CS 622: Machine Learning: Inductive Classification

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Classification (Categorization)

- Given:
  - A description of an instance, $x \in X$, where X is the ***instance language*** or ***instance space***.
  - A fixed set of categories: $C=\{c_1, c_2, \ldots c_n\}$
- Determine:
  - The category of x: $c(x) \in C$, where $c(x)$ is a categorization function whose domain is X and whose range is C.
  - If $c(x)$ is a binary function $C=\{0,1\}$ ({true,false}, {positive, negative}) then it is called a ***concept***.

Learning for Categorization

- A training example is an instance $x \in X$, paired with its correct category $c(x)$: $<x, c(x)>$ for an unknown categorization function, c.
- Given a set of training examples, D.
- Find a hypothesized categorization function, $h(x)$, such that:

$$\forall < x, c(x) > \in D : h(x) = c(x)$$

Consistency

Sample Category Learning Problem

- Instance language: <size, color, shape>
  - size ∈ {small, medium, large}
  - color ∈ {red, blue, green}
  - shape ∈ {square, circle, triangle}
- C = {positive, negative}
- D:

Example	Size	Color	Shape	Category
1	small	red	circle	positive
2	large	red	circle	positive
3	small	red	triangle	negative
4	large	blue	circle	negative

Hypothesis Selection

- Many hypotheses are usually consistent with the training data.
  - red & circle
  - (small & circle) or (large & red)
  - (small & red & circle) or (large & red & circle)
  - not [(red & triangle) or (blue & circle)]
  - not [(small & red & triangle) or (large & blue & circle)]
- Bias
  - Any criteria other than consistency with the training data that is used to select a hypothesis.

Generalization

- Hypotheses must generalize enough to correctly classify instances not in the training data.
- Simply memorizing training examples is a consistent hypothesis that does not generalize.
- *Occam's razor*:
  - Finding a *simple* hypothesis helps ensure generalization.

Hypothesis Space

- Restrict learned functions a priori to a given ***hypothesis space***, *H*, of functions *h*(*x*) that can be considered as definitions of *c*(*x*).
- For learning concepts on instances described by *n* discrete-valued features, consider the space of conjunctive hypotheses represented by a vector of *n* constraints

  $<c_1, c_2, \ldots c_n>$ where each c_i is either:
  - ?, a wild card indicating no constraint on the *i*th feature
  - A specific value from the domain of the *i*th feature
  - Ø indicating no value is acceptable
- Sample conjunctive hypotheses are
  - <big, red, ?>
  - <?, ?, ?> (most general hypothesis)
  - < Ø, Ø, Ø> (most specific hypothesis)

Inductive Learning Hypothesis

- Any function that is found to approximate the target concept well on a sufficiently large set of training examples will also approximate the target function well on unobserved examples.
- Assumes that the training and test examples are drawn independently from the same underlying distribution.
- This is a fundamentally unprovable hypothesis unless additional assumptions are made about the target concept and the notion of "approximating the target function well on unobserved examples" is defined appropriately (cf. computational learning theory).

Evaluation of Classification Learning

- Classification accuracy (% of instances classified correctly).
  - Measured on an independent test data.
- Training time (efficiency of training algorithm).
- Testing time (efficiency of subsequent classification).

Category Learning as Search

- Category learning can be viewed as searching the hypothesis space for one (or more) hypotheses that are consistent with the training data.
- Consider an instance space consisting of n binary features which therefore has 2^n instances.
- For conjunctive hypotheses, there are 4 choices for each feature: Ø, T, F, ?, so there are 4^n syntactically distinct hypotheses.
- However, all hypotheses with 1 or more Øs are equivalent, so there are 3^n+1 semantically distinct hypotheses.
- The target binary categorization function in principle could be any of the possible $2^{2\wedge n}$ functions on n input bits.
- Therefore, conjunctive hypotheses are a small subset of the space of possible functions, but both are intractably large.
- All reasonable hypothesis spaces are intractably large or even infinite.

Learning by Enumeration

- For any finite or countably infinite hypothesis space, one can simply enumerate and test hypotheses one at a time until a consistent one is found.

```
For each $h$ in $H$ do:
    If $h$ is consistent with the training data $D$,
        then terminate and return $h$.
```

- This algorithm is guaranteed to terminate with a consistent hypothesis if one exists; however, it is obviously computationally intractable for almost any practical problem.

