Data Mining

Practical Machine Learning Tools and Techniques

Slides for Chapter 3, Output: knowledge representation

of *Data Mining* by I. H. Witten, E. Frank,
M. A. Hall and C. J. Pal

Output: Knowledge representation

- Tables
- Linear models
- Trees
- Rules
- Classification rules
- Association rules
- Rules with exceptions
- More expressive rules
- Instance-based representation
- Clusters

Output: representing structural patterns

- Many different ways of representing patterns
  - Decision trees, rules, instance-based, …
- Also called “knowledge” representation
- Representation determines inference method
- Understanding the output is the key to understanding the underlying learning methods
- Different types of output for different learning problems (e.g., classification, regression, …)

Decision tables

- Simplest way of representing output:
  - Use the format that is used for representing the input!
- Decision table for the weather problem:

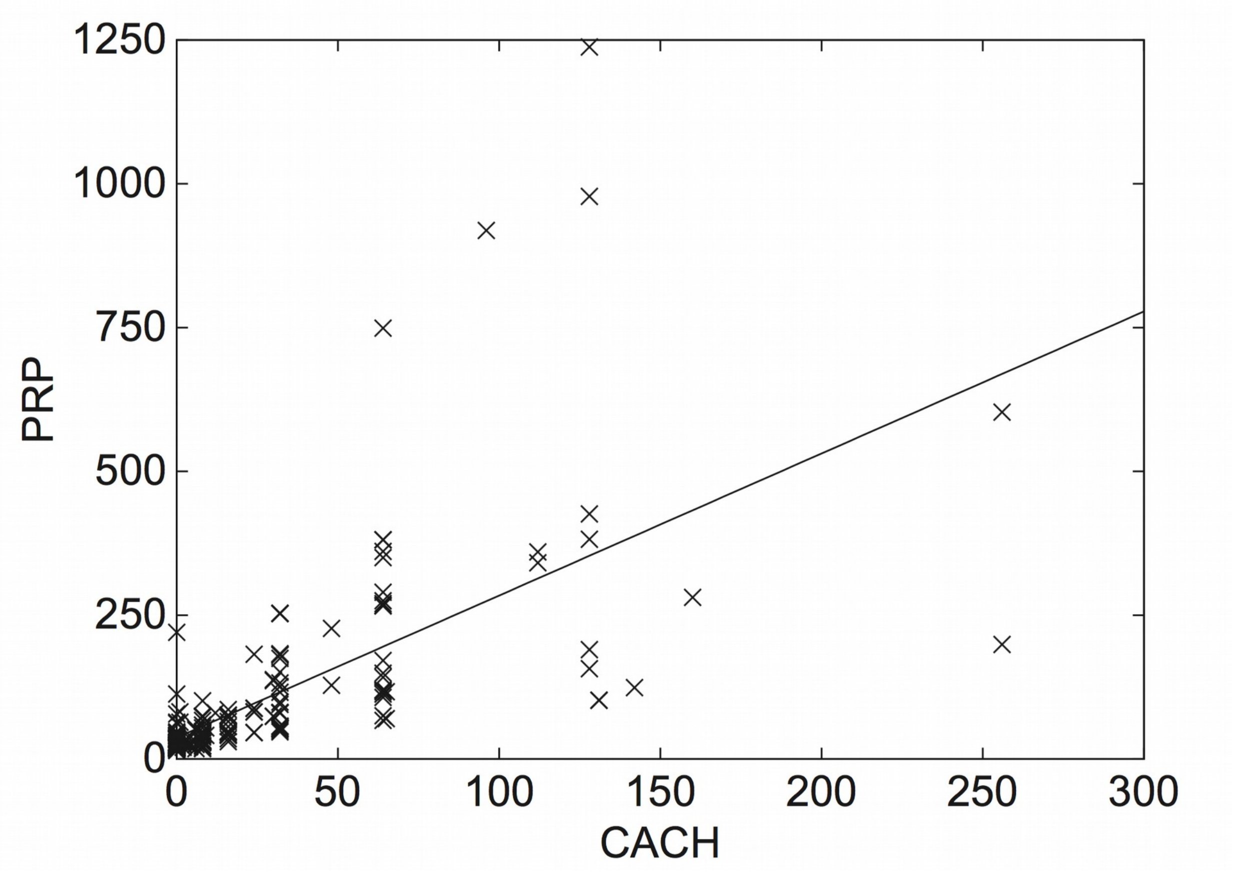
Outlook	Humidity	Play
Sunny	High	No
Sunny	Normal	Yes
Overcast	High	Yes
Overcast	Normal	Yes
Rainy	High	No
Rainy	Normal	No

- Main problem: selecting the right attributes

Linear models

- Another simple representation
- Traditionally primarily used for regression:
  - Inputs (attribute values) and output are all numeric
- Output is the sum of the weighted input attribute values
- The trick is to find good values for the weights
- There are different ways of doing this, which we will consider later; the most famous one is to minimize the squared error

