CMT311 Principles of Machine Learning

Concept Learning, ERM & PAC

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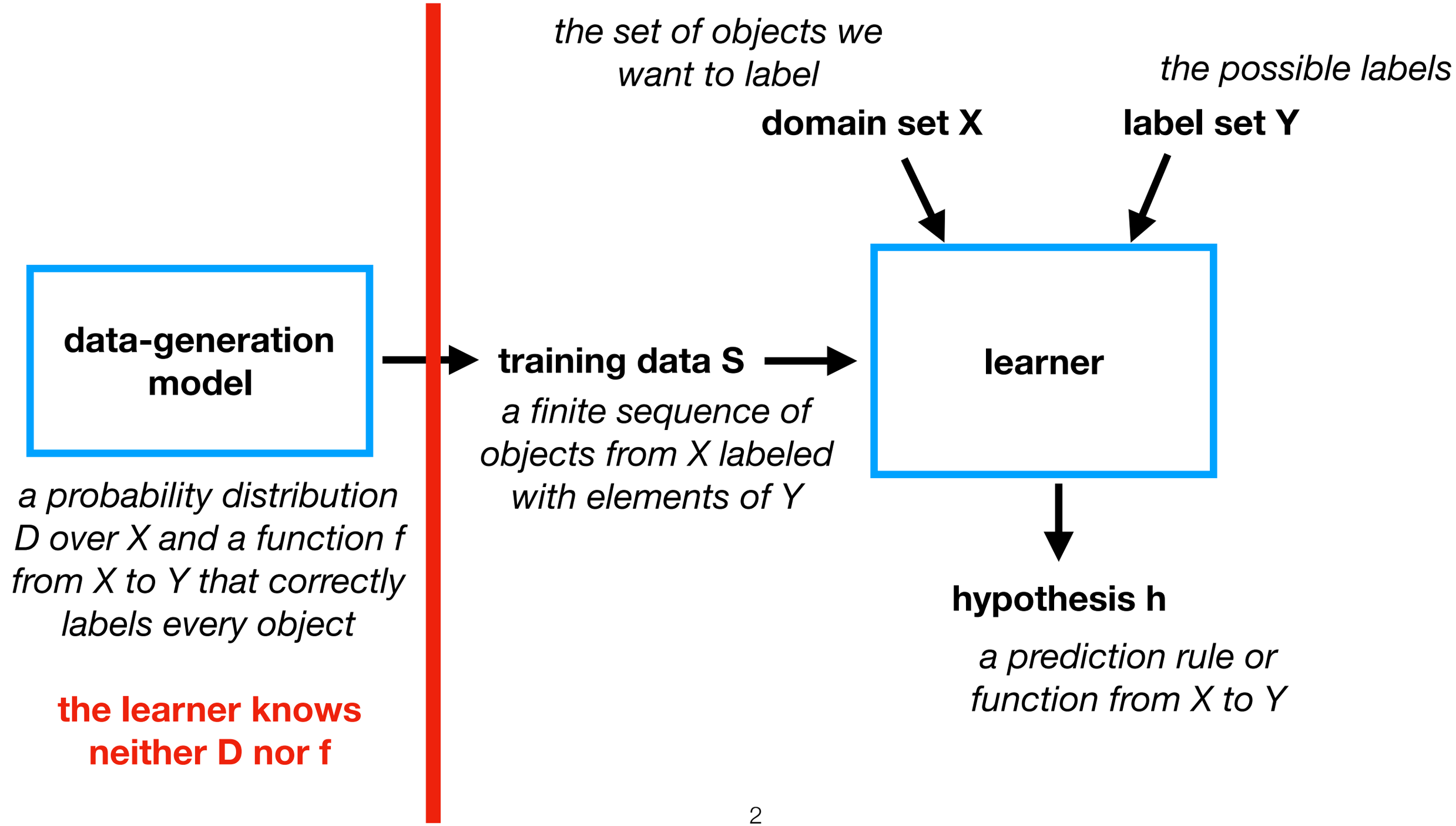
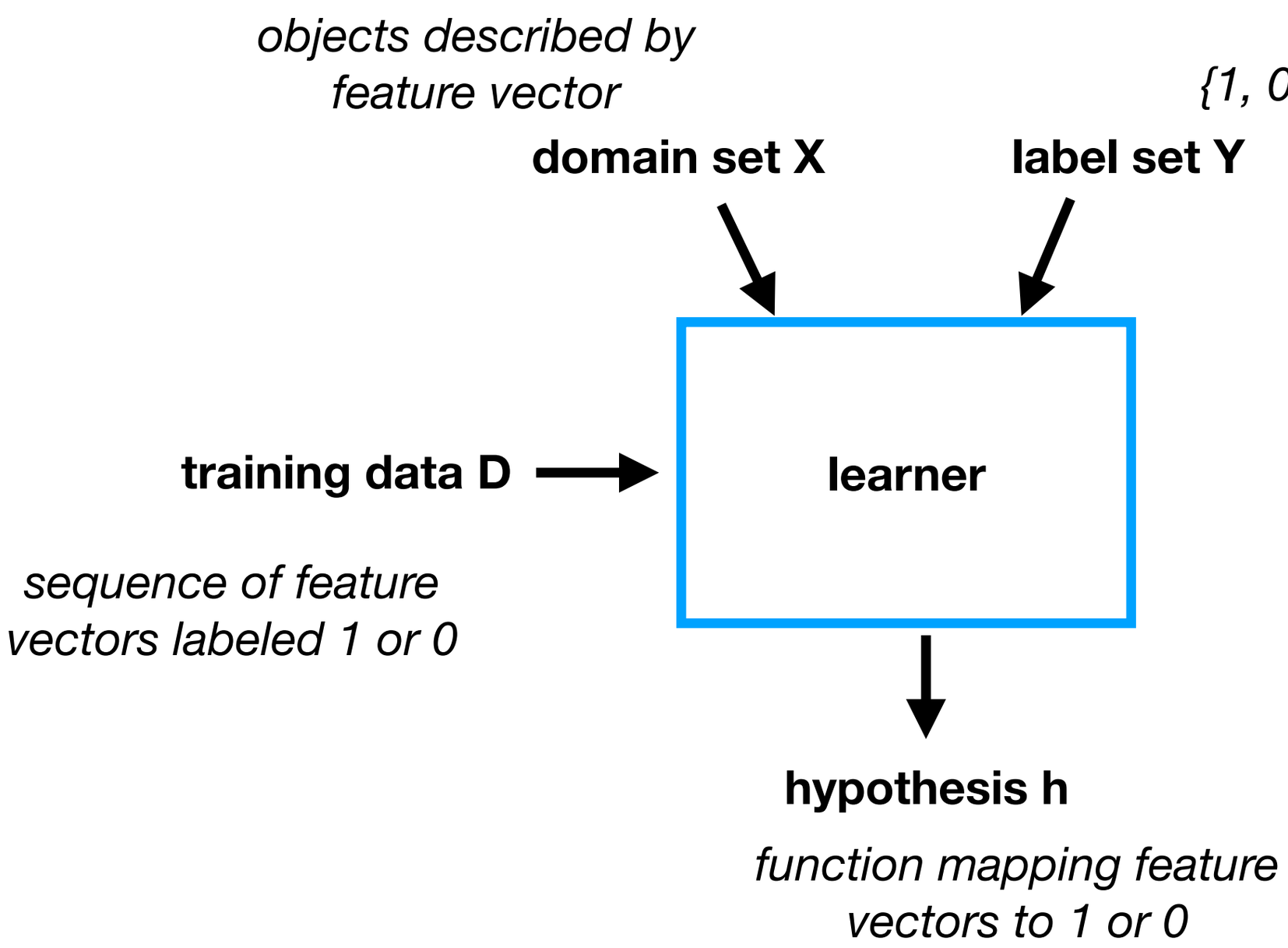
The Statistical Learning Framework