Efficient Learning

- Is there a way to learn conjunctive concepts without enumerating them?
- How do human subjects learn conjunctive concepts?
- Is there a way to efficiently find an unconstrained boolean function consistent with a set of discrete-valued training instances?
- If so, is it a useful/practical algorithm?

Conjunctive Rule Learning

- Conjunctive descriptions are easily learned by finding all commonalities shared by all positive examples.

Example	Size	Color	Shape	Category
1	small	red	circle	positive
2	large	red	circle	positive
3	small	red	triangle	negative
4	large	blue	circle	negative

Learned rule: red & circle → positive

- Must check consistency with negative examples. If inconsistent, **no** conjunctive rule exists.

Limitations of Conjunctive Rules

- If a concept does not have a single set of necessary and sufficient conditions, conjunctive learning fails.

Example	Size	Color	Shape	Category
1	small	red	circle	positive
2	large	red	circle	positive
3	small	red	triangle	negative
4	large	blue	circle	negative
5	medium	red	circle	negative

Learned rule: red & circle → positive

Inconsistent with negative example #5!

Disjunctive Concepts

- Concept may be disjunctive.

Example	Size	Color	Shape	Category
1	small	red	circle	positive
2	large	red	circle	positive
3	small	red	triangle	negative
4	large	blue	circle	negative
5	medium	red	circle	negative

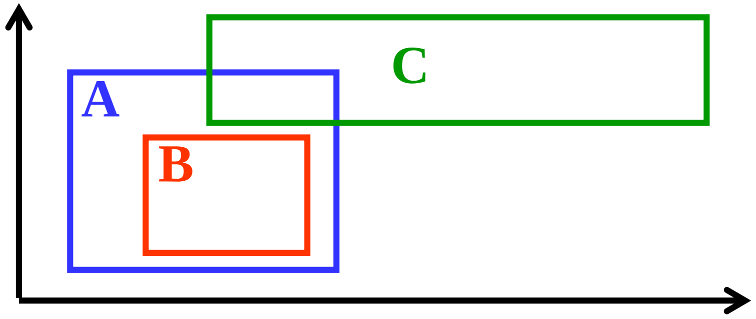
Learned rules: small & circle → positive
large & red → positive

Using the Generality Structure

- By exploiting the structure imposed by the generality of hypotheses, an hypothesis space can be searched for consistent hypotheses without enumerating or explicitly exploring all hypotheses.
- An instance, $x \in X$, is said to ***satisfy*** an hypothesis, h, iff $h(x)=1$ (positive)
- Given two hypotheses h_1 and h_2, h_1 is ***more general than or equal to*** h_2 ($h_1 \geq h_2$) iff every instance that satisfies h_2 also satisfies h_1.
- Given two hypotheses h_1 and h_2, h_1 is **(*strictly*) *more general than*** h_2 ($h_1 > h_2$) iff $h_1 \geq h_2$ and it is not the case that $h_2 \geq h_1$.
- Generality defines a partial order on hypotheses.