A linear regression function for the CPU performance data

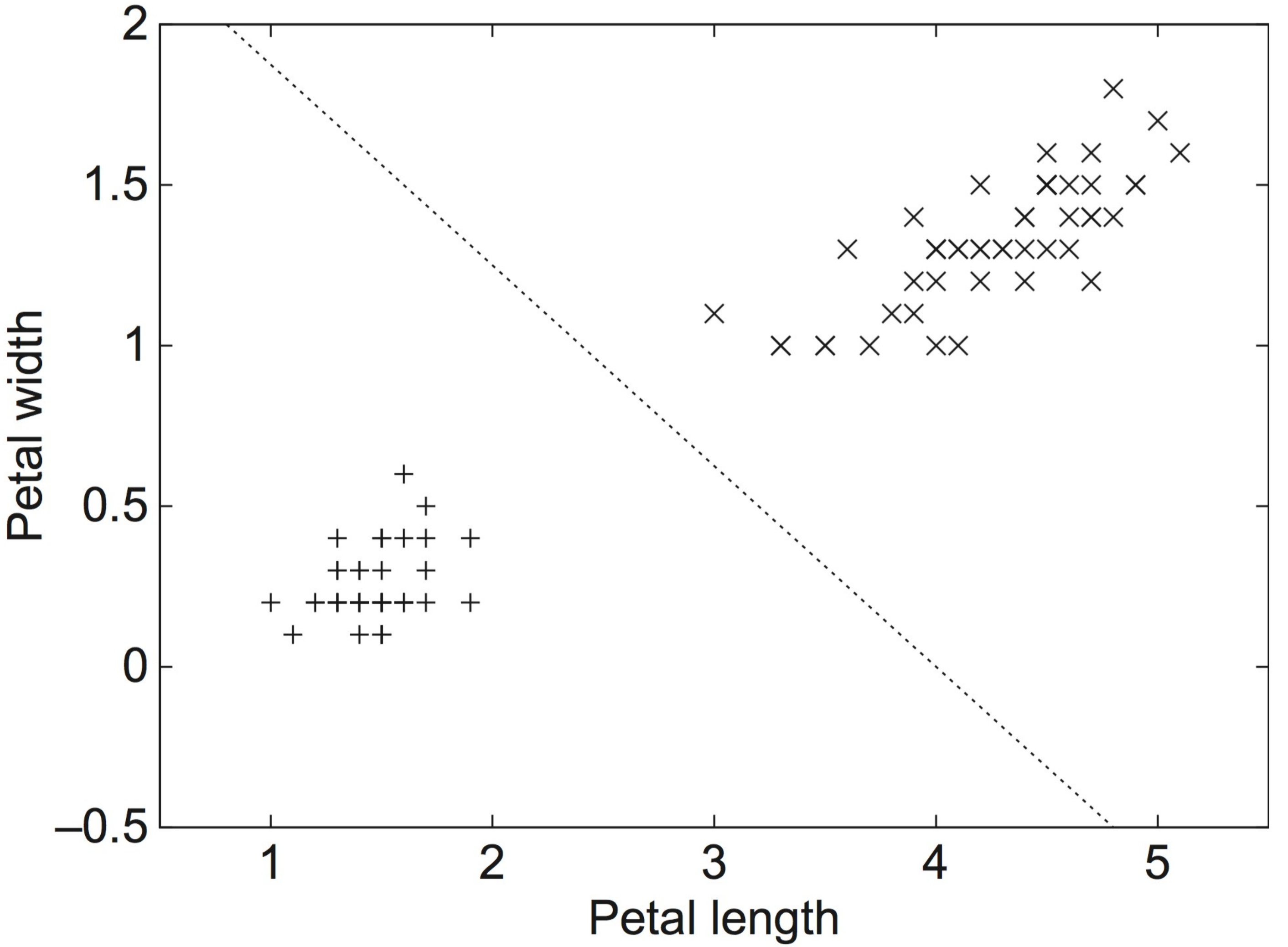


PRP = 37.06 + 2.47CACH

Linear models for classification

- Binary classification
- Line *separates* the two classes
  - Decision boundary - defines where the decision changes from one class value to the other
- Prediction is made by plugging in observed values of the attributes into the expression
  - Predict one class if output $\geqq 0$, and the other class if output < 0
- Boundary becomes a high-dimensional plane (*hyperplane*) when there are multiple attributes

Separating setosas from versicolors



`2.0 – 0.5PETAL-LENGTH – 0.8PETAL-WIDTH = 0`

Decision trees

- “Divide-and-conquer” approach produces tree
- Nodes involve testing a particular attribute
- Usually, attribute value is compared to constant
- Other possibilities:
  - Comparing values of two attributes
  - Using a function of one or more attributes
- Leaves assign classification, set of classifications, or probability distribution to instances
- Unknown instance is routed down the tree

Nominal and numeric attributes in trees

- Nominal:
  number of children usually equal to number values
  => attribute won’t get tested more than once
- Other possibility: division into two subsets
- Numeric:
  test whether value is greater or less than constant
  => attribute may get tested several times
  - Other possibility: three-way split (or multi-way split)
    - Integer: *less than, equal to, greater than*
    - Real: *below, within, above*

Missing values

- Does absence of value have some significance?
- Yes => "missing" is a separate value
- No => "missing" must be treated in a special way
  - Solution A: assign instance to most popular branch
  - Solution B: split instance into pieces
    - Pieces receive weight according to fraction of training instances that go down each branch
    - Classifications from leave nodes are combined using the weights that have percolated to them

Trees for numeric prediction

- *Regression*: the process of computing an expression that predicts a numeric quantity
- *Regression tree*: "decision tree" where each leaf predicts a numeric quantity
  - Predicted value is average value of training instances that reach the leaf
- *Model tree*: "regression tree" with linear regression models at the leaf nodes
  - Linear patches approximate continuous function

