Data Mining
Practical Machine Learning Tools and Techniques

Slides for Chapter 3 of Data Mining by I. H. Witten, E. Frank and M. A. Hall
Input: Concepts, instances, attributes

- Terminology
- What’s a concept?
  - Classification, association, clustering, numeric prediction
- What’s in an example?
  - Relations, flat files, recursion
- What’s in an attribute?
  - Nominal, ordinal, interval, ratio
- Preparing the input
  - ARFF, attributes, missing values, getting to know data
Components of the input:

- **Concepts**: kinds of things that can be learned
  - Aim: intelligible and operational concept description

- **Instances**: the individual, independent examples of a concept
  - Note: more complicated forms of input are possible

- **Attributes**: measuring aspects of an instance
  - We will focus on nominal and numeric ones
What’s a concept?

- **Styles of learning:**
  - Classification learning: predicting a discrete class
  - Association learning: detecting associations between features
  - Clustering: grouping similar instances into clusters
  - Numeric prediction: predicting a numeric quantity

- **Concept:** thing to be learned
- **Concept description:** output of learning scheme
Classification learning

- Example problems: weather data, contact lenses, irises, labor negotiations
- Classification learning is *supervised*
  - Scheme is provided with actual outcome
- Outcome is called the *class* of the example
- Measure success on fresh data for which class labels are known (*test data*)
- In practice success is often measured subjectively
Association learning

• Can be applied if no class is specified and any kind of structure is considered “interesting”

• Difference to classification learning:
  ♦ Can predict any attribute’s value, not just the class, and more than one attribute’s value at a time
  ♦ Hence: far more association rules than classification rules
  ♦ Thus: constraints are necessary
    • Minimum coverage and minimum accuracy
Clustering

- Finding groups of items that are similar
- Clustering is *unsupervised*
  - The class of an example is not known
- Success often measured subjectively

<table>
<thead>
<tr>
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<th>Sepal width</th>
<th>Petal length</th>
<th>Petal width</th>
<th>Type</th>
</tr>
</thead>
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<td>5.1</td>
<td>3.5</td>
<td>1.4</td>
<td>0.2</td>
<td>Iris setosa</td>
</tr>
<tr>
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<td>4.9</td>
<td>3.0</td>
<td>1.4</td>
<td>0.2</td>
<td>Iris setosa</td>
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<td>...</td>
</tr>
<tr>
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<td>3.2</td>
<td>4.7</td>
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<tr>
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<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
</tbody>
</table>

Iris virginica
Numeric prediction

- Variant of classification learning where “class” is numeric (also called “regression”)
- Learning is supervised
  - Scheme is being provided with target value
- Measure success on test data

<table>
<thead>
<tr>
<th>Outlook</th>
<th>Temperature</th>
<th>Humidity</th>
<th>Windy</th>
<th>Play-time</th>
</tr>
</thead>
<tbody>
<tr>
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<td>High</td>
<td>False</td>
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<td>Hot</td>
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<td>True</td>
<td>0</td>
</tr>
<tr>
<td>Overcast</td>
<td>Hot</td>
<td>High</td>
<td>False</td>
<td>55</td>
</tr>
<tr>
<td>Rainy</td>
<td>Mild</td>
<td>Normal</td>
<td>False</td>
<td>40</td>
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<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
</tbody>
</table>
What’s in an example?

- **Instance**: specific type of example
  - Thing to be classified, associated, or clustered
  - Individual, independent example of target concept
  - Characterized by a predetermined set of attributes

- **Input to learning scheme**: set of instances/dataset
  - Represented as a single relation/flat file