Examples of Generality

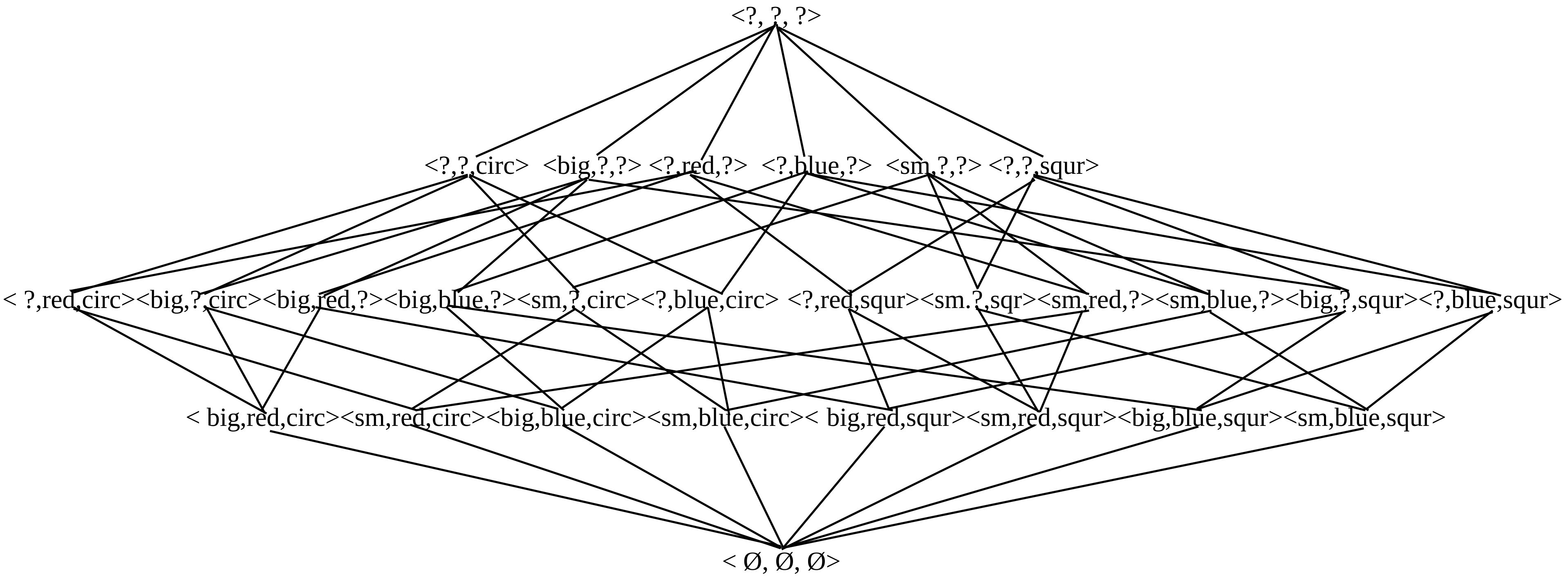
- Conjunctive feature vectors
  - <?, red, ?> is more general than <?, red, circle>
  - Neither of <?, red, ?> and <?, ?, circle> is more general than the other.
- Axis-parallel rectangles in 2-d space



  - A is more general than B
  - Neither of A and C are more general than the other.

Sample Generalization Lattice

Size: {sm, big}   Color: {red, blue}   Shape: {circ, squr}



<?, ?, ?>
<?,?,circ> <big,?,?> <?,red,?> <?,blue,?> <sm,?,?> <?,?,squr>
< ?,red,circ><big,?,circ><big,red,?><big,blue,?><sm,?,circ><?,blue,circ> <?,red,squr><sm.?,sqr><sm,red,?><sm,blue,?><big,?,squr><?,blue,squr>
< big,red,circ><sm,red,circ><big,blue,circ><sm,blue,circ>< big,red,squr><sm,red,squr><big,blue,squr><sm,blue,squr>
< Ø, Ø, Ø>

Number of hypotheses = $3^3 + 1 = 28$

Most Specific Learner (Find-S)

- Find the most-specific hypothesis (least-general generalization, LGG) that is consistent with the training data.
- Incrementally update hypothesis after every positive example, generalizing it just enough to satisfy the new example.
- For conjunctive feature vectors, this is easy:

```
Initialize $h$ = <Ø, Ø,… Ø>
For each positive training instance $x$ in $D$
    For each feature $f_i$
        If the constraint on $f_i$ in $h$ is **not** satisfied by $x$
            If $f_i$ in $h$ is Ø
                then set $f_i$ in $h$ to the value of $f_i$ in $x$
                else set $f_i$ in $h$ to “?”
If $h$ is consistent with the negative training instances in $D$
  then return $h$
  else no consistent hypothesis exists
```

Time complexity: $O(|D|\ n)$ if n is the number of features

Properties of Find-S

- For conjunctive feature vectors, the most-specific hypothesis is unique and found by Find-S.
- If the most specific hypothesis is not consistent with the negative examples, then there is no consistent function in the hypothesis space, since, by definition, it cannot be made more specific and retain consistency with the positive examples.
- For conjunctive feature vectors, if the most-specific hypothesis is inconsistent, then the target concept must be disjunctive.

Another Hypothesis Language

- Consider the case of two *unordered* objects each described by a fixed set of attributes.
  - {<big, red, circle>, <small, blue, square>}
- What is the most-specific generalization of:
  - Positive: {<big, red, triangle>, <small, blue, circle>}
  - Positive: {<big, blue, circle>, <small, red, triangle>}
- LGG is not unique, two incomparable generalizations are:
  - {<big, ?, ?>, <small, ?, ?>}
  - {<?, red, triangle>, <?, blue, circle>}
- For this space, Find-S would need to maintain a continually growing set of LGGs and eliminate those that cover negative examples.
- Find-S is no longer tractable for this space since the number of LGGs can grow exponentially.

