Nachtrag Organisatorisches

- Klausurtermin
  - Do 16.2.2017, 10-12h

- Tutorium!
  - Wir versuchen diesmal erstmals das Betreuungsangebot durch ein Tutorium bzw. Sprechstunde zu ergänzen
  - Termin jeden Mi 11.00-12.30h, A213
  - Im Tutorium werden
    - Fragen zur Übung vom Tutor beantwortet
    - Best-practice Demonstrationen vom Tutor gezeigt
  - Mehr Informationen bei der Vorbesprechung zur Übung am Dienstag

Data Mining and Machine Learning

TECHNISCHE UNIVERSITÄT DARMSTADT

Concept Learning and Version Spaces

- Introduction
  - Concept Learning
  - Generality Relations
  - Refinement Operators
  - Structured Hypothesis Spaces
- Simple algorithms
  - Find-S
  - Find-G
- Version Spaces
  - Version Spaces
  - Candidate-Elimination Algorithm

Why Rules?

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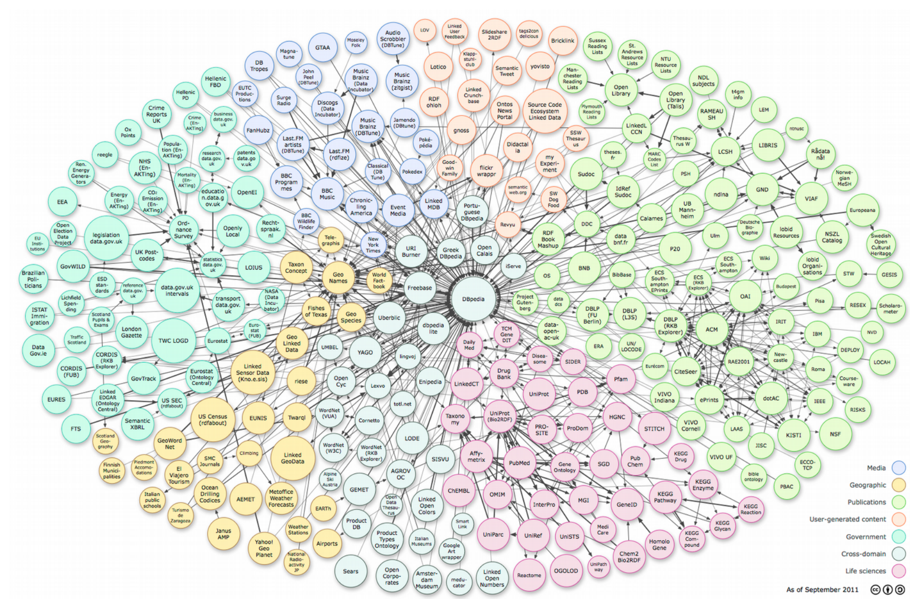
- Rules provide a good (the best?) trade-off between
  - human understandability
  - machine executability
- Used in many applications which will gain importance in the near future
  - Security
  - Spam Mail Filters
  - Semantic Web



- But they are not a universal tool
  - e.g., learned rules sometimes lack in predictive accuracy
    → challenge to close or narrow this gap

Concept

- Attribute-Value Representation
  - each object is represented with a finite number of attributes
- Concept
  - A *concept* is a subset of all possible objects
- Example 1:
  - objects are points in a 2-d plane
  - a concept can be any subarea in the plane
    - can have many disconnected components
  - # objects and # concepts is infinite
- Example 2:
  - all attributes are Boolean, objects are Boolean vectors
  - a concept can be any subset of the set of possible objects
  - # concepts and # objects is finite

Concept Learning

- Given:
  - Positive Examples E^+
    - examples for the concept to learn (e.g., days with golf)
  - Negative Examples E^-
    - counter-examples for the concept (e.g., days without golf)
  - Hypothesis Space H
    - a (possibly infinite) set of candidate hypotheses
    - e.g., rules, rule sets, decision trees, linear functions, neural networks, ...

- Find:
  - Find the target hypothesis $h \in H$
  - the target hypothesis is the concept that was used (or could have been used) to generate the training examples

Correctness

- What is a good rule?
  - Obviously, a correct rule would be good
  - Other criteria: interpretability, simplicity, efficiency, ...
- Problem:
  - We cannot compare the learned hypothesis to the target hypothesis because we don't know the target
    - Otherwise we wouldn't have to learn...
- Correctness on training examples
  - ***completeness***: Each positive example should be covered by the target hypothesis
  - ***consistency***: No negative example should be covered by the target hypothesis
- But what we want is correctness on *all* possible examples!

