CMT311 Principles of Machine Learning

ERM & PAC Learning

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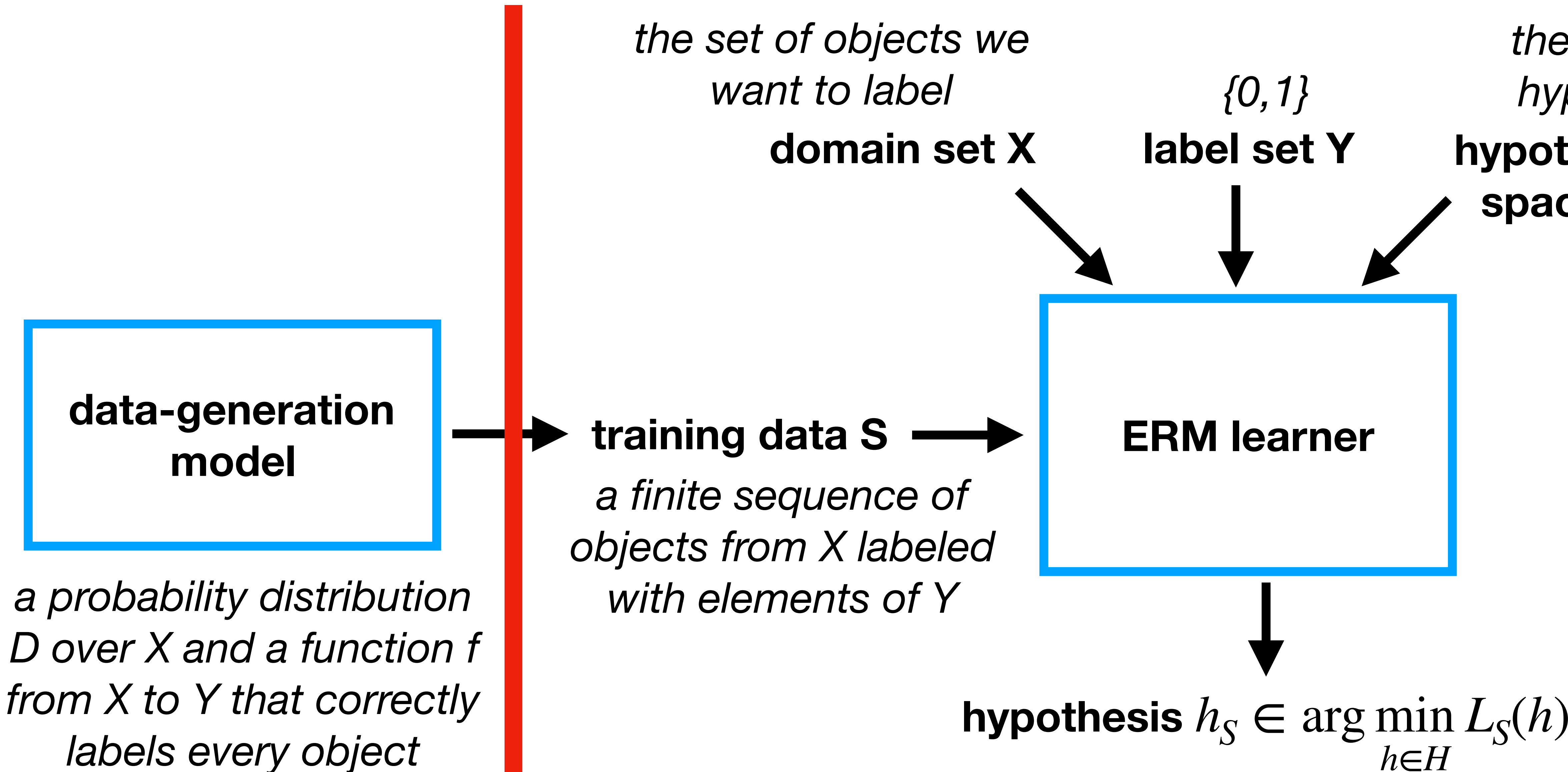
ERM Learning