Boolean Concept Learning



Example

days described by

< Sky, AirTemp, Humidity, Wind, Water, Forecast >

Sunny / Cloudy / Rainy

Warm / Cold

Normal / High

Strong / Weak

Warm / Cool

Same / Change

labels 1 / 0 indicating whether someone enjoys their favourite sport on that day

domain set X

label set Y

training data D

learner

<Sunny, Warm, Normal, Strong, Warm, Same> 1
<Sunny, Warm, High, Strong, Warm, Same> 1
<Rainy, Cold, High, Strong, Warm, Change> 0
<Sunny, Warm, High, Strong, Cool, Change> 1

hypothesis h

conjunction of attribute constraints using ?, -, specific values

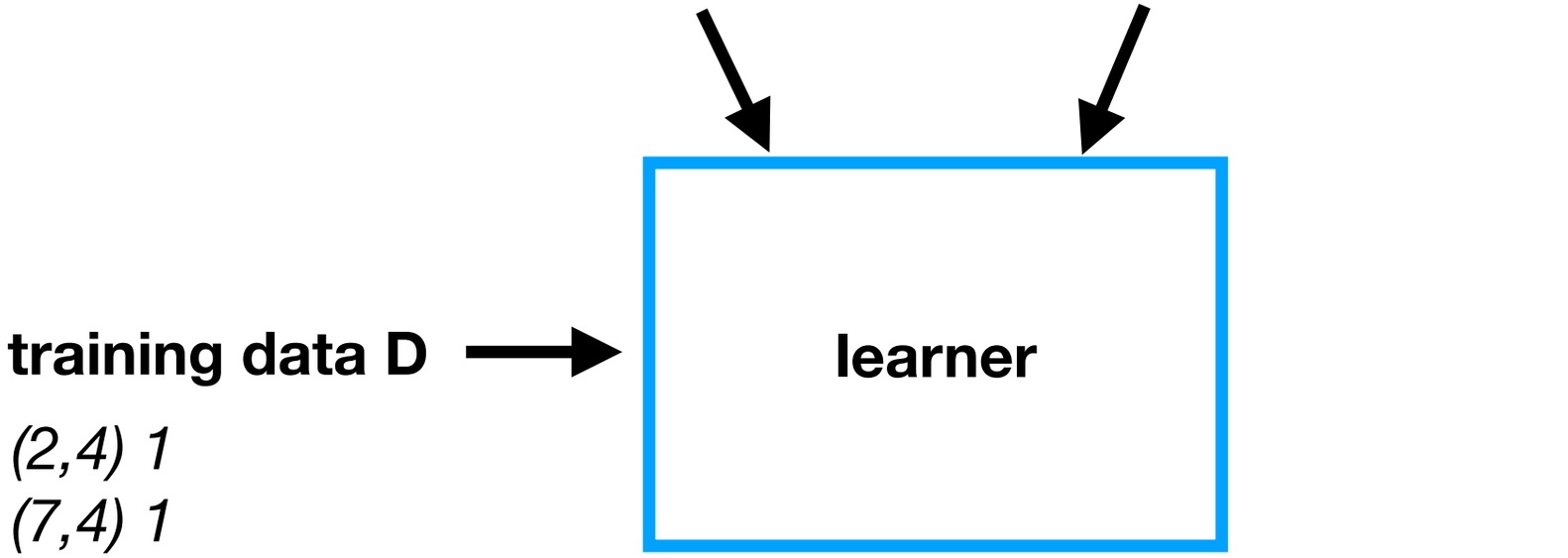
Example

points on a grid, described by coordinates (x,y) with $x \in [0,10]$, $y \in [0,10]$

labels 1 / 0

domain set X

label set Y



More-general-than

- Let h_j and h_k be two Boolean-valued functions defined over X.

- Then h_j is **more general than or equal to** h_k, $h_j \geq_g h_k$, if and only if
  $\forall x \in X : h_k(x) = 1 \rightarrow h_j(x) = 1$

- h_j is **strictly more general than** h_k, $h_j >_g h_k$, if and only if $h_j \geq_g h_k$ and $h_k \not\geq_g h_j$

- h_j is **more specific than** h_k if and only if h_k is more general than h_j

- note: these notions are **independent** of the target concept

General-to-specific ordering

$$h_j \geq_g h_k \text{ if and only if } \forall x \in X : h_k(x) = 1 \rightarrow h_j(x) = 1$$

< *Sky, AirTemp, Humidity, Wind, Water, Forecast* >

Sunny / Cloudy / Rainy

Warm / Cold

Normal / High

Strong / Weak

Warm / Cool

Same / Change

h_1	h_2
<?,Cold,?,?,?,?>	<?,Cold,High,?,?,?>
<?,Cold,?,Strong,Cool,?>	<?,?,?,?,?,?>
<?,Cold,?,Strong,Cool,?>	<?,Cold,High,?,?,?>
<?,Cold,?,?,?,?>	<-,-,-,-,-,->
<-,-,-,-,-,->	<?,Cold,High,-,?,?>
<Sunny,Cold,High,Weak,Warm,Same>	<Sunny,Cold,High,Weak,Cool,Same>

General-to-specific ordering

$$h_j \geq_g h_k \text{ if and only if } \forall x \in X : h_k(x) = 1 \rightarrow h_j(x) = 1$$

rectangle (a≤x≤b ∧ c≤y≤d)
with a,b,c,d integers in [0,10]

h_1	h_2
(0≤x≤10 ∧ 0≤y≤10)	(0≤x≤10 ∧ 1≤y≤5)
(0≤x≤10 ∧ 1≤y≤5)	(0≤x≤9 ∧ 1≤y≤5)
(10≤x≤10 ∧ 1≤y≤1)	(0≤x≤10 ∧ 1≤y≤5)
(0≤x≤10 ∧ 1≤y≤5)	(10≤x≤0 ∧ 1≤y≤5)
(10≤x≤0 ∧ 1≤y≤5)	(3≤x≤1 ∧ 10≤y≤5)
(2≤x≤4 ∧ 3≤y≤7)	(1≤x≤4 ∧ 3≤y≤8)

A basic learner: FIND-S

- set *h* to the most specific hypothesis in *H*
- for each positive *x* in *D*
  - for each constraint *a* in *h*
    - if *x* does not satisfy *a* then replace *a* in *h* by the next more general constraint *a'* that is satisfied by *x*
- return *h*

Example

days described by
< Sky, AirTemp, Humidity, Wind, Water, Forecast >

Sunny / Cloudy / Rainy

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labels 1 / 0 indicating whether someone enjoys their favourite sport on that day

domain set X

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training data D

learner

<Sunny, Warm, Normal, Strong, Warm, Same> 1
<Sunny, Warm, High, Strong, Warm, Same> 1
<Rainy, Cold, High, Strong, Warm, Change> 0
<Sunny, Warm, High, Strong, Cool, Change> 1

hypothesis h

conjunction of attribute constraints using ?, -, specific values

training example	current hypothesis h
-	<-,-,-,-,-,->
<Sunny, Warm, Normal, Strong, Warm, Same> 1	<Sunny, Warm, Normal, Strong, Warm, Same>
<Sunny, Warm, High, Strong, Warm, Same> 1	<Sunny, Warm, ?, Strong, Warm, Same>
<Rainy, Cold, High, Strong, Warm, Change> 0	<Sunny, Warm, ?, Strong, Warm, Same>
<Sunny, Warm, High, Strong, Cool, Change> 1	<Sunny, Warm, ?, Strong, ?, ?>

