

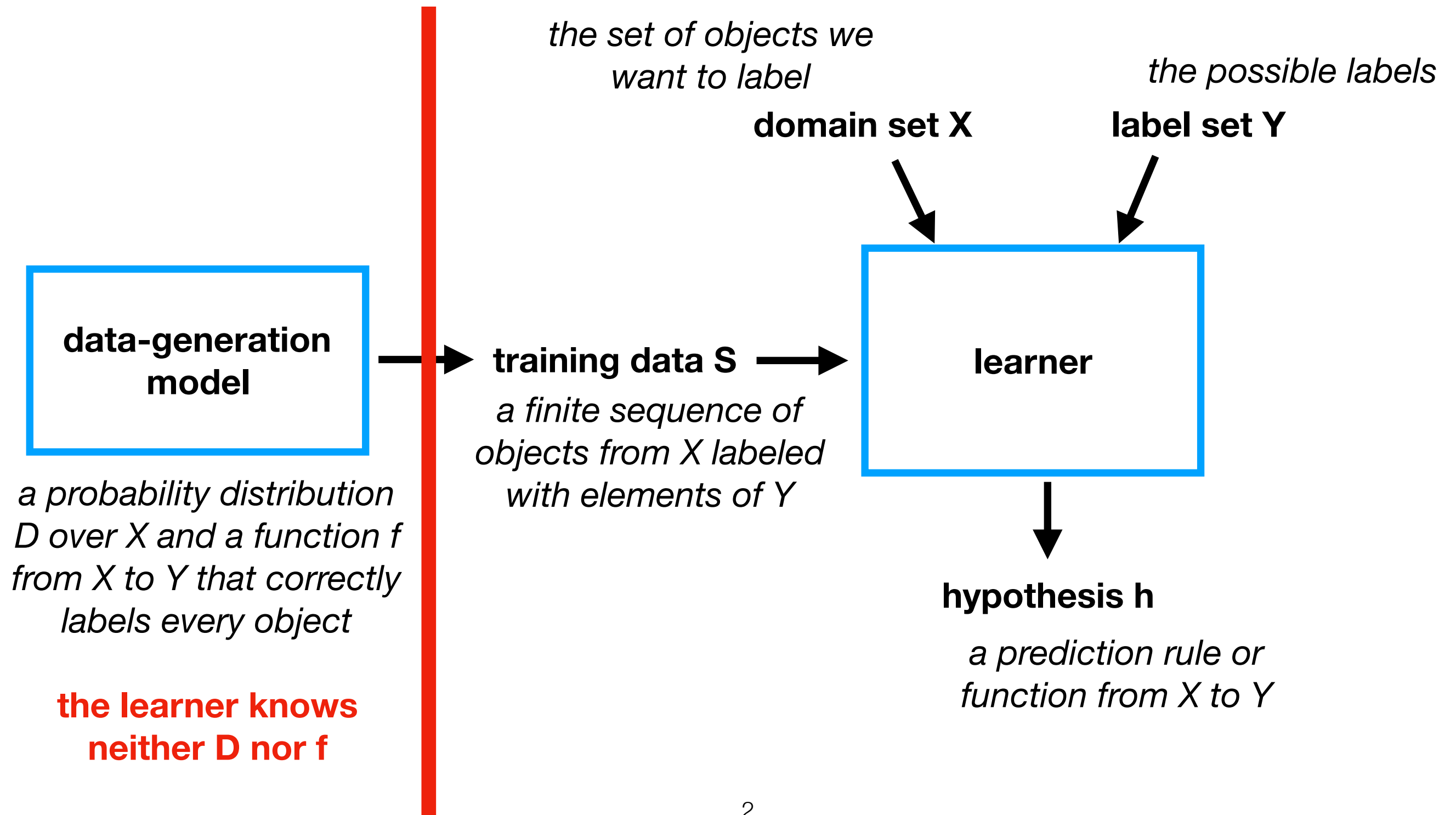
CMT311 Principles of Machine Learning

Concept Learning, ERM & PAC

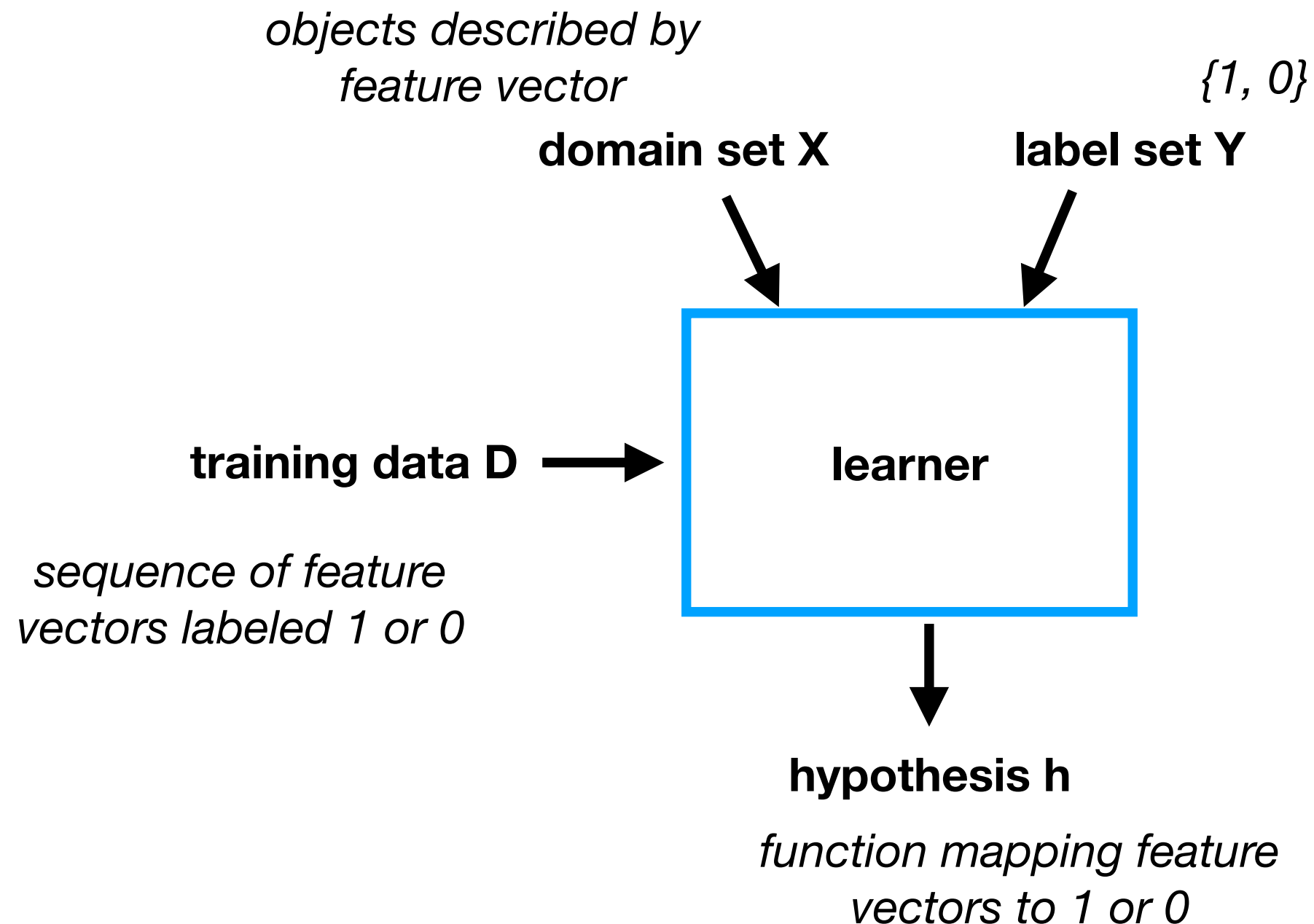
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11.10.2019

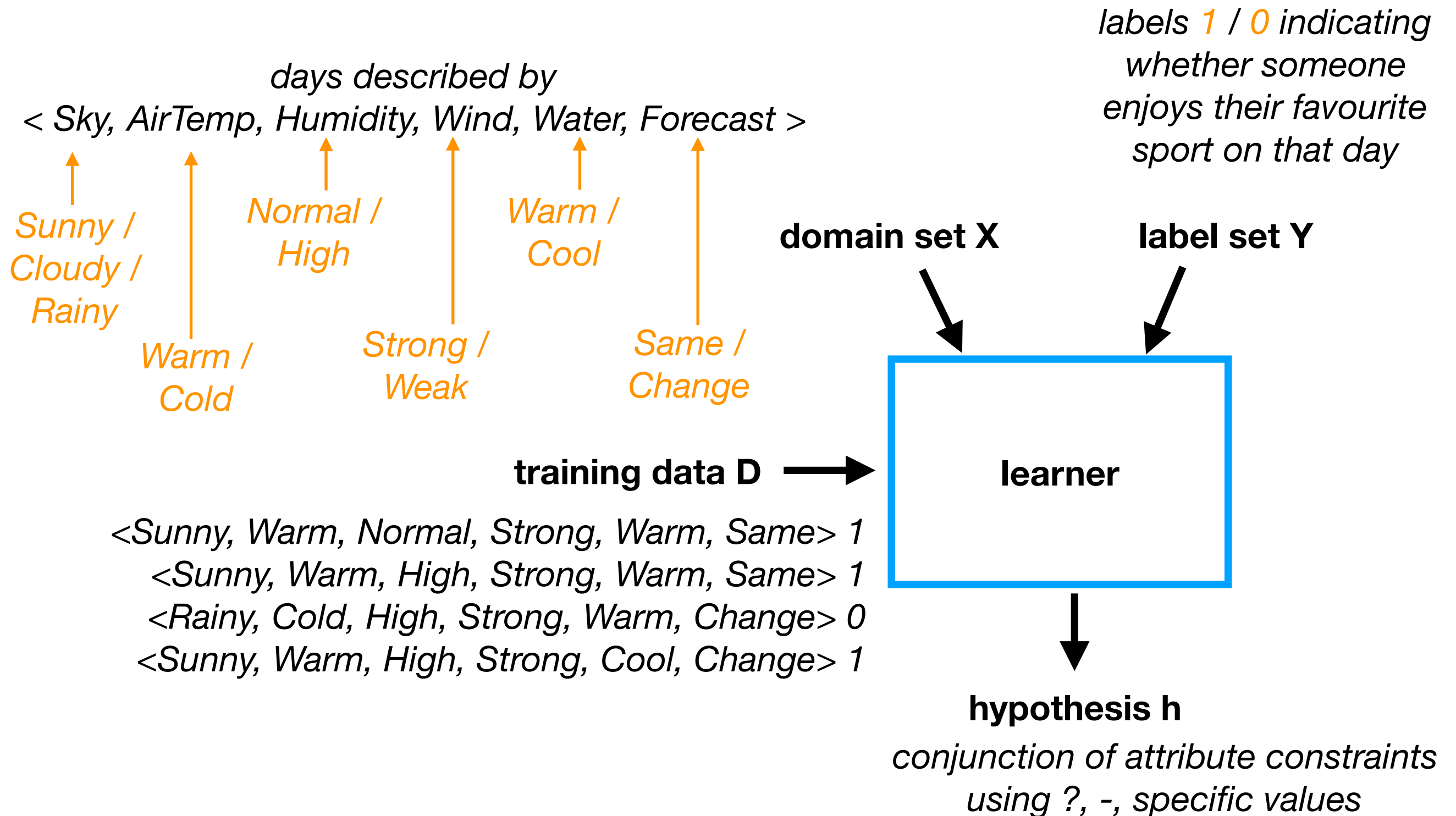
The Statistical Learning Framework



Boolean Concept Learning



Example



Example

points on a grid, described by coordinates

(x,y) with $x \in [0,10]$, $y \in [0,10]$

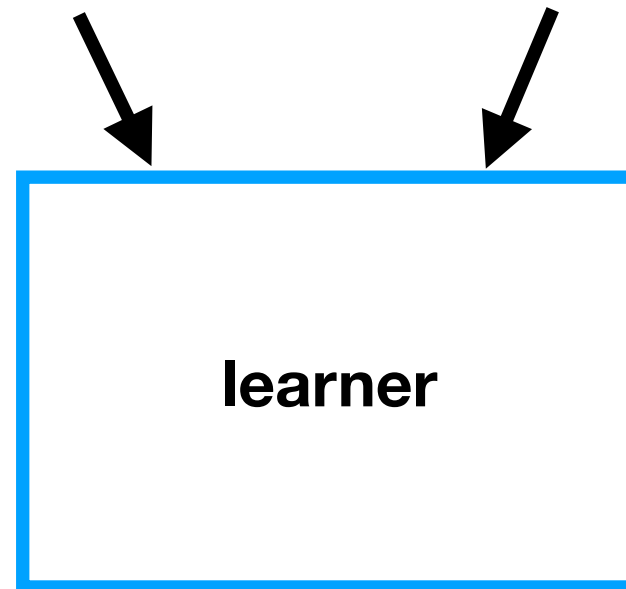
labels 1 / 0

domain set X

label set Y

training data D →

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



learner

hypothesis h

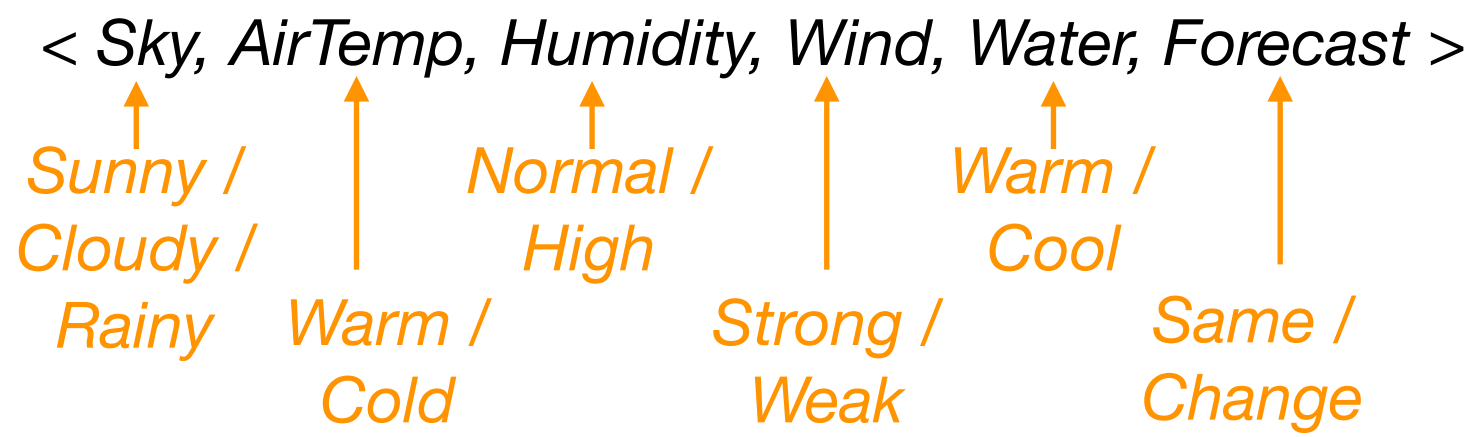
*rectangle $(a \leq x \leq b \wedge c \leq y \leq d)$
with a, b, c, d integers in $[0,10]$*

