Beyond Attribute-Value Data Mining

Lutz Hamel
Dept. of Computer Science and Statistics
University of Rhode Island

What is Data Mining?

Data mining is the application of *machine learning* techniques to large databases in order to extract *hidden knowledge*.

(KDD – Knowledge Discovery in Databases)

What is Machine Learning?

Programs that get better with *experience* given a task and some *performance measure*.

Most common is *inductive learning*, that is learning from a set of positive and negative examples.

- Learning to classify customers
- Learning to recognize spoken words
- Learning to play board games

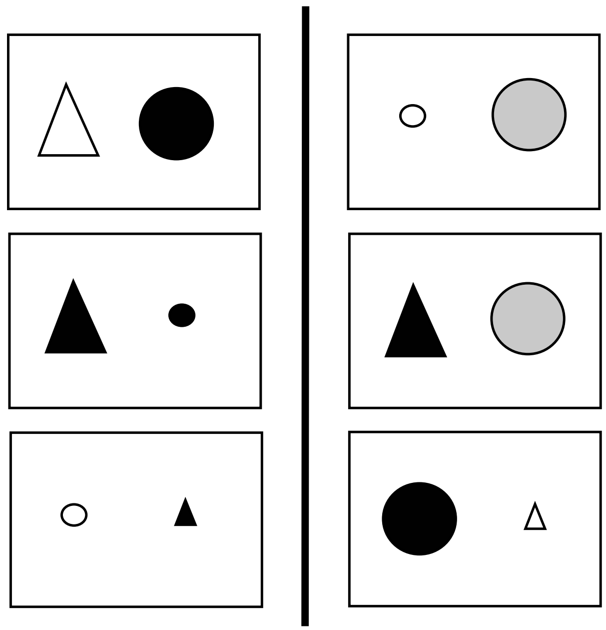
What is Knowledge?

- Structural descriptions of data (transparent)
  - If-then-else rules
  - Decision trees
  - First-order logic theories
- Models of data (non-transparent)
  - Neural networks
  - Clustering (self-organizing maps, k-Means)
  - Naive-Bayes classifiers

Data Mining Today

- Today's data mining tools are "single-table" oriented – *attribute-value oriented.*
- Basic assumption is that objects of a particular problem domain can be represented by a *fixed set* of attributes.

Attribute-Value Data Mining: Classification



ShapeLeft	SizeLeft	ColorLeft	ShapeRight	SizeRight	ColorRight	DiagramPosition
triangle	large	white	circle	large	black	left
triangle	large	black	circle	small	black	left
circle	small	white	triangle	small	black	left
circle	small	white	circle	large	grey	right
triangle	large	black	circle	large	grey	right
circle	large	black	triangle	small	white	right

Attribute-Value Data Mining: Classification

Given:

- A data universe X, here

  $X = ShapeLeft \times SizeLeft \times ColorLeft \times ShapeRight \times SizeRight \times ColorRight$

- A sample set S, where $S \subseteq X$
- A classification function $c\colon X \to \{\text{true, false}\}$, here

  $$DiagramPosition\colon X \to \{\text{left, right}\}$$

- Labeled training examples D, where

  $$D = \{(s, c(s)) | s \in S\}$$

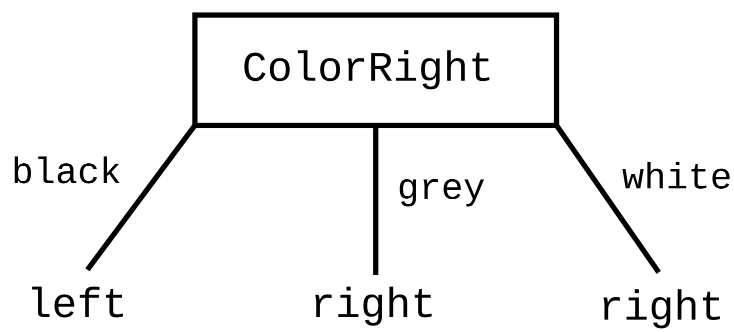
Use D to determine:

- A function or hypothesis c' such that $c'(x) \approx c(x)$ for all $x \in X$.