Conjunctive Rule

$$\texttt{if}\ (\text{att}_i = \text{val}_{iI})\ \texttt{and}\ (\text{att}_j = \text{val}_{jJ})\quad \texttt{then}\ +$$

Body of the rule (IF-part)
- contains a conjunction of conditions
- a condition typically consists of comparison of attribute values

Head of the rule (THEN-part)
- contains a prediction
- typically + if object belongs to concept, – otherwise

- Coverage
  - A rule is said to ***cover*** an example if the example satisfies the conditions of the rule.
- Prediction
  - If a rule covers an example, the rule's head is predicted for this example.

Propositional Logic

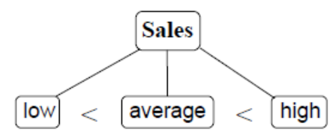
- simple logic of propositions
  - combination of simple facts (*features*)
  - no variables, no functions, no relations (→ predicate calculus)
  - Operators:
    - conjunction ∧, disjunction ∨, negation ¬, implication →, ...
- rules with attribute/value tests may be viewed as statements in propositional logic
    - because all statements in the rule implicitly refer to the same object
    - each attribute/value pair is one possible condition
- Example:
    - `if` windy = false `and` outlook = sunny `then` golf
    - in propositional logic: ¬ windy ∧ sunny_outlook → golf

Features

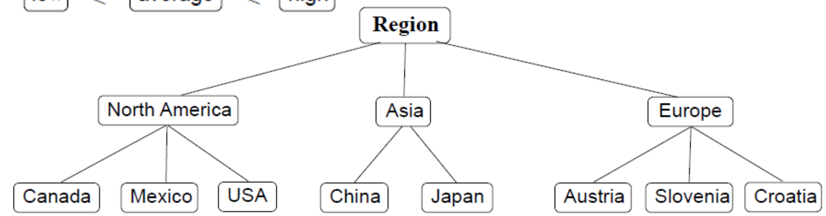
- A feature is a Boolean property of an object

Feature types

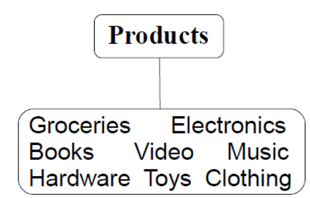
- Selectors
  - select a nominal value: **Sex** = female
  - compare to a numerical value: **Salary** > 100,000
- Ordered features
  - the nominal values form an ordered set



- Hierarchical features
  - the nominal values form a hierarchy



- Relational features
  - relate two or more values to each other **Length** > **Height**
- Set-valued features
  - compare to a set of values (e.g., a set of words)



Generality Relation

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- Intuitively:
  - A statement is more general than another statement if it refers to a superset of its objects
- Examples:

more general ↑

All students are good in Machine Learning.

All students who took a course in Machine Learning and Data Mining are good in Machine Learning

All students who took course DM&ML at the TU Darmstadt are good in Machine Learning

All students who took course DM&ML at the TU Darmstadt and passed with 2 or better are good in Machine Learning.

more specific ↓

Generality Relation for Rules

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- Rule r_1 is *more general* than r_2 $\qquad r_1 \geq r_2$
  - if it covers all examples that are covered by r_2.
- Rule r_1 is *more specific* than r_2 $\qquad r_1 \leq r_2$
  - if r_2 is more general than r_1.
- Rule r_1 is *equivalent* to r_2 $\qquad r_1 \equiv r_2$
  - if it is more specific and more general than r_2.