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

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



| 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

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

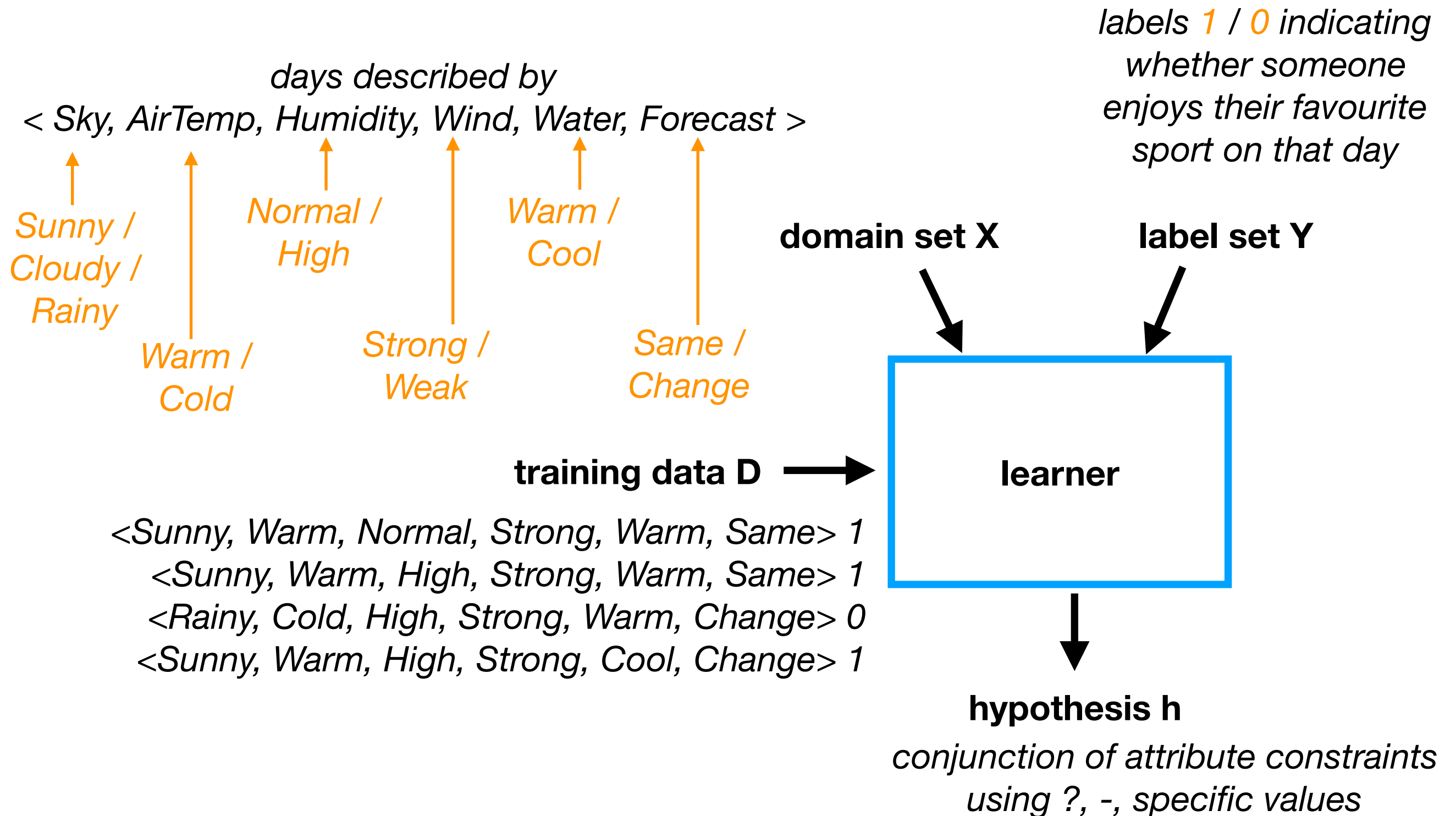
*rectangle ($a \leq x \leq b \wedge c \leq y \leq d$)
with a, b, c, d integers in $[0, 10]$*

| h_1 | h_2 |
|--|---|
| $(0 \leq x \leq 10 \wedge 0 \leq y \leq 10)$ | $(0 \leq x \leq 10 \wedge 1 \leq y \leq 5)$ |
| $(0 \leq x \leq 10 \wedge 1 \leq y \leq 5)$ | $(0 \leq x \leq 9 \wedge 1 \leq y \leq 5)$ |
| $(10 \leq x \leq 10 \wedge 1 \leq y \leq 1)$ | $(0 \leq x \leq 10 \wedge 1 \leq y \leq 5)$ |
| $(0 \leq x \leq 10 \wedge 1 \leq y \leq 5)$ | $(10 \leq x \leq 0 \wedge 1 \leq y \leq 5)$ |
| $(10 \leq x \leq 0 \wedge 1 \leq y \leq 5)$ | $(3 \leq x \leq 1 \wedge 10 \leq y \leq 5)$ |
| $(2 \leq x \leq 4 \wedge 3 \leq y \leq 7)$ | $(1 \leq x \leq 4 \wedge 3 \leq y \leq 8)$ |

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



| 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 | <div> <Sunny, Warm, ?, Strong, ?, ?> </div> <p>hypothesis returned by FIND-S</p> |

Exercise

- Consider again the space of rectangles ($a \leq x \leq b \wedge c \leq y \leq d$) on the $[0,10] \times [0,10]$ grid.
- Trace the FIND-S algorithm for the following sequence of examples:

(2,4) 1

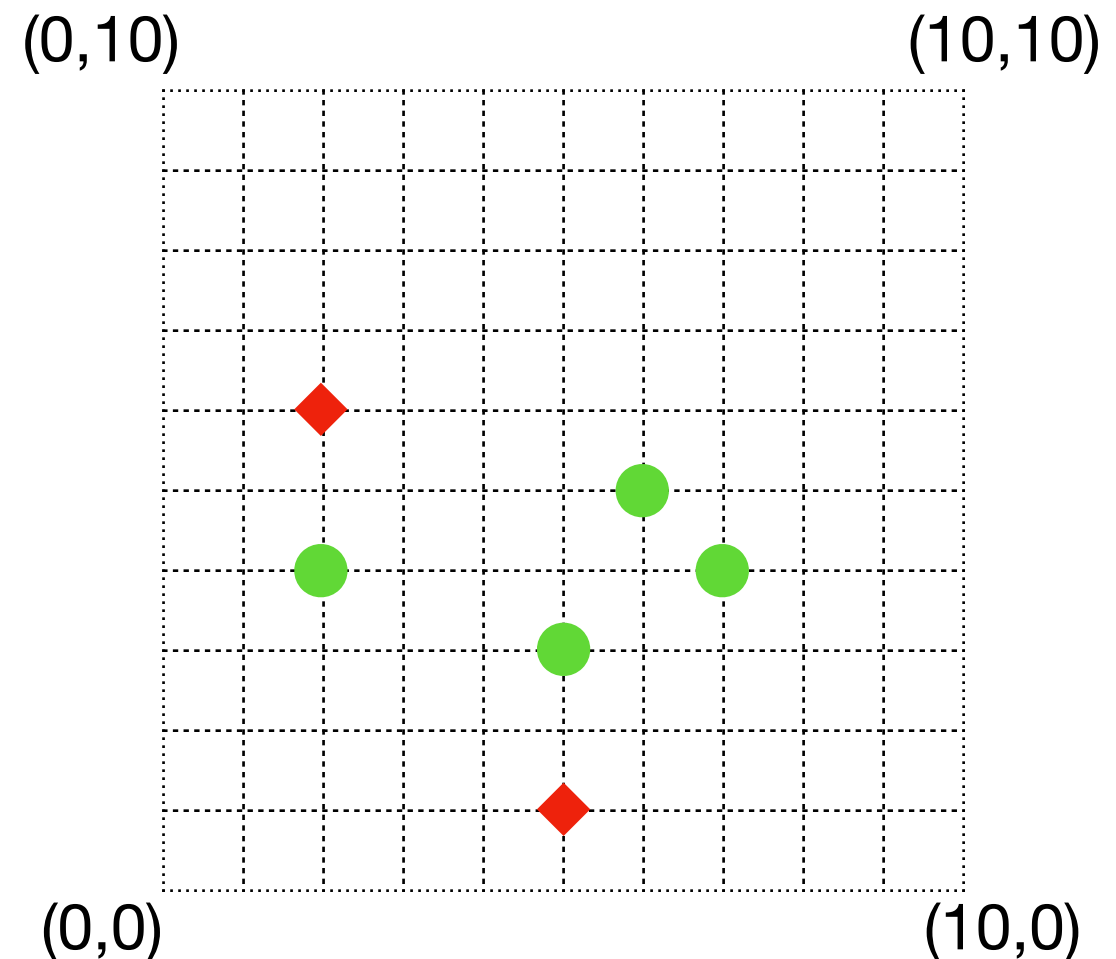
(7,4) 1

(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

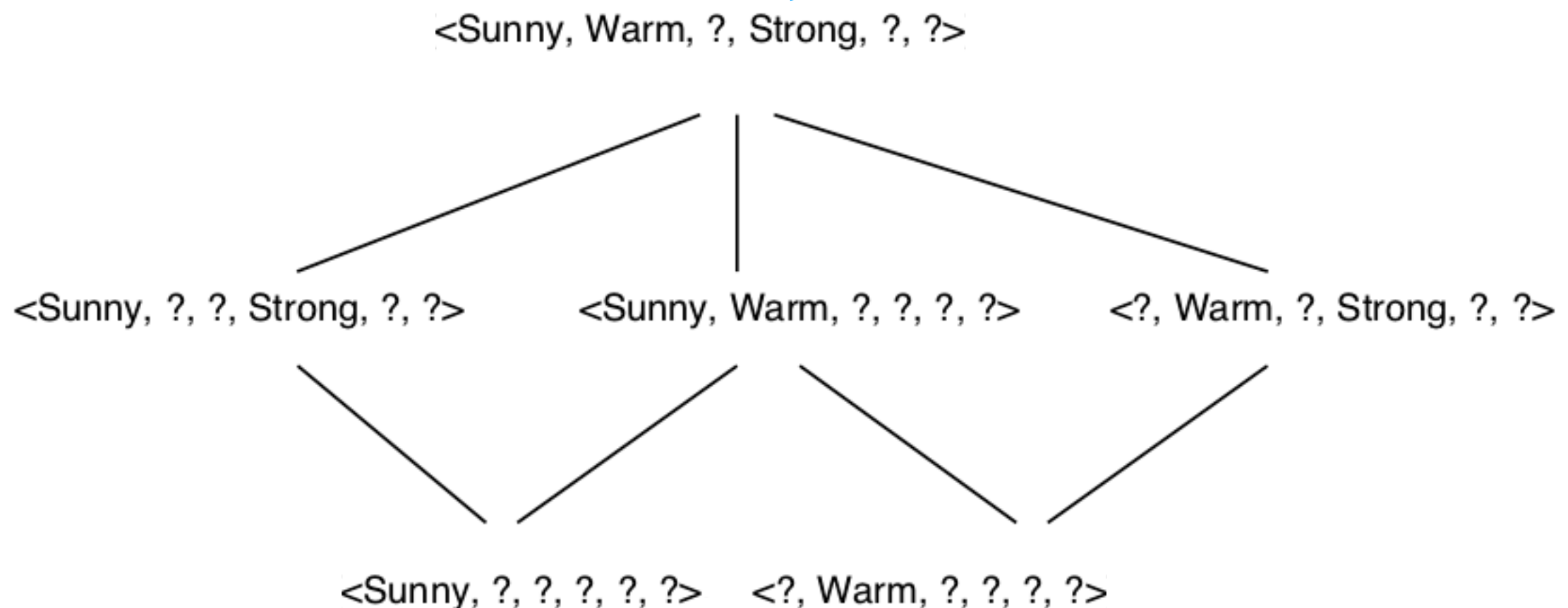
- A hypothesis h is **consistent** with training data D if and only if for all examples (x,y) in D , $h(x)=y$
- Goal: a learner that finds all hypotheses in H that are consistent with D , using the “more general than” order
- The **version space** $VS_{H,D}$ with respect to hypothesis space H and training data D is the set of all hypotheses in H consistent with D

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

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



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 $h(x) \neq y$
- 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 .

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

- 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 .