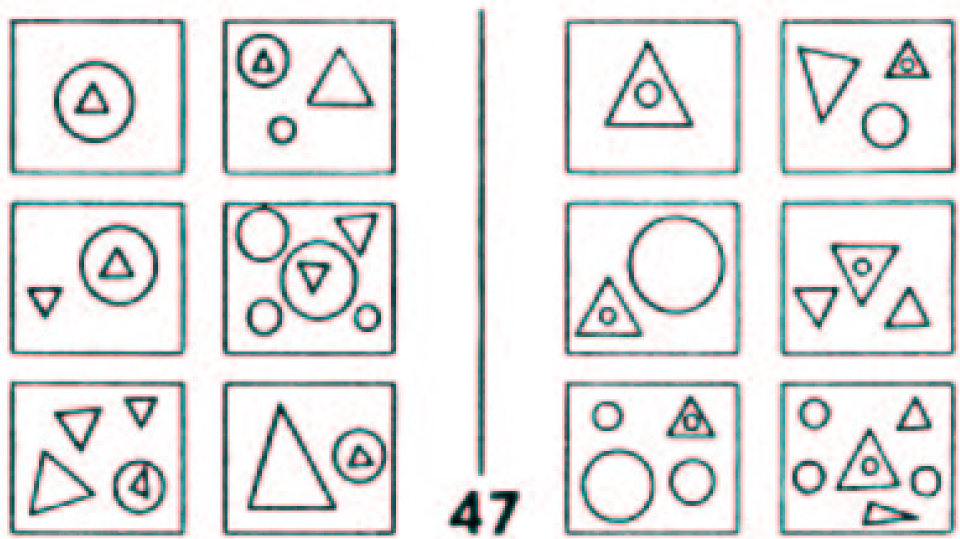
Attribute-Value Data Mining: Decision Trees

- In decision tree learning the hypothesis c' is represented as a tree.
- We can view decision tree learning as a heuristic search over all possible decision trees for the "best" tree.

A decision tree for our diagram problem would look like this:



A More Complicated Problem Domain



Difficult to represent with a fixed set of attributes:

- The scenes do not contain fixed numbers of objects.
- No inherent order of the objects in the scenes – difficult to express relations between objects.

Even if one forces an attribute-value representation – lots of "null" values in the table and exponential explosion of attributes.

First-Order Equational Logic

Equational logic is the logic of substituting equals for equals with algebras as models and term rewriting as the operational semantics.

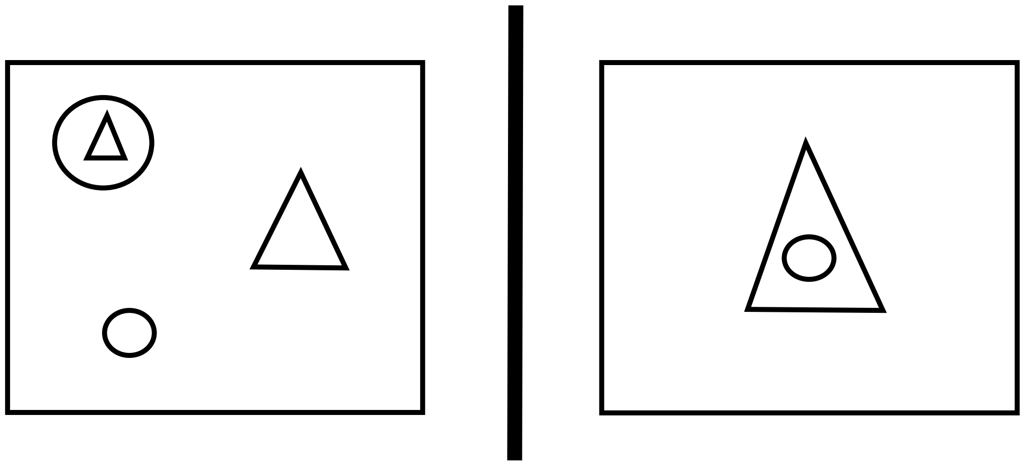
```
theory LIST is
  sort List .
  sort ListElement .
  subsort ListElement < List .

  op _,_ : ListElement List -> List .
  op length : List -> Int .

  var E : ListElement .
  var L : List .

  eq length(E) = 1 .
  eq length(E,L) = 1 + length(L) .
end
```