Issues with Find-S

- Given sufficient training examples, does Find-S converge to a correct definition of the target concept (assuming it is in the hypothesis space)?
- How de we know when the hypothesis has converged to a correct definition?
- Why prefer the most-specific hypothesis? Are more general hypotheses consistent? What about the most-general hypothesis? What about the simplest hypothesis?
- If the LGG is not unique
  - Which LGG should be chosen?
  - How can a single consistent LGG be efficiently computed or determined not to exist?
- What if there is noise in the training data and some training examples are incorrectly labeled?

Effect of Noise in Training Data

- Frequently realistic training data is corrupted by errors (noise) in the features or class values.
- Such noise can result in missing valid generalizations.
  - For example, imagine there are many positive examples like #1 and #2, but out of many negative examples, only one like #5 that actually resulted from a error in labeling.

Example	Size	Color	Shape	Category
1	small	red	circle	positive
2	large	red	circle	positive
3	small	red	triangle	negative
4	large	blue	circle	negative
5	medium	red	circle	negative

Version Space

- Given an hypothesis space, *H*, and training data, *D*, the ***version space*** is the complete subset of *H* that is consistent with *D*.
- The version space can be naively generated for any finite *H* by enumerating all hypotheses and eliminating the inconsistent ones.
- Can one compute the version space more efficiently than using enumeration?

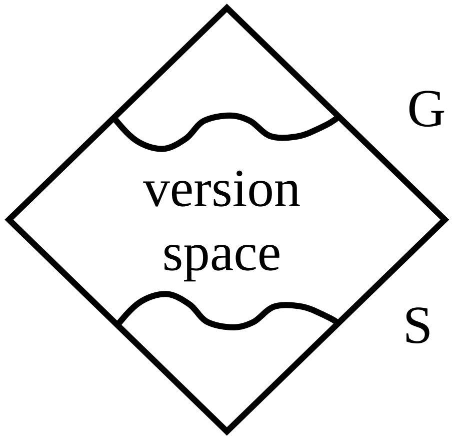
Version Space with S and G

- The version space can be represented more compactly by maintaining two boundary sets of hypotheses, *S*, the set of most specific consistent hypotheses, and *G*, the set of most general consistent hypotheses:

$$S = \{s \in H \mid Consistent(s, D) \wedge \neg\exists s' \in H[s > s' \wedge Consistent(s', D)]\}$$

$$G = \{g \in H \mid Consistent(g, D) \wedge \neg\exists g' \in H[g' > g \wedge Consistent(s', D)]\}$$

- S and G represent the entire version space via its boundaries in the generalization lattice:



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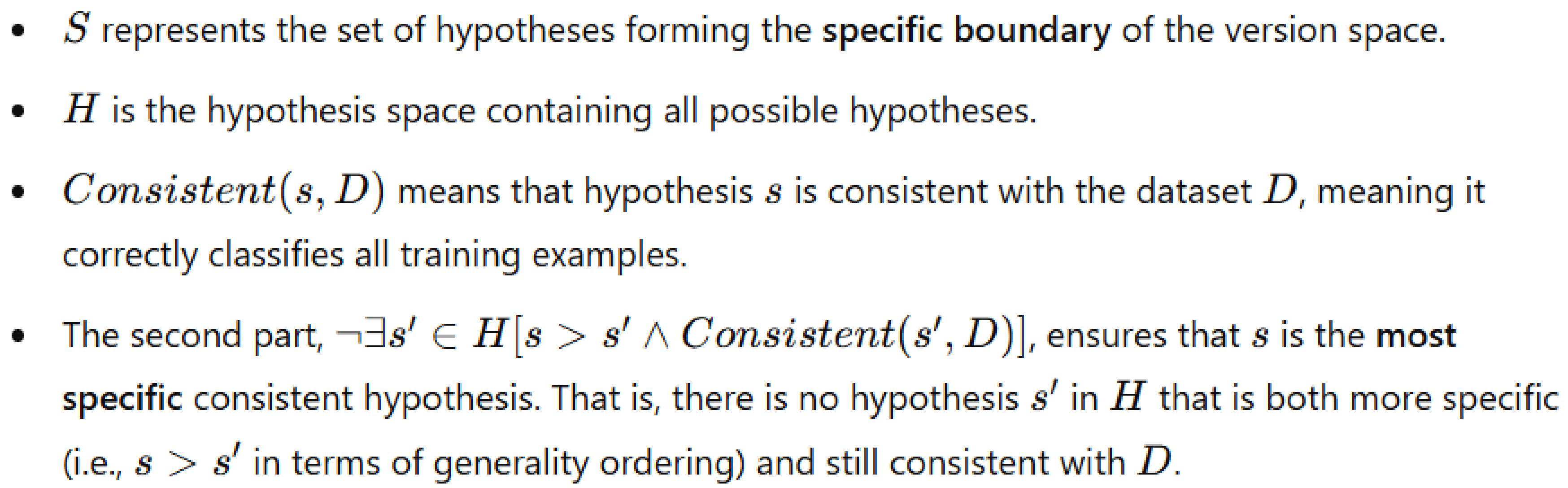
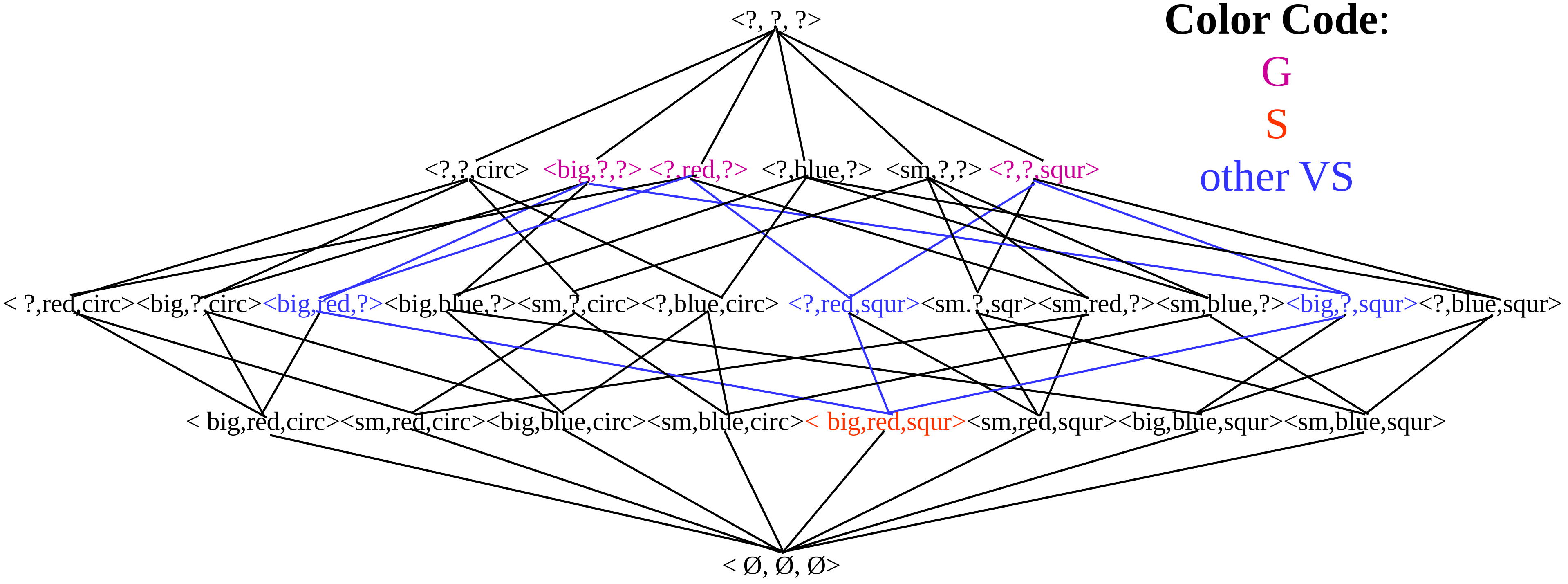


- S represents the set of hypotheses forming the **specific boundary** of the version space.
- H is the hypothesis space containing all possible hypotheses.
- $Consistent(s, D)$ means that hypothesis s is consistent with the dataset D, meaning it correctly classifies all training examples.
- The second part, $\neg \exists s' \in H[s > s' \wedge Consistent(s', D)]$, ensures that s is the **most specific** consistent hypothesis. That is, there is no hypothesis s' in H that is both more specific (i.e., $s > s'$ in terms of generality ordering) and still consistent with D.