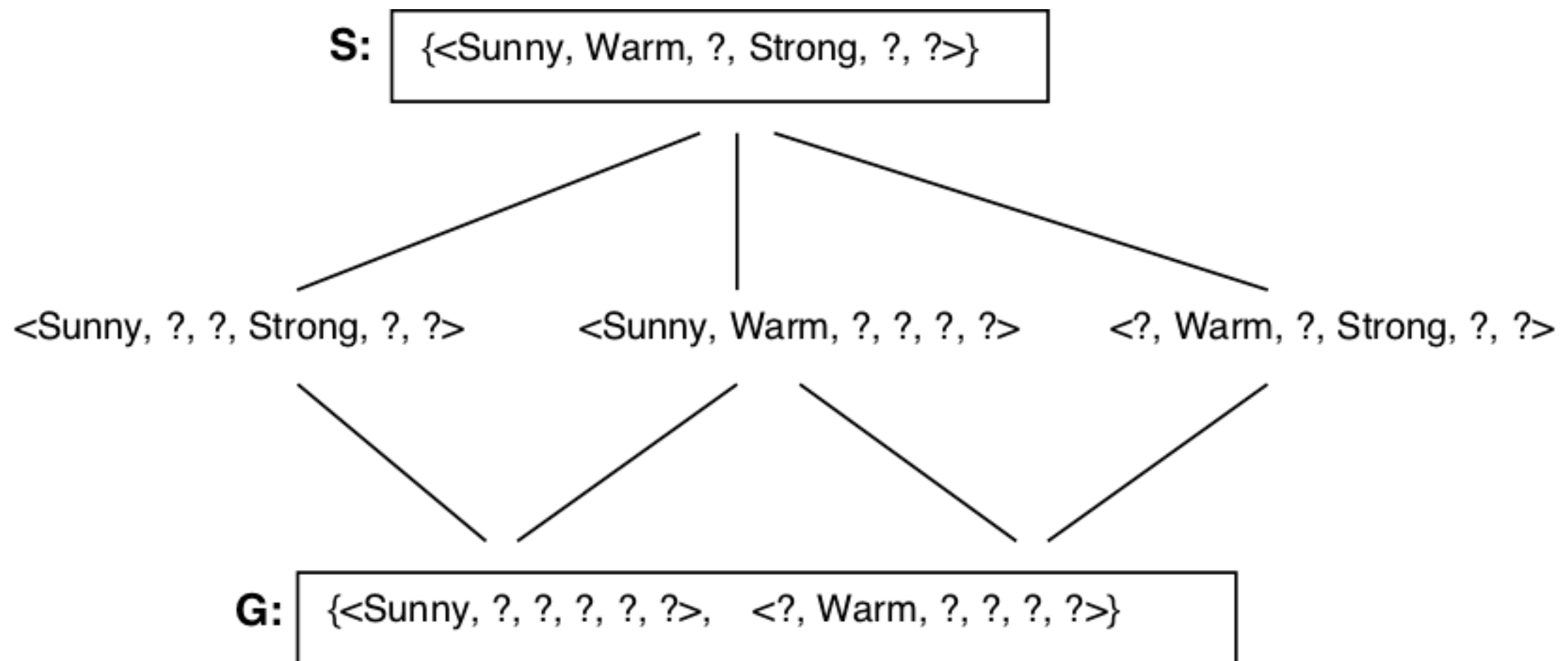
$$S \equiv \{s \in H \mid \text{consistent}(s, D) \wedge \neg \exists s' \in H : s >_g s' \wedge \text{consistent}(s', D)\}$$

- 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

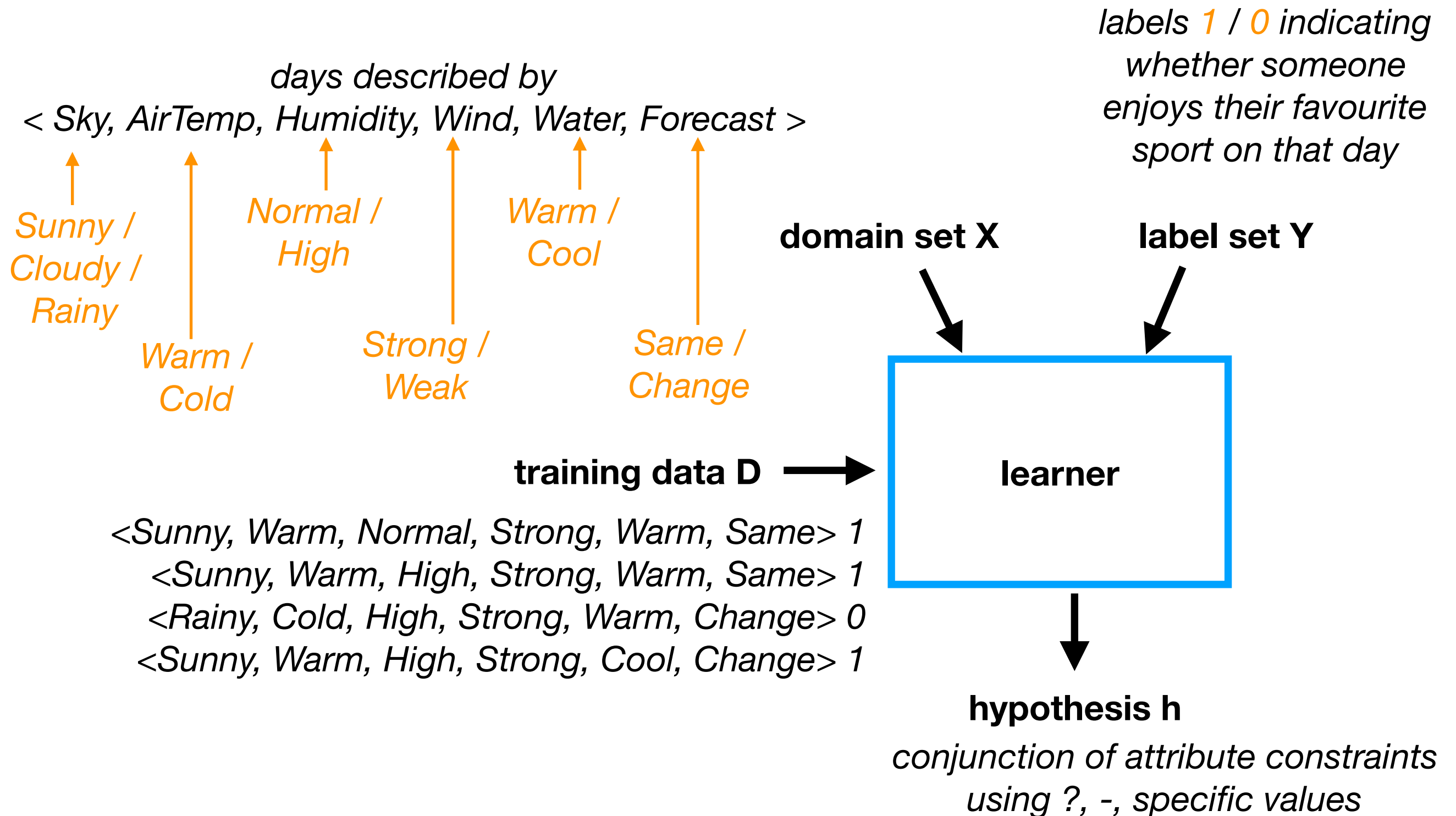
<Sunny, Warm, Normal, Strong, Warm, Same> 1
<Sunny, Warm, High, Strong, Warm, Same> 1
<Rainy, Cold, High, Strong, Warm, Change> 0
<Sunny, Warm, High, Strong, Cool, Change> 1



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

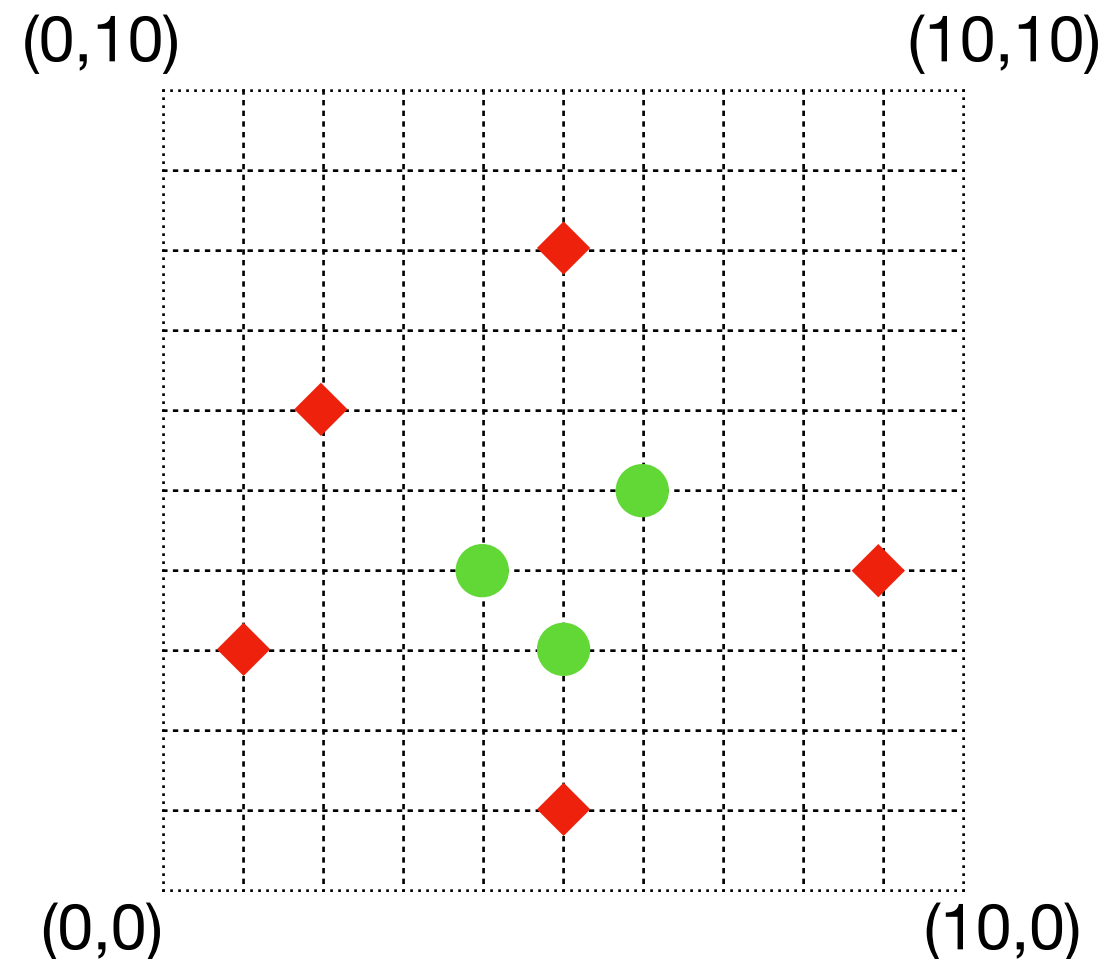
Example



<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

Exercise

- Consider again the space of rectangles ($a \leq x \leq b \wedge c \leq y \leq d$) on the $[0,10] \times [0,10]$ 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, $(2 \leq x \leq 8 \wedge 3 \leq y \leq 5)$?

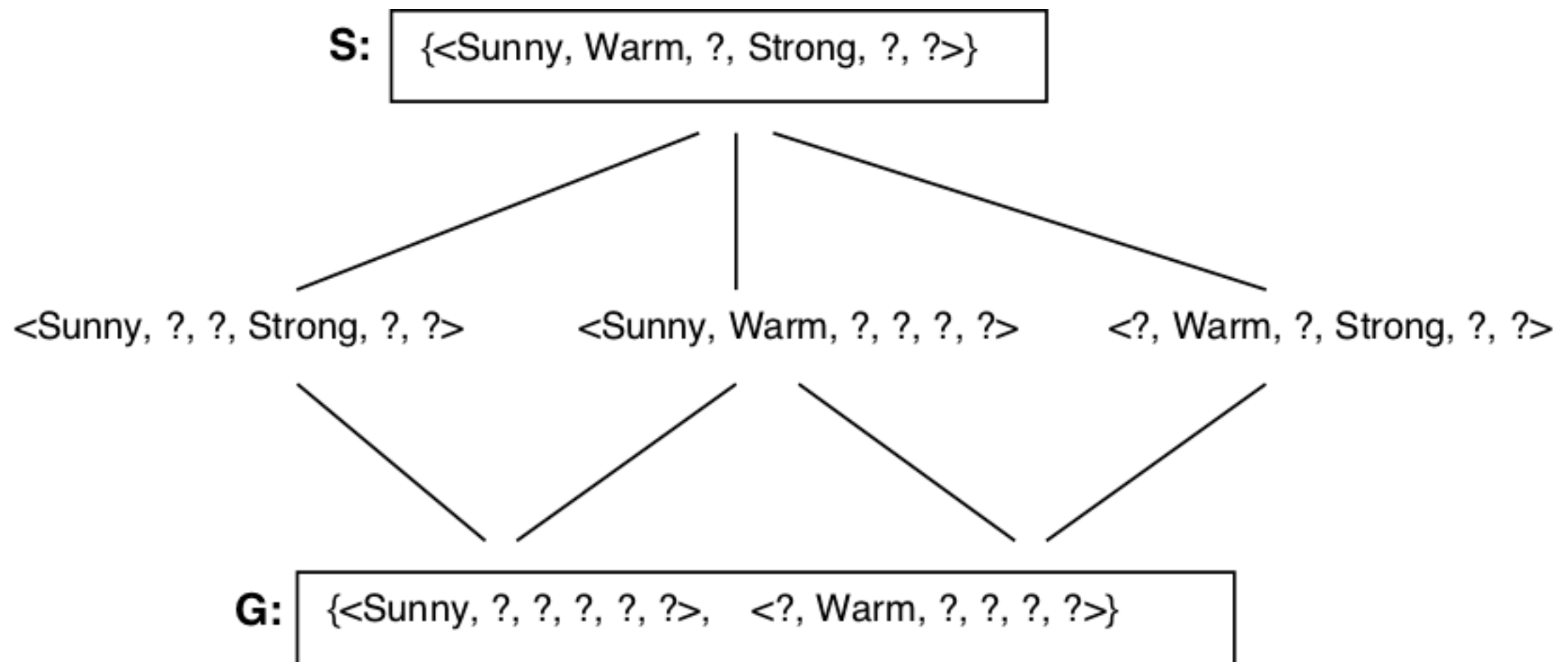


Discussion

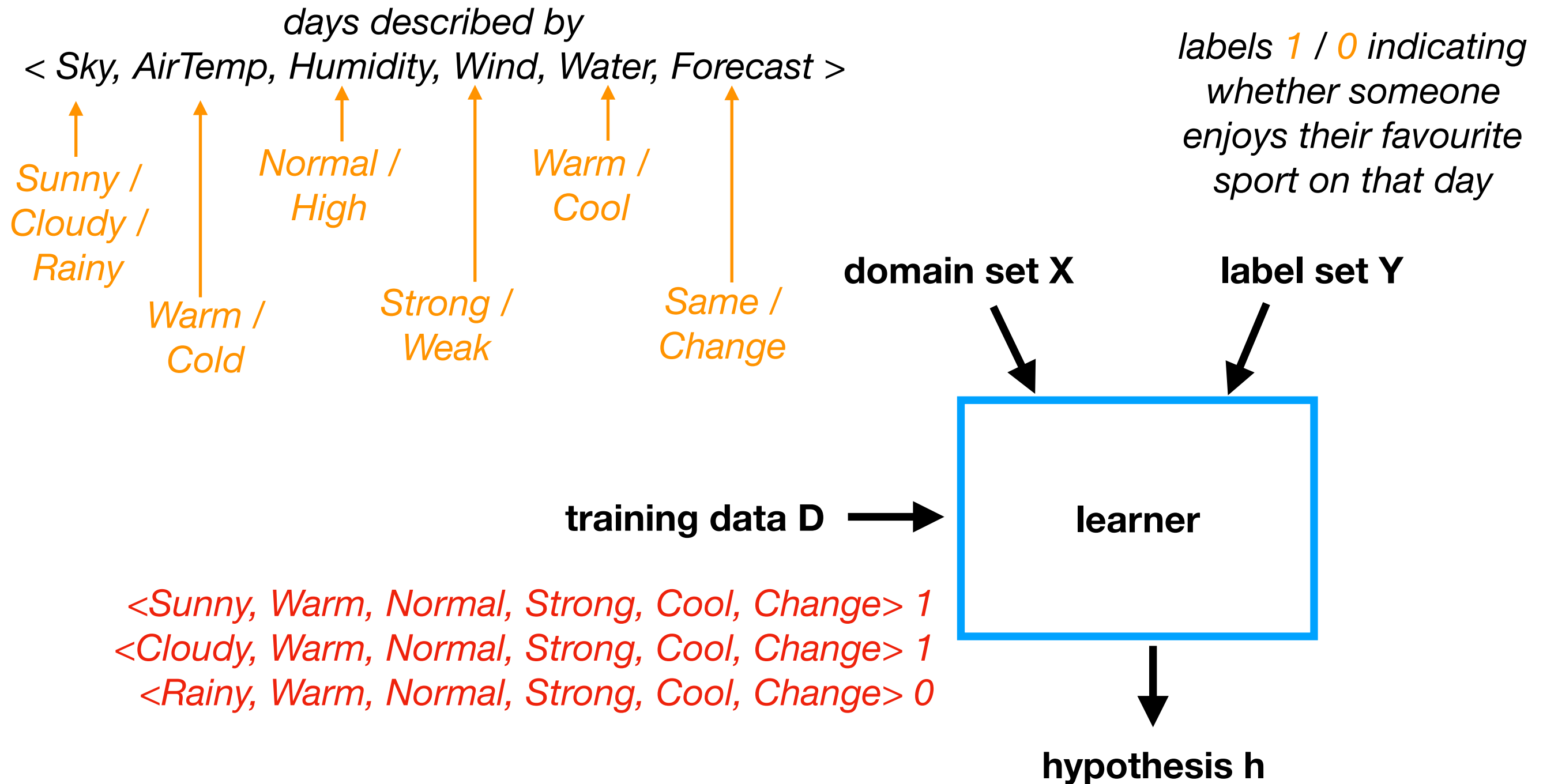
- The version space learned by CANDIDATE-ELIMINATION converges towards the hypothesis correctly describing the target concept, provided that
 - there is such a hypothesis in H , and
 - the training data is labeled correctly
- The size of the version space tells us how close we are
- What if we don't 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>



