# Partially Defined Boolean Functions, Classification, and Logical Analysis of Data 

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based on earlier presentations by Endre Boros

Based on numerous papers by E. Boros, Y. Crama, P.L. Hammer, T. Ibaraki, A. Kogan, K. Makino, etc.

## Outline

- Learning from Examples
- Partially Defined Boolean Functions
- Logical Analysis of Data


## Process of Learning ...

## Data: Examples



## Process of Learning ...



Data: Examples


## Testing:

Test point

## Process of Learning ...

## Data: Examples

Learning

$$
\Rightarrow \cdots \Rightarrow
$$

## Classifier



## Testing:

Test point:

> Trial
> $\Rightarrow \cdots \Rightarrow$

Result


## Process of Learning ...



Common measures of classifier quality involve new data:

- training - test partition, cross validation (assumes distribution of future examples follows that of data)


## Process of Learning ...

## Data: Examples

Classifier

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- training - test partition, cross validation (assumes distribution of future examples follows that of data)
- simulation (assumes knowledge of distribution of future examples)


## Process of Learning ...

## Data: Examples

Classifier

Learning

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\Rightarrow \cdots \Rightarrow
$$



Common measures of classifier quality involve new data:

- training - test partition, cross validation (assumes distribution of future examples follows that of data)
- simulation (assumes knowledge of distribution of future examples)
- clinical trial (done "in the future")

WHAT (ANNOT BE LEARNED FROM EXAMPLES!

"Just a darn minute! - Yesterday you said that $X$ equals two!"

## Some typical examples

- Credit approval. Data: attributes of applicants for credit card vs. decision.
- Customer targeting. Data: attributes of customers vs. decision to buy.
- Medical diagnosis. Data: symptoms or bio-medical features vs. diagnosis.


## Data Sets and Classifiers

Attributes: $\quad A, B, \ldots$ in domains $\mathrm{A}, \mathrm{B}, \ldots$
Data Set: $\quad \mathrm{D}=\left\{\mathbf{X}^{i}=\left(X_{A}^{i}, X_{B}^{i}, \ldots\right) \mid i=1, \ldots, M\right\}$
Class: $\quad c: \mathbf{D} \longrightarrow\{0,1\}$

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We usually expect: $f(\mathbf{X})=c(\mathbf{X})$ for all $\mathbf{X} \in \mathbf{D}$
There may be many classifiers for a same data set.

## A small example

7 patients in the training set with 4 test results for each

|  |  | Test Results |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $x_{1}$ | $x_{2}$ | $x_{3}$ | $x_{4}$ |
| $\mathbb{T}$ |  | 1 | 1 | 0 | 1 |
|  | B | 0 | 1 | 1 | 1 |
|  | C | 1 | 1 | 1 | 0 |
| $\mathbb{F}$ | T | 0 | 0 | 1 | 1 |
|  | U | 1 | 0 | 0 | 1 |
|  | V | 1 | 0 | 1 | 0 |
|  | W | 0 | 1 | 1 | 0 |

## A small example

7 patients in the training set with 4 test results for each

|  | Test Results |  |  |  | Dr. $F$ |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | ID | $x_{1}$ | $x_{2}$ | $x_{3}$ | $x_{4}$ | $\mathrm{x}_{1}+\mathrm{x}_{2}+\mathrm{x}_{3}+\mathrm{x}_{4} \geq 3$ |
| $\mathbb{T}$ | A | 1 | 1 | 0 | 1 | 1 |
|  | B | 0 | 1 | 1 | 1 | 1 |
|  | C | 1 | 1 | 1 | 0 | 1 |
| $\mathbb{F}$ | T | 0 | 0 | 1 | 1 | 0 |
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## A small example

7 patients in the training set with 4 test results for each

|  | Test Results |  |  |  | Dr. F | Dr. G |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | ID | $x_{1}$ | $x_{2}$ | $x_{3}$ | $x_{4}$ | $\mathrm{x}_{1}+\mathrm{x}_{2}+\mathrm{x}_{3}+\mathrm{x}_{4} \geq 3$ | $\mathrm{x}_{1}+2 \mathrm{x}_{2}+\mathrm{x}_{4} \geq 3$ |
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|  | V | 1 | 0 | 1 | 0 | 0 | 0 |
|  | W | 0 | 1 | 1 | 0 | 0 | 0 |


|  | Ms. Y | 1 | 1 | 0 | 0 |  |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
|  | Mr. Z | 1 | 0 | 1 | 1 |  |

## A small example

7 patients in the training set with 4 test results for each

|  | Test Results | Dr. F | Dr. G |  |  |  |  |
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| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
|  | Mr. Z | 1 | 0 | 1 | 1 | $\mathbf{1}$ | 0 |

## Partially Defined Boolean Functions

- Definition
- Support sets
- Patterns
- Theories


## Definitions

Attributes: $V=\{1,2, \ldots, n\}$.

Boolean function: $f:\{0,1\}^{V} \longrightarrow\{0,1\}$.
True vectors of $f: T(f)=\left\{\mathbf{x} \in\{0,1\}^{V} \mid f(\mathbf{x})=1\right\}$.

False vectors of $f: F(f)=\left\{\mathrm{x} \in\{0,1\}^{V} \mid f(\mathrm{x})=0\right\}$.

$$
T(f) \cap F(f)=\emptyset \quad \text { and } \quad T(f) \cup F(f)=\{0,1\}^{V}
$$

## Definitions

A term t is a Boolean function defined by an elementary conjunction

$$
\mathrm{t}(\mathrm{x})=\bigwedge_{j \in P} x_{j} \wedge \bigwedge_{j \in N} \bar{x}_{j}
$$

where $P, N \subseteq V$, and $\bar{x}=1-x$.

The conjunction takes value 1 (or "true") if and only if

$$
x_{j}=1 \text { for all } j \in P \text { and } x_{j}=0 \text { for all } j \in N
$$

The set of true vectors of a term forms a sub-cube of $\{0,1\}^{V}$, and viceversa, every sub-cube, is the set of true vectors of a Boolean function, defined by a unique term.