- **Rather restricted form of input**
  - No relationships between objects

- **Most common form in practical data mining**
A family tree

Peter M = Peggy F

Steven M Graham M Pam F = Ian M Pippa F

Ray M

Brian M

Anna F Nikki F
Family tree represented as a table

<table>
<thead>
<tr>
<th>Name</th>
<th>Gender</th>
<th>Parent1</th>
<th>parent2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peter</td>
<td>Male</td>
<td>?</td>
<td>?</td>
</tr>
<tr>
<td>Peggy</td>
<td>Female</td>
<td>?</td>
<td>?</td>
</tr>
<tr>
<td>Steven</td>
<td>Male</td>
<td>Peter</td>
<td>Peggy</td>
</tr>
<tr>
<td>Graham</td>
<td>Male</td>
<td>Peter</td>
<td>Peggy</td>
</tr>
<tr>
<td>Pam</td>
<td>Female</td>
<td>Peter</td>
<td>Peggy</td>
</tr>
<tr>
<td>Ian</td>
<td>Male</td>
<td>Grace</td>
<td>Ray</td>
</tr>
<tr>
<td>Pippa</td>
<td>Female</td>
<td>Grace</td>
<td>Ray</td>
</tr>
<tr>
<td>Brian</td>
<td>Male</td>
<td>Grace</td>
<td>Ray</td>
</tr>
<tr>
<td>Anna</td>
<td>Female</td>
<td>Pam</td>
<td>Ian</td>
</tr>
<tr>
<td>Nikki</td>
<td>Female</td>
<td>Pam</td>
<td>Ian</td>
</tr>
</tbody>
</table>
The “sister-of” relation

<table>
<thead>
<tr>
<th>First person</th>
<th>Second person</th>
<th>Sister of?</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peter</td>
<td>Peggy</td>
<td>No</td>
</tr>
<tr>
<td>Peter</td>
<td>Steven</td>
<td>No</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>Steven</td>
<td>Peter</td>
<td>No</td>
</tr>
<tr>
<td>Steven</td>
<td>Graham</td>
<td>No</td>
</tr>
<tr>
<td>Steven</td>
<td>Pam</td>
<td>Yes</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>Ian</td>
<td>Pippa</td>
<td>Yes</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>Anna</td>
<td>Nikki</td>
<td>Yes</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>Nikki</td>
<td>Anna</td>
<td>Yes</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>First person</th>
<th>Second person</th>
<th>Sister of?</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steven</td>
<td>Pam</td>
<td>Yes</td>
</tr>
<tr>
<td>Graham</td>
<td>Pam</td>
<td>Yes</td>
</tr>
<tr>
<td>Ian</td>
<td>Pippa</td>
<td>Yes</td>
</tr>
<tr>
<td>Brian</td>
<td>Pippa</td>
<td>Yes</td>
</tr>
<tr>
<td>Anna</td>
<td>Nikki</td>
<td>Yes</td>
</tr>
<tr>
<td>Nikki</td>
<td>Anna</td>
<td>Yes</td>
</tr>
</tbody>
</table>

*All the rest* No

Closed-world assumption
### A full representation in one table

| First person |  | Second person |  |
|--------------|-------------------------------|-------------------------------|
| **Name**     | **Gender** | **Parent1** | **Parent2** | **Name** | **Gender** | **Parent1** | **Parent2** | **Sister of?** |
| Steven Graham | Male       | Peter      | Peggy      | Pam       | Female     | Peter      | Peggy      | Yes          |
| Ian          | Male       | Grace      | Ray        | Pippa     | Female     | Grace      | Ray        | Yes          |
| Brian        | Male       | Grace      | Ray        | Pippa     | Female     | Grace      | Ray        | Yes          |
| Anna         | Female     | Pam        | Ian        | Nikki     | Female     | Pam        | Ian        | Yes          |
| Nikki        | Female     | Pam        | Ian        | Anna      | Female     | Pam        | Ian        | Yes          |

*All the rest*

If second person’s gender = female and first person’s parent = second person’s parent then sister-of = yes
Generating a flat file

- Process of flattening called “denormalization”
  - Several relations are joined together to make one
- Possible with any finite set of finite relations
- Problematic: relationships without pre-specified number of objects
  - Example: concept of *nuclear-family*
- Denormalization may produce spurious regularities that reflect structure of database
  - Example: “supplier” predicts “supplier address”
## The “ancestor-of” relation

