

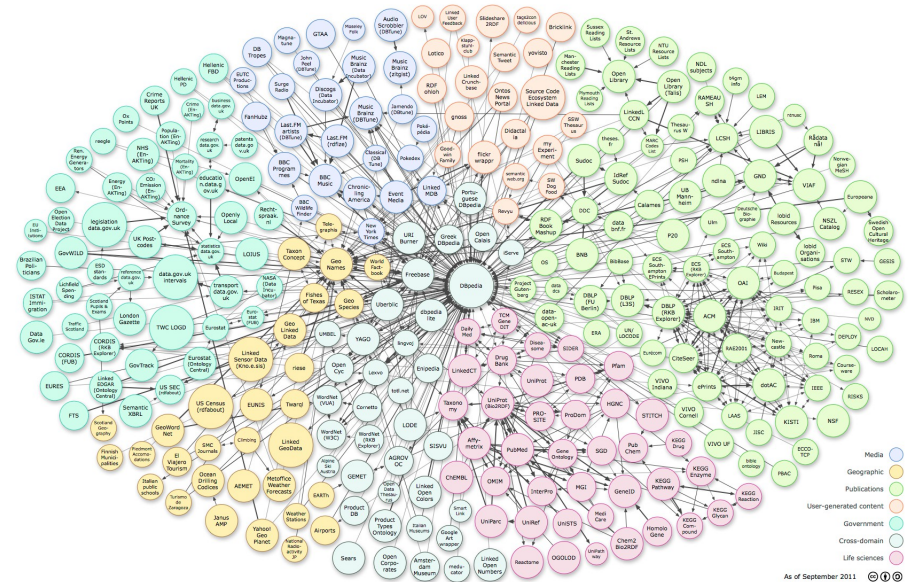
Data Mining and Machine Learning (Maschinelles Lernen: Symbolische Ansätze)

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?

- 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



- 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

- 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

if $(att_i = val_{iI})$ **and** $(att_j = val_{jJ})$

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.

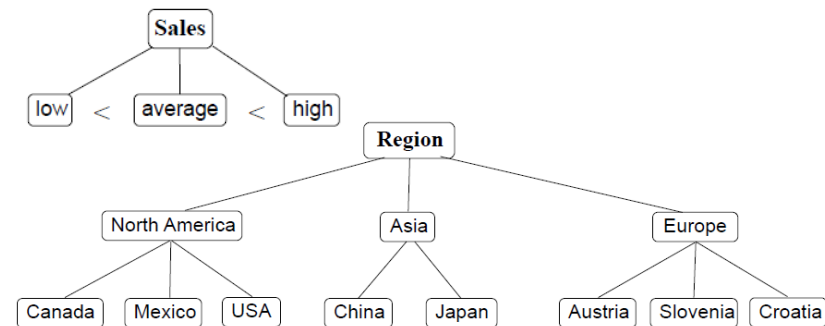
- simple logic of propositions
 - combination of simple facts (*features*)
 - no variables, no functions, no relations (\rightarrow predicate calculus)
 - Operators:
 - conjunction \wedge , disjunction \vee , negation \neg , implication \rightarrow , ...
- rules with attribute/value tests may be viewed 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: $\neg \text{windy} \wedge \text{sunny_outlook} \rightarrow \text{golf}$

Features

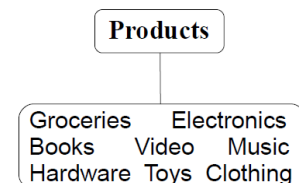
- A **feature** is a Boolean property of an object

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
- Set-valued features
 - compare to a set of values (e.g., a set of words)



Length > Height



Generality Relation

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

↓ more specific

Generality Relation for Rules

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

Examples:

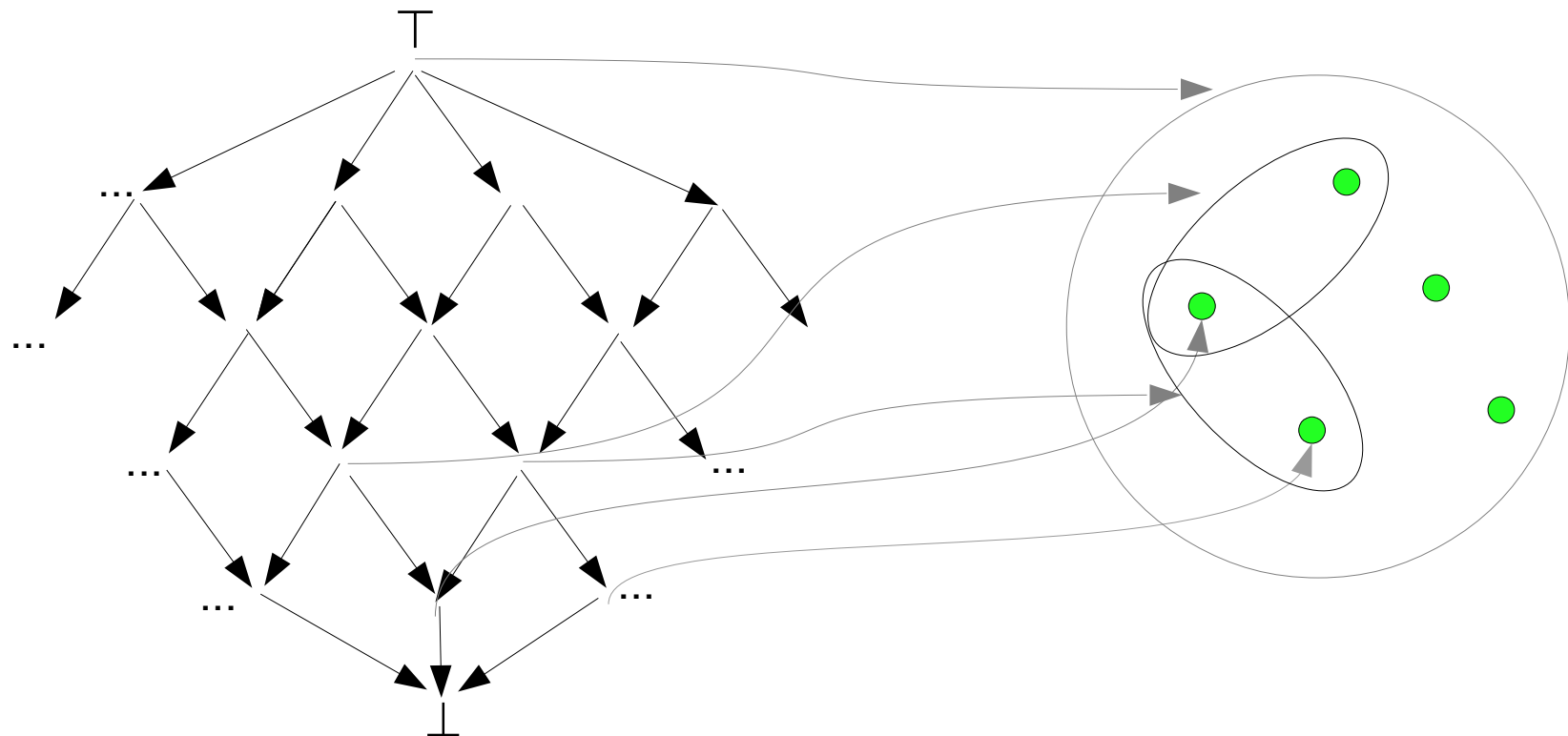
↓	<pre>if size > 5 then + if size > 3 then +</pre>	 	<pre>if animal = mammal then + if feeds_children = milk then +</pre>
↓	<pre>if outlook = sunny then + if outlook = sunny and windy = false then +</pre>		

Special Rules

- **Most general rule \top**
 - 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 \perp**
 - 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 \perp
 - 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 \rightarrow +
 \Rightarrow
color = blue \rightarrow +