Sub-cubes and Terms in $\{0,1\}^{3}$


Sub-cubes and Terms in $\{0,1\}^{3}$


## Definitions

Every Boolean function can be represented as a disjunctive normal form (DNF), that is, as a disjunction (OR) of terms (elementary conjunctions):

$$
f(\mathrm{x})=\bigvee_{(P, N) \in E}\left(\bigwedge_{j \in P} x_{j} \wedge \bigwedge_{j \in N} \bar{x}_{j}\right)
$$

where $P, N \subseteq V$, and $\bar{x}=1-x$.

The DNF takes value 1 (or "true") if and only if at least one of its terms takes value 1 .

Geometrically: the set of true vectors of $f$ is covered by a union of subcubes of $\{0,1\}^{V}$.

Boolean functions as DNFs


## Definitions

Training Data: a pair of subsets ( $\mathrm{T}, \mathrm{F}$ ) such that

$$
\mathbf{T} \subseteq\{0,1\}^{V}, \quad \mathrm{~F} \subseteq\{0,1\}^{V}, \quad \text { and } \quad \mathbf{T} \cap \mathbf{F}=\emptyset
$$

We call such a pair (T,F) a partially defined Boolean function (or pdBf in short).

Classifier: a Boolean function $f:\{0,1\}^{V} \longrightarrow\{0,1\}$, which is an extension of (T,F), i.e., for which

$$
\mathbf{T} \subseteq T(f) \quad \text { and } \quad \mathrm{F} \subseteq F(f)
$$

Let $\mathcal{E}(\mathrm{T}, \mathrm{F})$ denote the family of all extensions. Clearly, we have

$$
|\mathcal{E}(\mathrm{T}, \mathrm{~F})|=2^{2^{n}-|\mathrm{T} \cup \mathrm{~F}|}
$$

## What can guide learning?

If $|V|=20$ and $|(T, F)|=1000$, then

$$
|\mathcal{E}(\mathrm{T}, \mathrm{~F})|>2^{1,000,000}
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- Simplicity
- Essential attributes
- Function $f \in \mathcal{E}(\mathbf{T}, \mathbf{F})$
- Representation (DNF, CNF, decision tree, etc.)


## What can guide learning?

If $|V|=20$ and $|(T, F)|=1000$, then

$$
|\mathcal{E}(\mathrm{T}, \mathrm{~F})|>2^{1,000,000}
$$

- Simplicity
- Essential attributes
- Efficient representation (DNF, CNF, decision tree, etc.)
- Justifiability

Note on framework: we mostly speak here of building unspecified models, as opposed to specified models such as regression models (which assume a priori knowledge about the relation between inputs and outputs).

## Building reasonable extensions

Given ( $\mathbf{T}, \mathbf{F}$ ), how can we build a reasonable extension $f \in \mathcal{E}_{T}(\mathbf{T}, \mathbf{F})$ ?

> Many ways....

For example, nearest neiglhbor methods, decision trees, or neural networks build such classifiers.

## Nearest Neighbor classifiers

Define a notion of distance $\rho(X, Y)$ between any two points $X, Y$ in the input space.

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Data: Examples


Test point:

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Data: Examples


Test point:
Result

Closest example

$$
\Rightarrow \cdots \Rightarrow
$$

Nearest Neighbor classifiers

Example in the Boolean case.


Nearest Neighbor classifiers

Example in the Boolean case.

(111) is classified as red (false)
(000) is classified as blue (true)

## Decision Trees for pdBfs



$$
\begin{aligned}
& \mathrm{F}=\{(110),(101)\} \\
& \mathrm{T}=\{(010),(100)\}
\end{aligned}
$$

## Decision Trees for pdBfs



## Decision Trees for pdBfs



## Decision Trees for pdBfs



## Decision Trees for pdBfs



## Decision Trees for pdBfs



Note: (001) is classified differently by NN and by DT

## Linear separator



Decide whether T and F can be separated by a hyperplane.
This is a simple linear programming problem.
Similar to recognizing a weighted majority game.

## Logical Analysis of Data

LAD: Introduced in Crama, Hammer and Ibaraki (1988).

Based on the representation of extensions by DNFs and on selection of

- subsets of relevant variables (support sets)
- relevant terms (patterns)
- relevant disjunctions of terms (theories)


## Partially Defined Boolean Functions

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## Finding Essential Attributes

- Select relevant features.
- Eliminate noise.
- Compress data.


## Relevance and its evaluations

- Well defined for complete systems: an attribute is relevant, if changing its value changes the classification of some situations.
- Measures of relevance are based on counting such situations (with slight variations, e.g., coalitions' power in game theory; voters' influence in voting schemes, etc., Shapley (1954), Chow (1961), Banzhaf (1965), Winder (1971), Kahn, Kalai and Linial (1988), Hammer, Kogan and Rohtblum (2000))
- These definitions cannot be easily extended to incomplete data sets in a consistent way, see e.g., John, Kohavi and Pfleger (1994).


## Eliminate Noise: What is it?

- A random attribute?
- An irrelevant attribute?
- An (almost) constant attribute?
- A dependent attribute?


## Data compression

- The simpler, the better! - "Occam's Razor:"

Theories built on smaller attribute sets, generalize better. Blumer,Ehrenfeucht,Haussler and Warmuth (1987)

- Decreases the computational complexity of finding and using a classifier.
- Decreases the cost of future data collection.


## Feature selection based on separating power

Find a small (smallest, if possible) subset of the attributes which distinguishes the sets $\mathbb{T}$ and $\mathbb{F}$. Such a subset is called a support set.

Crama, Hammer and Ibaraki (1988).