<table>
<thead>
<tr>
<th>First person</th>
<th></th>
<th></th>
<th>Second person</th>
<th></th>
<th></th>
<th>Ancestor of?</th>
</tr>
</thead>
<tbody>
<tr>
<td>Name</td>
<td>Gender</td>
<td>Parent1</td>
<td>Parent2</td>
<td>Name</td>
<td>Gender</td>
<td>Parent1</td>
</tr>
<tr>
<td>Peter</td>
<td>Male</td>
<td>?</td>
<td>?</td>
<td>Steven</td>
<td>Male</td>
<td>Peter</td>
</tr>
<tr>
<td>Peter</td>
<td>Male</td>
<td>?</td>
<td>?</td>
<td>Pam</td>
<td>Female</td>
<td>Peter</td>
</tr>
<tr>
<td>Peter</td>
<td>Male</td>
<td>?</td>
<td>?</td>
<td>Anna</td>
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<td>Pam</td>
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<tr>
<td>Peter</td>
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<td>?</td>
<td>?</td>
<td>Nikki</td>
<td>Female</td>
<td>Pam</td>
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<tr>
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<td>Female</td>
<td>Peter</td>
<td>Peggy</td>
<td>Nikki</td>
<td>Female</td>
<td>Pam</td>
</tr>
<tr>
<td>Grace</td>
<td>Female</td>
<td>?</td>
<td>?</td>
<td>Ian</td>
<td>Male</td>
<td>Grace</td>
</tr>
<tr>
<td>Grace</td>
<td>Female</td>
<td>?</td>
<td>?</td>
<td>Nikki</td>
<td>Female</td>
<td>Pam</td>
</tr>
</tbody>
</table>

*Other positive examples here*

*All the rest*

<table>
<thead>
<tr>
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<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th>No</th>
</tr>
</thead>
</table>

Data Mining: Practical Machine Learning Tools and Techniques (Chapter 2)
Recursion

- Infinite relations require recursion

  If person1 is a parent of person2
  then person1 is an ancestor of person2

  If person1 is a parent of person2
  and person2 is an ancestor of person3
  then person1 is an ancestor of person3

- Appropriate techniques are known as “inductive logic programming”
  - (e.g. Quinlan’s FOIL)
  - Problems: (a) noise and (b) computational complexity
Multi-instance Concepts

• Each individual example comprises a set of instances
  ♦ All instances are described by the same attributes
  ♦ One or more instances within an example may be responsible for its classification
• Goal of learning is still to produce a concept description
• Important real world applications
  ♦ e.g. drug activity prediction
What’s in an attribute?

- Each instance is described by a fixed predefined set of features, its “attributes”
- But: number of attributes may vary in practice
  - Possible solution: “irrelevant value” flag
- Related problem: existence of an attribute may depend of value of another one
- Possible attribute types (“levels of measurement”):
  - Nominal, ordinal, interval and ratio
Nominal quantities

- Values are distinct symbols
  - Values themselves serve only as labels or names
  - *Nominal* comes from the Latin word for name
- Example: attribute “outlook” from weather data
  - Values: “sunny”, “overcast”, and “rainy”
- No relation is implied among nominal values (no ordering or distance measure)
- Only equality tests can be performed
Ordinal quantities

- Impose order on values
- But: no distance between values defined
- Example:
  attribute “temperature” in weather data
    - Values: “hot” > “mild” > “cool”
- Note: addition and subtraction don’t make sense
- Example rule:
  \[ \text{temperature} < \text{hot} \implies \text{play} = \text{yes} \]
- Distinction between nominal and ordinal not always clear (e.g. attribute “outlook”)
Interval quantities

- Interval quantities are not only ordered but measured in fixed and equal units.
- Example 1: attribute “temperature” expressed in degrees Fahrenheit.
- Example 2: attribute “year”.
- Difference of two values makes sense.
- Sum or product doesn’t make sense.
  - Zero point is not defined!
Ratio quantities

- Ratio quantities are ones for which the measurement scheme defines a zero point
- Example: attribute “distance”
  - Distance between an object and itself is zero
- Ratio quantities are treated as real numbers
  - All mathematical operations are allowed
- But: is there an “inherently” defined zero point?
  - Answer depends on scientific knowledge (e.g. Fahrenheit knew no lower limit to temperature)
Attribute types used in practice

- Most schemes accommodate just two levels of measurement: nominal and ordinal
- Nominal attributes are also called “categorical”, “enumerated”, or “discrete”
  - But: “enumerated” and “discrete” imply order
- Special case: dichotomoy (“boolean” attribute)
- Ordinal attributes are called “numeric”, or “continuous”
  - But: “continuous” implies mathematical continuity
Metadata

- Information about the data that encodes background knowledge
- Can be used to restrict search space
- Examples:
  - Dimensional considerations
    (i.e. expressions must be dimensionally correct)
  - Circular orderings
    (e.g. degrees in compass)
  - Partial orderings
    (e.g. generalization/specialization relations)
Preparing the input