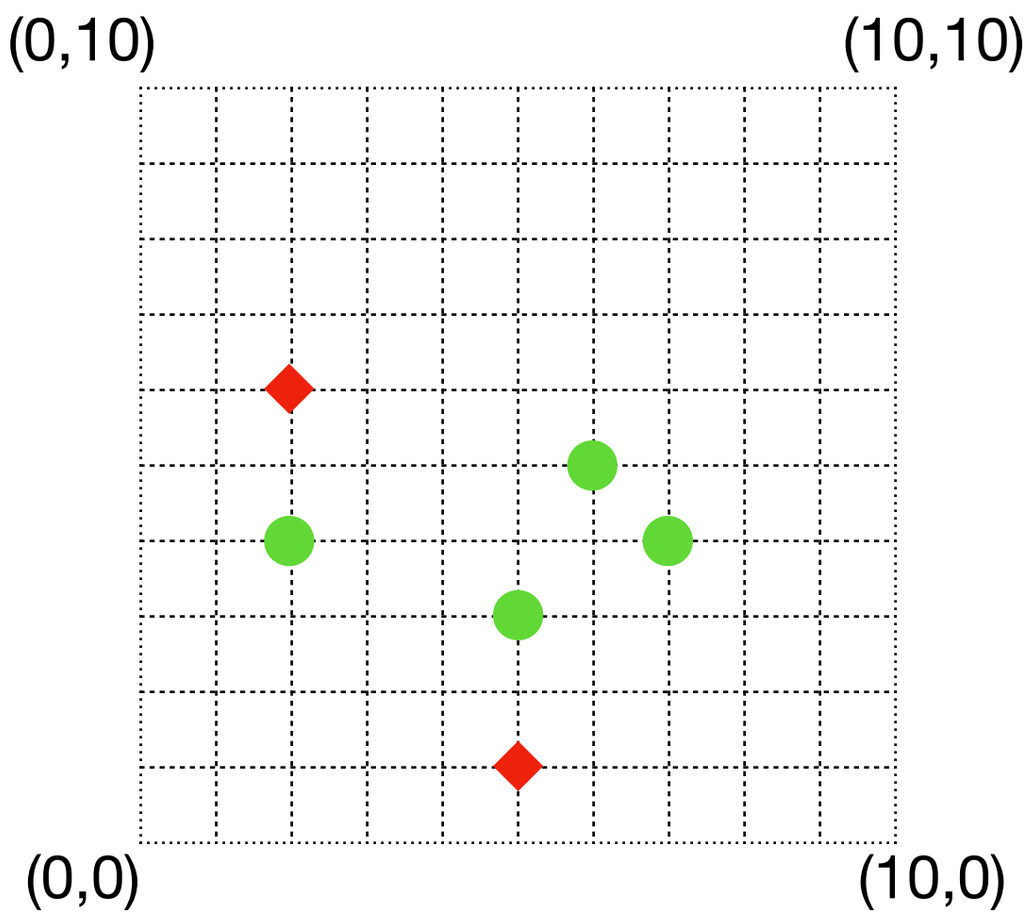
hypothesis returned by FIND-S

Exercise

- Consider again the space of rectangles ($a \le x \le b \wedge c \le y \le d$) on the [0,10]x[0,10] grid.

- Trace the FIND-S algorithm for the following sequence of examples:

(2,4) 1
(7,4) 1
(5,1) 0
(5,3) 1
(2,6) 0
(6,5) 1



FIND-S: Discussion

- the hypothesis returned by FIND-S is
  - the most specific one in H that correctly labels all positive training examples
  - correctly labels all negative training examples, provided that the correct target concept is in H and the training data is correct
- open questions:
  - has the learner converged to the correct answer?
  - why prefer the most specific h?
  - what if the training data is not labeled correctly?
  - what if there are several maximally specific hypotheses for the training data?

Using version spaces

- A hypothesis h is **consistent** with training data D if and only if for all examples (x,y) in D, h(x)=y

- Goal: a learner that finds all hypotheses in H that are consistent with D, using the “more general than” order

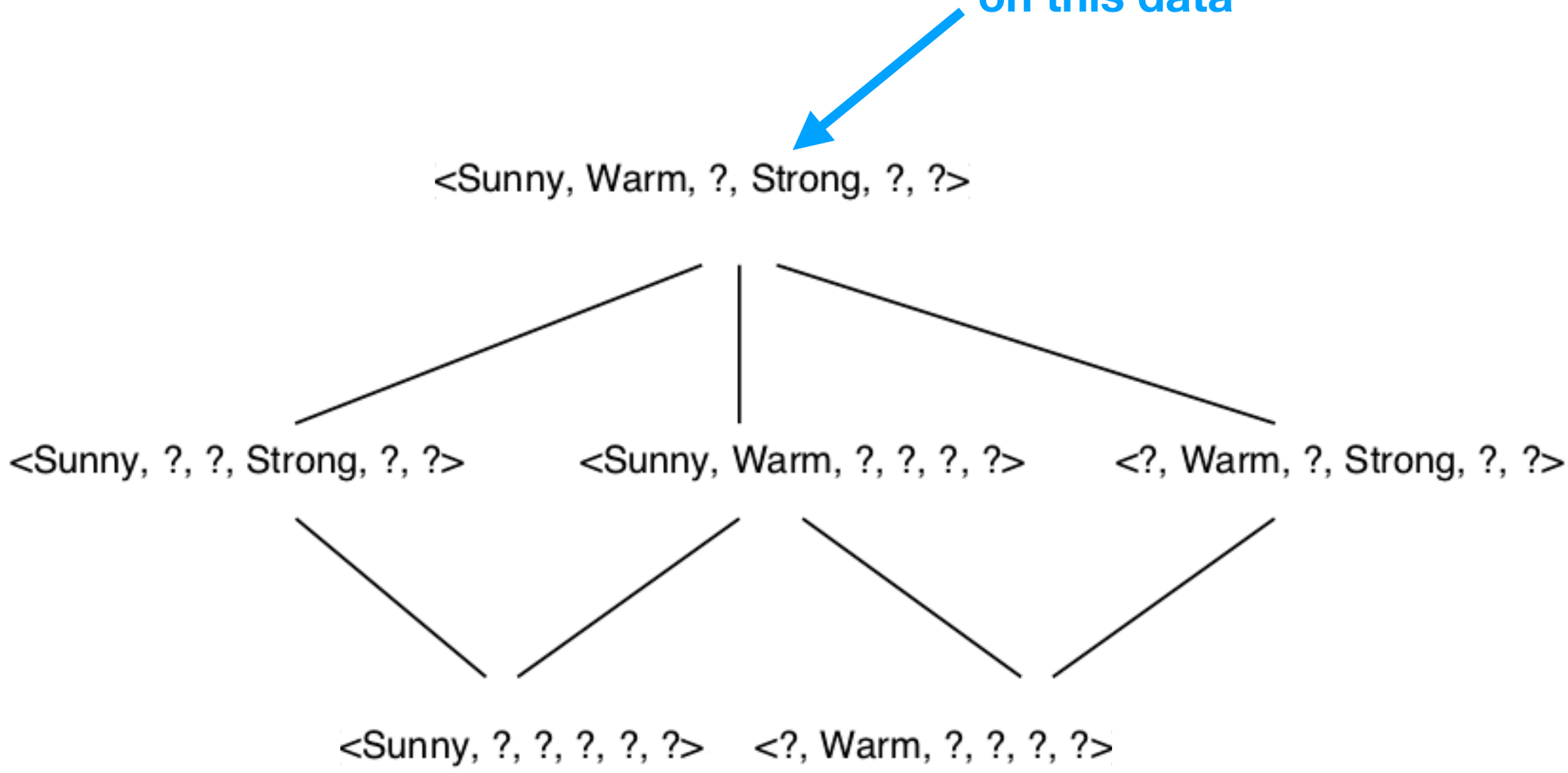
- The **version space** $VS_{H,D}$ with respect to hypothesis space H and training data D is the set of all hypotheses in H consistent with D

$$VS_{H,D} \equiv \{h \in H \mid consistent(h, D)\}$$

Example

<Sunny, Warm, Normal, Strong, Warm, Same> 1
<Sunny, Warm, High, Strong, Warm, Same> 1
<Rainy, Cold, High, Strong, Warm, Change> 0
<Sunny, Warm, High, Strong, Cool, Change> 1

the hypothesis returned by FIND-S on this data



[Figure: Mitchell]

another learner: LIST-THEN-ELIMINATE

- VS = list of all hypotheses in H
- for each example (x,y) in D
  - remove from VS all h with h(x)≠y
- return VS

Version space boundaries

- The **general boundary G** with respect to hypothesis space H and training data D is the set of maximally general members of H consistent with D.

$$G \equiv \{g \in H \mid consistent(g, D) \wedge \neg \exists g' \in H : g' >_g g \wedge consistent(g', D)\}$$

- The **specific boundary S** with respect to hypothesis space H and training data D is the set of minimally general members of H consistent with D.