Linear regression for the CPU data

PRP =

– 56.1

+ 0.049 MYCT

+ 0.015 MMIN

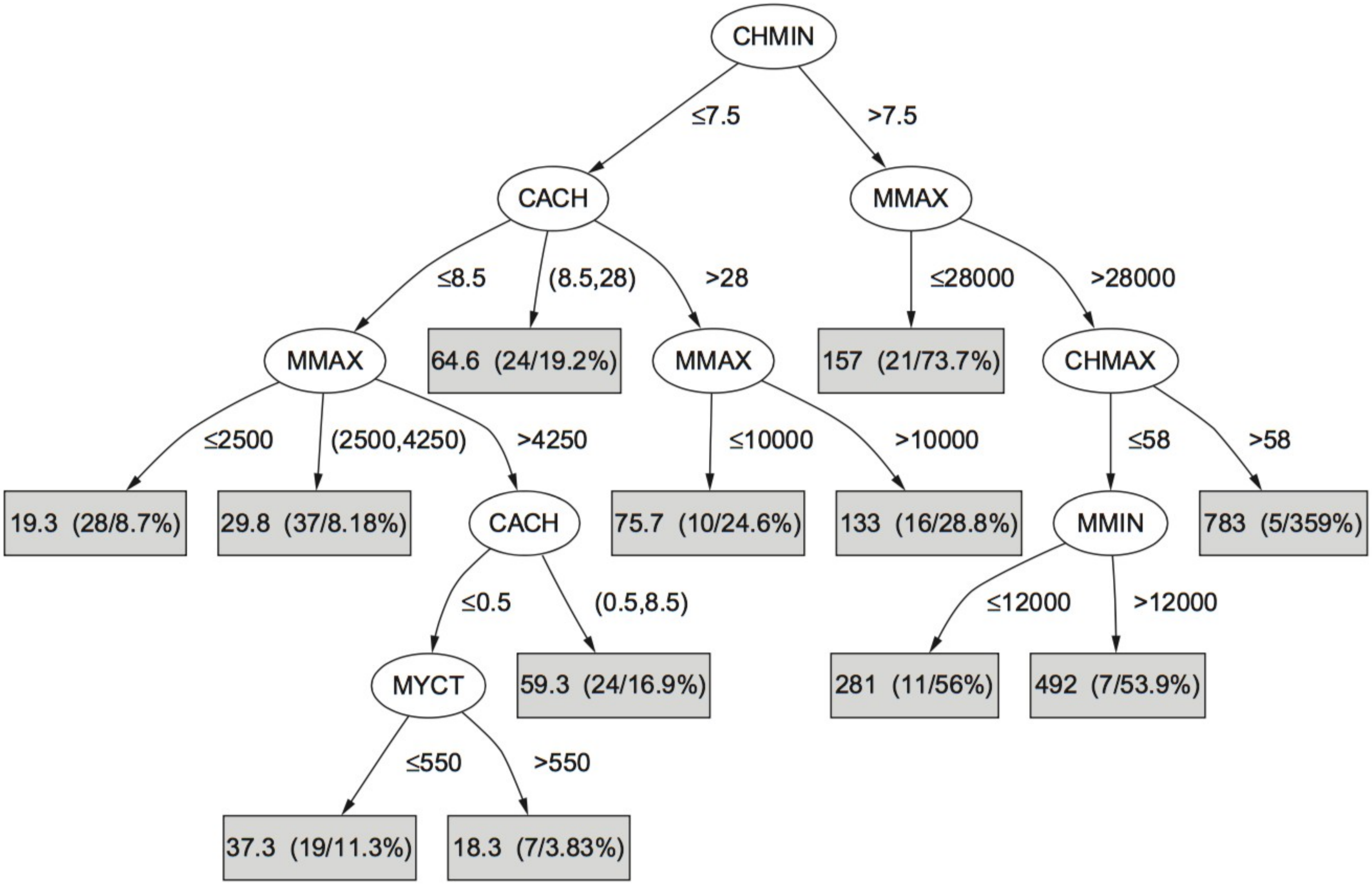
+ 0.006 MMAX

+ 0.630 CACH

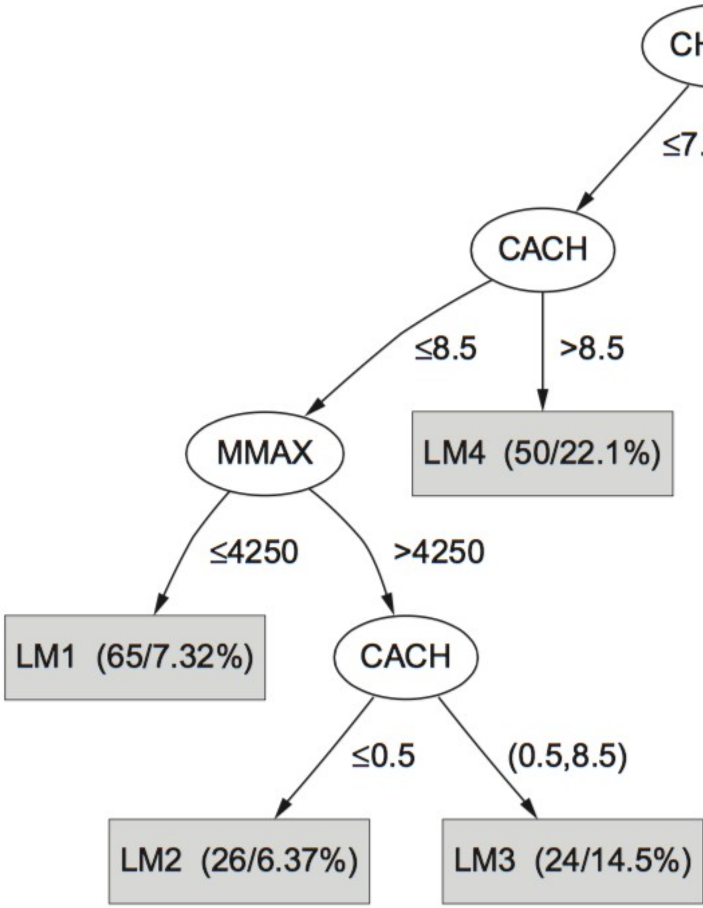
– 0.270 CHMIN

+ 1.46 CHMAX

Regression tree for the CPU data



Model tree for the CPU data



LM1 PRP = 8.29 + 0.004 MMAX + 2.77 CHMIN

LM2 PRP = 20.3 + 0.004 MMIN – 3.99 CHMIN
+ 0.946 CHMAX

LM3 PRP = 38.1 + 0.012 MMIN

LM4 PRP = 19.5 + 0.002 MMAX + 0.698 CACH
+ 0.969 CHMAX

LM5 PRP = 285 1.46 MYCT + 1.02 CACH
– 9.39 CHMIN

LM6 PRP = – 65.8 + 0.03 MMIN – 2.94 CHMIN
+ 4.98 CHMAX

Classification rules

- Popular alternative to decision trees
- *Antecedent* (pre-condition): a series of tests (just like the tests at the nodes of a decision tree)
- Tests are usually logically ANDed together (but may also be general logical expressions)
- *Consequent* (conclusion): classes, set of classes, or probability distribution assigned by rule