- Denormalization is not the only issue
- Problem: different data sources (e.g. sales department, customer billing department, …)
  - Differences: styles of record keeping, conventions, time periods, data aggregation, primary keys, errors
  - Data must be assembled, integrated, cleaned up
  - “Data warehouse”: consistent point of access
- External data may be required (“overlay data”)
- Critical: type and level of data aggregation
The ARFF format

% ARFF file for weather data with some numeric features
%
@relation weather

@attribute outlook {sunny, overcast, rainy}
@attribute temperature numeric
@attribute humidity numeric
@attribute windy {true, false}
@attribute play? {yes, no}

@data
sunny, 85, 85, false, no
sunny, 80, 90, true, no
overcast, 83, 86, false, yes
...
Additional attribute types

• ARFF supports *string* attributes:

  ```
  @attribute description string
  ```

  ✷ Similar to nominal attributes but list of values is not pre-specified

• It also supports *date* attributes:

  ```
  @attribute today date
  ```

  ✷ Uses the ISO-8601 combined date and time format `yyyy-MM-dd-THH:mm:ss`
Relational attributes

- Allow multi-instance problems to be represented in ARFF format
  - The value of a relational attribute is a *separate* set of instances

```plaintext
@attribute bag relational
  @attribute outlook { sunny, overcast, rainy }
  @attribute temperature numeric
  @attribute humidity numeric
  @attribute windy { true, false }
@end bag
```

- Nested attribute block gives the structure of the referenced instances
% Multiple instance ARFF file for the weather data
%
@relation weather

@attribute bag_ID { 1, 2, 3, 4, 5, 6, 7 }
@attribute bag relational
    @attribute outlook {sunny, overcast, rainy}
    @attribute temperature numeric
    @attribute humidity numeric
    @attribute windy {true, false}
    @attribute play? {yes, no}
@end bag

@data
1, "sunny, 85, 85, false\nsunny, 80, 90, true", no
2, "overcast, 83, 86, false\nrainy, 70, 96, false", yes
...
Sparse data

- In some applications most attribute values in a dataset are zero
  - E.g.: word counts in a text categorization problem
- ARFF supports sparse data

\[
\begin{align*}
0, &
26, 0, 0, 0, 0, 63, 0, 0, 0, "class A" \\
0, &
0, 0, 0, 42, 0, 0, 0, 0, 0, "class B" \\
\{1 &
26, 6 63, 10 "class A"\} \\
\{3 &
42, 10 "class B"\}
\end{align*}
\]

- This also works for nominal attributes (where the first value corresponds to “zero”)
Attribute types

- Interpretation of attribute types in ARFF depends on learning scheme
  - Numeric attributes are interpreted as
    - ordinal scales if less-than and greater-than are used
    - ratio scales if distance calculations are performed (normalization/standardization may be required)
  - Instance-based schemes define distance between nominal values (0 if values are equal, 1 otherwise)
- Integers in some given data file: nominal, ordinal, or ratio scale?
Nominal vs. ordinal

• Attribute “age” nominal

If age = young and astigmatic = no
   and tear production rate = normal
   then recommendation = soft

If age = pre-presbyopic and astigmatic = no
   and tear production rate = normal
   then recommendation = soft

• Attribute “age” ordinal
  (e.g. “young” < “pre-presbyopic” < “presbyopic”)

If age ≤ pre-presbyopic and astigmatic = no
   and tear production rate = normal
   then recommendation = soft
Missing values

- Frequently indicated by out-of-range entries
  - Types: unknown, unrecorded, irrelevant
  - Reasons:
    - malfunctioning equipment
    - changes in experimental design
    - collation of different datasets
    - measurement not possible

- Missing value may have significance in itself (e.g. missing test in a medical examination)
  - Most schemes assume that is not the case: “missing” may need to be coded as additional value
Inaccurate values

- Reason: data has not been collected for mining it
- Result: errors and omissions that don’t affect original purpose of data (e.g. age of customer)
- Typographical errors in nominal attributes $\Rightarrow$ values need to be checked for consistency
- Typographical and measurement errors in numeric attributes $\Rightarrow$ outliers need to be identified
- Errors may be deliberate (e.g. wrong zip codes)
- Other problems: duplicates, stale data
Getting to know the data

• Simple visualization tools are very useful
  ♦ Nominal attributes: histograms (Distribution consistent with background knowledge?)
  ♦ Numeric attributes: graphs (Any obvious outliers?)
• 2-D and 3-D plots show dependencies
• Need to consult domain experts
• Too much data to inspect? Take a sample!