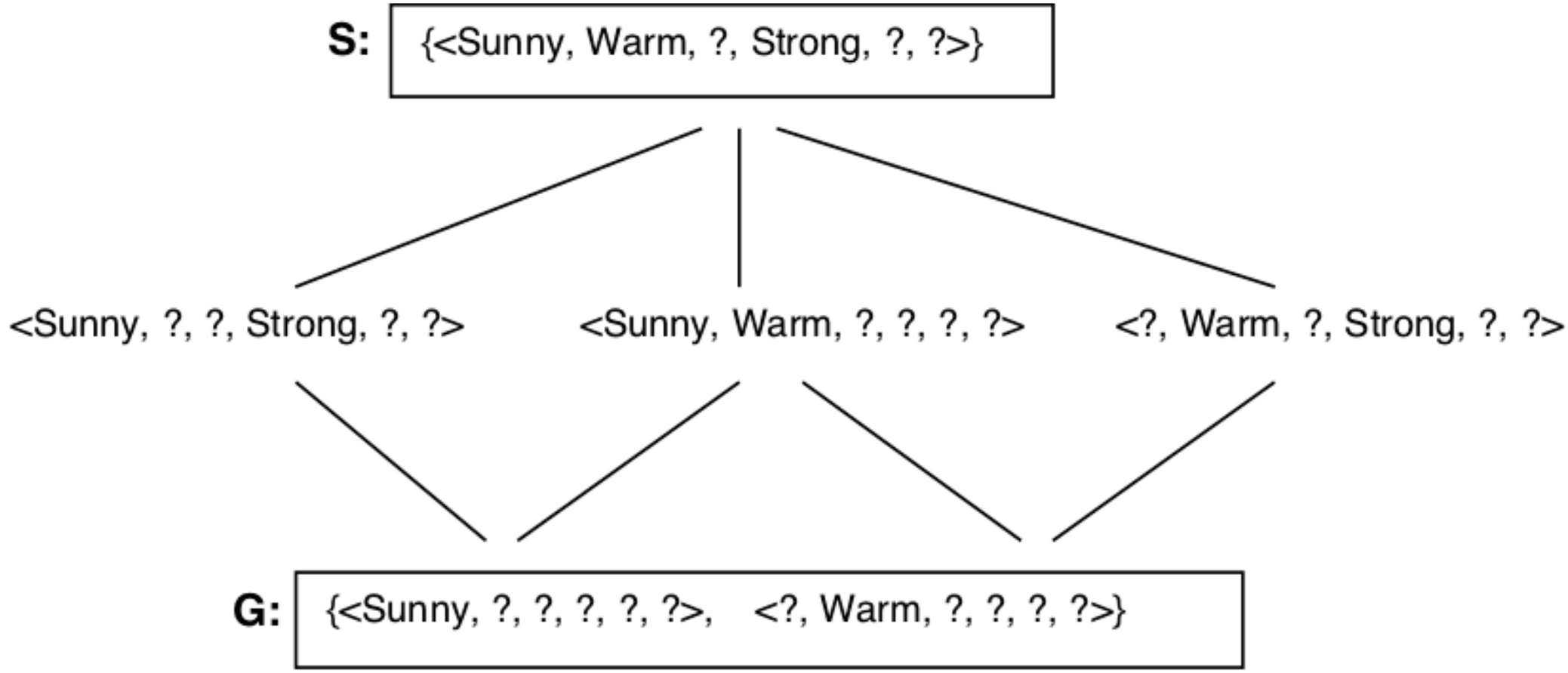
$$S \equiv \{s \in H \mid consistent(s, D) \wedge \neg \exists s' \in H : s >_g s' \wedge consistent(s', D)\}$$

- Every member of the version space lies between G and S:

$$VS_{H,D} = \{h \in H \mid \exists s \in S : \exists g \in G : g \geq_g h \geq_g s\}$$

Example

<Sunny, Warm, Normal, Strong, Warm, Same> 1
<Sunny, Warm, High, Strong, Warm, Same> 1
<Rainy, Cold, High, Strong, Warm, Change> 0
<Sunny, Warm, High, Strong, Cool, Change> 1



[Figure: Mitchell]

CANDIDATE-ELIMINATION

- G = set of maximally general hypotheses in H
- S = set of maximally specific hypotheses in H
- for each training example d
    - if d is positive
        - remove from G any h inconsistent with d
        - for each s in S that is not consistent with d
            - remove s from S
            - add to S all minimal generalisations h of s such that h is consistent with d and some member of G is more general than h
            - remove from S any h that is more general than some h’ in S
- if d is negative
    - remove from S any h inconsistent with d
    - for each g in G that is not consistent with d
        - remove g from G
        - add to G all minimal specialisations h of g such that h is consistent with d and some member of S is more specific than h
        - remove from G any h that is less general than some h’ in G

Example

days described by

< Sky, AirTemp, Humidity, Wind, Water, Forecast >

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Strong / Weak

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domain set X

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<Sunny, Warm, Normal, Strong, Warm, Same> 1
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hypothesis h

conjunction of attribute constraints using ?, -, specific values

G={<?,?,?,?,?,?>}

S={<-,-,-,-,-,->}

<Sunny, Warm, Normal, Strong, Warm, Same> 1

<Sunny, Warm, High, Strong, Warm, Same> 1

<Rainy, Cold, High, Strong, Warm, Change> 0

<Sunny, Warm, High, Strong, Cool, Change> 1

<Sunny, Warm, Normal, Strong, Warm, Same> 1

G={<?,?,?,?,?,?>}

S={<Sunny,Warm,Normal,Strong,Warm,Same>}

<Sunny, Warm, High, Strong, Warm, Same> 1

G={<?,?,?,?,?,?>}

S={<Sunny,Warm,?,Strong,Warm,Same>}

<Rainy, Cold, High, Strong, Warm, Change> 0

G={<Sunny,?,?,?,?,?>, <?,Warm,?,?,?,?>, <?,?,?,?,?,Same>}

S={<Sunny,Warm,?,Strong,Warm,Same>}

<Sunny, Warm, High, Strong, Cool, Change> 1

G={<Sunny,?,?,?,?,?>, <?,Warm,?,?,?,?>}

S={<Sunny,Warm,?,Strong,?,?>}

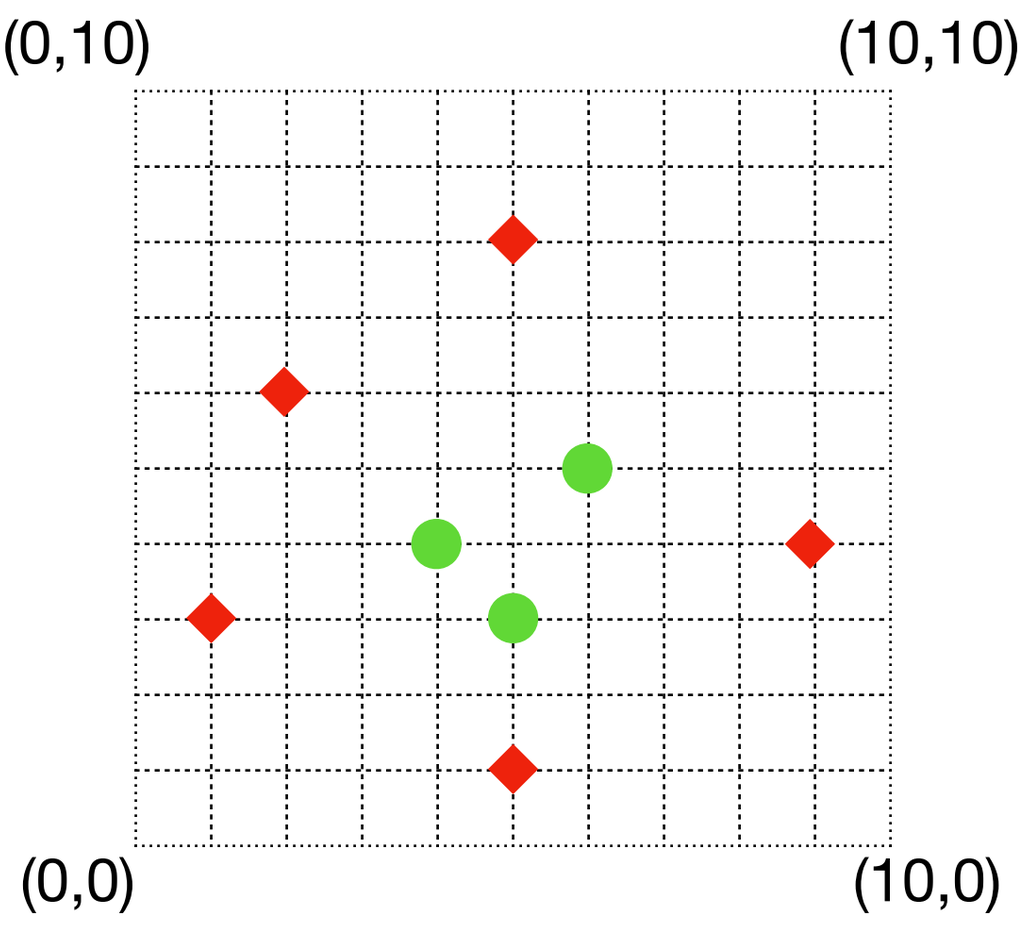
Exercise

- Consider again the space of rectangles ($a \le x \le b \wedge c \le y \le d$) on the [0,10]x[0,10] grid, and the positive ● and negative ◆ training examples in the figure.

