Finding Explanations: Rules!

- Propositional Rules:
  - Rules from Decision Trees
  - Rule Sets and Lists
  - Geometrical Rules
  - CN2

- First Order Rules:
  - Inductive Logic Programming
  - FOIL
Propositional Rules
Propositional Rules

Propositional\(^1\) Rules are simple:

\(^1\)proposition = truthbearer or statement. Either true or false (under an interpretation).

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Example:

\[
\text{IF } x_1 \leq 10 \text{ AND } x_3 = \text{red} \text{ THEN class A}
\]

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Example:

\[
\text{IF } x_1 \leq 10 \text{ AND } x_3 = \text{red} \quad \text{THEN } \text{class A}
\]

\text{antecedent} \quad \text{consequent}

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Either true or false (under an interpretation).
Propositional Rules

Atomic facts of propositional rules:

- constraints on numerical attributes, e.g. $<$, $\leq$, $=$, \ldots
- constraints on nominal attributes, e.g. $=$, $\in$ set
- constraints on ordinal attributes, e.g. $<$, $\in$ set, $\in$ range
Finding Propositional Rules in Data
Extracting Rules from Trees

- **temperature [°C]**
  - ≤ 20
  - > 20
    - cold
    - **humidity [%]**
      - ≤ 50
      - > 50
        - comfortable
        - **temperature [°C]**
          - ≤ 35
          - > 35
            - comfortable
            - unbearable
Extracting Rules from Trees

\[ R_a : \text{IF } \text{temperature} \leq 20 \text{ THEN class “cold”} \]
Extracting Rules from Trees

\[ R_a : \text{IF} \ \text{temperature} \leq 20 \ \text{THEN} \ \text{class “cold”} \]

\[ R_b : \text{IF} \ \text{temperature} > 20 \ \text{AND} \ \text{humidity} \leq 50 \ \text{THEN} \ \text{class “comf.”} \]
Extracting Rules from Trees

Temperature [°C]

≤ 20

> 20

Cold

Humidity [%]

≤ 50

> 50

Comfortable

Temperature [°C]

≤ 35

> 35

Comfortable

Unbearable

\( R_a : \) IF temperature \( \leq 20 \) THEN class “cold”

\( R_b : \) IF temperature \( > 20 \) AND humidity \( \leq 50 \) THEN class “comf.”

\( R_c : \) IF temperature \( \in (20, 35] \) AND humidity \( > 50 \) THEN class “comf.”
Extracting Rules from Trees

- $R_a$: IF temperature $\leq 20$ THEN class “cold”
- $R_b$: IF temperature $> 20$ AND humidity $\leq 50$ THEN class “comf.”
- $R_c$: IF temperature $\in (20, 35]$ AND humidity $> 50$ THEN class “comf.”
- $R_d$: IF temperature $> 35$ AND humidity $> 50$ THEN class “unbearable”
Extracting Rules from Trees

Rules from Decision Tree are:

- mutually exclusive (and therefore also conflict free)
- unordered
- complete
Extracting Rules from Trees

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Rules from Decision Tree have the usual problems
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Extracting Rules from Trees

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and (due to the recursive nature of the trees):

- redundancy

  (constraints on splits appear in several rules.)
Extracting Rules from Trees

Non-redundant rule set:
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\( R_1 : \text{IF temperature } \leq 20 \text{ THEN class “cold”} \)
Extracting Rules from Trees

Non-redundant rule set:

\( R_1 \): IF temperature \( \leq 20 \) THEN class “cold”

\( R_2 \): IF humidity \( \leq 50 \) THEN class “comfortable”
Non-redundant rule set:

\( R_1 : \text{IF} \ \text{temperature} \leq 20 \ \text{THEN} \ \text{class} \ "\text{cold}" \)

\( R_2 : \text{IF} \ \text{humidity} \leq 50 \ \text{THEN} \ \text{class} \ "\text{comfortable}" \)

\( R_3 : \text{IF} \ \text{temperature} \leq 35 \ \text{THEN} \ \text{class} \ "\text{comfortable}" \)
Extracting Rules from Trees

Non-redundant rule set:

\[ R_1 : \text{IF temperature } \leq 20 \text{ THEN class “cold”} \]
\[ R_2 : \text{IF humidity } \leq 50 \text{ THEN class “comfortable”} \]
\[ R_3 : \text{IF temperature } \leq 35 \text{ THEN class “comfortable”} \]
\[ R_4 : \text{class } = \text{ “unbearable”} \]
Extracting Ordered Rules from Trees