- Individual rules are often logically ORed together
    - Conflicts arise if different conclusions apply

From trees to rules

- Easy: converting a tree into a set of rules
  - One rule for each leaf:
    - Antecedent contains a condition for every node on the path from the root to the leaf
    - Consequent is class assigned by the leaf
- Produces rules that are unambiguous
  - Doesn’t matter in which order they are executed
- But: resulting rules are unnecessarily complex
  - Pruning to remove redundant tests/rules

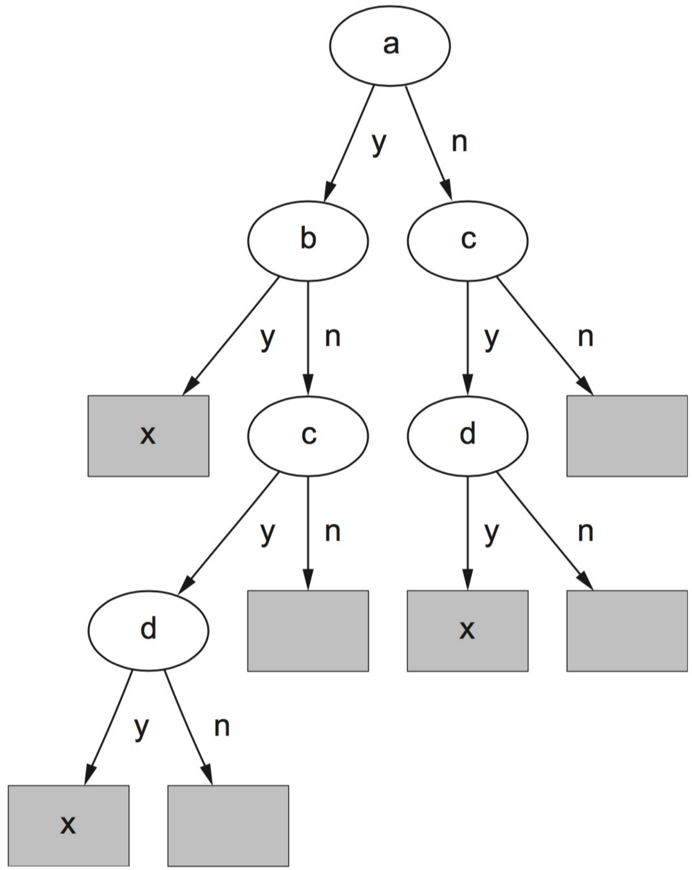
From rules to trees

- More difficult: transforming a rule set into a tree
  - Tree cannot easily express disjunction between rules
- Example: rules which test different attributes

```
If a and b then x
If c and d then x
```

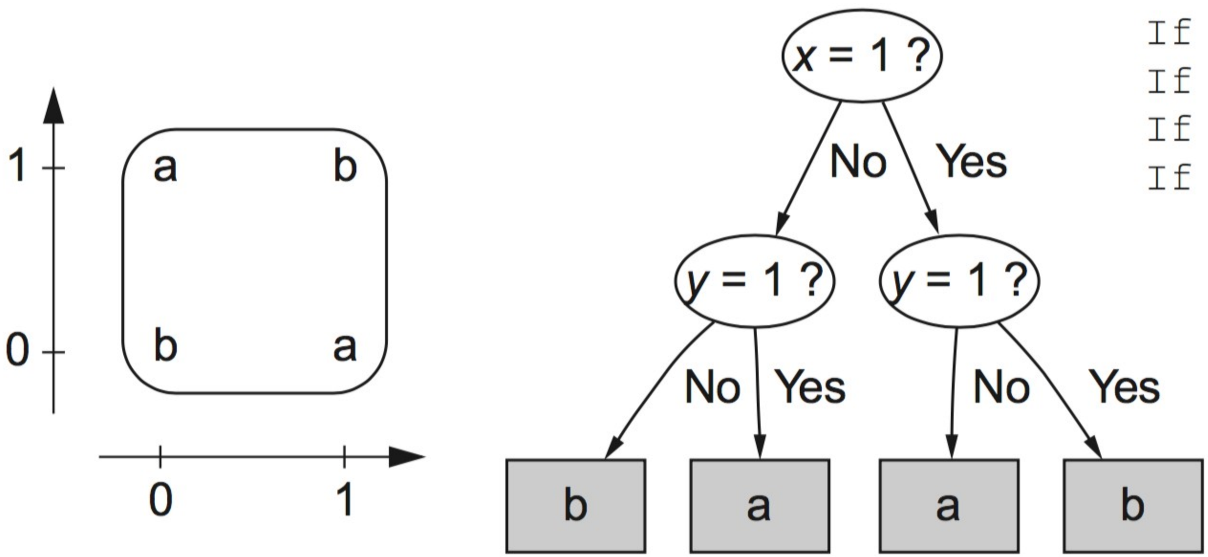
- Symmetry needs to be broken
- Corresponding tree contains identical subtrees (→ “replicated subtree problem”)