- What are the G and S boundaries of the version space? Write them down and draw them on the grid.

- Imagine the learner can ask the teacher to label a specific point as next training example. Suggest a point that would guarantee to shrink the version space independently of its label, and one that wouldn't.

- What is the smallest number of examples for which CANDIDATE-ELIMINATION can precisely learn any specific rectangle, say, ($2 \le x \le 8 \wedge 3 \le y \le 5$)?

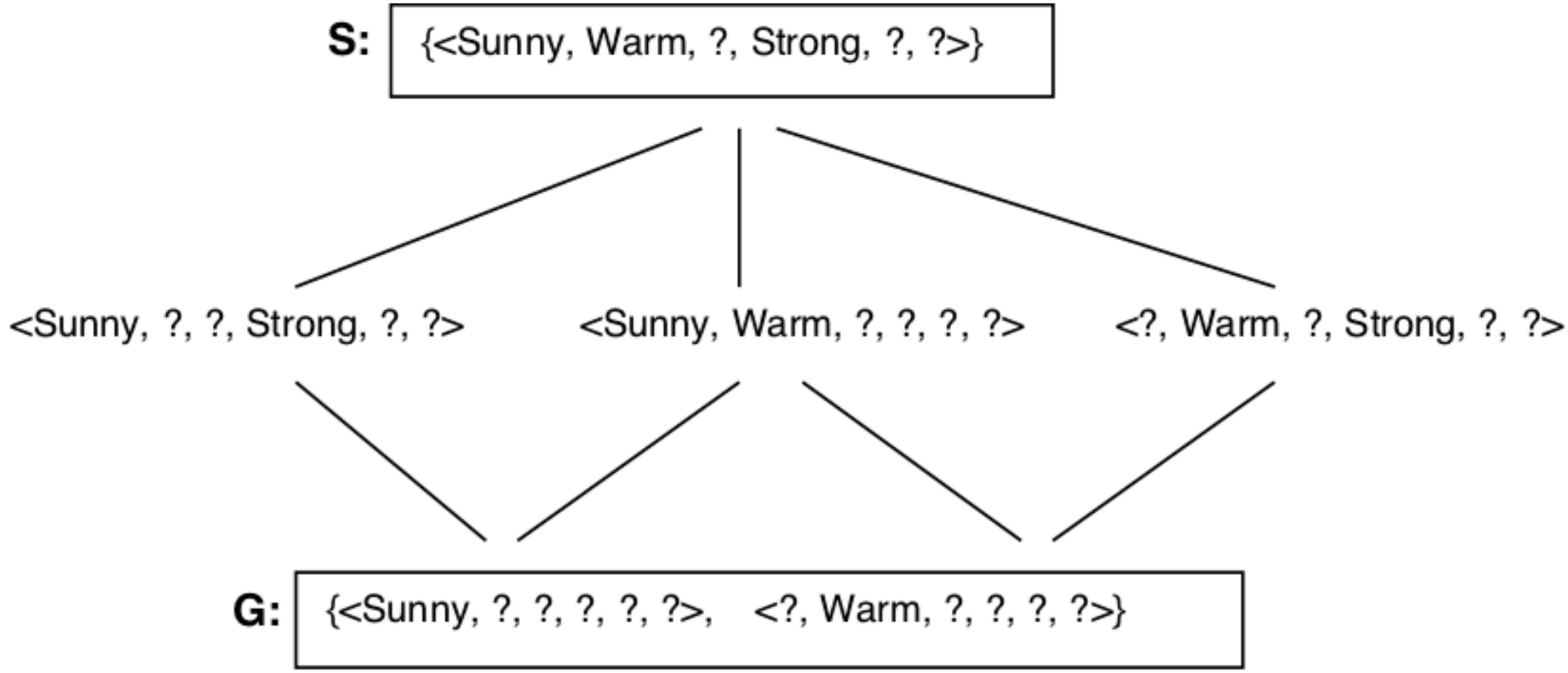


Discussion

- The version space learned by CANDIDATE-ELIMINATION converges towards the hypothesis correctly describing the target concept, provided that
  - there is such a hypothesis in H, and
  - the training data is labeled correctly
- The size of the version space tells us how close we are
- What if we don’t have enough data to converge?
- What if there is no correct h in H?

Using version spaces as classifiers

<Sunny, Warm, Normal, Strong, Cool, Change>
<Rainy, Cold, Normal, Light, Warm, Same>
<Sunny, Warm, Normal, Light, Warm, Same>
<Sunny, Cold, Normal, Strong, Warm, Same>



[Figure: Mitchell]

No correct h in H

days described by
< Sky, AirTemp, Humidity, Wind, Water, Forecast >

Sunny / Cloudy / Rainy

Warm / Cold

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Warm / Cool

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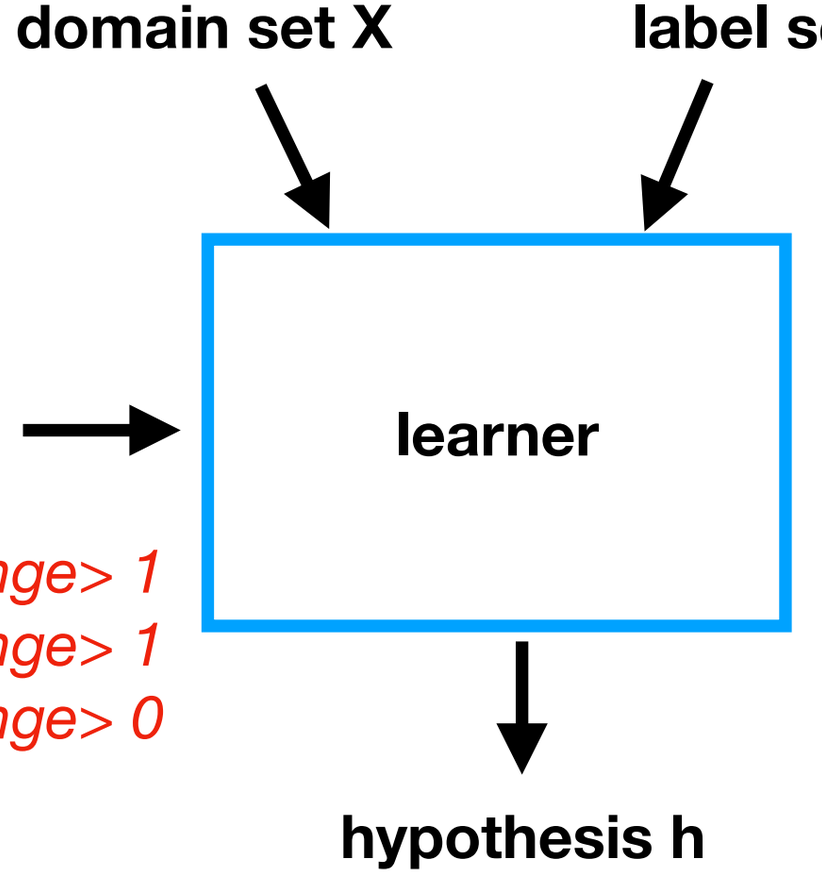
labels 1 / 0 indicating whether someone enjoys their favourite sport on that day



<Sunny, Warm, Normal, Strong, Cool, Change> 1
<Cloudy, Warm, Normal, Strong, Cool, Change> 1
<Rainy, Warm, Normal, Strong, Cool, Change> 0

conjunction of attribute constraints

No correct h in H

- Problem: there are many more Boolean functions over X than hypotheses in H, so the assumption that there is a good h in H is too strong

- What about including all these functions in H?