Version Space Lattice

Size: {sm, big}   Color: {red, blue}   Shape: {circ, squr}



Color Code:

G

S

other VS

<<big, red, squr> positive>

<<sm, blue, circ> negative>

Example

Example Dataset

•*Hypotheses must classify positive examples correctly while excluding negatives.*

Example	Color	Size	Shape	Label (Fruit?)
1	Red	Small	Round	Yes
2	Red	Medium	Round	Yes
3	Yellow	Small	Round	No

Specific Boundary (S) Construction

- Finding the Most Specific Hypothesis
  - Start with the first positive example: (Red, Small, Round).
  - Compare with the second positive example: (Red, Medium, Round).
  - Generalize Size to {Small, Medium}.
  - Negative example (Yellow, Small, Round) is ignored.
  - Final S-Boundary: (Red, {Small, Medium}, Round).

General Boundary (G) Construction

- Finding the Most General Hypothesis
  - Start with the most general form: (?, ?, ?).
  - Adjust based on the negative example (Yellow, Small, Round, No).
  - Exclude Yellow from Color.
  - General form remains for Size and Shape.
  - Final G-Boundary: (≠ Yellow, ?, ?)

Version Space Representation

- Hypothesis Ordering in Version Space
  - Version Space consists of all hypotheses between S and G.
  - S: (Red, {Small, Medium}, Round).
  - G: (≠ Yellow, ?, ?)
  - Example hypotheses:
  - (Red, ?, Round) → More general than S.
  - (≠ Yellow, {Small, Medium}, ?) → Between S and G.

Candidate Elimination (Version Space) Algorithm

```
Initialize $G$ to the set of most-general hypotheses in $H$
Initialize $S$ to the set of most-specific hypotheses in $H$
For each training example, $d$, do:
    If $d$ is a positive example then:
        Remove from $G$ any hypotheses that do not match $d$
        For each hypothesis $s$ in $S$ that does not match $d$
            Remove $s$ from $S$
            Add to $S$ all minimal generalizations, $h$, of $s$ such that:
                1)  $h$ matches $d$
                2) some member of $G$ is more general than $h$
        Remove from $S$ any $h$ that is more general than another hypothesis in $S$
    If $d$ is a negative example then:
        Remove from $S$ any hypotheses that match $d$
        For each hypothesis $g$ in $G$ that matches $d$
            Remove $g$ from $G$
            Add to $G$ all minimal specializations, $h$, of $g$ such that:
                1) $h$ does not match $d$
                2) some member of $S$ is more specific than $h$
        Remove from $G$ any $h$ that is more specific than another hypothesis in $G$
```

Required Subroutines

- To instantiate the algorithm for a specific hypothesis language requires the following procedures:
  - equal-hypotheses(h_1, h_2)
  - more-general(h_1, h_2)
  - match(h, i)
  - initialize-g()
  - initialize-s()
  - generalize-to(h, i)
  - specialize-against(h, i)

Minimal Specialization and Generalization

- Procedures generalize-to and specialize-against are specific to a hypothesis language and can be complex.
- For conjunctive feature vectors:
  - generalize-to: unique, see Find-S
  - specialize-against: not unique, can convert each "?" to an alernative non-matching value for this feature.
    - Inputs:
      - *h* = <?, red, ?>
      - *i* = <small, red, triangle>
    - Outputs:
      - <big, red, ?>
      - <medium, red, ?>
      - <?, red, square>
      - <?, red, circle>

Sample VS Trace

S= {< Ø, Ø, Ø>}; *G*= {<?, ?, ?>}

Positive: <big, red, circle>
Nothing to remove from *G*
Minimal generalization of only *S* element is <big, red, circle> which is more specific than *G*.
S={<big, red, circle>}; *G*={<?, ?, ?>}

Negative: <small, red, triangle>
Nothing to remove from *S*.
Minimal specializations of <?, ?, ?> are <medium, ?, ?>, <big, ?, ?>, <?, blue, ?>, <?, green, ?>, <?, ?, circle>, <?, ?, square> but most are not more general than some element of *S*
S={<big, red, circle>}; *G*={<big, ?, ?>, <?, ?, circle>}

Sample VS Trace (cont)

S={<big, red, circle>}; *G*={<big, ?, ?>, <?, ?, circle>}

Positive: <small, red, circle>
Remove <big, ?, ?> from *G*
Minimal generalization of <big, red, circle> is <?, red, circle>
S={<?, red, circle>}; *G*={<?, ?, circle>}

Negative: <big, blue, circle>
Nothing to remove from *S*
Minimal specializations of <?, ?, circle> are <small, ? circle>, <medium, ?, circle>, <?, red, circle>, <?, green, circle> but most are not more general than some element of *S*.
S={<?, red, circle>}; *G*={<?, red, circle>}

S=*G*; Converged!