A tree for a simple disjunction




```
If a and b then x
If c and d then x
```

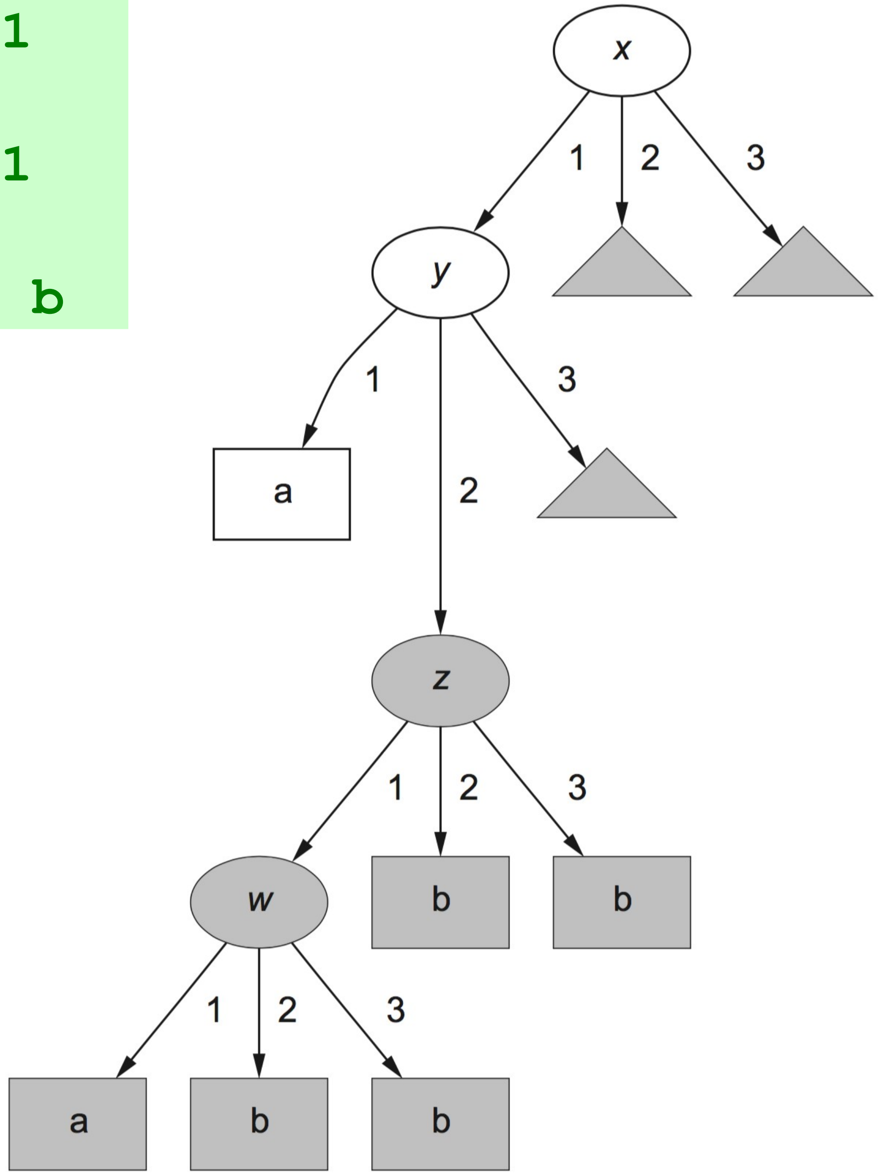
The exclusive-or problem



If x=1 and y=0 then class = a
If x=0 and y=1 then class = a
If x=0 and y=0 then class = b
If x=1 and y=1 then class = b

A tree with a replicated subtree

```
If x = 1 and y = 1
   then class = a
If z = 1 and w = 1
   then class = a
Otherwise class = b
```



“Nuggets” of knowledge

- Are rules independent pieces of knowledge? (It seems easy to add a rule to an existing rule base.)
- Problem: ignores how rules are executed
- Two ways of executing a rule set:
  - Ordered set of rules (“decision list”)
    - Order is important for interpretation
  - Unordered set of rules
    - Rules may overlap and lead to different conclusions for the same instance

Interpreting rules

- What if two or more rules conflict?
  - Give no conclusion at all?
  - Go with rule that is most popular on training data?
  - …
- What if no rule applies to a test instance?
  - Give no conclusion at all?
  - Go with class that is most frequent in training data?
  - …

Special case: Boolean class

- Assumption: if instance does not belong to class “yes”, it belongs to class “no”
- Trick: only learn rules for class “yes” and use default rule for “no”

```
If x = 1 and y = 1 then class = a
If z = 1 and w = 1 then class = a
Otherwise class = b
```

- Order of rules is not important. No conflicts!
- Rule can be written in *disjunctive normal form*