Non-redundant rule set:

\( R_1 \): IF temperature \( \leq 20 \) THEN class “cold”

\( R_2 \): IF humidity \( \leq 50 \) THEN class “comfortable”

\( R_3 \): IF temperature \( \leq 35 \) THEN class “comfortable”

\( R_4 \): class = “unbearable”

↑ order of rules matters!
previous example was heavily imbalanced tree.
more balanced tree results in nested ordering of rules.
in normal trees ordered rule extraction is considerably more complex.
Categorization of more general Propositional Rule Learners:

- **Supported Attribute Types**
  - **nominal only** ⇒ relatively small hypothesis space
  - **numerical only** ⇒ "geometrical" rule learners
  - **mixed attributes** ⇒ more complex heuristics needed
Categorization of more general Propositional Rule Learners:

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  - specializing
  - generalizing
Learning Propositional Rules: Generalizing

An example for a rule generalization:

Given a training instance \( (\vec{x}_1, k) \) with \( \vec{x}_1 = (12.3, 5, \text{red}) \), an initial, special rule could look like:

\[ \text{IF } x_1 = 12 \text{ AND } x_2 = 3.5 \text{ AND } x_3 = \text{red} \text{ THEN class } k \]

For a second example \( (\vec{x}_2, k) \) with \( \vec{x}_2 = (12.3, 3.5, \text{blue}) \), the rule is generalized:

\[ \text{IF } x_1 \in [12, 12.3] \text{ AND } x_2 = 3.5 \text{ AND } x_3 \in \{\text{red}, \text{blue}\} \text{ THEN class } k \]
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The resulting training algorithms generally are:
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The resulting training algorithms generally are:

- greedy (complete search of merge tree infeasible).
  (note difference to Find-S which explores entire space!)
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The resulting training algorithms generally are:

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- differ in
  - the choice of rules/patterns to merge
  - the used stopping criteria.
Remark: Specializing Propositional Rules

Specializing Rule Learners follow the same principle.
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Specializing Rule Learners follow the same principle.

- they start with very general rules

\[
\text{IF true THEN class } k.
\]
Remark: Specializing Propositional Rules

Specializing Rule Learners follow the same principle.

- they start with very general rules

  \[ \text{IF true THEN class } k. \]

- and iteratively specialize the rule.
Finding Sets of Rules

So far we only generalized/specialized one rule.
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- Most real world data sets are too complex to be explained by one rule only.
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Finding Sets of Rules

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- Most real world data sets are too complex to be explained by one rule only.
- Many rule learning algorithms wrap the learning of one rule into an outer loop based on set covering strategy (sequential covering):
  - attempts to build most important rules first
  - iteratively adds smaller / less important rules
Geometrical Rule Learners
Geometrical Rule Learners

- limited to numerical attributes (comparable ranges help, too)

Goal:
- Find rectangular (axes parallel) area(s) one by one that are occupied only by patterns of one class.
- each such area represents a rule:

\[ \text{IF } x_1 \in [a_1, b_1] \land \cdots \land x_n \in [a_n, b_n] \text{ THEN class } k \]

- Creates one rule after the other until no more useful rules can be built.

To find one rule:
- draw random starting point
- form most specific rectangular hypothesis covering this point
- While possible
  - find nearest neighbor of same class
  - generalize hypothesis (rectangle) to include this point
    (the latter may not be possible for all neighbors of the same class)
Geometrical Rule Learners

An example:
Geometrical Rule Learners: RecBF Learner

- Goal: Finding specific and general rules
  - Allows to estimate classification certainty
- RecBF algorithm: motivated by Neural Network Learning method
- Finds most specific within each (locally) most general rule
- Iterative algorithm
- (Much) faster than rule-by-rule approach.
**Algorithm RecBF(T)**