- Syntactically, this is easy: just allow any disjunctions, conjunctions and negations of our earlier hypotheses, e.g., <Sunny,?,?,?,?,?> v <Cloudy,?,?,?,?,?>

but…

- CANDIDATE-ELIMINATION now boils down to **memorisation**:
  - S = disjunction of all positive training examples
  - G = negated disjunction of all negative training examples
- only **converges** after **seeing all** instances
- every **unseen** instance is classified **positive by half** of the version space and **negative by the other half**

Inductive bias

- This tension is central to machine learning: we cannot learn **successfully** unless we **restrict** the hypothesis space

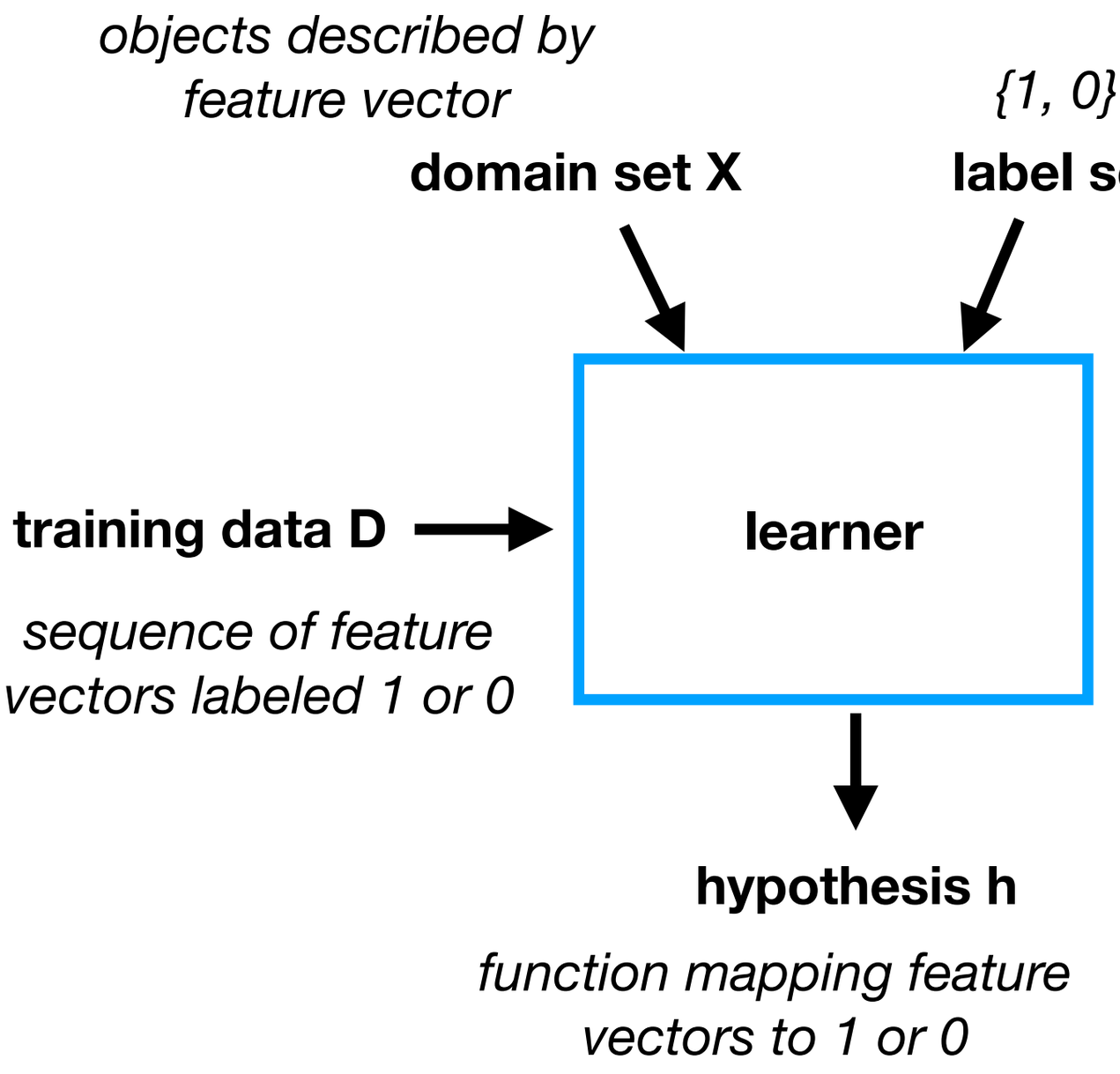
- Different learners make different assumptions to achieve learning; these assumptions are also called **inductive bias**

- Learners with stronger bias make more inductive leaps, classifying larger parts of the instance space

Inductive bias: example

	learning	classification	inductive bias
learner 1	store training data in memory	stored label if available, “unknown” otherwise	none
learner 2	CANDIDATE-ELIMINATION	agreed label if all members of the version space agree, “unknown” otherwise	target concept in hypothesis space
learner 3	FIND-S	label given by learned hypothesis	target concept in H & all examples negative unless there is reason to consider them positive

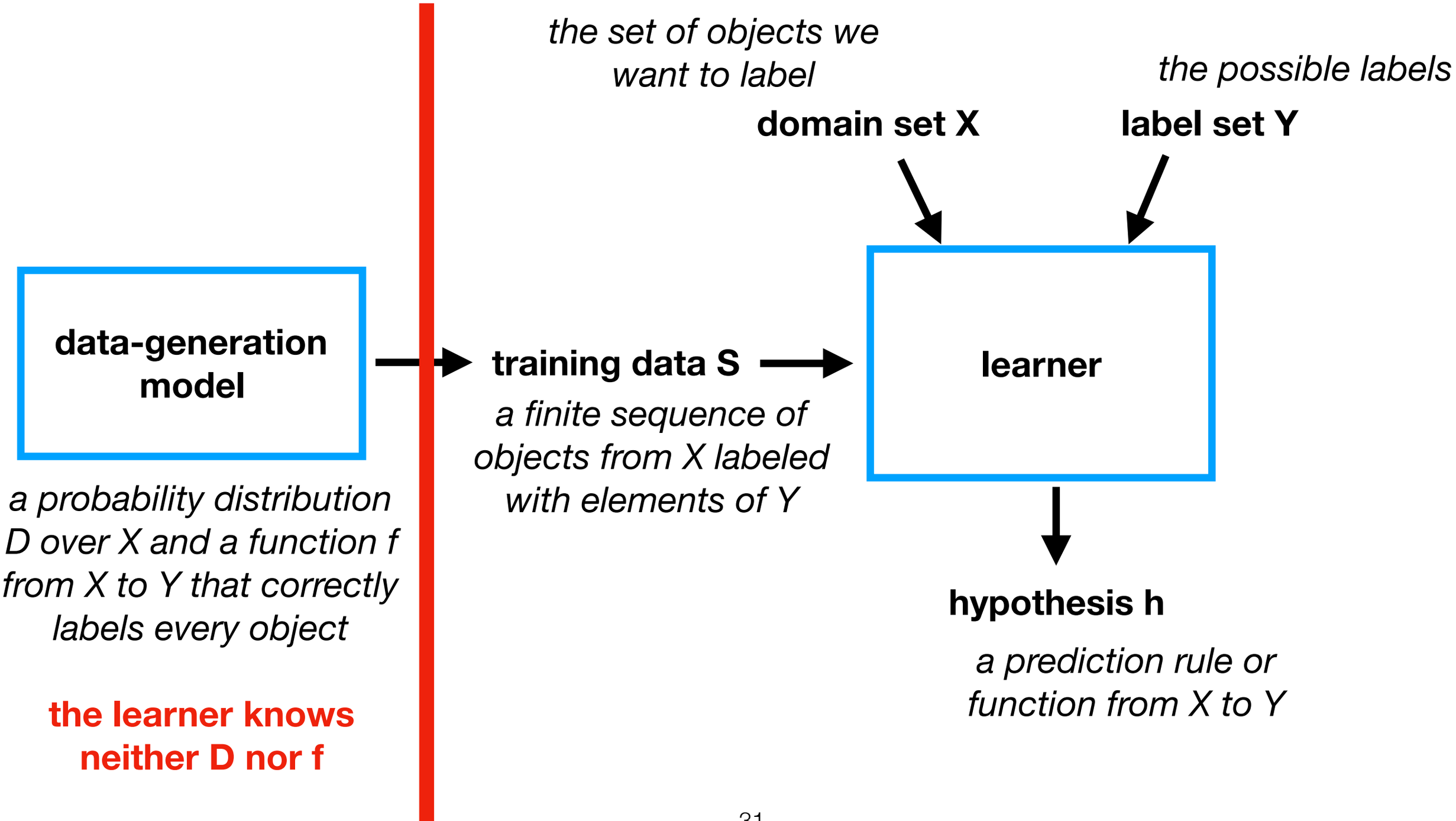
Boolean Concept Learning



Lots of choices when building a learner for a given problem:

- different feature vector representations
- different hypothesis spaces
- different learning algorithms with different inductive bias

The Statistical Learning Framework



Measure of success

- **error** of a hypothesis h = probability of h assigning a wrong label to a random object x drawn from D

- formally:

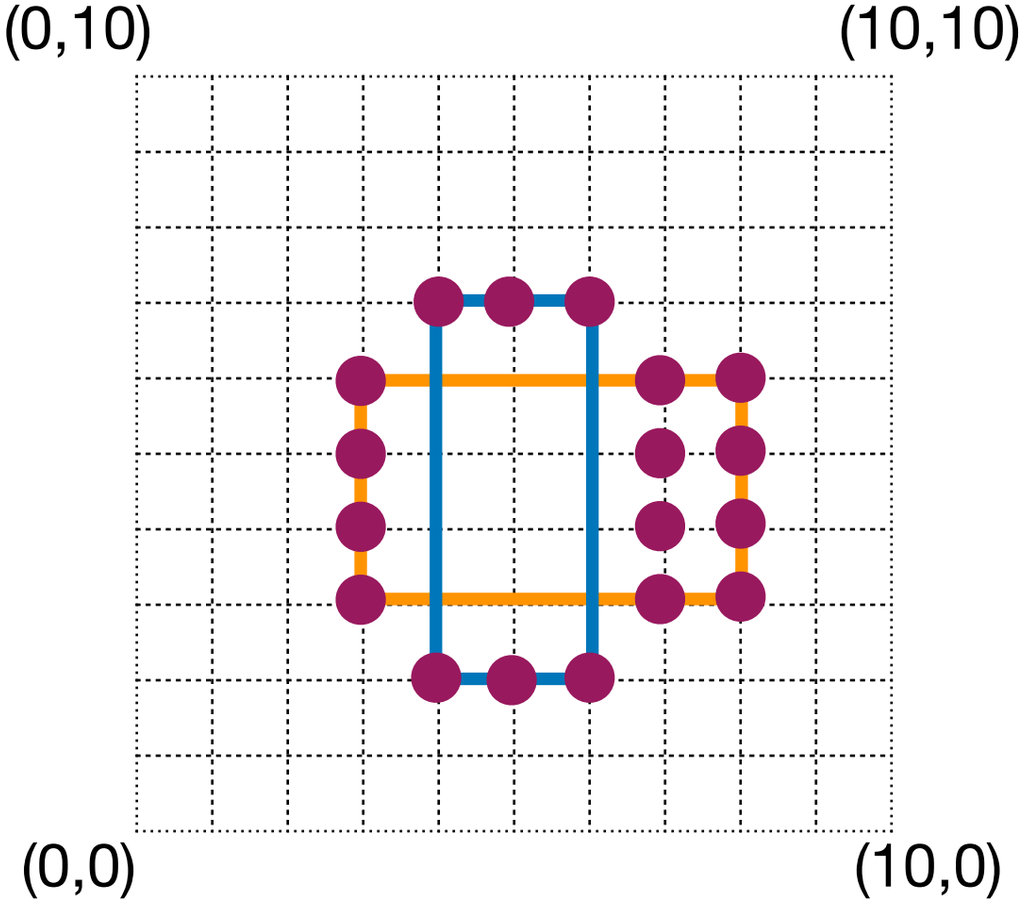
$$L_{D,f}(h) = D(\{x \in X \mid h(x) \neq f(x)\})$$

error (or loss) of hypothesis h with respect to distribution D and correct labeling function f

probability according to distribution D of the subset of X where hypothesis h and correct function f disagree

- If the learner would know D and f, it could simply search for the h with minimal $L_{D,f}(h)$

Example



assume D is uniform, i.e., each point on the grid has probability $\frac{1}{121}$

correct function f: $3 \leq x \leq 8 \wedge 3 \leq y \leq 6$

hypothesis h: $4 \leq x \leq 6 \wedge 2 \leq y \leq 7$

$$L_{D,f}(h) = D(\{x \in X \mid h(x) \neq f(x)\}) = \frac{18}{121} = 0.149$$

Empirical Risk Minimisation (ERM)

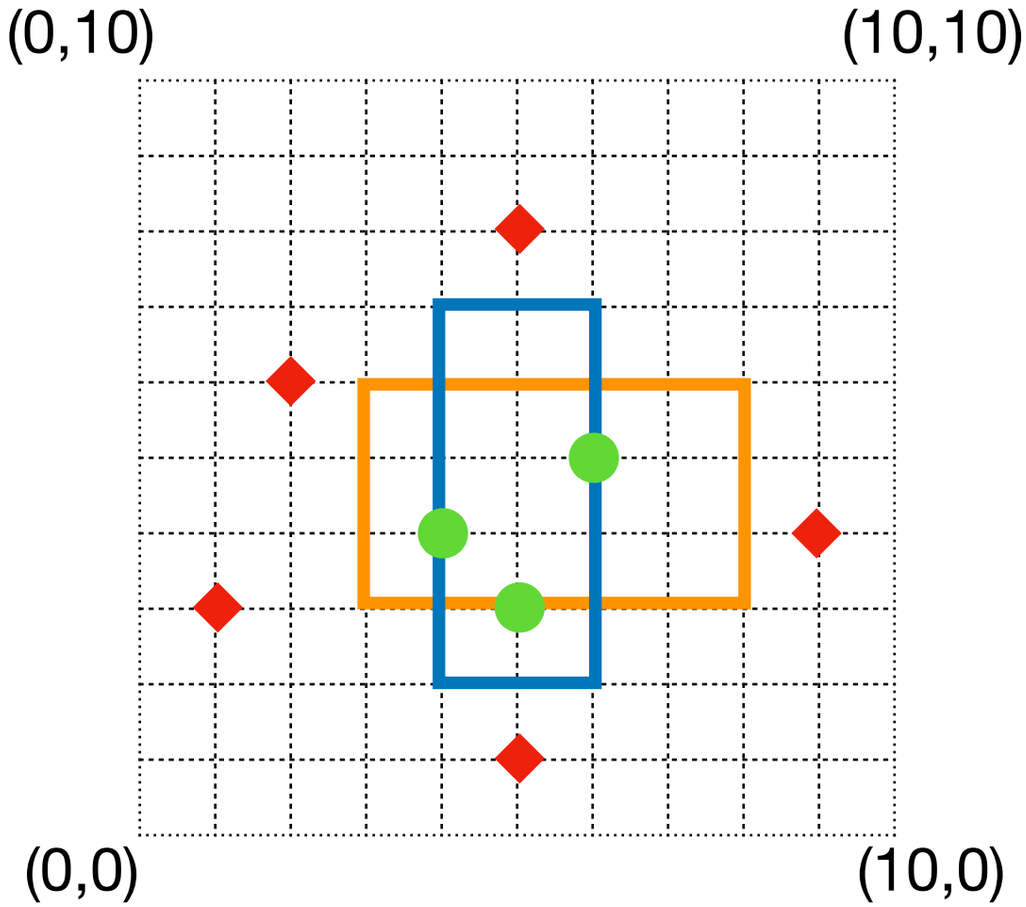
- The **training error** (also called **empirical error** or **empirical risk**) of hypothesis h with respect to training sample $S = ((x_1, y_1), \ldots, (x_m, y_m))$ is the **fraction** of the training sample h is **not consistent** with, i.e.,

$$L_S(h) = \frac{\left| \{ i \in \{1,\ldots,m\} \mid h(x_i) \neq y_i \} \right|}{m}$$

- The learner can compute this for any given hypothesis!