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|  | 1 | 0 | 0 | 1 | 1 | 0 | 0 | 0 | 0 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $\mathbb{T}$ | 1 | 1 | 1 | 1 | 0 | 0 | 1 | 0 | 0 |
|  | 0 | 1 | 1 | 0 | 1 | 1 | 1 | 0 | 0 |
|  | 1 | 0 | 1 | 0 | 0 | 1 | 1 | 1 | 1 |
| $\mathbb{F}$ | 0 | 0 | 1 | 1 | 1 | 1 | 0 | 0 | 1 |
|  | 0 | 1 | 0 | 1 | 1 | 1 | 1 | 1 | 1 |
|  | 0 | 0 | 0 | 0 | 1 | 1 | 0 | 1 | 0 |
|  | 1 | 1 | 0 | 0 | 0 | 0 | 0 | 1 | 0 |

## Feature selection based on separating power

Find a small (smallest, if possible) subset of the attributes which distinguishes the sets $\mathbb{T}$ and $\mathbb{F}$. Such a subset is called a support set.

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| $\mathbb{T}$ | $\mathbb{1}$ | 0 | 0 | $\mathbb{1}$ | 1 | 0 | 0 | 0 | 0 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
|  | $\mathbb{1}$ | 1 | 1 | $\mathbb{1}$ | 0 | 0 | $\mathbb{1}$ | 0 | 0 |
|  | 0 | 1 | 1 | 0 | 1 | 1 | $\mathbb{1}$ | 0 | 0 |
|  | $\mathbb{1}$ | 0 | 1 | 0 | 0 | 1 | $\mathbb{1}$ | 1 | 1 |
| $\mathbb{F}$ | 0 | 0 | 1 | $\mathbb{1}$ | 1 | 1 | 0 | 0 | 1 |
|  | 0 | 1 | 0 | $\mathbb{1}$ | 1 | 1 | $\mathbb{1}$ | 1 | 1 |
|  | 0 | 0 | 0 | 0 | 1 | 1 | 0 | 1 | 0 |
|  | $\mathbb{1}$ | 1 | 0 | 0 | 0 | 0 | 0 | 1 | 0 |

## Feature selection based on separating power

Finding a smallest support set is NP-hard.

Algorithmic Approaches to find a small(est) support set:

- complete enumeration: FOCUS (Almuallim and Dietterich, 1994)...
- greedy search: Rel-FSS (Bell and Wang, 2000) ...
- computing relevance index: (Kira and Rendell, 1992) ...
- etc., ... over 40 references in the past decade.

Note that decision trees automatically select a (small) support set.

## Feature selection based on separating power

A set covering model to find a small(est) support set:

- associate a 0-1 variable $a_{i}$ with each attribute $A_{i}$
- for every pair of false example $X$ and true example $Y$, express that at least one of the attributes differentiating $X$ from $Y$ must be chosen:

$$
\text { for all } X \in \mathbb{F}, Y \in \mathbb{T}, \quad \sum_{i: x_{i} \neq y_{i}} a_{i} \geq 1
$$

- minimize $\sum_{i} a_{i}$.

This model can be solved either exactly, or heuristically.

# Feature selection based on separating power 

## Questions to clarify

Why a small(est) feature set??

## Which one??

How to measure the quality of a support set?

## Why a small(est) feature set??

## Which one??

- Typically, there are many support sets of different sizes.


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- The larger the data set, the more surprising to have a small support set.


## Why a small(est) feature set??

## Which one??

- Typically, there are many support sets of different sizes.
- The larger the data set, the less likely to have a small support set.
- The larger the data set, the more surprising to have a small support set.
- OUR SURPRISE $\approx$ INFORMATION IN DATA


## The Good News

Boros, Horiyama, Ibaraki, Makino and Yagiura, 2003
Distribution of Support Sets in Randomly Generated Data

|  | $K$ | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
| :--- | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: |
| $n=10$ | $L B$ | 22 | 34 | 46 | 60 | 66 |  |  |  |
|  | $U B$ | 60 | 58 | 68 | 80 | 84 |  |  |  |
| $n=15$ | $L B$ | 26 | 42 | 62 | 90 | 126 | 176 | 238 | 312 |
|  | $U B$ | $\infty$ | 82 | 98 | 126 | 164 | 214 | 278 | 352 |
| $n=20$ | $L B$ | 30 | 46 | 70 | 102 | 150 | 216 | 306 | 432 |
|  | $U B$ | $\infty$ | 102 | 116 | 150 | 198 | 268 | 364 | 494 |
| $n=40$ | $L B$ | 34 | 54 | 84 | 126 | 198 | 278 | 408 | 594 |
|  | $U B$ | $\infty$ | $\infty$ | 156 | 196 | 262 | 358 | 498 | 694 |
| $n=100$ | $L B$ | 38 | 62 | 96 | 148 | 226 | 336 | 500 | 734 |
|  | $U B$ | $\infty$ | $\infty$ | 236 | 252 | 330 | 450 | 624 | 876 |
| $n=1000$ | $L B$ | 46 | 76 | 122 | 190 | 292 | 442 | 662 | 982 |
|  | $U B$ | $\infty$ | $\infty$ | $\infty$ | 420 | 480 | 672 | 874 | 1220 |

Lower and upper bounds on the threshold size of data sets (assuming $|\mathbb{T}|=|\mathbb{F}|$ and uniform random generation) above which support sets of size $K$ are unlikely to exists.

## The Good News

Distribution of Support Sets in Randomly Generated Data

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- If we have 20 attributes and less than 46 records, then it is very likely to have many support sets of size 6 or smaller.
- If we have more than 102 records, then it is very unlikely to have a support set of size 6 or smaller $\Longrightarrow$ If there is one ...


## The Good News

Distribution of Support Sets in Randomly Generated Data

|  | $K$ | 5 | 6 | 7 | 8 | 9 | $\mathbf{1 0}$ | 11 | 12 |
| :--- | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: |
| $n=10$ | $L B$ | 22 | 34 | 46 | 60 | 66 |  |  |  |
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|  | $U B$ | $\infty$ | $\infty$ | 236 | 252 | 330 | 450 | 624 | 876 |
| $n=1000$ | $L B$ | 46 | 76 | 122 | 190 | 292 | 442 | 662 | 982 |
|  | $U B$ | $\infty$ | $\infty$ | $\infty$ | 420 | 480 | $\mathbf{6 7 2}$ | 874 | 1220 |

- If, in a data set with 1000 attributes and more than 672 records, we find a support set of size 10 , then
- it might be a unique one;
- it is probably related to the structure of the data, and not to random noise.