■ Disjunctive Generalization

- another option is added to the test

shape = square & color = blue \rightarrow +
 \Rightarrow
shape = (square \vee rectangle)
& color = blue \rightarrow +

■ Hierarchical Generalization

- a generalization hierarchy is exploited

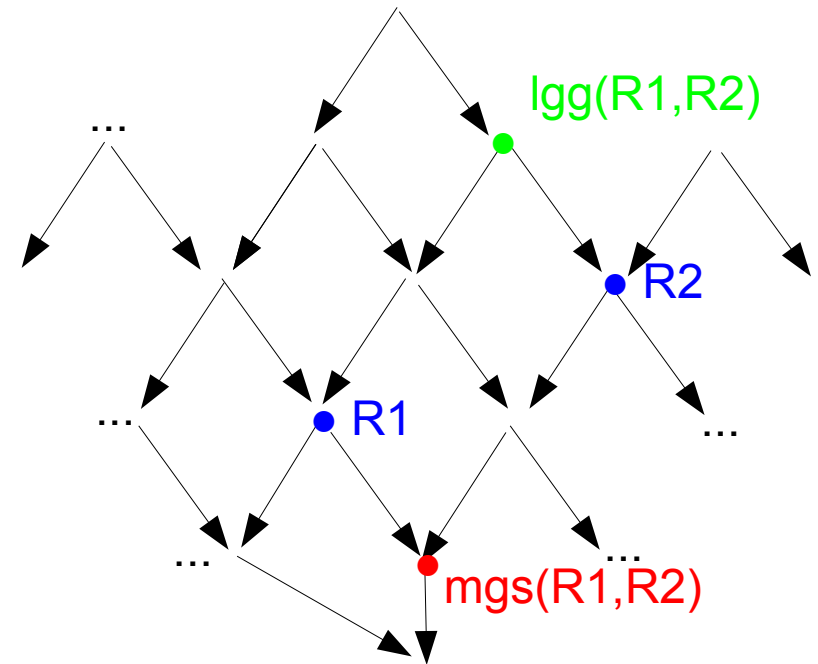
shape = square & color = blue \rightarrow +
 \Rightarrow
shape = quadrangle & color = blue \rightarrow +

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

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	sport?
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 +
< $\emptyset, \emptyset, \emptyset, \emptyset, \emptyset, \emptyset$ >

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
- \emptyset 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)

The hypothesis
if true then +

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

Minimal Subset
specialization
(other specializations
possible)

III. return h

Example

No.	Sky	Temperature	Humidity	Windy	Water	Forecast	sport?
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 || forecast = change) then +
 <?, ?, ?, ?, ?, ?>

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

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

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

H_4 : ?????

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

Other possibilities:

- <?, hot, ?, ?, ?, ?>
- <sunny, ?, ?, ?, ?, ?>

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	sport?
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

$G_0: \{ \langle ?, ?, ?, ?, ?, ? \rangle \}$

We now have a set of hypotheses!

$G_1: \{ \langle ?, ?, ?, ?, ?, ? \rangle \}$

$G_2: \{ \langle ?, ?, ?, ?, ?, ? \rangle \}$

Remember all possible refinements that exclude example 3

$G_3: \{ \langle \text{sunny}, ?, ?, ?, ?, ? \rangle, \langle ?, \text{hot}, ?, ?, ?, ? \rangle, \langle ?, ?, ?, ?, ?, \text{same} \rangle \}$