Examples:

`if` size > 5 `then` +
`if` size > 3 `then` +

`if` animal = mammal `then` +
`if` feeds_children = milk `then` +

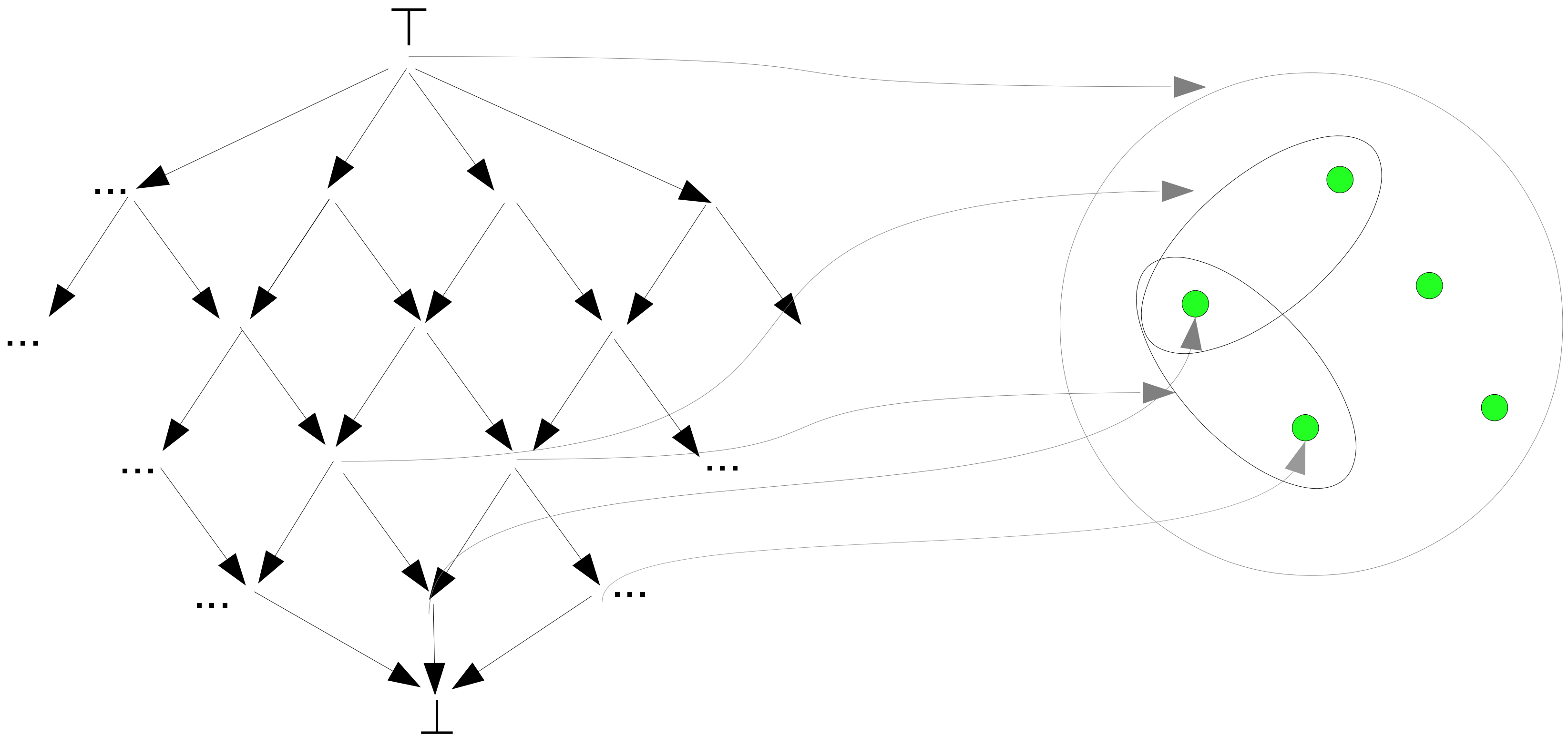
`if` outlook = sunny `then` +
`if` outlook = sunny `and` windy = false `then` +

Special Rules

- Most general rule ⊤
  - typically the rule that covers all examples
    - the rule with the body true
    - if disjunctions are allowed: the rule that allows all possible values for all attributes
- Most specific rule ⊥
  - typically the rule that covers no examples
    - the rule with the body false
    - the conjunction of all possible values of each attribute
      - evaluates to false (only one value per attribute is possible)
- Each training example can be interpreted as a rule
  - body: all attribute-value tests that appear inside the example
  - the resulting rule is an immediate generalization of ⊥
    - covers only a single example

Structured Hypothesis Space

The availability of a generality relation allows to structure the hypothesis space:



Structured Hypothesis Space
arrows to represent „is more general than“

Instance Space

Testing for Generality

- In general, we cannot check the generality of hypotheses
  - We do not have all examples of the domain available (and it would be too expensive to generate them)
- For single rules, we can approximate generality via a *syntactic generality check*:
  - **Example:** Rule r_1 is *more general* than r_2 if the set of conditions of r_1 forms a *subset* of the set of conditions of r_2.
  - Why is this only an approximation?
- For the general case, computable generality relations will rarely be available
  - E.g., rule sets
- Structured hypothesis spaces and version spaces are also a theoretical model for learning

Refinement Operators

- A refinement operator modifies a hypothesis
  - can be used to search for good hypotheses
- Generalization Operator:
  - Modify a hypothesis so that it becomes more general
    - e.g.: remove a condition from the body of a rule
  - necessary when a positive example is uncovered
- Specialization Operator:
  - Modify a hypothesis so that it becomes more specific
    - e.g., add a condition to the body of a rule
  - necessary when a negative examples is covered
- Other Refinement Operators:
  - in some cases, the hypothesis is modified in a way that neither generalizes nor specializes
    - e.g., stochastic or genetic search

Generalization Operators for Symbolic Attributes

There are different ways to generalize a rule, e.g.:

- **Subset Generalization**
  - a condition is removed
  - used by most rule learning algorithms

shape = square & color = blue → +
⇒
color = blue → +

- **Disjunctive Generalization**
  - another option is added to the test

shape = square & color = blue → +
⇒
shape = (square ∨ rectangle) & color = blue → +

- **Hierarchical Generalization**
  - a generalization hierarchy is exploited

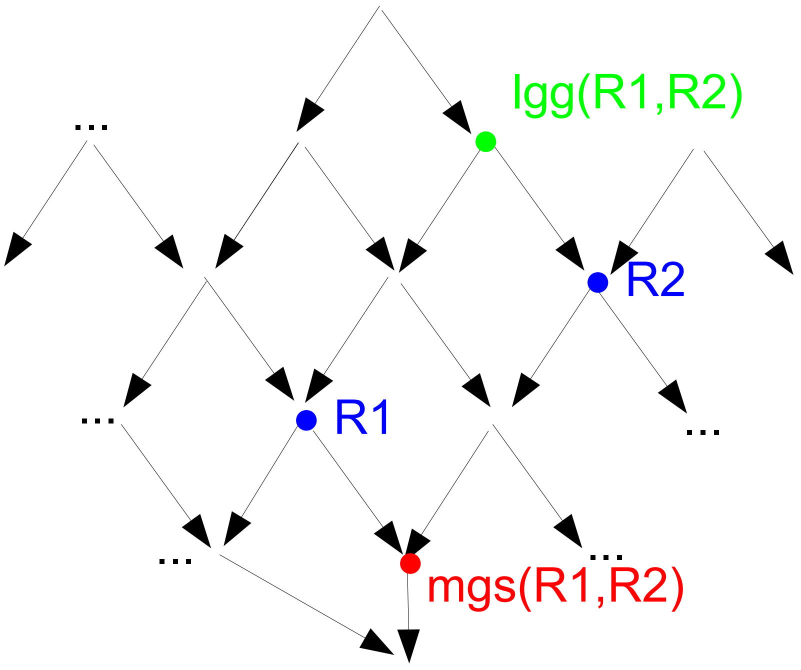
shape = square & color = blue → +
⇒
shape = quadrangle & color = blue → +

Minimal Refinement Operators

- In many cases it is desirable, to only make minimal changes to a hypothesis
  - specialize only so much as is necessary to uncover a previously covered negative example
  - generalize only so much as is necessary to cover a previously uncovered positive example
- Minimal Generalization of a rule r relative to an example e:
  - Find a generalization g of rule r and example e so that
    - g covers example e (r did not cover e)
    - there is no other rule g' so that $e \leq g' < g$ and $g' \geq r$
  - need not be unique
- Minimal Specialization of a rule r relative to an example e:
    - Analogously (specialize r so that it does not cover e)

Minimal Generalization/Specialization

- least general generalization (lgg) of two rules
  - *for Subset Generalization:* the intersection of the conditions of the rules (or a rule and an example)



- most general specialization (mgs) of two rules
  - *for Subset Generalization:* the union of the conditions of the rules

Algorithm Find-S

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I. h = most specific hypothesis in H
(covering no examples)

II. for each training example e

a) if e is negative
- do nothing

b) if e is positive
- for each condition c in h
  - if c does not cover e
    - delete c from h

III. return h

The hypothesis
`if` false `then +`

Minimal Subset generalization
(other generalizations possible)

Note: when the first positive example is encountered, step II.b) amounts to converting the example into a rule
(The most specific hypothesis can be written as a conjunction of all possible values of each attribute.)