## Partially Defined Boolean Functions

- Definition
- Support sets
- Patterns
- Theories


## Definitions

A term $t$ is a pattern of $(T, F)$ if

$$
\mathbf{T} \cap T(\mathbf{t}) \neq \emptyset \quad \text { and } \quad \mathbf{F} \subseteq F(\mathbf{t})
$$

or

$$
t(x)=1 \text { for at least one } x \in T \quad \text { and } \quad t(x)=0 \text { for all } x \in F
$$

A pattern corresponds to a combination of attributes which has been observed at least once in a true data point, but which never occurs in a false data point.

A pattern of $(\mathbf{F}, \mathrm{T})$ is called a co-pattern of $(\mathbf{T}, \mathrm{F})$.
$\operatorname{Pat}(\mathrm{T}, \mathrm{F})$ and co-Pat(T,F) denote the families of all patterns and copatterns of ( $\mathbf{T}, \mathbf{F}$ ), respectively.

## Returning to the medical example

|  |  | Test Results |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $x_{1}$ | $x_{2}$ | $x_{3}$ | $x_{4}$ |
| $\mathbb{T}$ |  | 1 | 1 | 0 | 1 |
|  | B | 0 | 1 | 1 | 1 |
|  | C | 1 | 1 | 1 | 0 |
|  | T | 0 | 0 | 1 | 1 |
|  | U | 1 | 0 | 0 | 1 |
|  | V | 1 | 0 | 1 | 0 |
|  | W | 0 | 1 | 1 | 0 |
|  | $\mathrm{Ms} Y$. | 1 | 1 | 0 | 0 |
|  | $\mathrm{Mr} . \mathrm{Z}$ | 1 | 0 | 1 | 1 |

Some patterns:

$$
x_{1} x_{2}, x_{2} \bar{x}_{3}, x_{2} x_{4}, \ldots
$$

Some co-patterns:

$$
\bar{x}_{1} \bar{x}_{2}, \bar{x}_{2}, \bar{x}_{1} \bar{x}_{4}, \ldots
$$

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## Theories and Co-Theories

An extension $f \in \mathcal{E}(\mathbf{T}, \mathbf{F})$ is called a theory of ( $\mathbf{T}, \mathbf{F})$ if it can be represented as a disjunction of some of the patterns of ( $\mathbf{T}, \mathbf{F}$ ).

A theory $g$ of ( $\mathbf{F}, \mathbf{T}$ ) is called a co-theory of ( $\mathbf{T}, \mathbf{F}$ ) (it can be represented by a disjunction of some of the co-patterns of (T,F)).

Denote by $\mathcal{E}_{T}(\mathbf{T}, \mathbf{F})$ and $\mathcal{E}_{T}(\mathbf{F}, \mathbf{T})$ the families of theories and co-theories of a given $\operatorname{pdBf}(\mathbf{T}, \mathbf{F})$.

Typically we have

$$
\left|\mathcal{E}_{T}(\mathrm{~T}, \mathrm{~F})\right| \ll|\mathcal{E}(\mathrm{T}, \mathrm{~F})|
$$

## Examples

Nearest Neighbor classifier


## Examples

## Decision Trees for pdBfs


$f_{D}$ is a theory and $\bar{f}_{D}$ is a co-theory.

## Theories as justifiable classifiers

Theory $f$ classifies an example x as a "positive" example if $f(\mathrm{x})=1$.

This is the case only if (at least) one pattern of $f$ is "triggered" by $\mathbf{x}$, meaning that we have observed earlier another positive example displaying the same features, and we have never observed a negative example displaying these features.

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Similarly, co-theory $g$ classifies an example $\mathbf{x}$ as a "negative" example if $g(\mathrm{x})=1$.

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But we don't necessarily have a good justification for the opposite classification.

Similarly, co-theory $g$ classifies an example x as a "negative" example if $g(\mathrm{x})=1$.

In both cases, we can provide some explanation or justification for the classification, but not for the opposite one.

## Theories, Co-Theories and Bi-Theories

A pair of a theory $f \in \mathcal{E}_{T}(\mathbf{T}, \mathbf{F})$ and a co-theory $g \in \mathcal{E}_{T}(\mathbf{F}, \mathrm{~T})$ can be used to define a classifier $F$ :

$$
F_{f, g}(\mathbf{x})= \begin{cases}1 & \text { if } f(\mathbf{x})=1 \text { and } g(\mathbf{x})=0 \\ 0 & \text { if } f(\mathbf{x})=0 \text { and } g(\mathbf{x})=1 \\ ? & \text { otherwise }\end{cases}
$$

Such a classifier can justify all its definite answers with evidence from (T, F), however, it may not be able to give an answer for all $\mathbf{x} \in\{0,1\}^{V}$ !

To avoid such uncertainties, ideally we would like to use a pair for which

$$
\bar{g}=f
$$

## Theories, Co-Theories and Bi-Theories

A theory $f \in \mathcal{E}_{T}(\mathbf{T}, \mathbf{F})$ is called a bi-theory of $(\mathbf{T}, \mathbf{F})$ if $\bar{f}$ is a co-theory of (T, F).

Then, the pair $(f, \bar{f})$ defines a classifier $F_{f, \bar{f}}$ which always provides evidence to support its answers.

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Do we always have bi-theories?

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Do we always have bi-theories?

YES, in fact (most) nearest neighbor approaches and decision tree based methods build a classifier $F_{f, \bar{f}}$ for some bi-theory $f \in \mathcal{E}_{B}(\mathbf{T}, \mathbf{F})$.