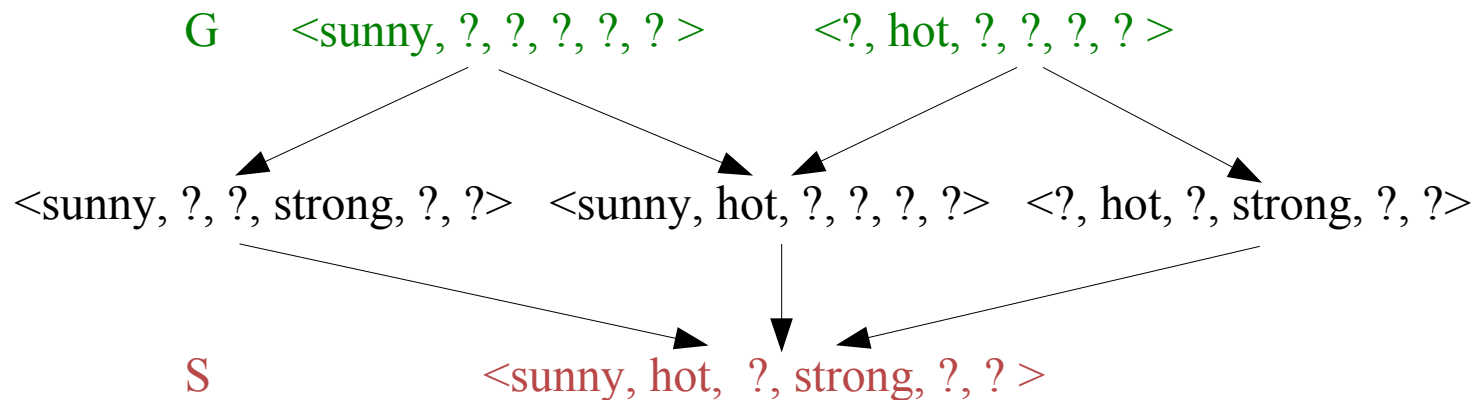
$G_4: \{ \langle \text{sunny}, ?, ?, ?, ?, ? \rangle, \langle ?, \text{hot}, ?, ?, ?, ? \rangle \}$

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 in our example consists of 6 hypotheses
 - i.e. 6 rules are complete and consistent with the 4 seen examples



- **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

- 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	sport?
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

$S_0: \{ \langle \emptyset, \emptyset, \emptyset, \emptyset, \emptyset, \emptyset \rangle \}$

$G_0: \{ \langle ?, ?, ?, ?, ?, ? \rangle \}$

$S_1: \{ \langle \text{sunny}, \text{hot}, \text{normal}, \text{strong}, \text{warm}, \text{same} \rangle \}$

$G_1: \{ \langle ?, ?, ?, ?, ?, ? \rangle \}$

$S_2: \{ \langle \text{sunny}, \text{hot}, ?, \text{strong}, \text{warm}, \text{same} \rangle \}$

$G_2: \{ \langle ?, ?, ?, ?, ?, ? \rangle \}$

$S_3: \{ \langle \text{sunny}, \text{hot}, ?, \text{strong}, \text{warm}, \text{same} \rangle \}$