No correct h in H



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., $\langle \text{Sunny}, ?, ?, ?, ?, ? \rangle \vee \langle \text{Cloudy}, ?, ?, ?, ?, ? \rangle$

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**

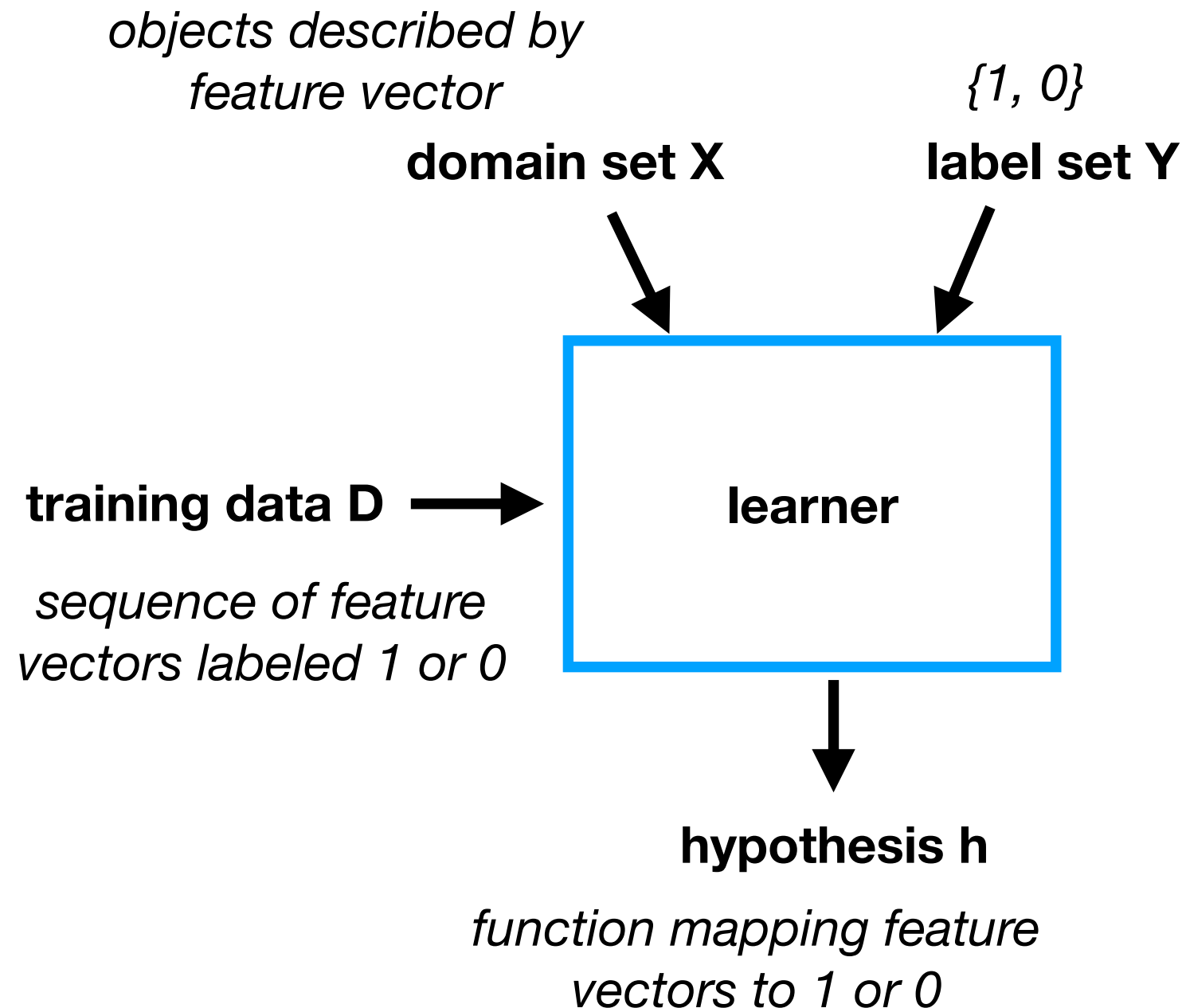
Inductive bias

- 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 |

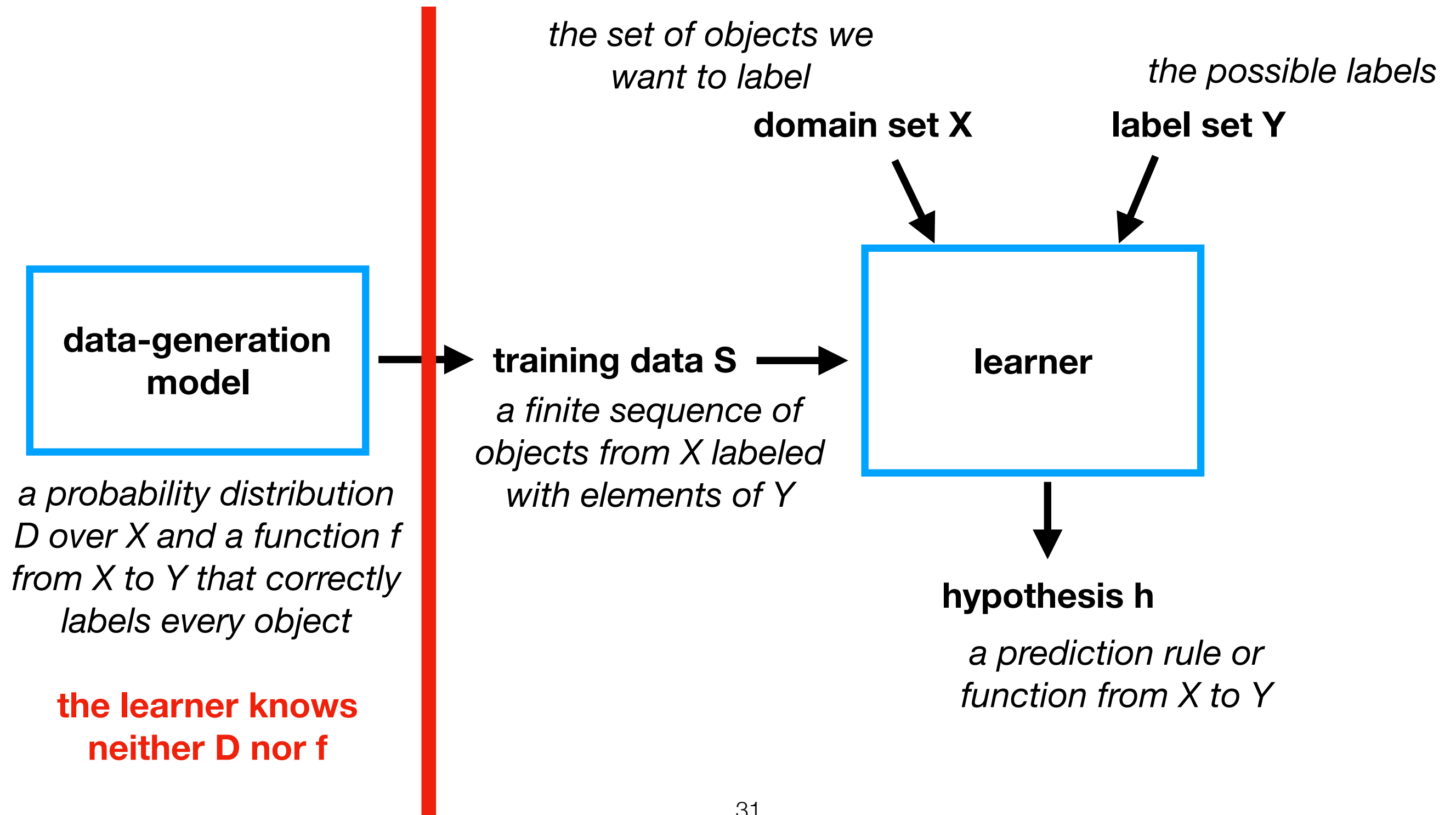
Boolean Concept Learning



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:

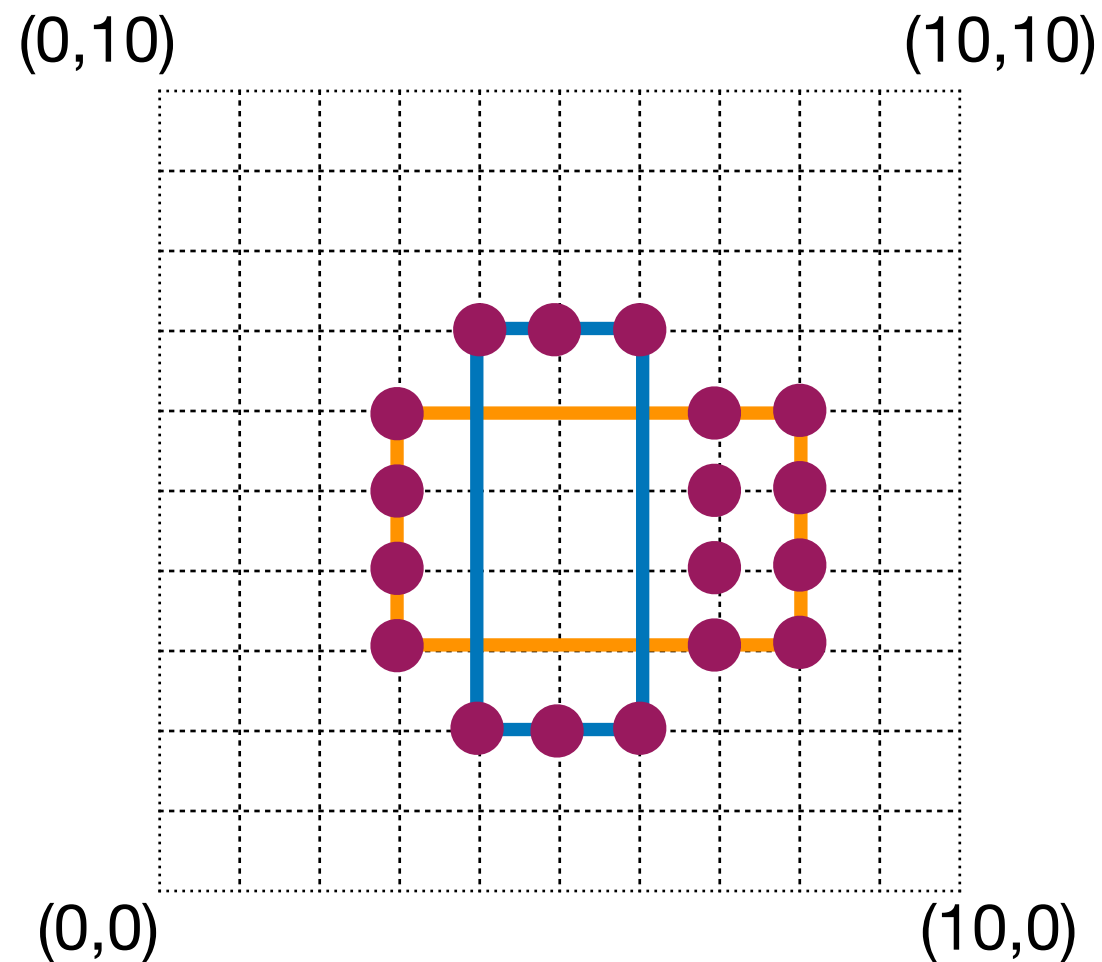
$$L_{D,f}(h) = D(\{x \in X \mid h(x) \neq f(x)\})$$

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

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

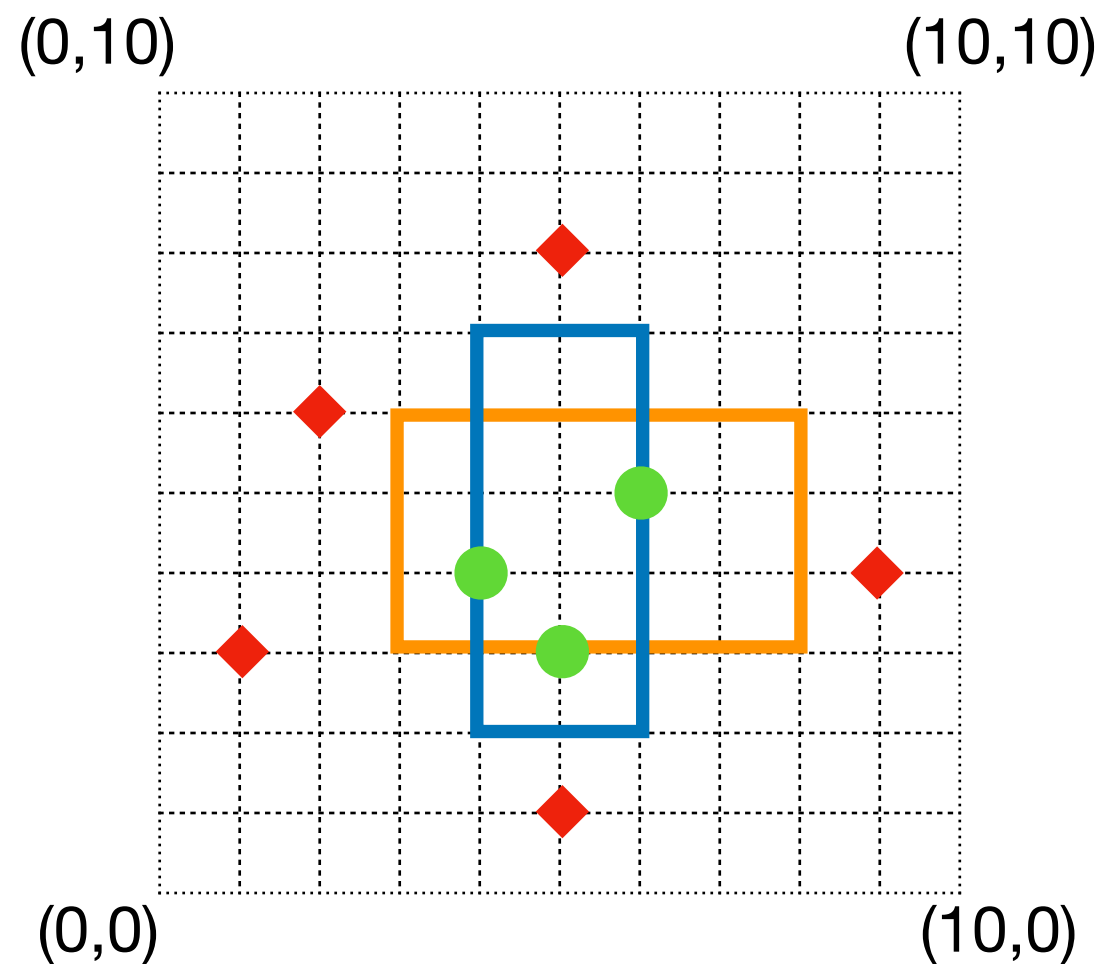
Empirical Risk Minimisation (ERM)