Example

No	Sky	Temperature	Humidity	Windy	Water	Forecast	Golf?
1	sunny	hot	normal	strong	warm	same	yes
2	sunny	hot	high	strong	warm	same	yes
3	rainy	cool	high	strong	warm	change	no
4	sunny	hot	high	strong	cool	change	yes

Example

No	Sky	Temperature	Humidity	Windy	Water	Forecast	Golf?
1	sunny	hot	normal	strong	warm	same	yes
2	sunny	hot	high	strong	warm	same	yes
3	rainy	cool	high	strong	warm	change	no
4	sunny	hot	high	strong	cool	change	yes

H_0: `if` false `then` +

`if` (sky = sunny & sky = rainy & ... & forecast = same & forecast = change) `then` +

<Ø,Ø,Ø,Ø,Ø,Ø>

H_1: <sunny, hot, normal, strong, warm, same>

H_2: <sunny, hot, ?, strong, warm, same>

H_3: <sunny, hot, ?, strong, warm, same>

H_4: <sunny, hot, ?, strong, ?, ? >

Short-hand notation:

- only body (head is +)
- one value per attribute
- ∅ for `false` (full conjunction)
- ? for `true` (full disjunction)

Properties of Find-S

- completeness:
  - h covers all positive examples
- consistency:
  - h will not cover any negative training examples
  - but only if the hypothesis space contains a target concept
    (i.e., there is a single conjunctive rule that describes the target concept)
- Properties:
  - no way of knowing whether it has found the target concept
    (there might be more than one theory that are complete and consistent)
  - it only maintains one specific hypothesis
    (in other hypothesis languages there might be more than one)
  - Find-S prefers more specific hypotheses (hence the name)
    (it will never generalize unless forced by a training example)

Can we also find the most general hypothesis?

Algorithm Find-G

I. h = most general hypothesis in H
(covering all examples)

II. for each training example e
  a) if e is positive
    - do nothing
  b) if e is negative
    - for some condition c in e
      - if c is not part of h
        - add a condition that negates c and covers all previous positive examples to h

III. return h

The hypothesis
`if` true `then +`

Minimal Subset specialization
(other specializations possible)

Example

No	Sky	Temperature	Humidity	Windy	Water	Forecast	Golf?
1	sunny	hot	normal	strong	warm	same	yes
2	sunny	hot	high	strong	warm	same	yes
3	rainy	cool	high	strong	warm	change	no
4	sunny	hot	high	strong	cool	change	yes

Example

No	Sky	Temperature	Humidity	Windy	Water	Forecast	Golf?
1	sunny	hot	normal	strong	warm	same	yes
2	sunny	hot	high	strong	warm	same	yes
3	rainy	cool	high	strong	warm	change	no
4	sunny	hot	high	strong	cool	change	yes

H_0: `if` true `then` +

`if` (sky = sunny || sky = rainy) & ... & (forecast = same || forecaset = change) `then` +

<?, ?, ?, ?, ?, ?>

H_1: <?, ?, ?, ?, ?, ?>

H_2: <?, ?, ?, ?, ?, ?>

H_3: <?, ?, ?, ?, ?, same>

Other possibilities:
- <?, hot, ?, ?, ?, ?>
- <sunny, ?, ?, ?, ?, ?>

H_4: ????

There is no way to refine H_3 so that it covers example 4.