Properties of VS Algorithm

- *S* summarizes the relevant information in the positive examples (relative to *H*) so that positive examples do not need to be retained.
- *G* summarizes the relevant information in the negative examples, so that negative examples do not need to be retained.
- Result is not affected by the order in which examples are processes but computational efficiency may.
- Positive examples move the *S* boundary up; Negative examples move the *G* boundary down.
- If *S* and *G* converge to the same hypothesis, then it is the only one in *H* that is consistent with the data.
- If *S* and *G* become empty (if one does the other must also) then there is no hypothesis in *H* consistent with the data.

Correctness of Learning

- Since the entire version space is maintained, given a continuous stream of noise-free training examples, the VS algorithm will eventually converge to the correct target concept if it is in the hypothesis space, *H*, or eventually correctly determine that it is not in *H*.
- Convergence is correctly indicated when S=G.

Computational Complexity of VS

- Computing the *S* set for conjunctive feature vectors is linear in the number of features and the number of training examples.
- Computing the *G* set for conjunctive feature vectors is exponential in the number of training examples in the worst case.
- In more expressive languages, both *S* and *G* can grow exponentially.
- The order in which examples are processed can significantly affect computational complexity.

Active Learning

- In ***active learning***, the system is responsible for selecting good training examples and asking a teacher (oracle) to provide a class label.
- In ***sample selection***, the system picks good examples to query by picking them from a provided pool of unlabeled examples.
- In ***query generation***, the system must generate the description of an example for which to request a label.
- Goal is to minimize the number of queries required to learn an accurate concept description.

Active Learning with VS

- An ideal training example would eliminate half of the hypotheses in the current version space regardless of its label.
- If a training example matches half of the hypotheses in the version space, then the matching half is eliminated if the example is negative, and the other (non-matching) half is eliminated if the example is positive.
- Example:
  - Assume training set
    - Positive: <big, red, circle>
    - Negative: <small, red, triangle>
  - Current version space:
    - {<big, red, circle>, <big, red, ?>, <big, ?, circle>, <?, red, circle> <?, ?, circle> <big, ?, ?>}
  - An optimal query: <big, blue, circle>
- Given a ceiling of $\log_2|VS|$ such examples will result in convergence. This is the best possible guarantee in general.

Using an Unconverged VS

- If the VS has not converged, how does it classify a novel test instance?
- If all elements of *S* match an instance, then the entire version space much (since it is more general) and it can be confidently classified as positive (assuming target concept is in *H*).
- If no element of *G* matches an instance, then the entire version space must not (since it is more specific) and it can be confidently classified as negative (assuming target concept is in *H*).
- Otherwise, one could vote all of the hypotheses in the VS (or just the *G* and *S* sets to avoid enumerating the VS) to give a classification with an associated confidence value.
- Voting the entire VS is probabilistically optimal assuming the target concept is in *H* and all hypotheses in *H* are equally likely *a priori*.

Learning for Multiple Categories

- What if the classification problem is not concept learning and involves more than two categories?
- Can treat as a series of concept learning problems, where for each category, C_i, the instances of C_i are treated as positive and all other instances in categories C_j, $j \neq i$ are treated as negative (***one-versus-all***).
- This will assign a unique category to each training instance but may assign a novel instance to zero or multiple categories.
- If the binary classifier produces confidence estimates (e.g. based on voting), then a novel instance can be assigned to the category with the highest confidence.
- Other approaches exist, such as learning to discriminate all pairs of categories (***all-pairs***) and combining decisions appropriately during test.

Inductive Bias

- Inductive bias refers to the set of assumptions a learning algorithm makes to generalize beyond the observed training data. Since machine learning models cannot learn from infinite data, they rely on prior knowledge to make predictions on unseen instances.

Inductive Bias

- Final S: (Red,{Small,Medium},Round)
- Final G: (≠Yellow,?,?)
- Here, the inductive bias assumes:
  - Color is important (since Yellow is excluded).
  - Size can vary among fruits.
  - Shape remains unchanged.

Inductive Bias

- How Inductive Bias Affects Learning
- Stronger Bias (more restrictive assumptions): Faster learning but less flexibility.
- Weaker Bias (fewer assumptions): More flexibility but requires more data to generalize correctly.
- Incorrect Bias: Can lead to overgeneralization or overspecialization.