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

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

- 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 : $4 \leq x \leq 6 \wedge 2 \leq y \leq 7$

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

$$= \frac{18}{121} = 0.149$$

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

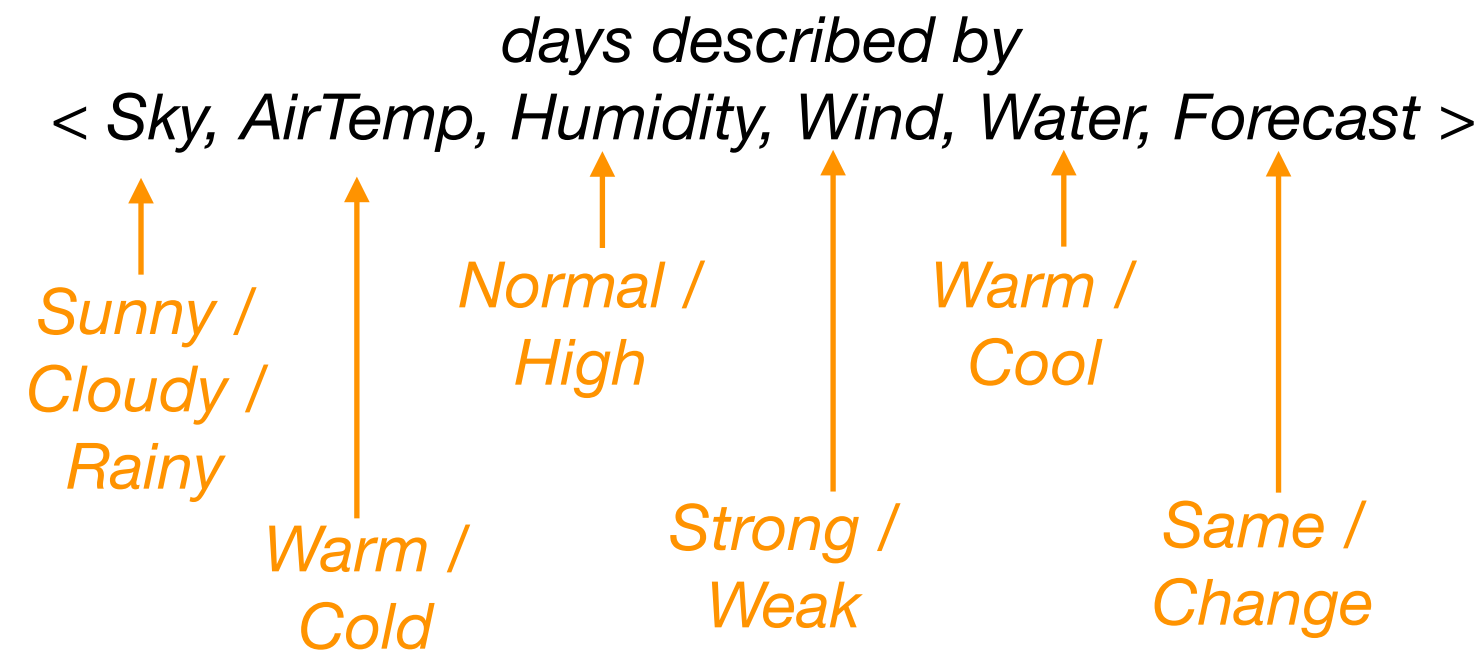
$$= \frac{0}{8} = 0$$

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?

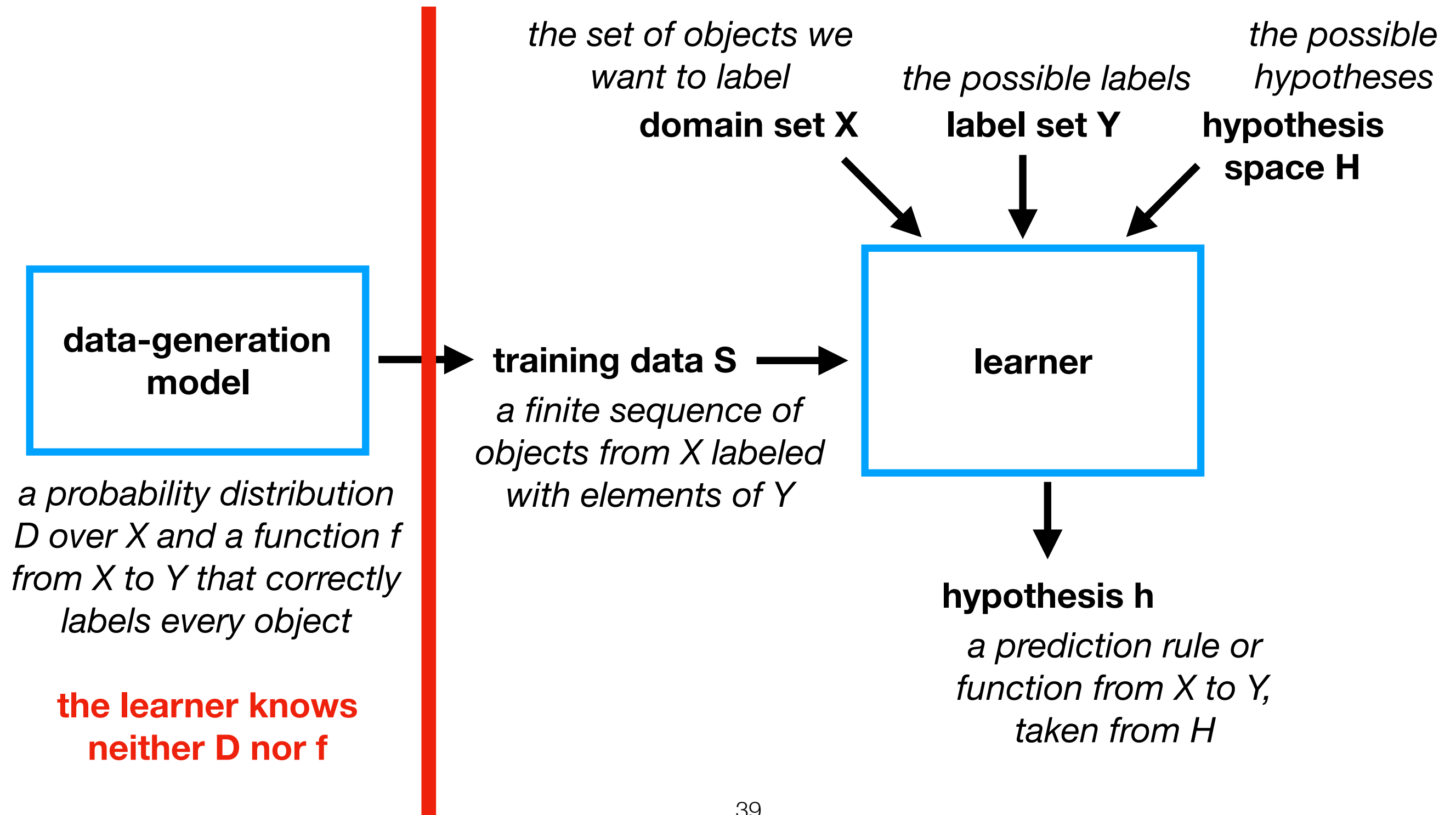
what is the **true error** of h?

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

Overfitting

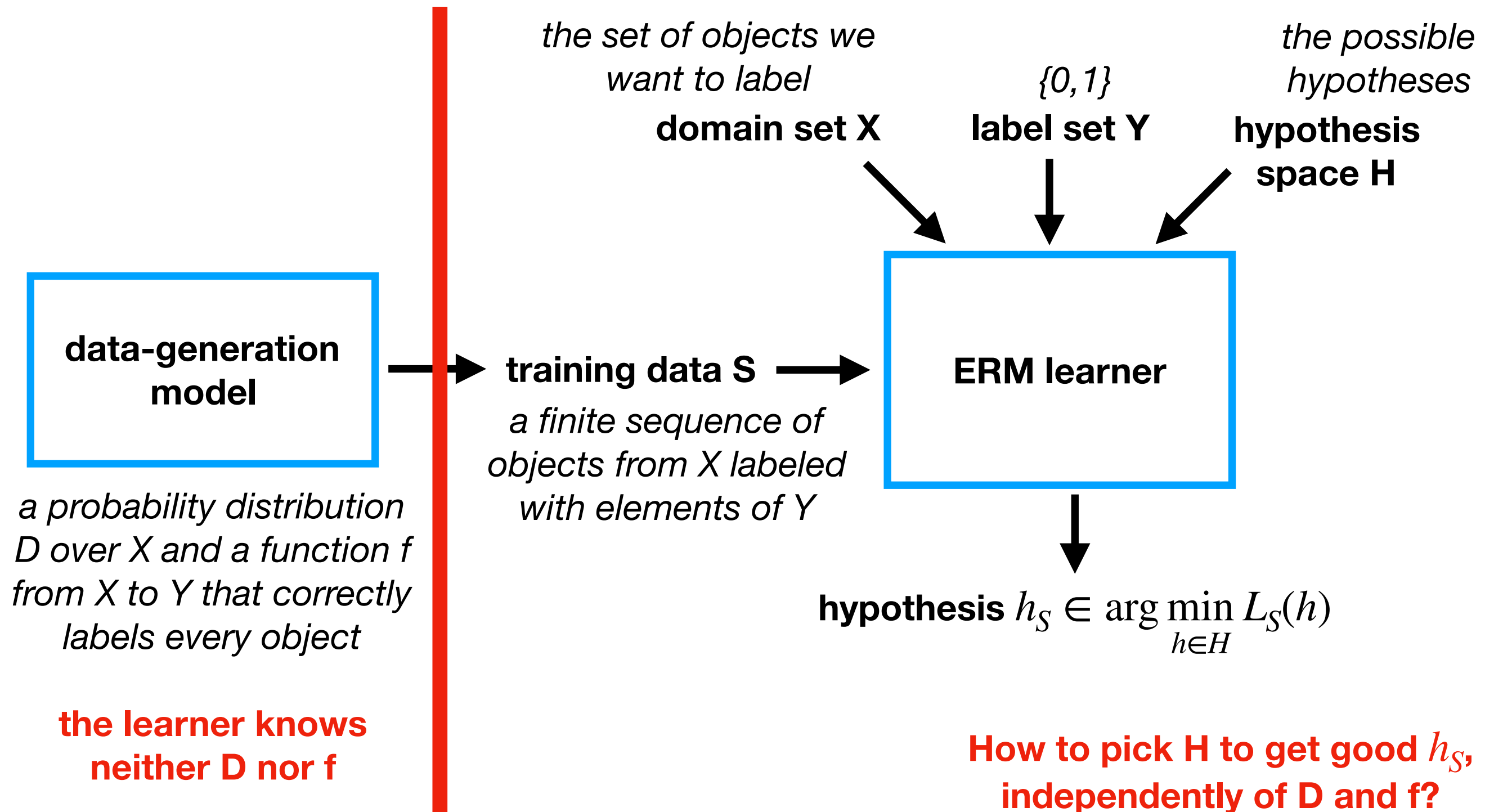
- We saw another example of overfitting earlier: CANDIDATE-ELIMINATION memoizes training examples if we allow it to learn arbitrary Boolean functions
- One way to avoid overfitting is to restrict the hypothesis space before seeing the data