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A theory $f \in \mathcal{E}_{T}(\mathbf{T}, \mathbf{F})$ is called a bi-theory of $(\mathbf{T}, \mathbf{F})$ if $\bar{f}$ is a co-theory of ( $\mathrm{T}, \mathrm{F}$ ).

Then, the pair $(f, \bar{f})$ defines a classifier $F_{f, \bar{f}}$ which always provides evidence to support its answers.

Do we always have bi-theories?

YES, in fact (most) nearest neighbor approaches and decision tree based methods build a classifier $F_{f, \bar{f}}$ for some bi-theory $f \in \mathcal{E}_{B}(\mathbf{T}, \mathbf{F})$.

But in general, some bi-theories do not correspond to any decision tree nor to any nearest neighbor classifier.

## Conclusions

- Bi-theories and decision trees are very strongly related.


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- Bi-theories and nearest neighbor approaches are very strongly related.


## Conclusions

- Bi-theories and decision trees are very strongly related.
- Bi-theories and nearest neighbor approaches are very strongly related.
- Patterns and co-patterns are the basic building blocks in all these methods.


## Logical Analysis of Data

Extensions and applications of LAD

- Binarization of numerical attributes
- Binarization of categorical attributes
- Pattern generation
- Theory building


## Binarization - Numerical Attributes

|  | ID | Attributes |  | ID | Binarized Attributes |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | A |  |  | $\mathrm{A} \geq 2.9$ | ... |
| $\mathbb{S}^{+}$ | 001 | 1.7 | $\mathbb{T}$ | 001 | 0 |  |
|  | 002 | 3.5 |  | 002 | 1 |  |
|  | 003 | 4.2 |  | 003 | 1 |  |
|  | 004 | 9.3 |  | 004 | 1 |  |
| $\mathbb{S}^{-}$ | 991 | 2.3 | $\mathbb{F}$ | 991 | 0 |  |
|  | 992 | 6.2 |  | 992 | 1 |  |
|  | 993 | 7.5 |  | 993 | 1 |  |



## Binarization - Numerical Attributes

|  |  | Attributes |  |
| :--- | :---: | :---: | :---: |
|  |  | A |  |
| $+\cdots$ |  |  |
|  | 001 | 1.7 |  |
|  | 002 | 3.5 |  |
|  | 003 | 4.2 |  |
|  | 004 | 9.3 |  |
| - | 991 | 2.3 |  |
|  | 992 | 6.2 |  |
|  | 993 | 7.5 |  |


|  |  | Binarized Attributes |  |
| :---: | :---: | :---: | :---: |
|  |  | $\mathbf{A} \geq 2.9$ | $\mathbf{A} \geq 5.2$ |
| $\mathbb{T}$ | 001 | 0 | 0 |
|  | 002 | 1 | 0 |
|  | 003 | 1 | 0 |
|  | 004 | 1 | 1 |
| $\mathbb{F}$ | 991 | 0 | 0 |
|  | 992 | 1 | 1 |
|  | 993 | 1 | 1 |



Binarization - Numerical Attributes

|  | ID | Attributes |  | ID | Binarized Attributes |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | A |  |  | $\mathrm{A} \geq 2.9$ | $\mathrm{A} \geq 5$. |  |
| $\mathbb{S}^{+}$ | 001 | 1.7 | $\mathbb{T}$ | 001 | 0 | 0 |  |
|  | 002 | 3.5 |  | 002 | 1 | 0 |  |
|  | 003 | 4.2 |  | 003 | 1 | 0 |  |
|  | 004 | 9.3 |  | 004 | 1 | 1 |  |
| $\mathbb{S}^{-}$ | 991 | 2.3 | $\mathbb{F}$ | 991 | 0 | 0 |  |
|  | 992 | 6.2 |  | 992 | 1 | 1 |  |
|  | 993 | 7.5 |  | 993 | 1 | 1 |  |



Linear time generation; up to 40 cut points per attribute

## Binarization

| $c(\mathbf{X})$ | $A$ | $B$ | $C$ |
| :---: | :---: | :---: | :---: |
| 1 | 5.7 | 3.1 | blue |
| 1 | 1.2 | 4.2 | green |
| 1 | 3.1 | 5.1 | blue |
| 1 | 2.8 | 3.2 | green |
| 0 | 7.1 | 7.3 | red |
| 0 | 5.9 | 3.6 | yellow |
| 0 | 6.4 | 4.2 | blue |
| 0 | 3.4 | 1.6 | green |

Binarization

| $c(\mathbf{X})$ | $A$ | $B$ | $C$ |
| :---: | :---: | :---: | :---: |
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| 1 | 2.8 | 3.2 | green |
| 0 | 7.1 | 7.3 | red |
| 0 | 5.9 | 3.6 | yellow |
| 0 | 6.4 | 4.2 | blue |
| 0 | 3.4 | 1.6 | green |$\quad$| $A \geq 6$ | $\cdots$ | $B \geq 3$ | $\cdots$ | $C=$ blue | $\cdots$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 0 |  | 1 |  | 1 |  |
| 0 |  | 1 |  | 0 |  |
| 0 | $\cdots$ | 1 | $\cdots$ | 1 | $\cdots$ |
| 0 |  | 1 |  | 0 |  |
| 1 |  | 1 |  | 0 |  |
| 0 |  | 1 |  | 0 |  |
| 1 | $\cdots$ | 1 | $\cdots$ | 1 | $\cdots$ |
| 0 |  | 0 |  | 0 |  |

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| :---: | :---: | :---: | :---: | :---: | :---: |
| 0 |  | 1 |  | 1 |  |
| 0 |  | 1 |  | 0 |  |
| 0 | $\cdots$ | 1 | $\cdots$ | 1 | $\cdots$ |
| 0 |  | 1 |  | 0 |  |
| 1 |  | 1 |  | 0 |  |
| 0 |  | 1 |  | 0 |  |
| 1 | $\cdots$ | 1 | $\cdots$ | 1 | $\cdots$ |
| 0 |  | 0 |  | 0 |  |

$$
c(\mathbf{X})=(A<6) \wedge(B \geq 3) \wedge(C \in\{b l u e, \text { green }\})
$$