Uniqueness of Refinement Operators

- Subset Specialization is not unique
  - we could specialize any condition in the rule that currently covers the negative example
  - we could specialize it to any value other than the one that is used in the example

  → a wrong choice may lead to an impasse
- Possible Solutions:
  - more expressive hypothesis language (e.g., disjunctions of values)
  - backtracking
  - remember all possible specializations and remove bad ones later → Find-GSet algorithm
- Note: Generalization operators also need not be unique!
  - depends on the hypothesis language

Algorithm Find-GSet

I. h = most general hypothesis in H (covering all examples)

II. $G = \{ h \}$

III. for each training example e

  a) if e is positive

  - remove all $h \in G$ that do not cover e

  b) if e is negative

  - for all hypotheses $h \in G$ that cover e
    - $G = G \setminus \{h\}$
    - for every condition c in e that is not part of h
      - for all conditions c' that negate c
        - $h' = h \cup \{c'\}$
        - if h' covers all previous positive examples
          - $G = G \cup \{h'\}$

IV. return G

Example

No	Sky	Temperature	Humidity	Windy	Water	Forecast	Golf?
1	sunny	hot	normal	strong	warm	same	yes
2	sunny	hot	high	strong	warm	same	yes
3	rainy	cool	high	strong	warm	change	no
4	sunny	hot	high	strong	cool	change	yes

G_0: { <?, ?, ?, ?, ?, ?> }

We now have a set of hypotheses!

G_1: { <?, ?, ?, ?, ?, ?> }

G_2: { <?, ?, ?, ?, ?, ?> }

Remember all possible refinements that exclude example 3

G_3: { <sunny, ?, ?, ?, ?, ?>, <?, hot, ?, ?, ?, ?>, <?, ?, ?, ?, ?, same>}

G_4: { <sunny, ?, ?, ?, ?, ?>, <?, hot, ?, ?, ?, ?>}

Correct Hypotheses

- Find-GSet:
  - finds most general hypotheses that are correct on the data

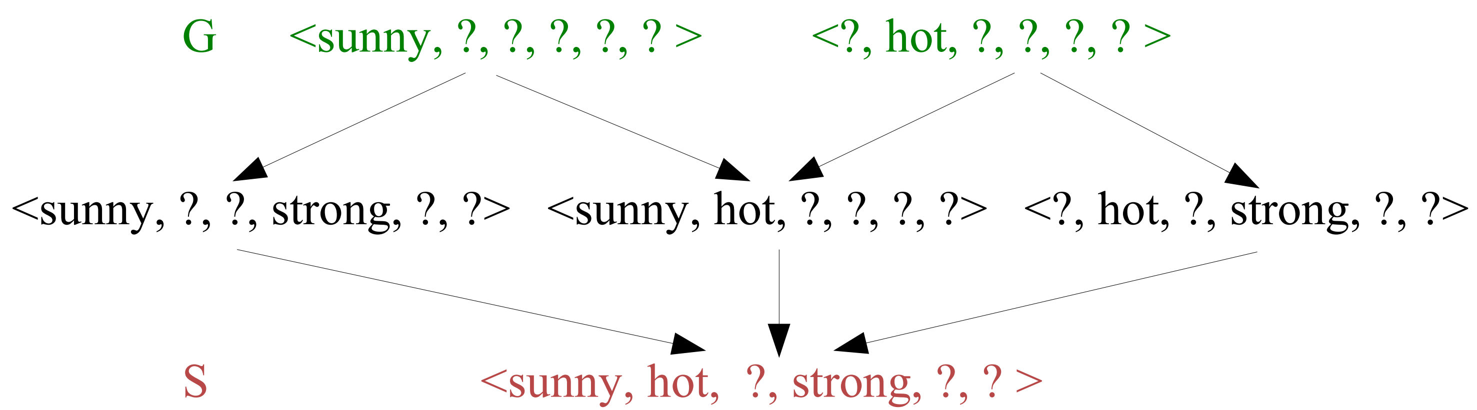
  → has a bias towards general hypotheses
- Find-SSet:
  - can be defined analogously
  - finds most specific hypotheses that are correct on the data

  → has a bias towards specific hypotheses
- Thus, the hypotheses found by Find-GSet or Find-SSet are not necessarily identical!

→ Could there be hypotheses that are correct but are neither found by Find-GSet nor by Find-SSet?