The Statistical Learning Framework


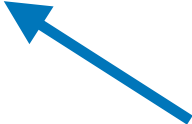



ERM Learning

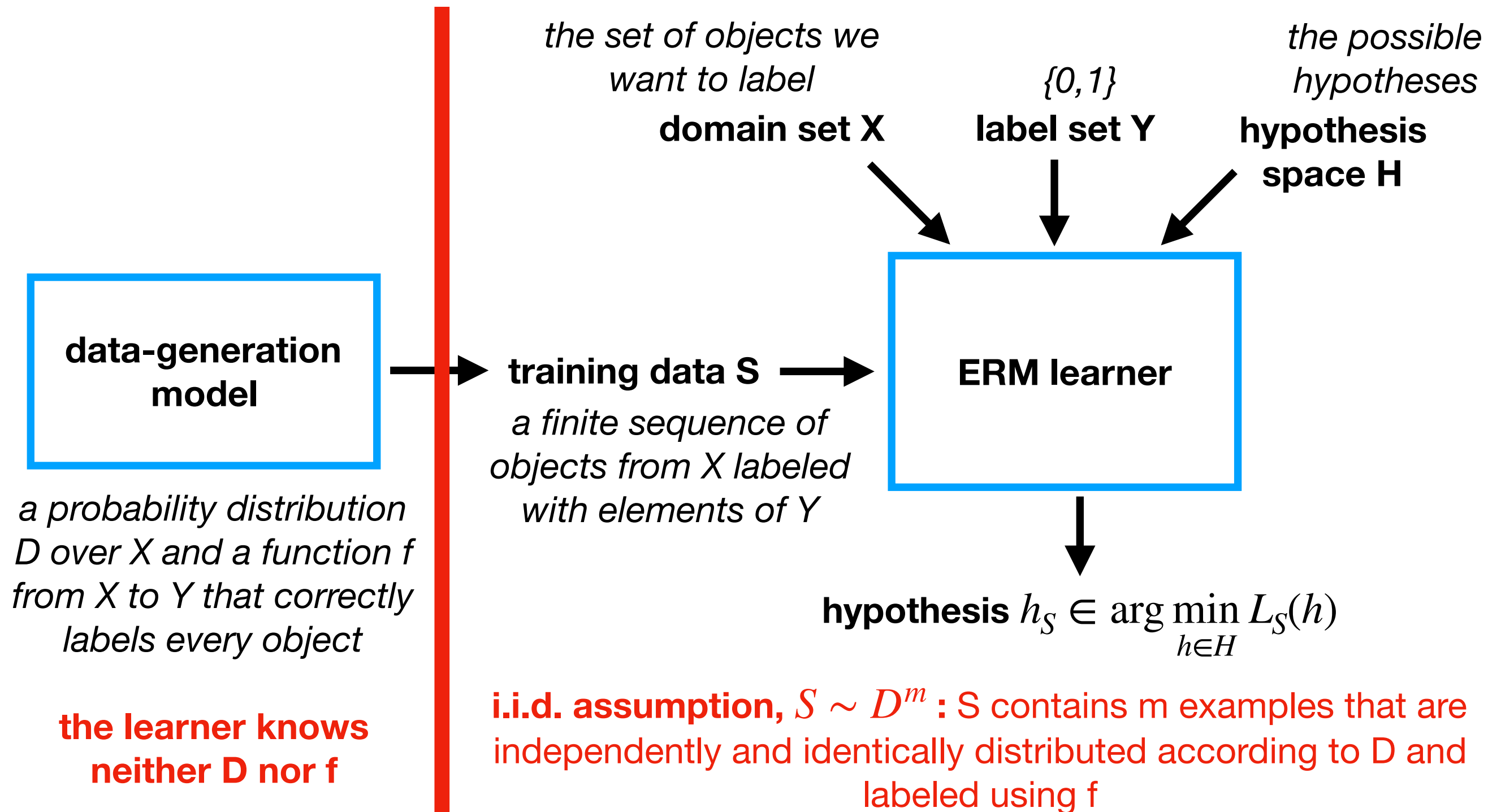
(Boolean functions)



ERM Learning

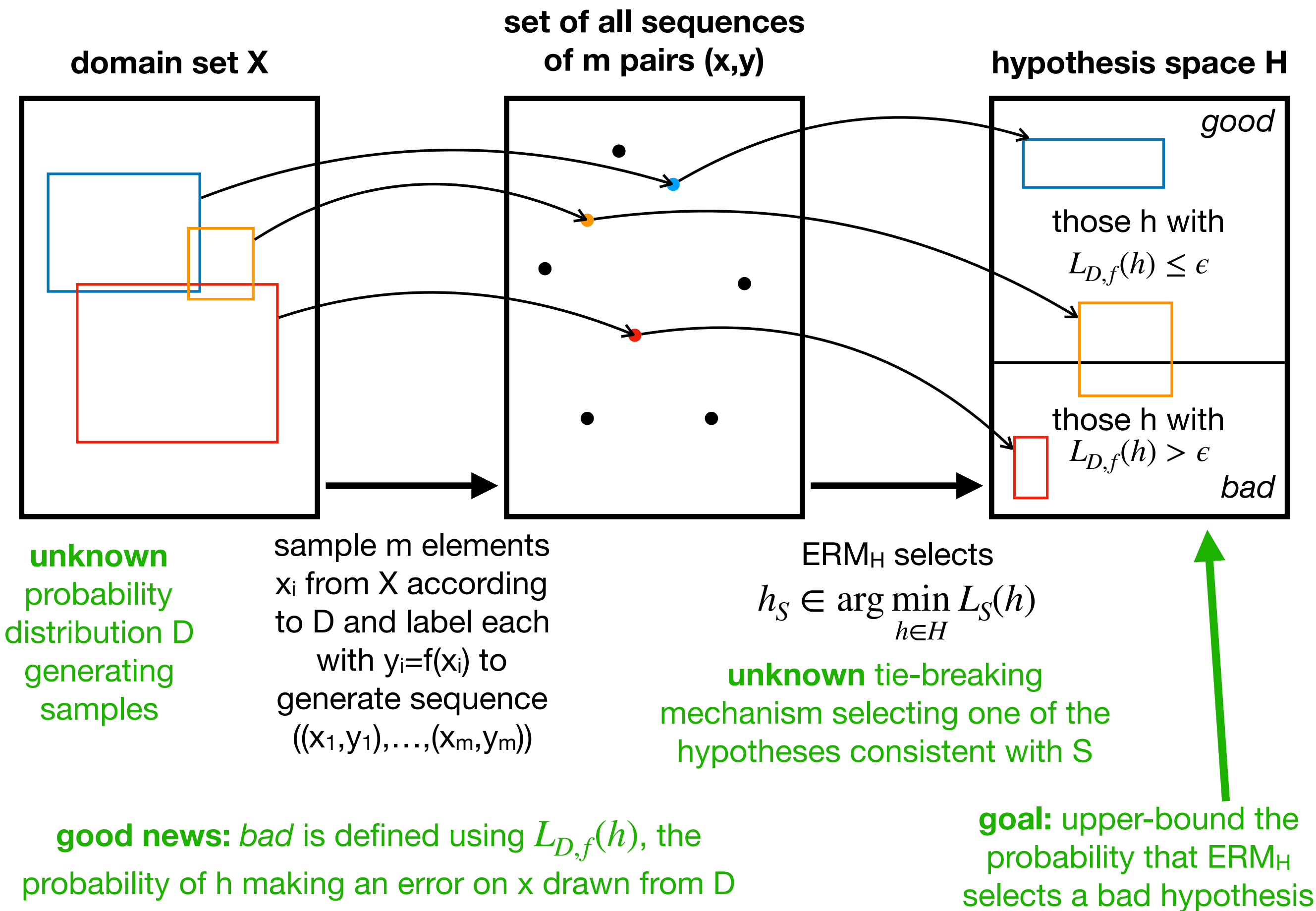
- Under the following conditions, ERM will not overfit:
 - H is finite  not a necessary condition (more later)
 - there is a $h \in H$ such that $L_{D,f}(h) = 0$  the **realisability** assumption
note: realisability implies $L_S(h_S) = 0$
 - S is “large enough”  we'll make this precise next

ERM Learning



ERM Learning

- ideally, we'd want ERM to return h_S with $L_{D,f}(h_S) = 0$
- this is not realistic: the random process may give us a misleading S
- instead, we aim for h_S that is **probably approximately correct**, i.e., for which it is very likely that $L_{D,f}(h_S)$ is small for a randomly selected S



Formally

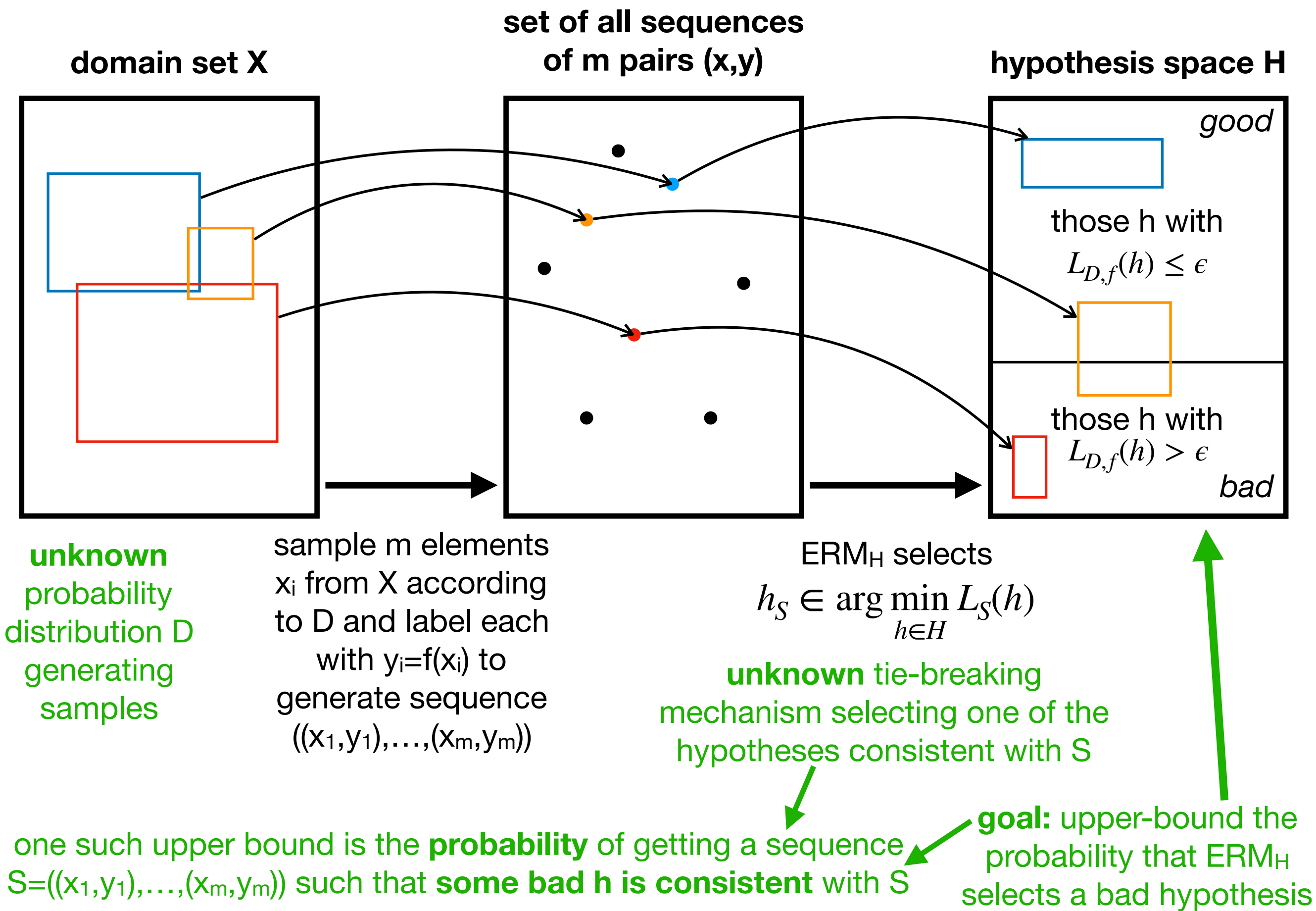
- Fix an **accuracy parameter** ϵ , and consider $L_{D,f}(h_S) > \epsilon$ a **failure** of the learner.
- **Goal:** ensure that the probability of failure (over samples S drawn from D and labeled by f) is at most δ , where we call $(1 - \delta)$ the **confidence parameter**.
- That is, given parameters ϵ and δ , we want $P(L_{D,f}(h_S) > \epsilon) \leq \delta$ or equivalently $P(L_{D,f}(h_S) \leq \epsilon) > 1 - \delta$
- Question: how large should S be for this to hold?

Basic process

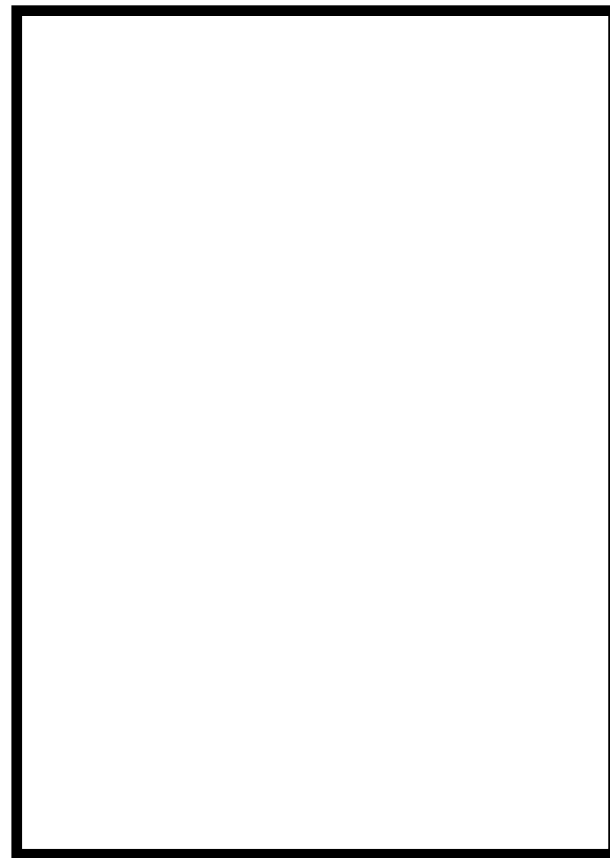
- The learner knows the object set X and hypothesis space H .
- The learner chooses the parameters ϵ and δ .
- The learner does not know the distribution D and function f , but can request an arbitrary but fixed number m of training examples drawn i.i.d. from D and labeled using f .
- How many examples should the learner ask for to achieve $P(L_{D,f}(h_S) > \epsilon) \leq \delta$?

Which m to choose?