First-Order Equational Logic



```
theory DIAGRAMS is
     ...
  eq diagram{ size(c1,medium)
              size(c2,small)
              size(t1,small) pointing(t1,up)
              size(t2,medium) pointing(t2,up)
              in(t1,c1) } = left .

  eq diagram{ size(c1,small)
              size(t1,large) pointing(t1,up)
              in(c1,t1) } = right .
end
```

First-Order Equational Logic

- First-order equational logic allows us to describe the diagrams in a very natural way.
- We can easily capture all the important aspects of object existence, characteristics, and relationships.

Why choose Equational Logic as the Representation Language?

- Precise semantics.
- Logical reasoning capabilities.
- Well developed module and type systems.

Deductive vs. Inductive Logic

- In (deductive) logic we deduce specific facts from general theories.
- In inductive logic we induce general theories from specific facts.

$$\begin{tikzcd} \text{Theories} \arrow[r, shift left, "\text{Deduction}"] & \text{Facts} \arrow[l, shift left, "\text{Induction}"] \end{tikzcd}$$

Inductive Equational Logic

- In inductive equational logic we induce equational theories (hypotheses) from equations which represent the facts.
- Inductive equational logic admits the use of domain theories or background knowledge.

$\Rightarrow$ Inductive equational logic allows us to generalize from given facts and background knowledge.

$\Rightarrow$ In this setting we can consider inductive reasoning in equational logic to be *data mining over first-order structures*.

Inductive Equational Logic

Given:

- An observation universe O, here

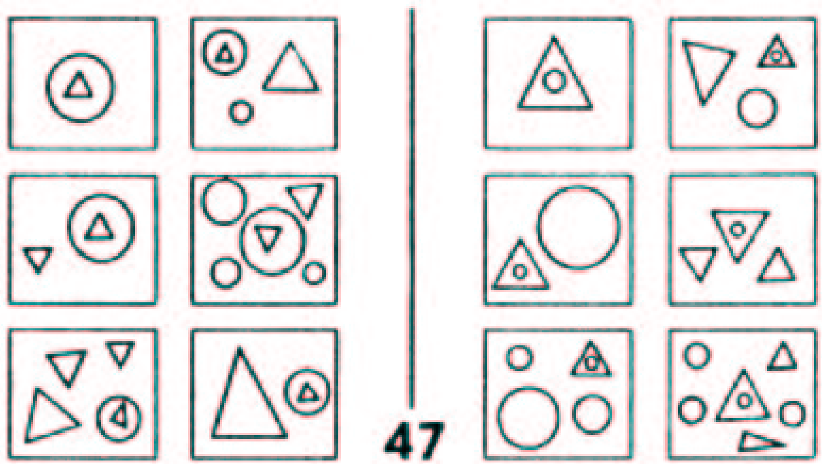
$$O = \{d \,|\, d \text{ is a left or right diagram description}\}.$$

- A fact theory F, where $F \subseteq O$.
- A (possibly empty) background theory B.

Use F and B to determine hypothesis H:

- Use the relation $H \cup B \vdash f$, for all $f \in F$, to estimate an H such that $H \cup B \vdash o$ for all $o \in O$.
- $H \cup B \vdash f$ means fact f is *derivable* from H and B.

Inducing a Hypothesis




```
theory DIAGRAM-HYPOTHESIS is
     ...
  eq diagram{ D } = left
           if outside-is-circle(get-in(D)) and
              inside-is-triangle(get-in(D)) .

  eq diagram{ D } = right
           if outside-is-triangle(get-in(D)) and
              inside-is-circle(get-in(D)) .
end
```

NOTE: the "helper functions" are elements of background theory B.