Association rules

- Association rules…
  - … can predict any attribute and combinations of attributes
  - … are not intended to be used together as a set
- Problem: immense number of possible associations
  - Output needs to be restricted to show only the most predictive associations
    → only those with high *support* and high *confidence*

Support and confidence of a rule

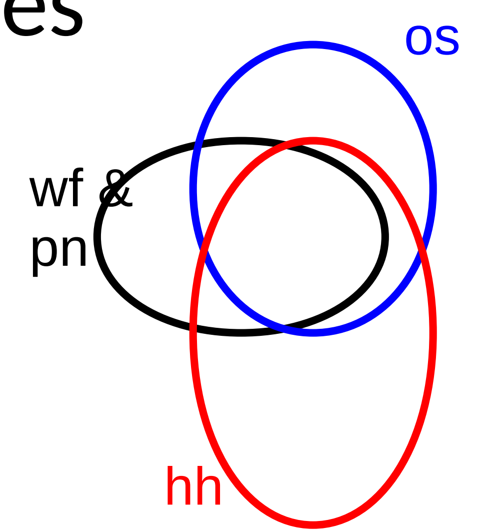
- Support: number of instances predicted correctly
- Confidence: number of correct predictions, as proportion of all instances that rule applies to
- Example: 4 cool days with normal humidity

```
If temperature = cool then humidity = normal
```

→ Support = 4, confidence = 100%

- Normally: minimum support and confidence pre-specified (e.g. 58 rules with support $\geqq$ 2 and confidence $\geqq$ 95% for weather data)

Interpreting association rules



- Interpretation is not obvious:

```
If windy = false and play = no then
outlook = sunny and humidity = high
```

is *not* the same as

```
If windy = false and play = no then outlook = sunny
If windy = false and play = no then humidity = high
```

- It means that the following also holds:

```
If humidity = high and windy = false and play = no
    then outlook = sunny
```

Rules with exceptions

- Idea: allow rules to have *exceptions*
- Example: rule for iris data

```
If petal-length ≥ 2.45 and petal-length < 4.45 then Iris-versicolor
```

- New instance:

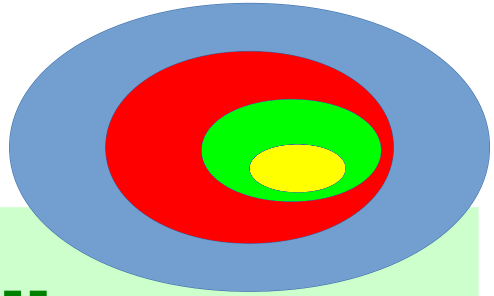
Sepal Length	Sepal Width	Petal Length	Petal Width	Type
5.1	3.5	2.6	0.2	?

- Modified rule:

```
If petal-length ≥ 2.45 and petal-length < 4.45 then Iris-versicolor
  EXCEPT if petal-width < 1.0 then Iris-setosa
```

A more complex example

- Exceptions to exceptions to exceptions …



```
default: Iris-setosa
except if petal-length ≥ 2.45 and petal-length < 5.355
          and petal-width < 1.75
       then Iris-versicolor
            except if petal-length >= 4.95 and petal-width < 1.55
                   then Iris-virginica
                   else if sepal-length < 4.95 and sepal-width ≥ 2.45
                        then Iris-virginica
       else if petal-length >= 3.35
            then Iris-virginica
                 except if petal-length < 4.85 and sepal-length < 5.95
                        then Iris-versicolor
```

Advantages of using exceptions

- Rules can be updated incrementally
  - Easy to incorporate new data
  - Easy to incorporate domain knowledge
- People often think in terms of exceptions
- Each conclusion can be considered just in the context of rules and exceptions that lead to it
  - Locality property is important for understanding large rule sets
  - “Normal” rule sets do not offer this advantage

More on exceptions

- `Default X except if C then Y`

  is logically equivalent to

  `if C then Y else X`

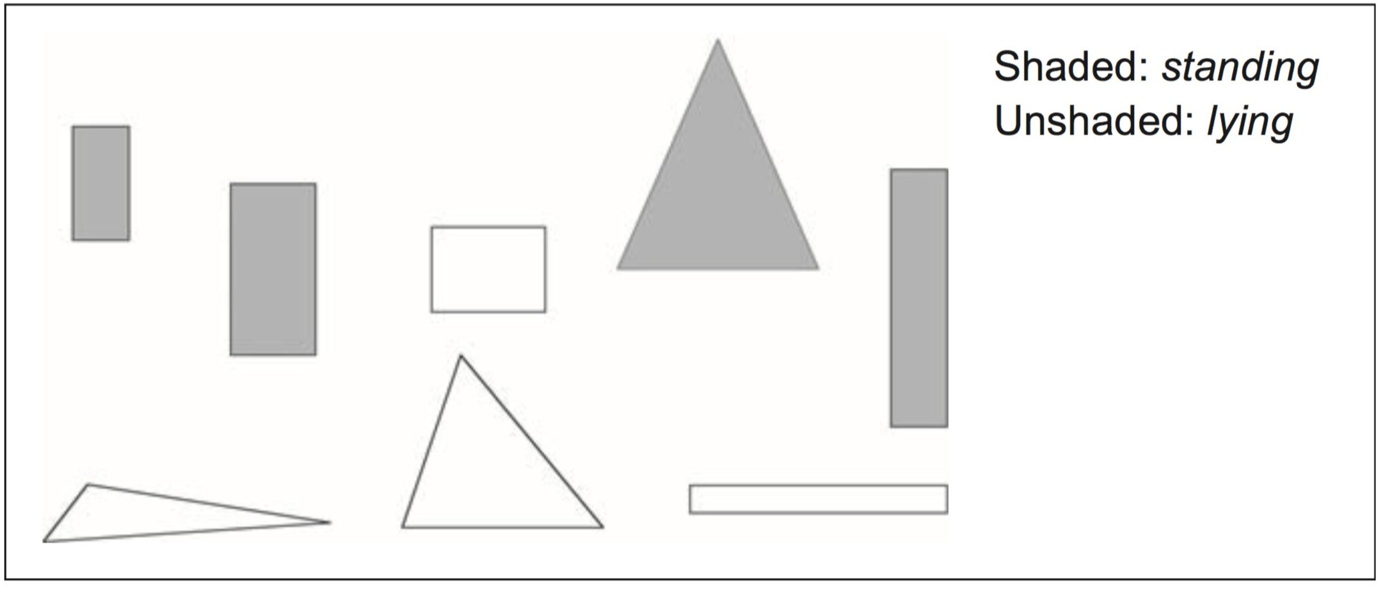
  (where the "else" specifies what the "default" does)
- But: exceptions offer a psychological advantage
  - Assumption: defaults and tests early on apply more widely than exceptions further down
  - Exceptions reflect special cases