- How many examples should the learner ask for to achieve $P(L_{D,f}(h_S) > \epsilon) \leq \delta$?
- We'll answer this question by
 - providing a function $g(m)$ such that $P(L_{D,f}(h_S) > \epsilon) \leq g(m)$
preview: $g(m) = |H| e^{-\epsilon m}$
 - rearranging $g(m) \leq \delta$ to obtain an inequality with just m on one side
preview: $m \geq \frac{\log(|H|/\delta)}{\epsilon}$

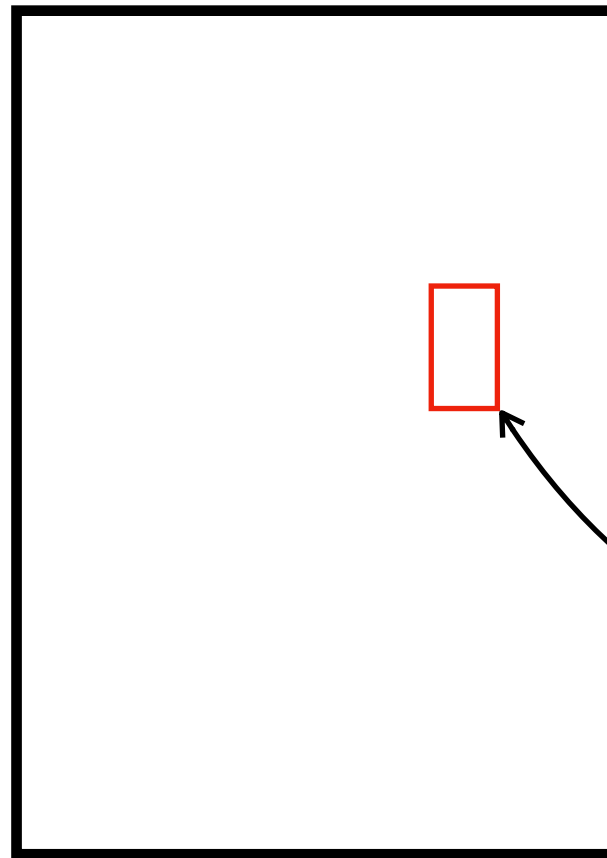


domain set X

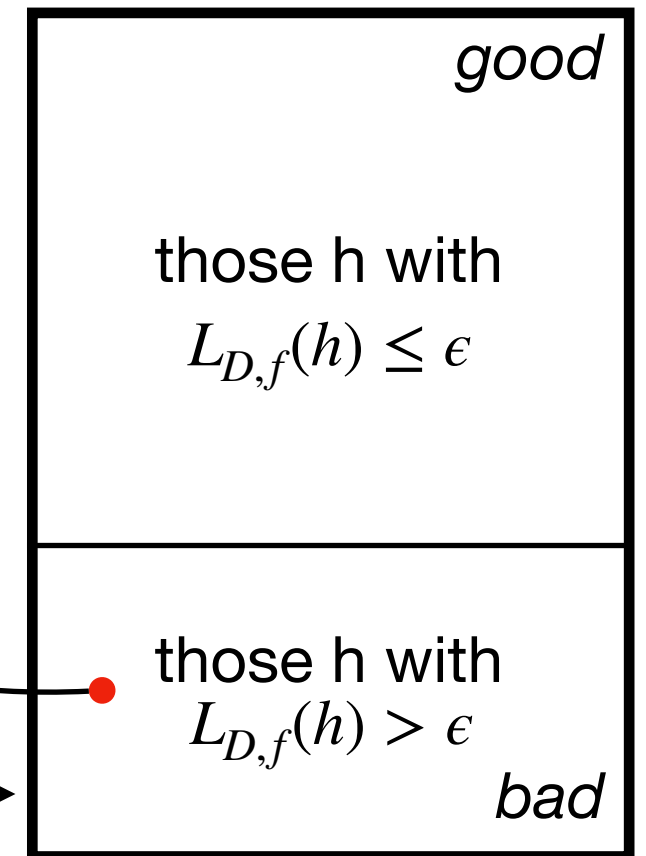


sample m elements x_i from X
according to D and label each
with $y_i=f(x_i)$ to generate
sequence $((x_1, y_1), \dots, (x_m, y_m))$

set of all sequences
of m pairs (x, y)



hypothesis space H



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

for a specific bad hypothesis h , what is the probability of getting a sequence $S=((x_1, y_1), \dots, (x_m, y_m))$ such that this h is consistent with S ?

for a specific bad hypothesis h , what is the probability of getting a sequence $S=((x_1,y_1),\dots,(x_m,y_m))$ such that this h is consistent with S ?

↑
for each x_i , $h(x_i)=y_i$

↑
for each x_i , $h(x_i)=f(x_i)$

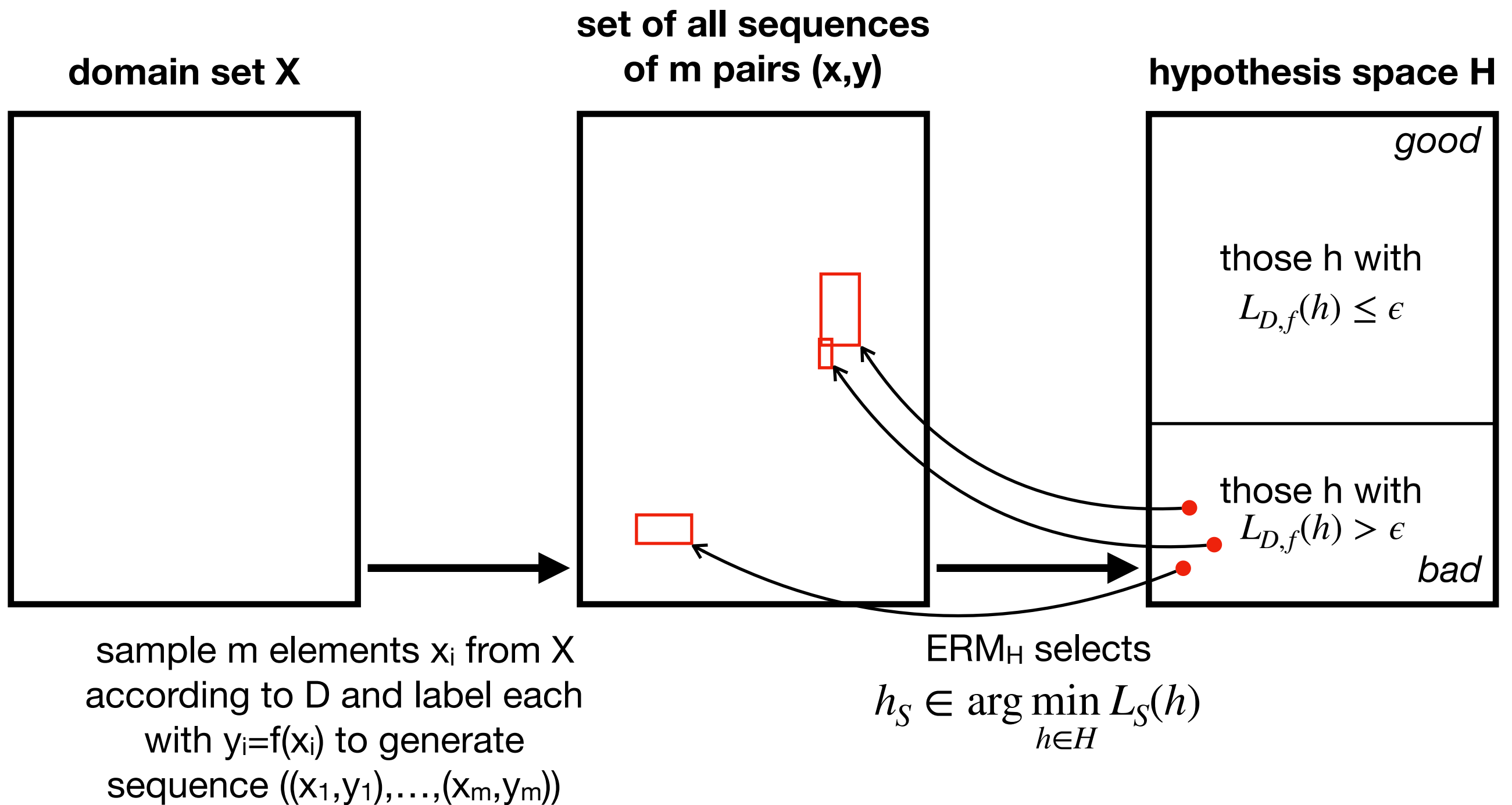
recall that $L_{D,f}(h)$ is the probability that for x drawn from D , $h(x) \neq f(x)$

thus, $1 - L_{D,f}(h)$ is the probability that for x drawn from D , $h(x) = f(x)$

as each x_i in S is drawn i.i.d. from D ,

the **probability of getting S consistent with h** is $(1 - L_{D,f}(h))^m \leq (1 - \epsilon)^m$

↖ h is bad



for a specific bad hypothesis h , what is the probability of getting a sequence $S=((x_1,y_1), \dots, (x_m,y_m))$ such that this h is consistent with S ? $\leq (1 - \epsilon)^m$

the probability of getting S consistent with some bad h is $\leq |H_{bad}| (1 - \epsilon)^m$

$\leq |H| (1 - \epsilon)^m \leq |H| e^{-\epsilon m}$

holds for all $\epsilon \in [0,1]$

Which m to choose?

- How many examples should the learner ask for to achieve $P(L_{D,f}(h_S) > \epsilon) \leq \delta$?
- We'll answer this question by
 - providing a function $g(m)$ such that $P(L_{D,f}(h_S) > \epsilon) \leq g(m)$
preview: $g(m) = |H| e^{-\epsilon m}$
 - rearranging $g(m) \leq \delta$ to obtain an inequality with just m on one side
preview: $m \geq \frac{\log(|H|/\delta)}{\epsilon}$

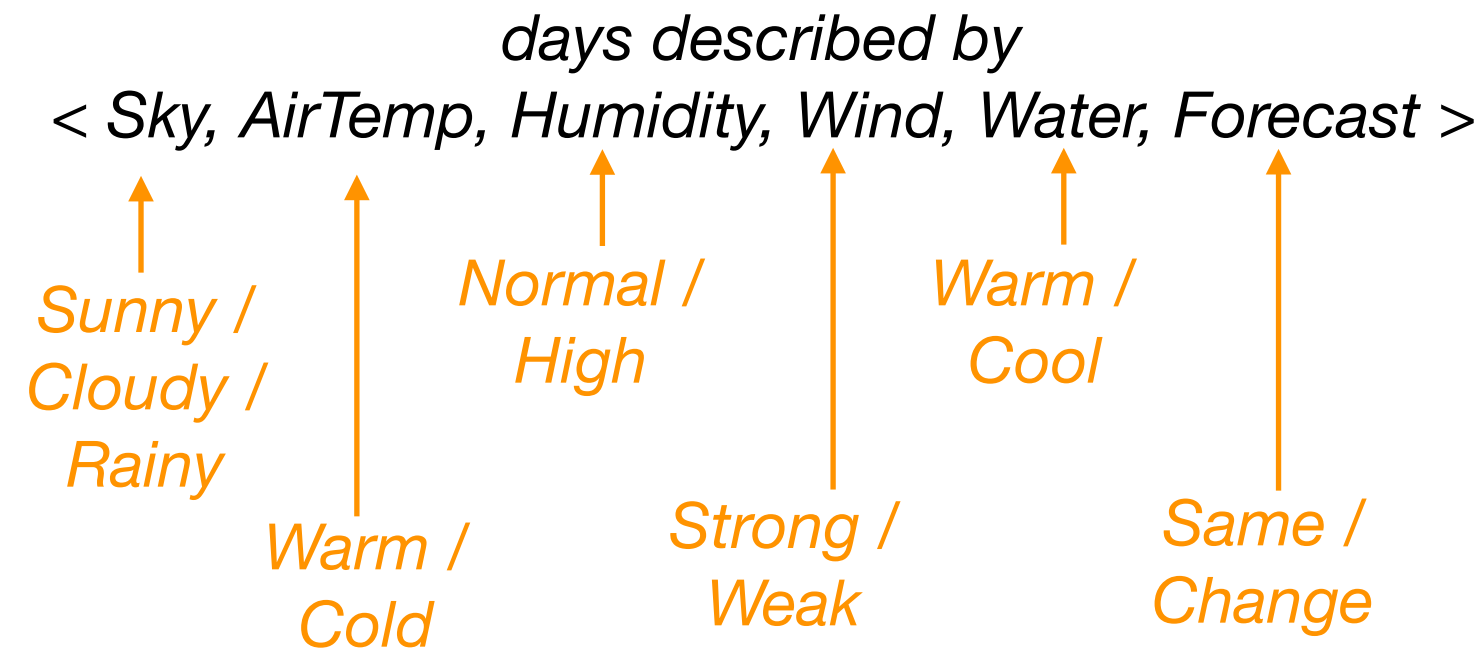
ERM Learning

- Let H be a finite hypothesis space of Boolean functions on X , $\delta \in [0,1]$, $\epsilon \in [0,1]$, and m an integer satisfying
$$m \geq \frac{\log(|H|/\delta)}{\epsilon}.$$
- Then, for any distribution D over X and any labeling function f for which the realisability assumption holds, with probability of at least $1 - \delta$ over the choice of an i.i.d. sample S of size m , we have that for every ERM hypothesis h_S it holds that $L_{D,f}(h_S) \leq \epsilon$.

*That is, for sufficiently large m , any ERM hypothesis is **probably** (with confidence $1 - \delta$) **approximately** (up to an error of ϵ) **correct**.*

Example

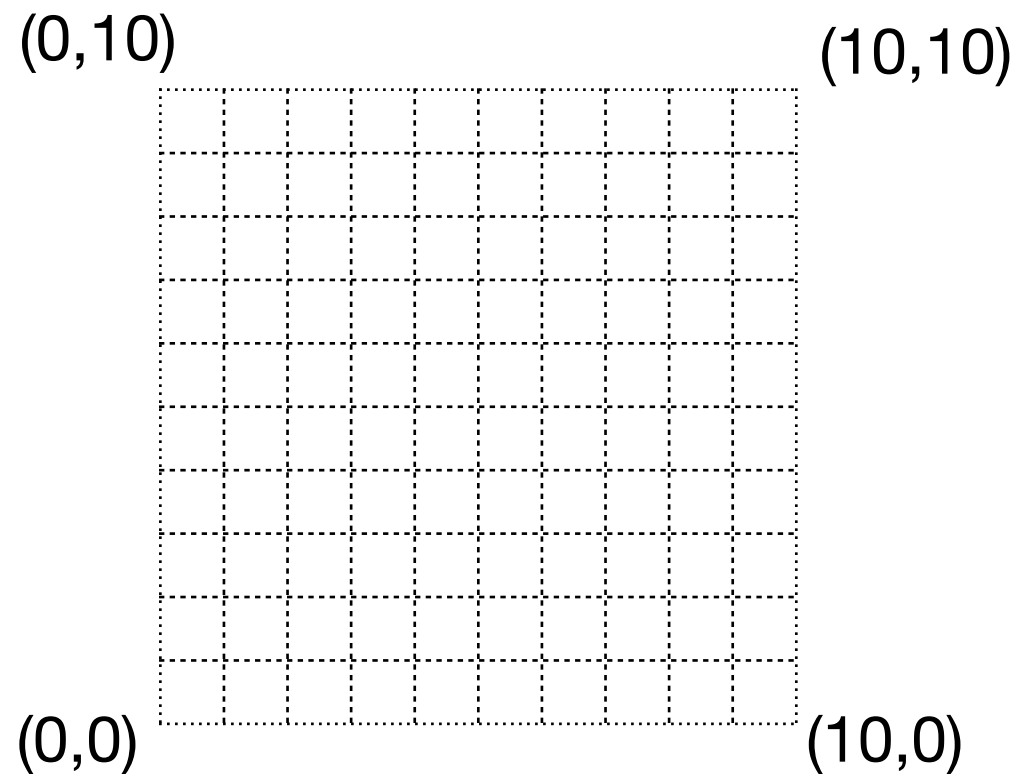
$$m \geq \frac{\log(|H|/\delta)}{\epsilon}$$



| ϵ | | | |
|------------|------|------|------|
| δ | | 0.05 | 0.01 |
| | 0.05 | | |
| | 0.01 | | |

Example

$$m \geq \frac{\log(|H|/\delta)}{\epsilon}$$



| ϵ | | | |
|------------|------|------|------|
| δ | | 0.05 | 0.01 |
| | 0.05 | | |
| | 0.01 | | |