Inductive Bias

- A hypothesis space that does not include all possible classification functions on the instance space incorporates a bias in the type of classifiers it can learn.
- Any means that a learning system uses to choose between two functions that are both consistent with the training data is called ***inductive bias***.
- Inductive bias can take two forms:
  - ***Language bias***: The language for representing concepts defines a hypothesis space that does not include all possible functions (e.g. conjunctive descriptions).
  - ***Search bias***: The language is expressive enough to represent all possible functions (e.g. disjunctive normal form) but the search algorithm embodies a preference for certain consistent functions over others (e.g. syntactic simplicity).

Unbiased Learning

- For instances described by *n* features each with *m* values, there are m^n instances. If these are to be classified into *c* categories, then there are $c^{m\wedge n}$ possible classification functions.
  - For n=10, m=c=2, there are approx. 3.4x10^{38} possible functions, of which only 59,049 can be represented as conjunctions (an incredibly small percentage!)
- However, unbiased learning is futile since if we consider all possible functions then simply memorizing the data without any real generalization is as good an option as any.
- Without bias, the version-space is always trivial. The unique most-specific hypothesis is the disjunction of the positive instances and the unique most general hypothesis is the negation of the disjunction of the negative instances:

$$S = \{(p_1 \vee p_2 \vee \ldots \vee p_k)\}$$

$$G = \{\neg(n_1 \vee n_2 \vee \ldots \vee n_j)\}$$

Futility of Bias-Free Learning

- A learner that makes no *a priori* assumptions about the target concept has no rational basis for classifying any unseen instances.
- Inductive bias can also be defined as the assumptions that, when combined with the observed training data, logically entail the subsequent classification of unseen instances.
  - Training-data + inductive-bias |— novel-classifications
- The bias of the VS algorithm (assuming it refuses to classify an instance unless it is classified the same by all members of the VS), is simply that *H* contains the target concept.
- The rote learner, which refuses to classify any instance unless it has seen it during training, is the least biased.
- Learners can be partially ordered by their amount of bias
  - Rote-learner < VS Algorithm < Find-S

No Panacea

- No Free Lunch (NFL) Theorem (Wolpert, 1995)

  Law of Conservation of Generalization Performance (Schaffer, 1994)
  - One can prove that improving generalization performance on unseen data for some tasks will always decrease performance on other tasks (which require different labels on the unseen instances).
  - Averaged across all possible target functions, no learner generalizes to unseen data any better than any other learner.
- There does not exist a learning method that is uniformly better than another for all problems.
- Given any two learning methods *A* and *B* and a training set, *D*, there always exists a target function for which *A* generalizes better (or at least as well) as *B*.
  - Train both methods on *D* to produce hypotheses h_A and h_B.
  - Construct a target function that labels all unseen instances according to the predictions of h_A.
  - Test h_A and h_B on any unseen test data for this target function and conclude that h_A is better.

Logical View of Induction

- Deduction is inferring sound specific conclusions from general rules (axioms) and specific facts.
- Induction is inferring general rules and theories from specific empirical data.
- Induction can be viewed as inverse deduction.
  - Find a hypothesis *h* from data *D* such that
    - $h \cup B \vdash D$

      where *B* is optional background knowledge
- ***Abduction*** is similar to induction, except it involves finding a specific hypothesis, *h*, that best *explains* a set of evidence, *D*, or inferring cause from effect. Typically, in this case *B* is quite large compared to induction and *h* is smaller and more specific to a particular event.

Induction and the Philosophy of Science

- Bacon (1561-1626), Newton (1643-1727) and the sound deductive derivation of knowledge from data.
- Hume (1711-1776) and the ***problem of induction***.
  - Inductive inferences can never be proven and are always subject to disconfirmation.
- Popper (1902-1994) and ***falsifiability***.
  - Inductive hypotheses can only be falsified not proven, so pick hypotheses that are most subject to being falsified.
- Kuhn (1922-1996) and ***paradigm shifts***.
  - Falsification is insufficient, an alternative paradigm must be available that is clearly elegant and more explanatory must be available.
    - Ptolmaic epicycles and the Copernican revolution
    - Orbit of Mercury and general relativity
    - Solar neutrino problem and neutrinos with mass
- Postmodernism: Objective truth does not exist; relativism; science is a social system of beliefs that is no more valid than others (e.g. religion).