## Logical Analysis of Data

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## Pattern Generation

|  |  | Test |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  |  |  |  |
|  | $\mathrm{x}_{\mathbf{1}}$ | $\mathbf{x}_{\mathbf{2}}$ | $\mathrm{x}_{\mathbf{3}}$ | $\mathbf{x}_{\mathbf{4}}$ |  |
| $\mathbb{T}$ | A | 1 | 1 | 0 | 1 |
|  | B | 0 | 1 | 0 | 1 |
|  | C | 1 | 0 | 0 | 0 |
|  | T | 0 | 0 | 0 | 1 |
|  | U | 1 | 0 | 1 | 1 |
|  | V | 1 | 1 | 0 | 0 |
|  | W | 0 | 1 | 0 | 0 |

Pattern: $\quad \mathrm{P}(\mathrm{x})=x_{2} x_{4}$

$$
\mathrm{P}(\mathrm{~b})=0 \quad \forall \mathrm{~b} \in \mathbb{F}
$$

## Pattern Generation

|  | Test Results |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  | ID | $\mathbf{x}_{\mathbf{1}}$ | $\mathbf{x}_{\mathbf{2}}$ | $\mathbf{x}_{\mathbf{3}}$ | $\mathbf{x}_{\mathbf{4}}$ |
| $\mathbb{T}$ | A | 1 | 1 | 0 | 1 |
|  | B | 0 | 1 | 0 | 1 |
|  | C | 1 | 0 | 0 | 0 |
|  | T | 0 | 0 | 0 | 1 |
|  | U | 1 | 0 | 1 | 1 |
|  | V | 1 | 1 | 0 | 0 |
|  | W | 0 | 1 | 0 | 0 |

Pattern: $\quad \mathrm{P}(\mathrm{x})=x_{2} x_{4}$

$$
\mathrm{P}(\mathrm{~b})=0 \quad \forall \mathrm{~b} \in \mathbb{F}
$$

Coverage: $\operatorname{cov}(\mathrm{P})=2>0$
number of positive examples covered
Precision: $\pi(\mathrm{P})=2 / 7 \quad>\quad 0$
fraction of data correctly classified

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|  | Test Results |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
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| $\mathbb{T}$ | A | 1 | 1 | 0 | 1 |
|  | B | 0 | 1 | 0 | 1 |
|  | C | 1 | 0 | 0 | 0 |
|  | T | 0 | 0 | 0 | 1 |
|  | U | 1 | 0 | 1 | 1 |
|  | V | 1 | 1 | 0 | 0 |
|  | W | 0 | 1 | 0 | 0 |

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Generating efficiently all patterns is possible (in total time).

## Pattern Generation

|  | Test |  |  |  | Results |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  | ID | $\mathrm{x}_{\mathbf{1}}$ | $\mathrm{x}_{\mathbf{2}}$ | $\mathrm{x}_{\mathbf{3}}$ | $\mathrm{x}_{\mathbf{4}}$ |
| $\mathbb{T}$ | A | 1 | 1 | 0 | 1 |
|  | B | 0 | 1 | 0 | 1 |
|  | C | 1 | 0 | 0 | 0 |
|  | T | 0 | 0 | 0 | 1 |
|  | U | 1 | 0 | 1 | 1 |
|  | V | 1 | 1 | 0 | 0 |
|  | W | 0 | 1 | 0 | 0 |

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TOO MANY!

## Pattern Generation

|  | Test Results |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  | ID | $\mathbf{x}_{\mathbf{1}}$ | $\mathbf{x}_{\mathbf{2}}$ | $\mathbf{x}_{\mathbf{3}}$ | $\mathbf{x}_{\mathbf{4}}$ |
| $\mathbb{T}$ | A | 1 | 1 | 0 | 1 |
|  | B | 0 | 1 | 0 | 1 |
|  | C | 1 | 0 | 0 | 0 |
|  | T | 0 | 0 | 0 | 1 |
|  | U | 1 | 0 | 1 | 1 |
|  | V | 1 | 1 | 0 | 0 |
|  | W | 0 | 1 | 0 | 0 |

Pattern: $\quad \mathrm{P}(\mathrm{x})=x_{2} x_{4}$
$\mathrm{P}(\mathrm{b})=0 \quad \forall \mathrm{~b} \in \mathbb{F}$
Coverage: $\operatorname{cov}(\mathrm{P})=2>0$
number of positive examples covered
Precision: $\pi(\mathrm{P})=2 / 7 \quad>0$
fraction of data correctly classified

Ideally, we would like to generate all patterns with high coverage:

$$
\mathcal{P}(\mathbf{T}, \mathbf{F}, \gamma)=\{\mathbf{P}|\operatorname{cov}(\mathbf{P}) \geq \gamma| \mathbf{T} \mid\}
$$

## Pattern Generation

|  | Test |  |  |  | Results |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  | ID | $\mathrm{x}_{\mathbf{1}}$ | $\mathrm{x}_{\mathbf{2}}$ | $\mathrm{x}_{\mathbf{3}}$ | $\mathrm{x}_{\mathbf{4}}$ |
| $\mathbb{T}$ | A | 1 | 1 | 0 | 1 |
|  | B | 0 | 1 | 0 | 1 |
|  | C | 1 | 0 | 0 | 0 |
|  | T | 0 | 0 | 0 | 1 |
|  | U | 1 | 0 | 1 | 1 |
|  | V | 1 | 1 | 0 | 0 |
|  | W | 0 | 1 | 0 | 0 |

Pattern: $\quad \mathbf{P}(\mathbf{x})=x_{2} x_{4}$
$\mathrm{P}(\mathrm{b})=0 \quad \forall \mathrm{~b} \in \mathbb{F}$
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number of positive examples covered
Precision: $\pi(\mathrm{P})=2 / 7 \quad>\quad 0$
fraction of data correctly classified

Ideally, we would like to generate all patterns with high coverage:

$$
\mathcal{P}(\mathbf{T}, \mathbf{F}, \gamma)=\{\mathbf{P}|\operatorname{cov}(\mathbf{P}) \geq \gamma| \mathbf{T} \mid\}
$$

NP-hard!