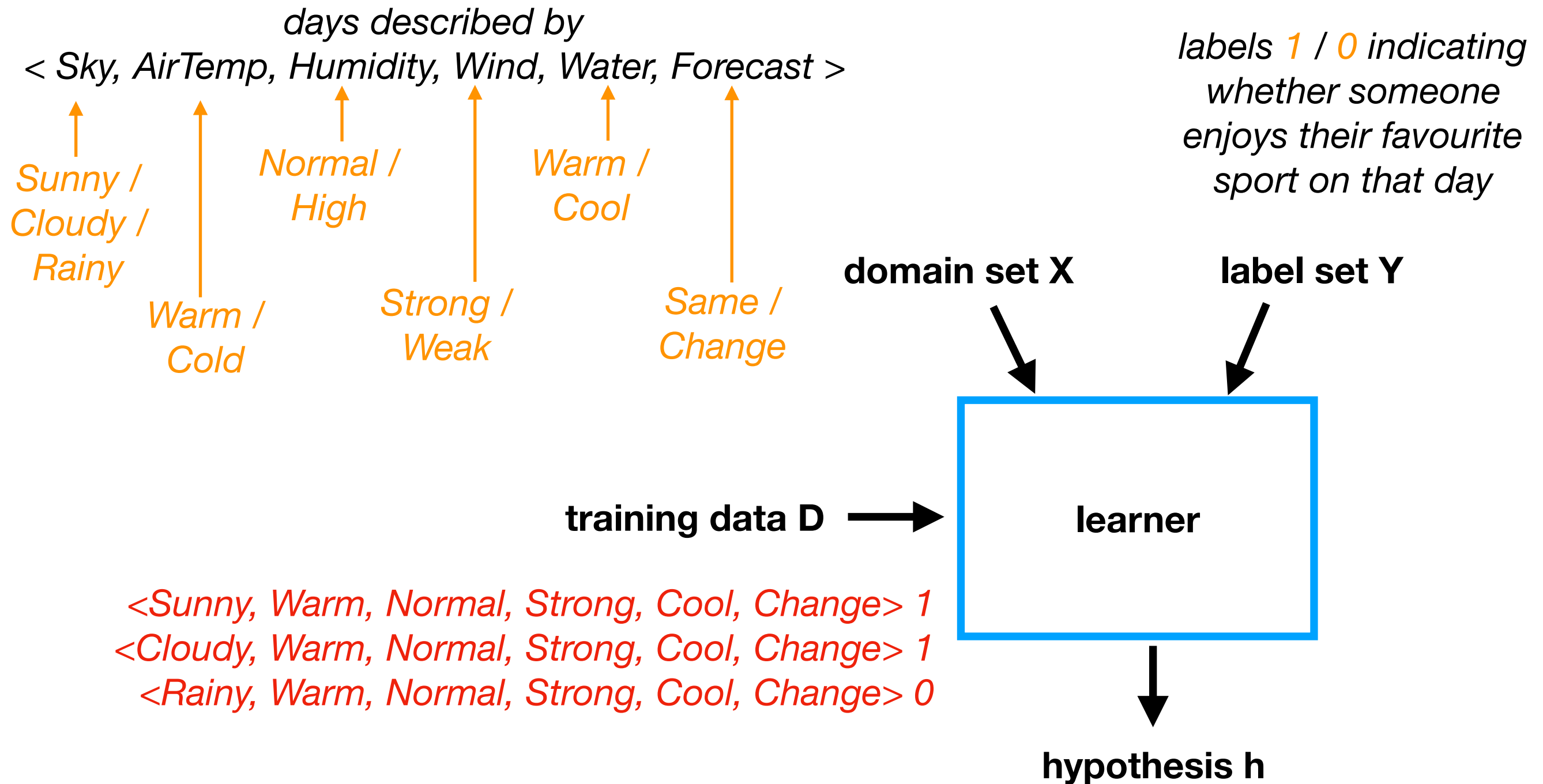
PAC Learnability

- PAC = **P**robably **A**pproximately **C**orrect
- A hypothesis class H is **PAC learnable** if there exists a function $m_H : (0,1)^2 \rightarrow \mathbb{N}$ and a learning algorithm with the following property: For every $\epsilon, \delta \in (0,1)$, for every distribution D over X , and for every function $f : X \rightarrow \{0,1\}$, if the realisability assumption holds w.r.t. H, D, f , then if given $m \geq m_H(\epsilon, \delta)$ i.i.d. examples generated by D and labeled by f , the algorithm returns a hypothesis h such that with probability at least $1 - \delta$ over the choice of the examples, the true error $L_{D,f}(h)$ is at most ϵ .

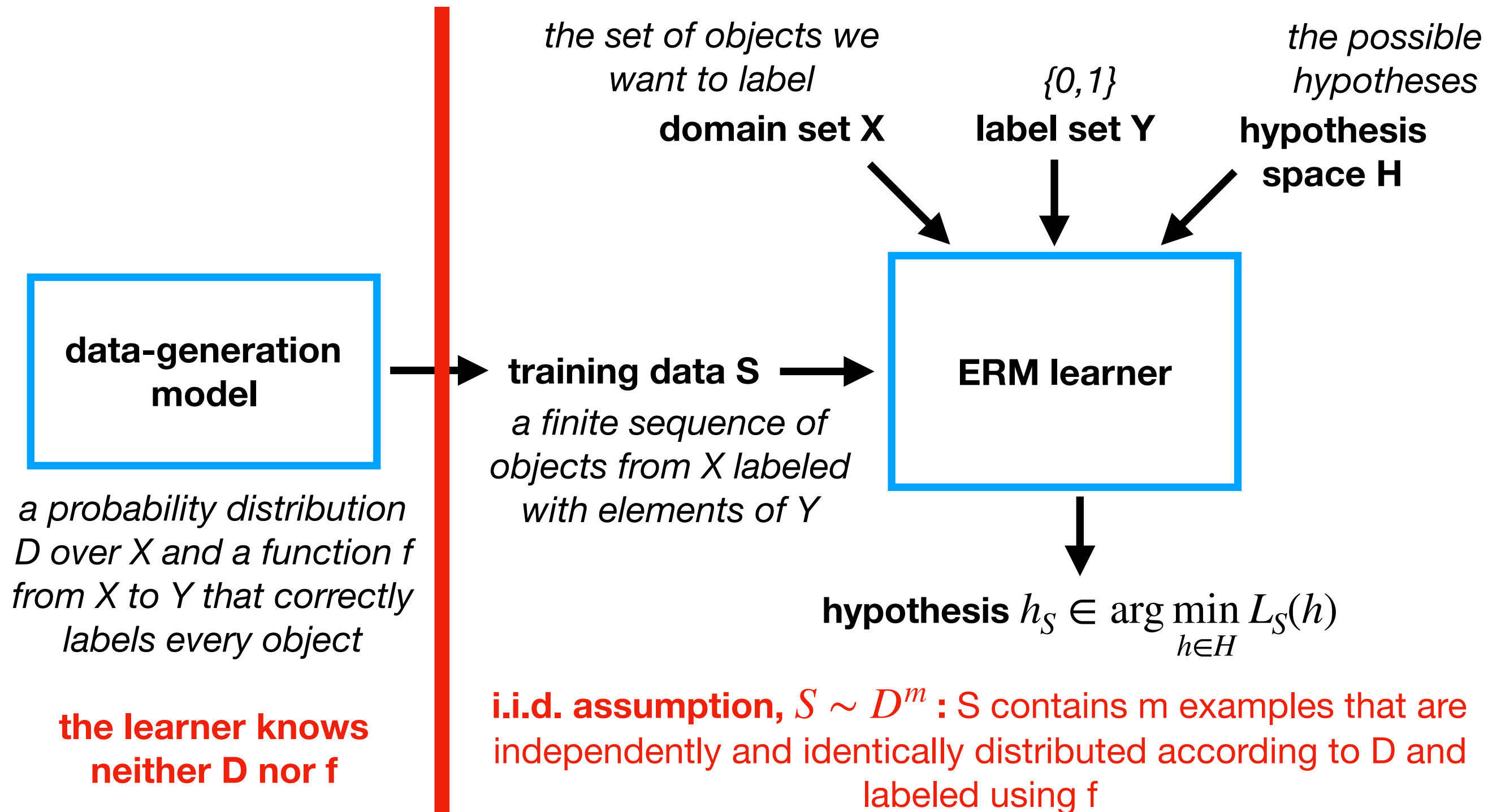
Sample Complexity

- The function $m_H : (0,1)^2 \rightarrow \mathbb{N}$ determines the **sample complexity** of learning H , i.e., the number of samples needed to guarantee a probably approximately correct solution.
- More precisely, $m_H(\epsilon, \delta)$ is the minimal integer that satisfies the requirements of PAC learning
- Thus: every finite H is PAC learnable with sample complexity
$$m_H(\epsilon, \delta) \leq \left\lceil \frac{\log(|H|/\delta)}{\epsilon} \right\rceil$$

No correct h in H

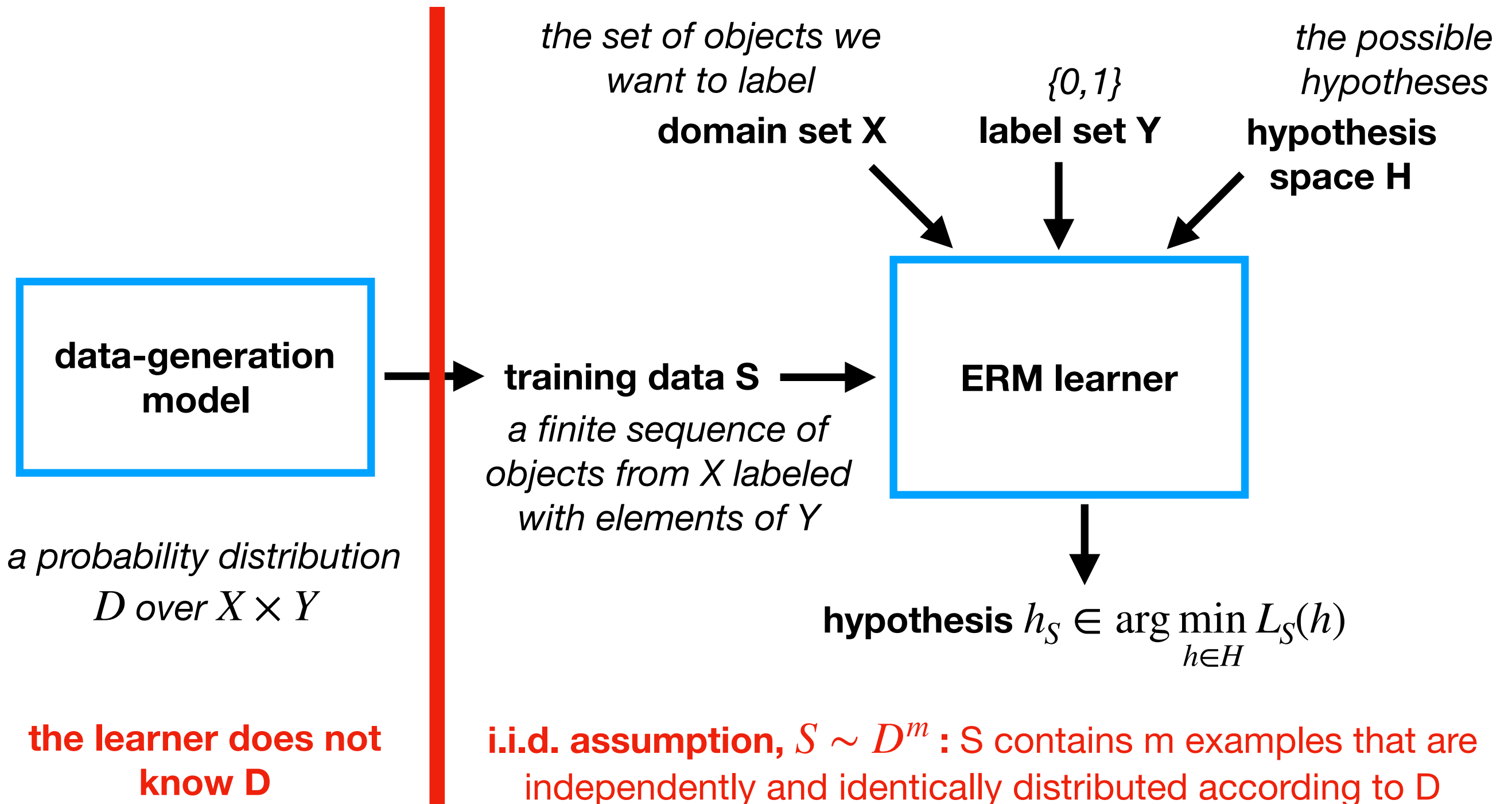


ERM Learning



ERM Learning

with randomly labeled examples



New data generation model

- We now consider a distribution D over labeled objects, e.g.,
 $D((x, y)) = D_X(x) \cdot D_Y(y \mid x)$
- Advantages:
 - can be a more realistic model of the world
 - can handle cases violating the realisability assumption
- Adapt the definition of true error to $L_D(h) = D(\{(x, y) \mid h(x) \neq y\})$
- Goal: a hypothesis that probably approximately minimises $L_D(h)$

The Bayes optimal predictor

- For any D over $X \times \{0,1\}$, the best labeling function is

$$f_D(x) = \begin{cases} 1 & \text{if } P(y = 1 \mid x) \geq 0.5 \\ 0 & \text{otherwise} \end{cases}$$

- best = no other $g : X \rightarrow \{0,1\}$ has lower error
- but we do not know D ...
- instead, we'll aim to learn a predictor whose error is not much larger than the best error in a given class of predictors

Agnostic PAC Learnability

- A hypothesis class H is **agnostic PAC learnable** if there exists a function $m_H : (0,1)^2 \rightarrow \mathbb{N}$ and a learning algorithm with the following property: For every $\epsilon, \delta \in (0,1)$, for every distribution D over $X \times Y$, if given $m \geq m_H(\epsilon, \delta)$ i.i.d. examples generated by D , the algorithm returns a hypothesis h such that with probability at least $1 - \delta$ over the choice of the examples, the true error $L_D(h)$ is at most ϵ larger than the lowest true error of any hypothesis in H , i.e., $L_D(h) \leq \min_{h' \in H} L_D(h') + \epsilon$.

Remarks

- Agnostic PAC learnability generalises PAC learnability beyond the realisability assumption.
- The whole setup can also be generalised beyond Boolean concept learning (*see the book if interested*)
- The original definition of PAC learnability by Valiant also imposes conditions on the time the algorithm needs to find an answer (*we'll get back to this*)

For next week

- **Mandatory:** revise today's material
 - relevant textbook chapters:
 - Shalev-Shwartz & Ben-David: chapters 2 & 3
 - Mitchell: chapter 2
- **Optional:** look forward
 - Read Shalev-Shwartz & Ben-David, chapters 5 and 6 (excluding proofs), with the following questions in mind:
 - What are the key concepts and ideas introduced?
 - How do they relate to the material covered already?