Version Space

- The version space is the set of hypothesis that are correct (complet and consistent) on the training examples
  - in our example consists of 6 hypotheses



- Find-GSet will find the rules in G
  - G are the most general rules in the version space
- Find-SSet will find the rules in S
  - S are the most specific rules in the version space

Version Space

- The Version Space V is the set of all hypotheses that
  - cover all positive examples (*completeness*)
  - do not cover any negative examples (*consistency*)
- For structured hypothesis spaces there is an efficient representation consisting of
  - the general boundary G
    - all hypotheses in V for which no generalization is in V
  - the specific boundary S
    - all hypotheses in V for which no specialization is in V
- a hypothesis in V that is neither in G nor in S is
  - a generalization of at least one hypothesis in S
  - a specialization of at least one hypothesis in G

Candidate Elimination Algorithm

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- G = set of maximally general hypotheses
  S = set of maximally specific hypotheses
- For each training example e
  - if e is positive
    - For each hypothesis g in G that does not cover e
      - remove g from G
    - For each hypothesis s in S that does not cover e
      - remove s from S
      - $S = S \cup$ all hypotheses h such that
        - h is a minimal generalization of s
        - h covers e
        - some hypothesis in G is more general than h
      - remove from S any hypothesis that is more general than another hypothesis in S

Candidate Elimination Algorithm (Ctd.)

- if e is negative
  - For each hypothesis s in S that covers e
    - remove s from S
  - For each hypothesis g in G that covers e
    - remove g from G
    - $G = G \cup$ all hypotheses h such that
      - h is a minimal specialization of g
      - h does not cover e
      - some hypothesis in S is more specific than h
    - remove from G any hypothesis that is less general than another hypothesis in G

Example

No	Sky	Temperature	Humidity	Windy	Water	Forecast	Golf?
1	sunny	hot	normal	strong	warm	same	yes
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3	rainy	cool	high	strong	warm	change	no
4	sunny	hot	high	strong	cool	change	yes

S_0: { <Ø,Ø,Ø,Ø,Ø,Ø> }

G_0: { <?, ?, ?, ?, ?, ?> }

S_1: { <sunny, hot, normal, strong, warm,same> }

G_1: { <?, ?, ?, ?, ?, ?> }

S_2: { <sunny, hot, ?, strong, warm,same> }

G_2: { <?, ?, ?, ?, ?, ?> }

S_3: { <sunny, hot, ?, strong, warm,same> }

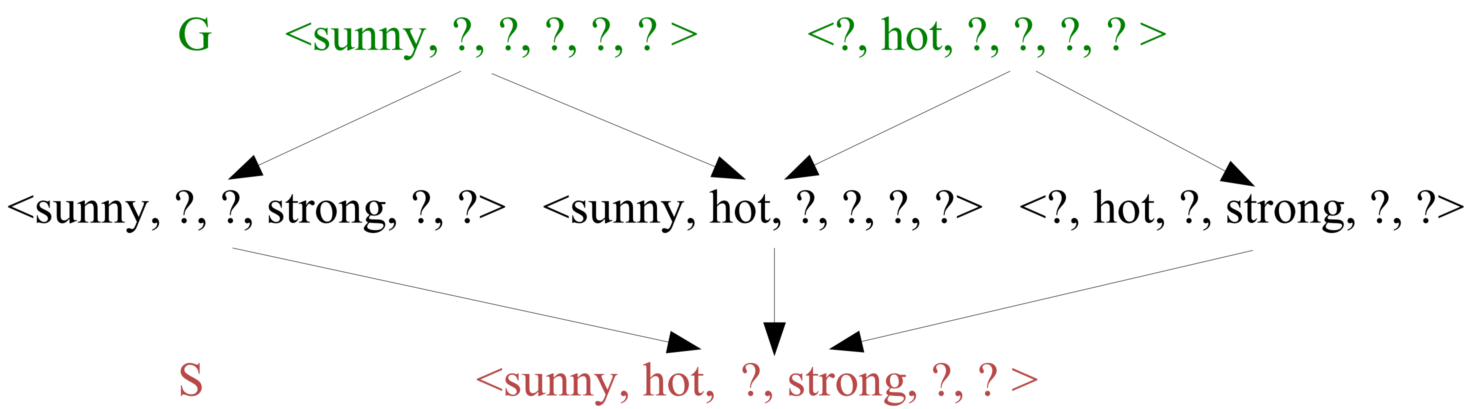
G_3: { <sunny, ?, ?, ?, ?, ? >
<?, hot, ?, ?, ?, ? >
<?, ?, ?, ?, ?, same > }

S_4: { <sunny, hot, ?, strong, ?, ? > }

G_4: { <sunny, ?, ?, ?, ?, ? >
<?, hot, ?, ?, ?, ? >}

How to Classify these Examples?