Even if $|\mathcal{P}(\mathbf{T}, \mathbf{F}, \gamma)|$ is small, we cannot guarantee finding them all, unless $P=N P!$

## Patterns

In practice, generation heuristics concentrate for instance on patterns of small degree, high coverage, high precision.

Remember:
$\operatorname{cov}(\mathrm{P})=$ number of positive examples covered by P
$\pi(\mathrm{P})=$ fraction of examples correctly classified by P

| $c(\mathbf{X})$ | $A_{1}$ | $A_{2}$ | $A_{3}$ | $A_{4}$ | $A_{5}$ | $\mathbf{P}(\mathbf{X})=\overline{\mathbf{A}}_{1} \wedge \mathbf{A}_{3} \wedge \mathbf{A}_{4}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | $\mathbf{0}$ | 0 | $\mathbf{1}$ | $\mathbf{1}$ | 1 | $\mathbf{1}$ |
| 1 | 0 | 1 | 1 | 0 | 1 | $\mathbf{0}$ |
| 1 | 0 | 0 | $\mathbf{1}$ | $\mathbf{1}$ | 0 | $\mathbf{1}$ |
| 1 | 0 | 0 | 1 | 0 | 1 | $\mathbf{0}$ |
| 1 | 0 | 1 | $\mathbf{1}$ | $\mathbf{1}$ | 0 | $\mathbf{1}$ |
| 0 | $\mathbf{1}$ | 0 | 1 | 1 | 0 | 0 |
| 0 | $\mathbf{1}$ | 1 | 1 | 1 | 1 | 0 |
| 0 | 0 | 1 | 1 | $\mathbf{0}$ | 0 | 0 |
| 0 | 0 | 0 | $\mathbf{0}$ | $\mathbf{0}$ | 0 | 0 |
| 0 | 0 | 1 | $\mathbf{0}$ | $\mathbf{1}$ | 1 | 0 |

Coverage: $\operatorname{cov}(\mathrm{P})=3 \quad$ Precision: $\pi(\mathrm{P})=0.8$

## Patterns

There is considerable empirical evidence that patterns with high precision on a training (data) set generalize well, in the sense that they provide classifiers with high precision on subsequent test sets.

## Wisconsin Breast Cancer Data Set

http://www.ics.uci.edu/ mlearn/MLRepository.html
O. L. Mangasarian and W. H. Wolberg: "Cancer diagnosis via linear programming", SIAM News, Volume 23, Number 5, September 1990, pp. 1-18.

- Number of Instances: 699 (status of 15 July 1992)
- Number of Attributes: 9 with integer values between 1 and 10
- Missing attribute values: 16, all for attribute "Bare-nuclei".
- Class distribution:
- Benign: 458 (65.5\%)
- Malignant: 241 (34.5\%)


## Wisconsin Breast Cancer Data Set

- Training set: 63 records ( $\approx 10 \%$ )
- Attributes: 13 binary
- Number of patterns P with $\pi(\mathrm{P}) \geq 0.7: 36$ (of degrees $2-5$ )


## Wisconsin Breast Cancer Data Set

Performance of the Best Patterns on the Wisconsin Breast Cancer Data Set (10\%, 0.6)


## Wisconsin Breast Cancer Data Set

- Training set: 63 records ( $\approx 10 \%$ )
- Attributes: $\mathbf{1 3}$ binary
- Number of patterns P with $\pi(\mathrm{P}) \geq 0.7: 36$ (of degrees $2-5$ )
- Single best pattern: 95.1\%-Classifier!!

$$
P_{1}(X)=(\text { Clump-Thickness } \leq 6) \wedge(\text { Bare-Nuclei } \leq 4) \wedge(\text { Normal-Nucleoli } \leq 3)
$$

- Misclassifies only 5 malignant cases (all with missing data!)
- Best results reported in literature: 95 - 98\%


## Mushroom Database

http://www.ics.uci.edu/ mlearn/MLRepository.html

- Number of Instances: 8124 (status of April 27, 1987)
- Number of Attributes: 22 with nominal values (126 categories)
- Missing attribute values: 2480, all for attribute stalk-root.
- Class distribution:
- edible: 4208 (51.8\%)
- poisonous: 3916 (48.2\%)


## Mushroom Database

- Training set: 161 records ( $\approx 2 \%$ )
- Attributes: 56 binary
- Number of patterns P with $\pi(\mathrm{P}) \geq 0.85$ : 218 (of degrees $2-9$ )


## Mushroom Database



## Mushroom Database

- Training set: 161 records ( $\approx 2 \%$ )
- Attributes: 56 binary
- Number of patterns P with $\pi(\mathrm{P}) \geq 0.85$ : 218 (of degrees $2-9$ )
- Single best pattern: 98.5\%-classifier!!

$$
\mathrm{P}(\mathrm{X})=(\text { Odor } \neq \text { none }) \wedge(\text { Odor } \neq \text { anise }) \wedge(\text { Odor } \neq \text { almond })
$$

- Best results reported in literature: 95 - 99\%


## Australian Credit Card Data Set

STATLOG: http://www.ncc.up.pt/liacc/ML/statlog/datasets.html

- Number of Instances: 690
- Number of Attributes: 14 (6 numerical and 8 categorical)
- Missing attribute values: none
- Class distribution:
- positive: 307 (44.5\%)
- negative: 383 (55.5\%)


## Australian Credit Card Data Set

- Training set: 36 records ( $\approx 5 \%$ )
- Attributes: 12 binary
- Number of patterns P with $\pi(\mathrm{P}) \geq 0.60$ : 26 (of degrees $1-4$ )