- An **ERM (empirical risk minimisation) learner** returns a hypothesis h that minimises $L_S(h)$ given S

Example



positive training example

negative training example

assume D is uniform, i.e., each point on the grid has probability $\frac{1}{121}$

correct function f: $3 \leq x \leq 8 \wedge 3 \leq y \leq 6$

hypothesis h: $4 \leq x \leq 6 \wedge 2 \leq y \leq 7$

$$L_{D,f}(h) = D(\{x \in X \mid h(x) \neq f(x)\}) = \frac{18}{121} = 0.149$$

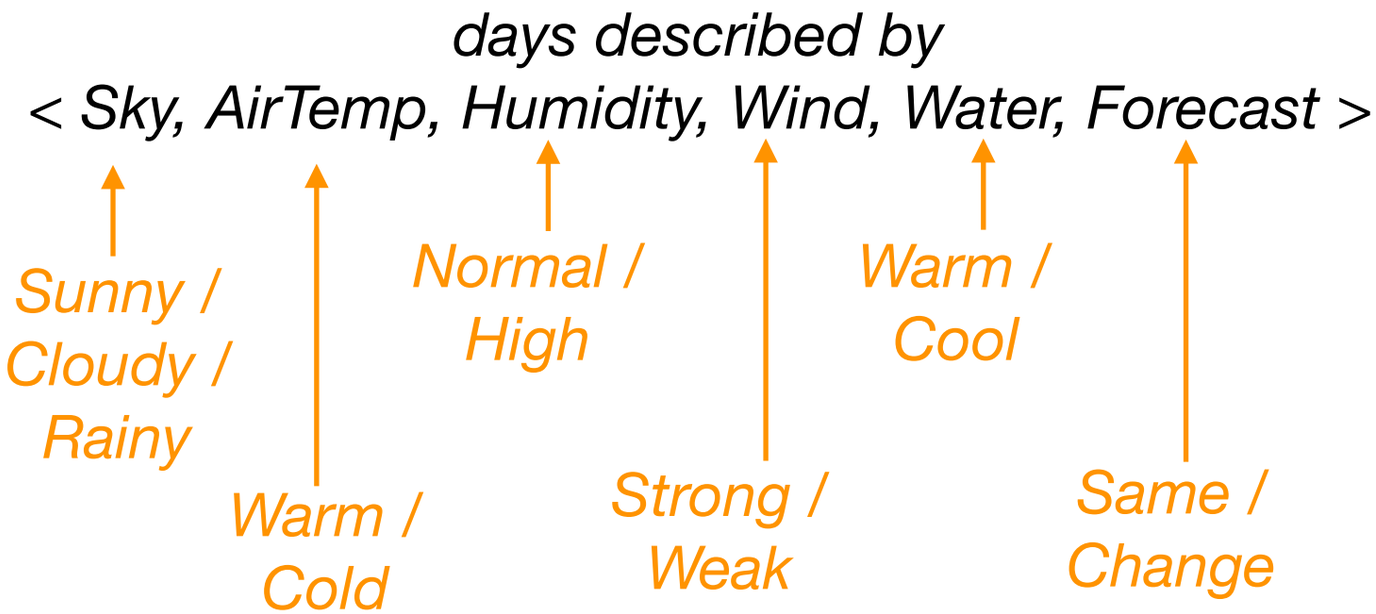
$$L_S(h) = \frac{\left|\{i \in \{1,\ldots,m\} \mid h(x_i) \neq y_i\}\right|}{m} = \frac{0}{8} = 0$$

Example ERM learners

	learning	classification
learner 1	store training data in memory	stored label if available, 0 otherwise
learner 2	CANDIDATE-ELIMINATION	agreed label if all members of the version space agree, 0 otherwise
learner 3	FIND-S	label given by learned hypothesis

all have empirical error $L_S(h)=0$, but true error $L_{D,F}(h)$ depends on the **unseen positive examples**

Example



assume
- **uniform** distribution over days,
- true function **f = <?,Warm,?,?,?,?>**,
- training data S: <Sunny,Warm,High,Weak,Warm,Same> 1
  <Sunny,Warm,High,Weak,Warm,Change> 1
- learned hypothesis **h = <Sunny,Warm,High,Weak,Warm,?>**

what is the **empirical error** of h?
what is the **true error** of h?

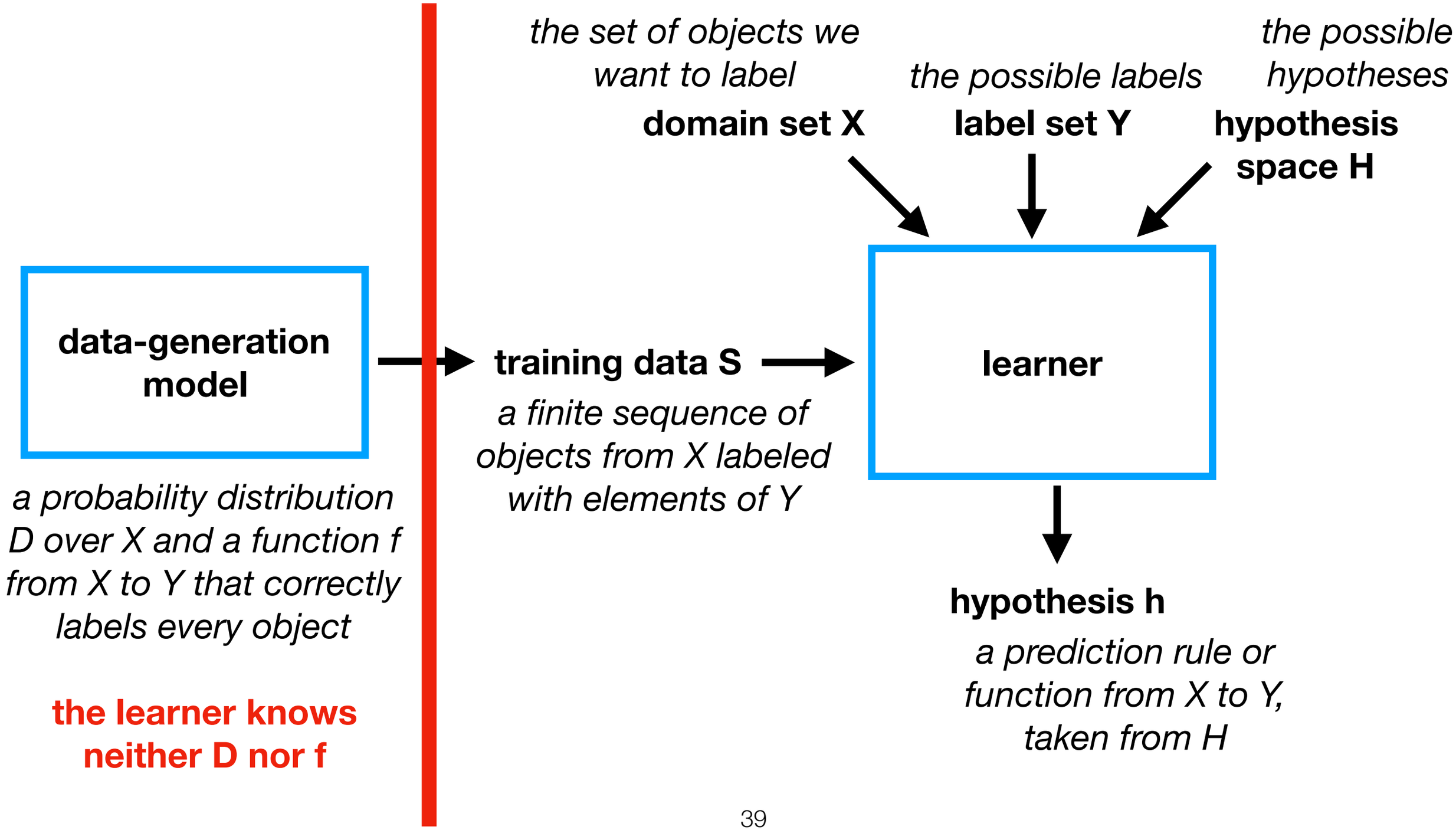
this is called **overfitting**: h fits the training data very well, but generalises poorly to unseen examples

Overfitting

- We saw another example of overfitting earlier: CANDIDATE-ELIMINATION memoizes training examples if we allow it to learn arbitrary Boolean functions

- One way to avoid overfitting is to restrict the hypothesis space before seeing the data

The Statistical Learning Framework



ERM Learning

(Boolean functions)

the set of objects we want to label

domain set X

{0,1}

label set Y

the possible hypotheses

hypothesis space H

data-generation model

a probability distribution D over X and a function f from X to Y that correctly labels every object

the learner knows neither D nor f

training data S

a finite sequence of objects from X labeled with elements of Y

ERM learner

hypothesis $h_S \in \arg\min_{h \in H} L_S(h)$

How to pick H to get good h_S, independently of D and f?