<table>
<thead>
<tr>
<th>Line</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( R = \emptyset )</td>
</tr>
<tr>
<td>2</td>
<td>while rules ( R ) are not stable</td>
</tr>
<tr>
<td>3</td>
<td>( \forall (\vec{x}, k) \in T )</td>
</tr>
<tr>
<td>4</td>
<td>if ( \exists R^k \in R : \text{covers}(R^k, \vec{x}) ) then</td>
</tr>
<tr>
<td>5</td>
<td>// Covered:</td>
</tr>
<tr>
<td>6</td>
<td>( R^k.w + + ) // increase weight</td>
</tr>
<tr>
<td>7</td>
<td>cover((R^k, \vec{x}))</td>
</tr>
<tr>
<td>8</td>
<td>else</td>
</tr>
<tr>
<td>9</td>
<td>// Commit:</td>
</tr>
<tr>
<td>10</td>
<td>( R \leftarrow R \cup \text{newRule}(\vec{x}) )</td>
</tr>
<tr>
<td>11</td>
<td>endif</td>
</tr>
<tr>
<td>12</td>
<td>( \forall R^{k'} \in R : k \neq k' \land \text{covers}(R^k, \vec{x}) ):</td>
</tr>
<tr>
<td>13</td>
<td>shrink((R^{k'}, \vec{x}))</td>
</tr>
</tbody>
</table>
RecBF Learner

An example:
RecBF Learner: Operations

- **Rule stability:**
  - Algorithm converges guaranteed if training data is conflict free
    (Maximum: $n$ iterations for $n$ training patterns)

- **Covered:**
  - simple boundary test
    Make sure specific rule $R$ covers new $\vec{x}$: boundary expansion

- **Commit:**
  - Simple insert of most general rule $R$ with corresponding most specific rule, centered on new training pattern

- **Shrink:**
  - Reducing rectangle to exclude conflicting pattern: $n$ choices.
  - Heuristics:
    - maximize remaining volume
    - Avoid shrinkage of specific rule of $R$
RecBF Learner: Shrink

Options for Specialization of specialized rules:

(a,b): entire region considered,
(c,d): regions to anchor considered.
RecBF Learner: Shrink

Options for Specialization of general rules:

(a,b): entire region considered,
(c,d): regions to anchor considered,
(e,f): regions to “core” considered.
RecBF Learner: Operations

- **Problems:**
  - Depends on order of training examples
  - Shrink-procedure based on heuristics

- **Properties**
  - Explains all training patterns correctly
  - Most general rules depend on few attributes only
  - Most specific rules depend on all attributes
Examples\(^2\) of Specialized and Generalized Rules:

\(^2\)images from Peter Flach

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Examples\(^2\) of Specialized and Generalized Rules:

Are there more general (or special) rule sets?

\(^2\)images from Peter Flach

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Back to Propositional Rules: CN2
The CN2 Rule Learning Algorithm


- prominent, early example of rule learning algorithm
- set covering approach
- greedy algorithm rule specialization
- simple heuristic for “most important” rule selection.
BuildRuleSet

**Algorithm** BuildRuleSet(D, p_{min})

<table>
<thead>
<tr>
<th>input:</th>
<th>training data D</th>
</tr>
</thead>
<tbody>
<tr>
<td>parameter:</td>
<td>performance threshold p_{min}</td>
</tr>
<tr>
<td>output:</td>
<td>a rule set R matching D with performance ( \geq p_{min} )</td>
</tr>
</tbody>
</table>

1. \( R = \emptyset \)
2. \( D_{\text{rest}} = D \)
3. **while** \( (\text{Performance}(R, D_{\text{rest}}) < p_{min}) \)
4. \( r = \text{FindOneGoodRule}(D_{\text{rest}}) \)
5. \( R = R \cup \{r\} \)
6. \( D_{\text{rest}} = D_{\text{rest}} - \text{covered}(r, D_{\text{rest}}) \)
7. **endwhile**
8. **return** R

Alternative implementations by varying:

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Algorithm BuildRuleSet($D, p_{\text{min}}$)

<table>
<thead>
<tr>
<th>input:</th>
<th>training data $D$</th>
</tr>
</thead>
<tbody>
<tr>
<td>parameter:</td>
<td>performance threshold $p_{\text{min}}$</td>
</tr>
<tr>
<td>output:</td>
<td>a rule set $R$ matching $D$ with performance $\geq p_{\text{min}}$</td>
</tr>
</tbody>
</table>

1. $R = \emptyset$
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Alternative implementations by varying:
- performance measure?
BuildRuleSet

Algorithm BuildRuleSet(\(D, p_{\text{min}}\))

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Alternative implementations by varying:
- performance measure?
- strategy for rule finding?
**BuildRuleSet**

**Algorithm** \( \text{BuildRuleSet}(D, p_{\text{min}}) \)

- **input:** training data \( D \)
- **parameter:** performance threshold \( p_{\text{min}} \)
- **output:** a rule set \( R \) matching \( D \) with performance \( \geq p_{\text{min}} \)

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   6. \( D_{\text{rest}} = D_{\text{rest}} - \text{covered}(r, D_{\text{rest}}) \)
4. **endwhile**
5. **return** \( R \)

Alternative implementations by varying:
- **performance measure**?
- **strategy for rule finding**?