Rules involving relations

- So far: all rules involved comparing an attribute-value to a constant (e.g. temperature < 45)
- These rules are called “propositional” because they have the same expressive power as propositional logic
- What if problem involves relationships between examples (e.g. family tree problem from above)?
  - Can’t be expressed with propositional rules
  - More expressive representation required

The shapes problem

- Target concept: *standing up*
- Shaded: *standing*
  Unshaded: *lying*



A propositional solution

Width	Height	Sides	Class
2	4	4	Standing
3	6	4	Standing
4	3	4	Lying
7	8	3	Standing
7	6	3	Lying
2	9	4	Standing
9	1	4	Lying
10	2	3	Lying

```
If width ≥ 3.5 and height < 7.0
   then lying
If height ≥ 3.5 then standing
```

Using relations between attributes

- Comparing attributes with each other enables rules like this:

```
If width > height then lying
If height > width then standing
```

- This description generalizes better to new data
- Standard relations: =, <, >
- But: searching for relations between attributes can be costly
- Simple solution: add extra attributes (e.g., a binary attribute "*is width < height?*")

Rules with variables

- Using variables and multiple relations:

```
If height_and_width_of(x,h,w) and h > w
   then standing(x)
```

- The top of a tower of blocks is standing:

```
If height_and_width_of(x,h,w) and h > w
      and is_top_of(y,x)
   then standing(x)
```

- The whole tower is standing:

```
If is_top_of(x,z) and
   height_and_width_of(z,h,w) and h > w
   and is_rest_of(x,y)and standing(y)
   then standing(x)
If empty(x) then standing(x)
```

- Recursive definition!

Inductive logic programming

- Recursive definition can be seen as logic program
- Techniques for learning logic programs stem from the area of “inductive logic programming” (ILP)
- But: recursive definitions are hard to learn
  - Also: few practical problems require recursion
  - Thus: many ILP techniques are restricted to non-recursive definitions to make learning easier

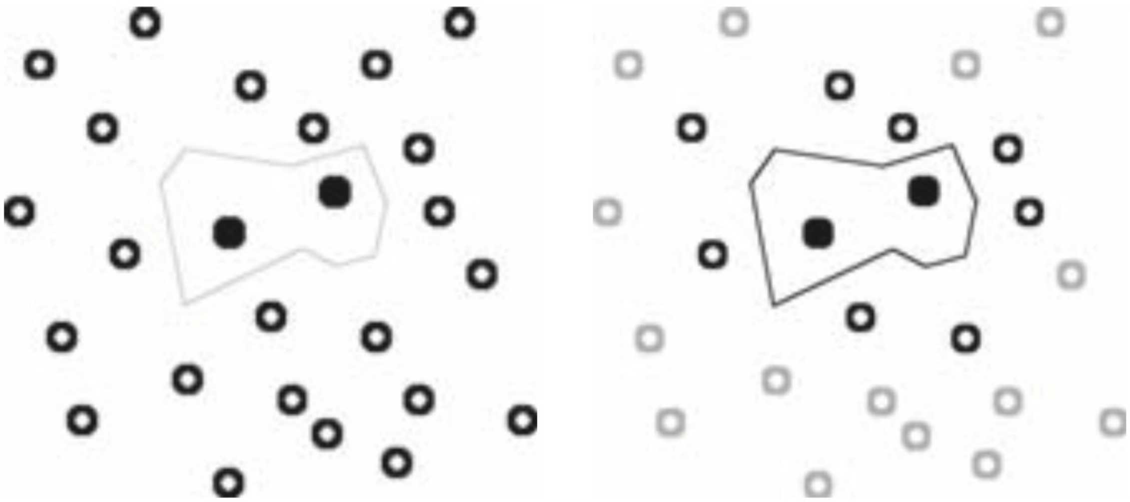
Instance-based representation

- Simplest form of learning: *rote learning*
  - Training instances are searched for instance that most closely resembles new instance
  - The instances themselves represent the knowledge
  - Also called *instance-based* learning
- Similarity function defines what's "learned"
- Instance-based learning is *lazy* learning
- Methods: *nearest-neighbor*, *k-nearest-neighbor*, …