- Version Space:

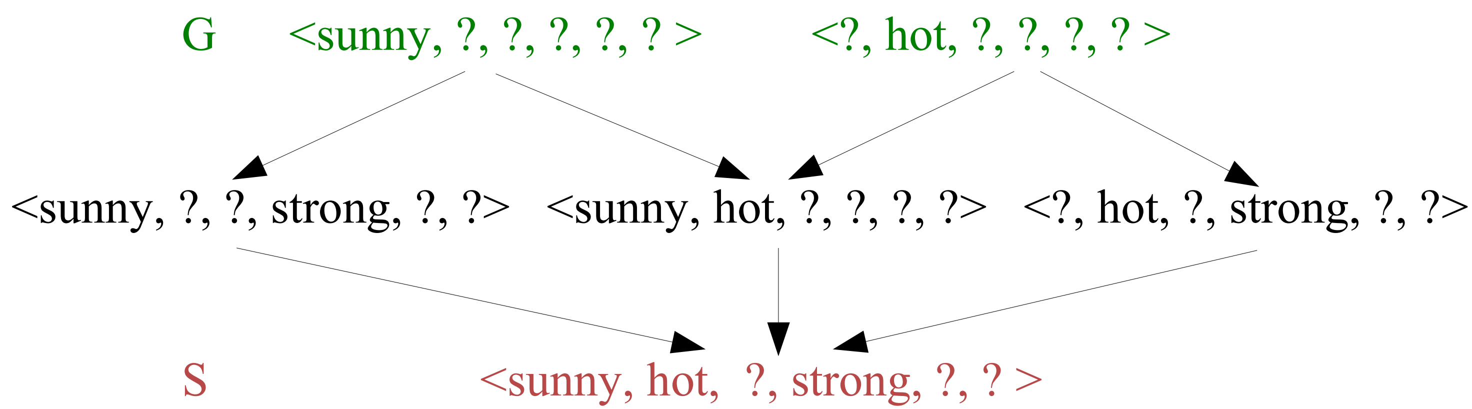


- How to Classify these Examples?

No	Sky	Temperature	Humidity	Windy	Water	Forecast	Golf?
1	sunny	hot	normal	strong	cool	change	?
2	rainy	cool	normal	light	warm	same	?
3	sunny	hot	normal	light	warm	same	?
4	sunny	cool	normal	strong	warm	same	?

How to Classify these Examples?

- Version Space:



- How to Classify these Examples?

No	Sky	Temperature	Humidity	Windy	Water	Forecast	Golf?
1	sunny	hot	normal	strong	cool	change	yes
2	rainy	cool	normal	light	warm	same	no
3	sunny	hot	normal	light	warm	same	?
4	sunny	cool	normal	strong	warm	same	maybe no

Properties

- Convergence towards target theory
  - convergence as soon as $S = G$
- Reliable classification with partially learned concepts
  - an example that matches all elements in S must be a member of the target concept
  - an example that matches no element in G cannot be a member of the target concept
  - examples that match parts of S and G are undecidable
- no need to remember examples (*incremental learning*)
- Assumptions
  - no errors in the training set
  - the hypothesis space contains the target theory
  - practical only if generality relation is (efficiently) computable

Generalization Operators for Numerical Attributes

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- Subset Generalization
  - generalization works as in symbolic case
  - specialization is difficult as there are infinitely many different values to specialize to
- Disjunctive Generalization
  - specialization and generalization as in symbolic case
  - problematic if no repetition of numeric values can be expected
    - generalization will only happen on training data
    - no new unseen examples are covered after a generalization
- Interval Generalization
  - the range of possible values is represented by an open or a closed interval
  - generalize by widening the interval to include the new point
  - specialize by shortening the interval to exclude the new point

Other Generality Relations

- First-Order
  - generalize the arguments of each pair of literals of the same relation
- Hierarchical Values
  - generalization and specialization for individual attributes follows the ontology

Summary

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- The hypothesis space of rules (typically) consists of conjunctions of propositional features
  - Other rule representations are possible (e.g., disjunctive rules)
- It can be structured via a generality relation between rules, which can in many cases be checked syntactically
  - i.e., without explicitly looking at the covered examples
- The version space is the set of theories that are complete and consistent with the training examples
- In a structured search space it can be found by identifying the set of most general and most specific hypotheses
  - The candidate elimination algorithm does that
- Not all concepts can be represented with single rules