(We could just use a decision tree learner and build only the ‘best branch...')
Following (more than) one branch resembles a general-to-specific beam search:

- Hypothesis (rule) is increasingly specified
- At each branching point all possible specializations are considered
- Choice of best branch can be made based on information gain, coverage, or mix of both
- Class (rule post condition) depends on majority class at each point

Greedy algorithm can produce sub-optimal solution

- Beam search produces $k$ candidate solutions (at each level only the $k$ best branches are kept)

Sometimes only learning rules of one class is sufficient (e.g. to model a minority class), default class $=$ majority class.
Algorithm FindOneGoodRule($D_{\text{rest}}$)

input: (subset of) training data $D_{\text{rest}}$

output: one good rule $r$ explaining some instances of the training data

1. $h_{\text{best}} = \text{true}$  // most general hypothesis
2. $H_{\text{candidates}} = \{h_{\text{best}}\}$
3. while $H_{\text{candidates}} \neq \emptyset$
4. \hspace{1em} $H_{\text{candidates}} = \text{specialize}(H_{\text{candidates}})$
5. \hspace{1em} $h_{\text{best}} = \arg \max_{h \in H_{\text{candidates}} \cup \{h_{\text{best}}\}} \{\text{Performance}(h, D_{\text{rest}})\}$
6. \hspace{1em} update($H_{\text{candidates}}$)  // clean up
7. endwhile
8. return 'IF $h_{\text{best}}$ THEN $\arg \max_k \{|\text{covered}_k(h_{\text{best}}, D_{\text{rest}})|\}'
Heuristics for FindOneGoodRule

How do we evaluate the accuracy \( A \) of a rule?
Heuristics for FindOneGoodRule

How do we evaluate the accuracy $A$ of a rule?

- Base Assumption:

$$A('\text{IF Conditions THEN class } k') = p(k|\text{Conditions})$$
Heuristics for FindOneGoodRule

How do we evaluate the accuracy $A$ of a rule?

- **Base Assumption:**

  $$A('\text{IF Conditions THEN class } k') = p(k|\text{Conditions})$$

- **Estimating the probability using relative frequencies:**

  $$p(k|\text{Conditions}) = \frac{\#\text{covered correct}}{\#\text{covered total}}$$
Probability Estimates

Relative frequency of covered correctly:
\[ p(k|R) = \frac{\text{#covered correct}}{\text{#covered total}} \]

Problems with small samples.
Laplace estimate:
\[ p(k|R) = \frac{\text{#covered correct} + 1}{\text{#covered total} + \text{#classes}} \]
Assumes uniform prior distribution of classes.

\[ p(k|R) = \frac{\text{#covered correct} + m \cdot p(k)}{\text{#covered total} + m} \]
Probability Estimates

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- \( m \)-estimate:

\[ p(k|R) = \frac{\#\text{covered correct} + m \cdot p(k)}{\#\text{covered total} + m} \]

...
m-estimate:

\[ p(k|R) = \frac{\#\text{covered correct} + m \cdot p(k)}{\#\text{covered total} + m} \]

- special case: \( p(k) = 1/\#\text{classes}, m = \#\text{classes} \)
- takes into account prior class probabilities
- independent of number of classes
- \( m \) is domain dependent (more noise, larger \( m \))
Other Search Heuristics

- Expected accuracy on positives:

\[ A(R) = p(k|R) \]
Other Search Heuristics

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- Weighted measures in order to favor more general rules:
  \[ W_G(R', R) = \frac{\#\text{correct covered by } R'}{\#\text{correct covered by } R} \cdot G(R', R) \]
Propositional Rule Induction

Issues with most propositional rule learners:

- Heuristics for real-world data often fail.
- Too many dimensions make greedy constraint picking difficult.
- In real-world feature spaces, often patterns of the same class are not "axes parallel".
- Sharp boundaries for noisy data are unsuited.