$G_3: \{ \langle \text{sunny}, ?, ?, ?, ?, ? \rangle \}$

$\langle ?, \text{hot}, ?, ?, ?, ? \rangle$

$\langle ?, ?, ?, ?, ?, \text{same} \rangle \}$

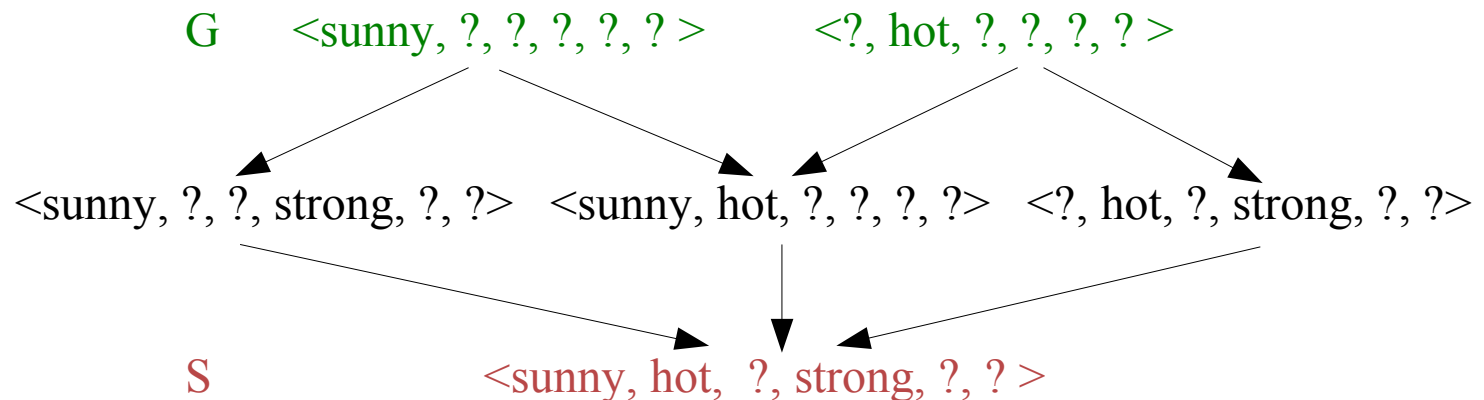
$S_4: \{ \langle \text{sunny}, \text{hot}, ?, \text{strong}, ?, ? \rangle \}$

$G_4: \{ \langle \text{sunny}, ?, ?, ?, ?, ? \rangle \}$

$\langle ?, \text{hot}, ?, ?, ?, ? \rangle \}$

How to Classify these Examples?

- Version Space:

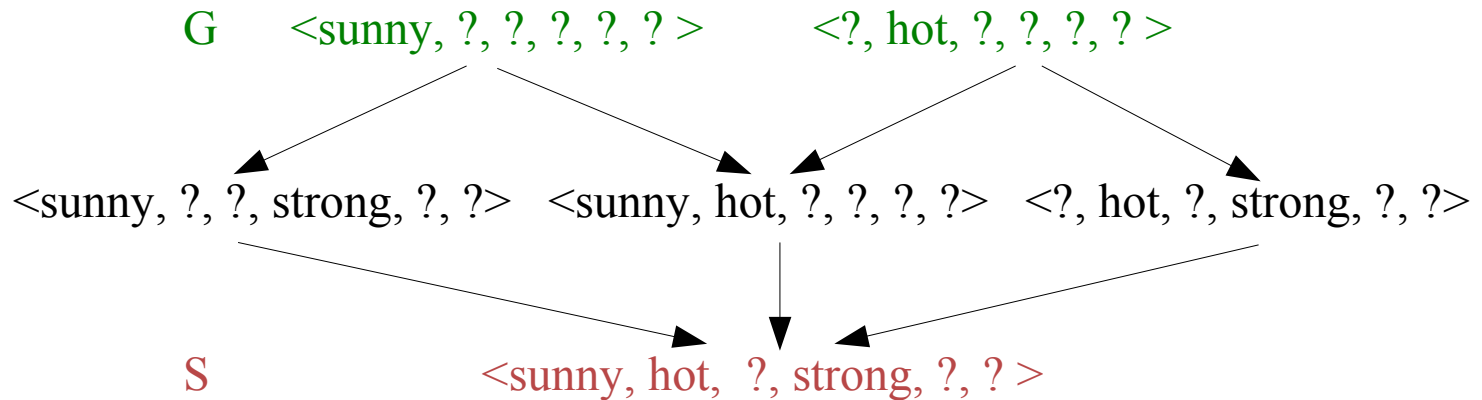


- How to Classify these Examples?

No.	Sky	Temperature	Humidity	Windy	Water	Forecast	sport?
5	sunny	hot	normal	strong	cool	change	?
6	rainy	cool	normal	light	warm	same	?
7	sunny	hot	normal	light	warm	same	?
8	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	sport?
5	sunny	hot	normal	strong	cool	change	yes
6	rainy	cool	normal	light	warm	same	no
7	sunny	hot	normal	light	warm	same	?
8	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

- **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

- 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