Implementation of Inductive Equational Logic

- Determining the hypothesis H can be considered a *search* over all possible hypotheses for the "best" hypothesis.
- Typically, the "best" hypothesis is the *shortest* theory from which all the facts in F can be derived – the theory that "explains" all the facts.
- We have implemented an experimental inductive equational logic programming system which utilizes evolutionary search techniques to search the hypotheses space for the "best" hypothesis.
- Evolutionary algorithms perform global searches rather than local, greedy searches, this results in very stable search results in the presence of noise in the fact theories.
- On the down side, evolutionary searches tend to be slow.

Mining Program Observations

- An interesting application of this technology is the mining of program observations or tests.
- Given a set of observations, we can construct a hypothesis that describes the behavior of the program in very concise terms.
- In general, it would be extremely difficult to capture program behavior in an attribute-value approach.

$\Rightarrow$ Reverse Engineering

$\Rightarrow$ Software Testing

Example: Even Predicate

Find a hypothesis describing the behavior of the predicate `even`:

```
theory EVEN-OBSERVATIONS is

  sort Int .
  op 0 : -> Int .
  op s : Int -> Int .
  op even : Int -> Bool .

  eq even(0) = true .
  eq even(s(s(0))) = true .
  eq even(s(s(s(s(0))))) = true .
  eq even(s(0)) = false .
  eq even(s(s(s(0)))) = false .
  eq even(s(s(s(s(s(0)))))) = false .

end
```

Example: Even Predicate

Hypothesis:

```
theory EVEN is

  sort Int .
  op 0 : -> Int .
  op s : Int -> Int .
  op even : Int -> Bool .
  var X : Int .

  eq even(s(s(X))) = even(X) .
  eq even(0) = true .

end
```

Example: Stack

Find a hypothesis describing the behavior of a stack module:

```
theory STACK-OBSERVATIONS is

  sorts Stack Element .
  ops a b c d: -> Element .
  op v : -> Stack .
  op top : Stack -> Element .
  op pop : Stack -> Stack .
  op push : Stack Element -> Stack .

  eq top(push(v,a)) = a .
  eq top(push(push(v,a),b)) = b .
  eq top(push(push(v,b),a)) = a .
  eq top(push(push(v,d),c)) = c .
  eq pop(push(v,a))= v .
  eq pop(push(push(v,a),b)) = push(v,a) .
  eq pop(push(push(v,b),a)) = push(v,b) .
  eq pop(push(push(v,d),c)) = push(v,d) .

end
```

Example: Stack

Hypothesis:

```
theory STACK is

  sorts Stack Element .
  op top : Stack -> Element .
  op pop : Stack -> Stack .
  op push : Stack Element -> Stack .
  var S : Stack .
  var E : Element .

  eq top(push(S,E)) = E .
  eq pop(push(S,E)) = S .

end
```

Summary

- Today's attribute-value data mining tools cannot capture the rich structure inherent in some interesting problem domains.
- Moving from an attribute-value representation to a first-order representation solves many of these representation problems.
- Equational logic is particularly well suited as a representation language due to its concise semantics and its well developed module and type systems.
- Our current, experimental implementation of inductive equational logic uses evolutionary search techniques and tends to be robust even in the presence of noise.
- Next steps include the move to a more efficient implementation based on C++ and the investigation of some large real-world problems.

Relevant Publications

Towards Inductive Equational Logic Programming, Lutz Hamel, submitted for publication, 2003.

Genetic Operators and Inductive Logic Programming: Fisher's Theorem of Natural Selection, Lutz Hamel, in preparation, 2003.

Breeding Algebraic Structures–An Evolutionary Approach To Inductive Equational Logic Programming, Lutz Hamel, GECCO 2002: Proceedings of the Genetic and Evolutionary Computation Conference, 2002, pp 748-755, Morgan Kaufmann Publishers.

Data Mining and Knowledge Discovery with Evolutionary Algorithms, Alex Freitas, 2002, Springer-Verlag.

Relational Data Mining, Sašo Džeroski, Nada Lavrač (eds.), 2001, Springer-Verlag.