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IF $x$ is Father of $y$ AND $y$ is female THEN $y$ is Daughter of $x$
Limitations of Propositional Rules

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They would need to “cover” training examples for all possible \((x, y)\) combinations.
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For this, other types of rules are more appropriate.
First Order Rules
First Order Rules differ from propositional logic by their use of variables. FOL is also based on a number of base constructs:
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( Reminder:
  - $\forall$: the universal quantifier, e.g. $\forall x, y : \text{Daughter}(x, y) \rightarrow \text{female}(x)$
  - $\exists$: existential quantifier, e.g. $\forall x : \exists y : \text{female}(x) \rightarrow \text{Daughter}(x, y)$
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- **horn clauses**: clauses with at most one positive literal.
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Horn clauses are especially interesting because any disjunction with at most one positive literal can be written as

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Horn clauses are also used to express Prolog programs \( \Rightarrow \) Learning First Order Rules is often called “Inductive Logic Programming” (ILP).
First Order Rule Types

A rule body is satisfied if at least one binding exists that satisfies all literals.

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A few examples:

- **simple rules:**
  
  IF \( x \) is Parent of \( y \) AND \( y \) is male
  
  THEN \( x \) is Father of \( y \)
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- **existentially qualified variables** (\( z \) in this case):
  
  IF \( y \) is Parent of \( z \) AND \( z \) is Parent of \( x \)
  
  THEN \( x \) is Grandchild of \( y \)
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- existentially qualified variables (z in this case):
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  THEN $x$ is Grandchild of $y$

- Recursive rules:
  IF $x$ is Parent of $z$ AND $z$ is Anchestor of $y$
  THEN $x$ is Anchestor of $y$
  IF $x$ is Parent of $y$ THEN $x$ is Anchestor of $y$

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- one (dramatic) restriction: no functions!
- one (easy) extension: literals in body can be negated.
Learning First Order Rules: FOIL

- **Algorithm** BuildRuleSet(·): remains the same (sequential set covering)

  - Adding $P(v_1,\ldots,v_r)$, where $P$ is any predicate name occurring in the set of available predicates. At least one of the variables must already be present in the original rule, the others can be either new or existing;
  - Adding $Equal(x,y)$, where $x$ and $y$ are variables already present in the rule; or
  - Negating of either of the above forms of literals.

  How does FOIL pick the "best" specialization?
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FOIL: Guiding the Search

FoilGain used to evaluation contribution of new literal $L$ to rule $R$:

$$\text{FoilGain}(L, R) = t \left( - \log_2 \frac{p'}{p' + n'} - \log_2 \frac{p}{p + n} \right)$$

- $R$: rule
- $p$: number of positive bindings of $R$
- $n$: number of negative bindings of $R$
- $L$: new literal
- $R'$: new rule ($R$ with added $L$)
- $p'$: number of positive bindings of $R'$
- $n'$: number of negative bindings of $R'$

If $L$ introduces a new variable, any original binding is considered to be covered if at least some of the (extended) binding of $R$ is present in the bindings of $R'$. 
FOIL: Example

- Target literal: GrandDaughter($x, y$)
  (the grand daughter of $x$ is $y$)
- Training “data” (assertions):
  - GrandDaughter(Victor, Sharon)
  - Father(Sharon, Bob)
  - Father(Tom, Bob)
  - Female(Sharon)
  - Father(Bob, Victor)

- Closed world assumption:
  all other bindings of predicates above are implicitly false, e.g.
  - ¬Father(Bob, Tom)
  - ¬Female(Victor)
  - ¬GrandDaughter(Bob, Sharon), ...

- Available predicates:
  - Father($x, y$)
  - Female($x$)
FOIL: Example

- Starting Point: Most general rule: GrandDaughter(x,y) :- .
  With $4 \times 4$ possible bindings for $x$ and $y$.
  (1 positive binding, 15 negative bindings)
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- Final result:
  GrandDaughter(x,y) :- Father(y,z), Father(z,x), Female(y)
**FOIL: Summary**

- FOIL combines

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Extensions of FOIL also handle noisy data

Stopping criteria considers description-length principle to avoid adding lengthy rules to explain few examples.
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- Most existing algorithms scale poorly (FOIL is a good example).
- Applicable for special types of data (e.g. structured or mainly nominal values).