The distance function

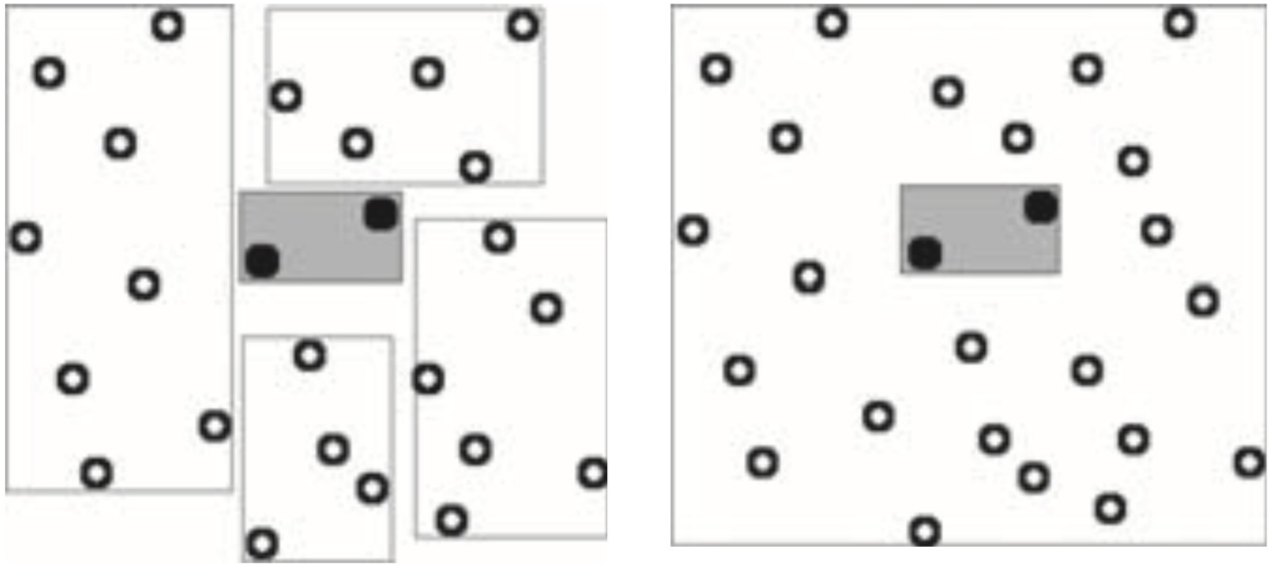
- Simplest case: one numeric attribute
  - Distance is the difference between the two attribute values involved (or a function thereof)
- Several numeric attributes: normally, Euclidean distance is used and attributes are normalized
- Nominal attributes: distance is set to 1 if values are different, 0 if they are equal
- Are all attributes equally important?
  - Weighting the attributes might be necessary

Learning prototypes



- Only those instances involved in a decision need to be stored
- Noisy instances should be filtered out
- Idea: only use *prototypical* examples

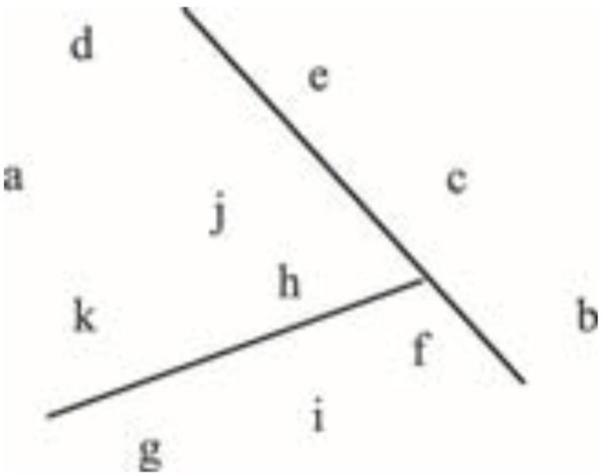
Rectangular generalizations



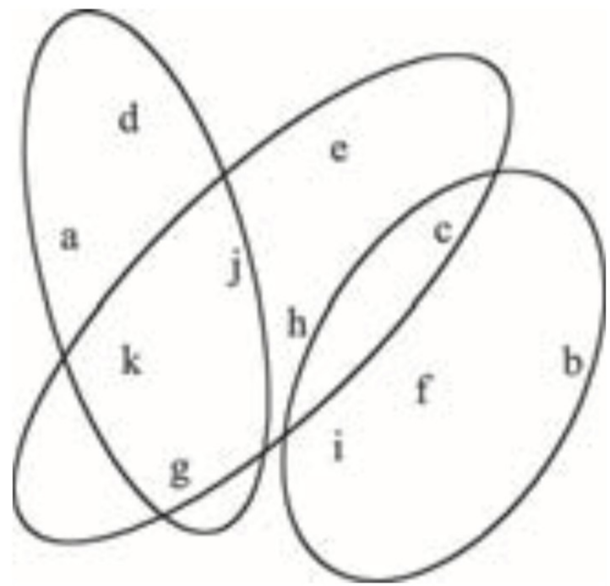
- Nearest-neighbor rule is used outside rectangles
- Rectangles are rules! (But they can be more conservative than “normal” rules, since they impose upper and lower bounds in each dimension.)
- Nested rectangles are rules with exceptions

Representing clusters I

Simple 2-D representation



Venn diagram



Representing clusters II

Probabilistic assignment

	1	2	3
a	0.4	0.1	0.5
b	0.1	0.8	0.1
c	0.3	0.3	0.4
d	0.1	0.1	0.8
e	0.4	0.2	0.4
f	0.1	0.4	0.5
g	0.7	0.2	0.1
h	0.5	0.4	0.1
…			

Dendrogram