## Australian Credit Card Data Set



- Training set: 36 records ( $\approx 5 \%$ )
- Attributes: 12 binary
- Number of patterns P with $\pi(\mathrm{P}) \geq 0.60$ : 26 (of degrees $1-4$ )
- Single best pattern: 85.4\%-classifier!!

$$
P(X)=(A 8=0)
$$

- Best results reported in literature: 80 - 87\%


## STATLOG Results: Australian Credit Card

|  | Error Rate |  |
| :--- | :--- | :--- |
| Algorithm | on training | on test |
| Cal5 | 0.132 | 0.131 |
| Itrule | 0.162 | 0.137 |
| LogDisc | 0.125 | 0.141 |
| Discrim | 0.139 | 0.141 |
| Dipol92 | 0.139 | 0.141 |
| Radial | 0.107 | 0.145 |
| Cart | 0.145 | 0.145 |
| Best Pattern | $\mathbf{0 . 1 1 1}$ | $\mathbf{0 . 1 4 6}$ |
| Castle | 0.144 | 0.148 |
| Bayes | 0.136 | 0.151 |
| IndCart | 0.081 | 0.152 |
| BackProp | 0.087 | 0.154 |
| C4.5 | 0.099 | 0.155 |
| Smart | 0.090 | 0.158 |
| BayTree | 0.000 | 0.171 |
| KNN | 0.000 | 0.181 |
| Ac2 | 0.000 | 0.181 |
| NewId | 0.000 | 0.181 |
| LVQ | 0.065 | 0.197 |
| Alloc80 | 0.194 | 0.201 |
| Cn2 | 0.001 | 0.204 |
| QuaDisc | 0.185 | 0.207 |
| Default | 0.440 | 0.440 |
| Cascade | $?$ | 100.0 |
| Kohonen | $?$ | 100.0 |

STATLOG: http://www.ncc.up.pt/liacc/ML/statlog/datasets.html

- Number of Instances: 846
- Number of Attributes: 18 numerical
- Missing attribute values: none
- Class distribution:
- OPEL: 212 (25.06\%)
- SAAB: 217 (25.65\%)
- BUS: 218 (25.77\%)
- VAN: 199 (23.52\%)


## STATLOG: Vehicle Data Set

Averages over the 4 classes

|  | Error Rate |  |
| :--- | :--- | :--- |
| Algorithm | on training | on test |
| QuaDisc | 0.085 | 0.150 |
| Dipol92 | 0.079 | 0.151 |
| Alloc80 | 0.000 | 0.173 |
| Best Patterns | 0.068 | 0.192 |
| LogDisc | 0.167 | 0.192 |
| BackProp | 0.168 | 0.207 |
| Discrim | 0.202 | 0.216 |
| Smart | 0.062 | 0.217 |
| Cart | 0.284 | 0.235 |
| C4.5 | 0.065 | 0.266 |
| BayTree | 0.079 | 0.271 |
| KNN | 0.000 | 0.275 |
| Cal5 | 0.068 | 0.279 |
| Cascade | 0.263 | 0.280 |
| LVQ | 0.171 | 0.287 |
| Ac2 | $?$ | 0.296 |
| IndCart | 0.047 | 0.298 |
| NewId | 0.030 | 0.298 |
| Radial | 0.098 | 0.307 |
| Cn2 | 0.018 | 0.314 |
| Itrule | $?$ | 0.324 |
| Kohonen | 0.115 | 0.340 |
| Castle | 0.545 | 0.505 |
| Bayes | 0.519 | 0.558 |
| Default | 0.750 | 0.750 |

When Best is Good

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© A best pattern alone is a very good, simple and robust classifier.

## Logical Analysis of Data

- Binarization of numerical attributes
- Binarization of categorical attributes
- Pattern generation
- Theory building


## Theory Building

Theories can be built by selecting enough patterns to cover all positive examples.

This can be done for instance by solving an optimization problem, either exactly or in a greedy way.

Similarly for co-theories.

Many applications in the literature...

## Theory Building

Theory formation: for each vector $\mathrm{a} \in \mathrm{T}$ we choose at most 5 patterns with the highest coverage from $\mathcal{P}(\mathrm{a}, \mathrm{T}, \mathrm{F}, \gamma)$.

| Results of 10 -fold cross validation |  |  |
| :--- | ---: | ---: |
| Data Set | Training | Test |
| AU CREDIT* | $88.9 \%$ | $85.4 \%$ |
| BCW | $99.7 \%$ | $97.4 \%$ |
| BUPA | $97.4 \%$ | $90.1 \%$ |
| DNA | $87.2 \%$ | $87.5 \%$ |
| HEART | $100.0 \%$ | $96.3 \%$ |
| HEPATITIS | $100.0 \%$ | $87.0 \%$ |
| IONOSPHERE | $99.9 \%$ | $95.2 \%$ |
| PIMA | $81.3 \%$ | $77.9 \%$ |
| VEHICLE* | $93.2 \%$ | $80.8 \%$ |
| VOTES | $100.0 \%$ | $98.3 \%$ |
| WINE | $100.0 \%$ | $97.9 \%$ |

* STATLOG Data Collection
$\dagger 4$ classes


## Conclusions

In conclusion

A A best pattern alone is a very good, simple and robust classifier.
$\bigcirc$ Theories built as disjunctions of good patterns provide excellent classifiers for a large variety of applications.
\& Theories provide classifications that are both understandable and justifiable.
$\diamond$ Several software packages have been developed.

## Software

Software available from Christhophe Meyer's LAD site
http://www.gerad.ca/~christop/LAD_en.html

1) Datascope (package written by Sorin Alexe in Visual Basic for Windows)
2) LADTools (program in C++ written by Eddy Mayoraz; may need CPLEX)
3) Ladoscope Gang (a set of programs written in Objective Caml by Pierre Lemaire)

Software available by request from E. Boros
4) PLAD (a PERL LAD Tool package, "use at your own risk researchware")

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