Sort the instances according to P(+|A) in decreasing order

- Apply threshold at each unique value of P(+|A)

- Count the number of TP, FP, TN, FN at each threshold

- TP rate, TPR = TP/(TP+FN)

- FP rate, FPR = FP/(FP + TN)
How to construct an ROC curve

<table>
<thead>
<tr>
<th>Class</th>
<th>+</th>
<th>-</th>
<th>+</th>
<th>-</th>
<th>-</th>
<th>-</th>
<th>+</th>
<th>-</th>
<th>-</th>
<th>+</th>
<th>+</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.25</td>
<td>0.43</td>
<td>0.53</td>
<td>0.76</td>
<td>0.85</td>
<td>0.85</td>
<td>0.85</td>
<td>0.87</td>
<td>0.93</td>
<td>0.95</td>
<td>1.00</td>
</tr>
<tr>
<td>TP</td>
<td>5</td>
<td>4</td>
<td>4</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>2</td>
<td>2</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>FP</td>
<td>5</td>
<td>5</td>
<td>4</td>
<td>4</td>
<td>3</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>TN</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>4</td>
<td>5</td>
<td>5</td>
<td>5</td>
</tr>
<tr>
<td>FN</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>5</td>
<td>5</td>
<td>5</td>
</tr>
<tr>
<td>TPR</td>
<td>1</td>
<td>0.8</td>
<td>0.8</td>
<td>0.6</td>
<td>0.6</td>
<td>0.6</td>
<td>0.6</td>
<td>0.4</td>
<td>0.4</td>
<td>0.2</td>
<td>0</td>
</tr>
<tr>
<td>FPR</td>
<td>1</td>
<td>1</td>
<td>0.8</td>
<td>0.8</td>
<td>0.6</td>
<td>0.4</td>
<td>0.2</td>
<td>0.2</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Threshold >=

ROC Curve:
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?
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
Methods of Estimation

- **Holdout**
  - 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
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
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?
Test of Significance

Given two models:
- Model $M_1$: accuracy = 85%, tested on 30 instances
- Model $M_2$: accuracy = 75%, tested on 5000 instances

Can we say $M_1$ is better than $M_2$?
- How much confidence can we place on accuracy of $M_1$ and $M_2$?
- Can the difference in performance measure be explained as a result of random fluctuations in the test set?
Confidence Interval for Accuracy

- Prediction can be regarded as a Bernoulli trial
  - A Bernoulli trial has 2 possible outcomes
  - Possible outcomes for prediction: correct or wrong
  - Collection of Bernoulli trials has a Binomial distribution:
    - \( x \sim \text{Bin}(N, p) \) \( x \): number of correct predictions
    - e.g.: Toss a fair coin 50 times, how many heads would turn up?
      Expected number of heads = \( N \times p = 50 \times 0.5 = 25 \)

- Given \( x \) (# of correct predictions) or equivalently, \( \text{acc}=x/N \), and \( N \) (# of test instances),

  Can we predict \( p \) (true accuracy of model)?
Confidence Interval for Accuracy

- For large test sets (N > 30),
  - acc has a normal distribution with mean p and variance p(1-p)/N

\[
P\left(Z_{\frac{\alpha}{2}} < \frac{\text{acc} - p}{\sqrt{p(1-p)/N}} < Z_{1-\frac{\alpha}{2}} \right) = 1 - \alpha
\]

- Confidence Interval for p:

\[
p = \frac{2 \times N \times \text{acc} + Z_{\frac{\alpha}{2}}^2 \pm \sqrt{Z_{\frac{\alpha}{2}}^2 + 4 \times N \times \text{acc} - 4 \times N \times \text{acc}^2}}{2(N + Z_{\frac{\alpha}{2}}^2)}
\]
Consider a model that produces an accuracy of 80% when evaluated on 100 test instances:

- N=100, acc = 0.8
- Let 1-\(\alpha\) = 0.95 (95% confidence)
- From probability table, \(Z_{\alpha/2}=1.96\)

<table>
<thead>
<tr>
<th>N</th>
<th>50</th>
<th>100</th>
<th>500</th>
<th>1000</th>
<th>5000</th>
</tr>
</thead>
<tbody>
<tr>
<td>p(lower)</td>
<td>0.670</td>
<td>0.711</td>
<td>0.763</td>
<td>0.774</td>
<td>0.789</td>
</tr>
<tr>
<td>p(upper)</td>
<td>0.888</td>
<td>0.866</td>
<td>0.833</td>
<td>0.824</td>
<td>0.811</td>
</tr>
</tbody>
</table>
Comparing Performance of 2 Models

Given two models, say $M_1$ and $M_2$, which is better?

- $M_1$ is tested on $D_1$ (size=$n_1$), found error rate = $e_1$
- $M_2$ is tested on $D_2$ (size=$n_2$), found error rate = $e_2$
- Assume $D_1$ and $D_2$ are independent
- If $n_1$ and $n_2$ are sufficiently large, then

$$e_1 \sim N(\mu_1, \sigma_1)$$
$$e_2 \sim N(\mu_2, \sigma_2)$$

- Approximate:

$$\hat{\sigma}_i = \frac{e_i (1-e_i)}{n_i}$$
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To test if performance difference is statistically significant: \( d = e_1 - e_2 \)
- \( d \sim \mathcal{N}(d_t, \sigma_t) \) where \( d_t \) is the true difference
- Since \( D_1 \) and \( D_2 \) are independent, their variance adds up:

\[
\sigma_t^2 = \sigma_1^2 + \sigma_2^2 \approx \hat{\sigma}_1^2 + \hat{\sigma}_2^2
\]

\[
= \frac{e_1(1-e_1)}{n_1} + \frac{e_2(1-e_2)}{n_2}
\]

- At \((1-\alpha)\) confidence level, \( d_t = d \pm Z_{\alpha/2} \hat{\sigma}_t \)
An Illustrative Example

- Given: $M_1: n_1 = 30, e_1 = 0.15$
- $M_2: n_2 = 5000, e_2 = 0.25$
- $d = |e_2 - e_1| = 0.1$ (2-sided test)

\[
\hat{\sigma}_d = \frac{0.15(1-0.15)}{30} + \frac{0.25(1-0.25)}{5000} = 0.0043
\]

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

\[
d_t = 0.100 \pm 1.96 \times \sqrt{0.0043} = 0.100 \pm 0.128
\]

=> Interval contains 0 => difference may not be statistically significant
Comparing Performance of 2 Algorithms

● Each learning algorithm may produce k models:
  – L1 may produce M11, M12, …, M1k
  – L2 may produce M21, M22, …, M2k

● If models are generated on the same test sets D1, D2, …, Dk (e.g., via cross-validation)
  – For each set: compute \( d_j = e_{1j} - e_{2j} \)
  – \( d_j \) has mean \( d_t \) and variance \( \sigma_t \)
  – Estimate:
    \[
    \hat{\sigma}_t^2 = \frac{\sum_{j=1}^{k} (d_j - \bar{d})^2}{k(k-1)}
    \]
    \[
    d_t = d + t \left[ 1 - \alpha, k-1 \right] \hat{\sigma}_t
    \]