(Boolean functions)



the learner knows neither D nor f

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

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

ERM Learning

- Under the following conditions, ERM will not overfit:
  - H is finite
  - there is a $h \in H$ such that $L_{D,f}(h) = 0$
  - S is "large enough"

not a necessary condition (more later)

the **realisability** assumption

note: realisability implies $L_S(h_S) = 0$

we'll make this precise next

ERM Learning

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

the set of objects we want to label

domain set X

{0,1}

label set Y

the possible hypotheses

hypothesis space H

training data S

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

ERM learner

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

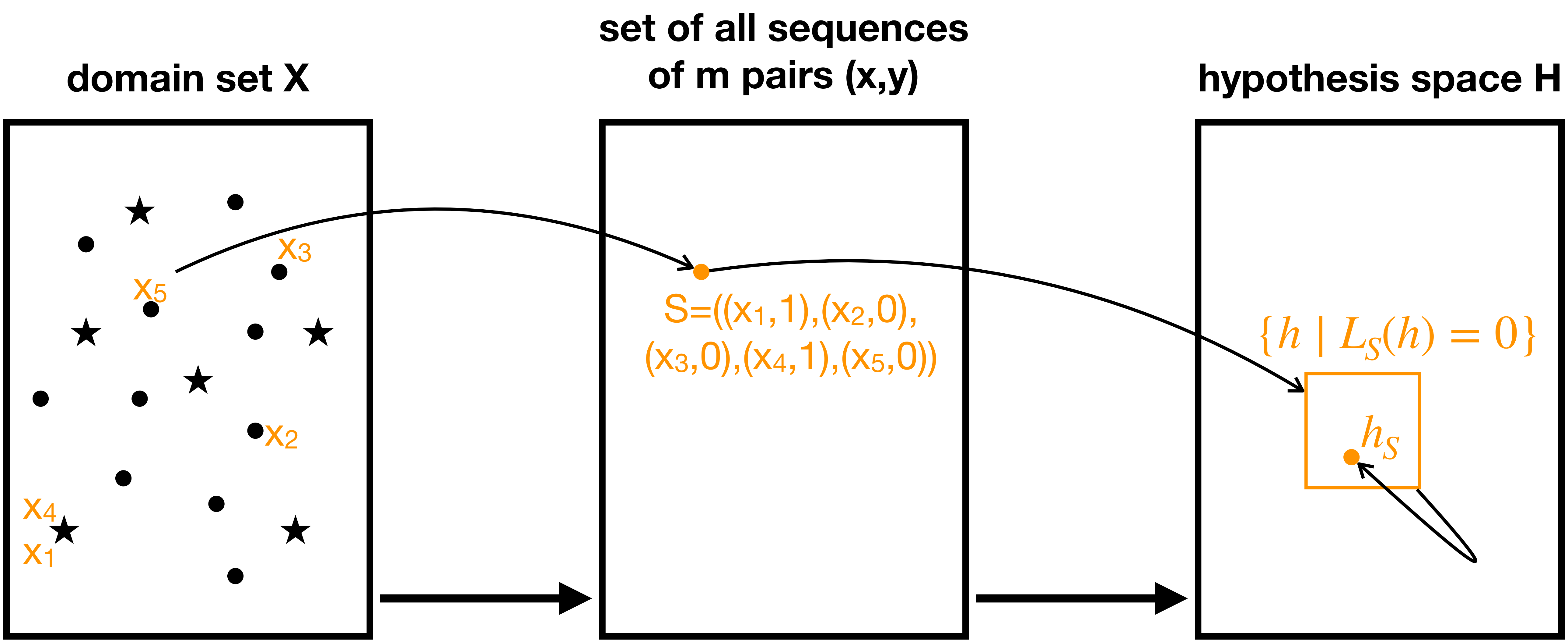
i.i.d. assumption, $S \sim D^m$ **:** S contains m examples that are independently and identically distributed according to D and labeled using f

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

probability $> 1 - \delta$

$\leq \epsilon$



★ f(x)=1

● f(x)=0

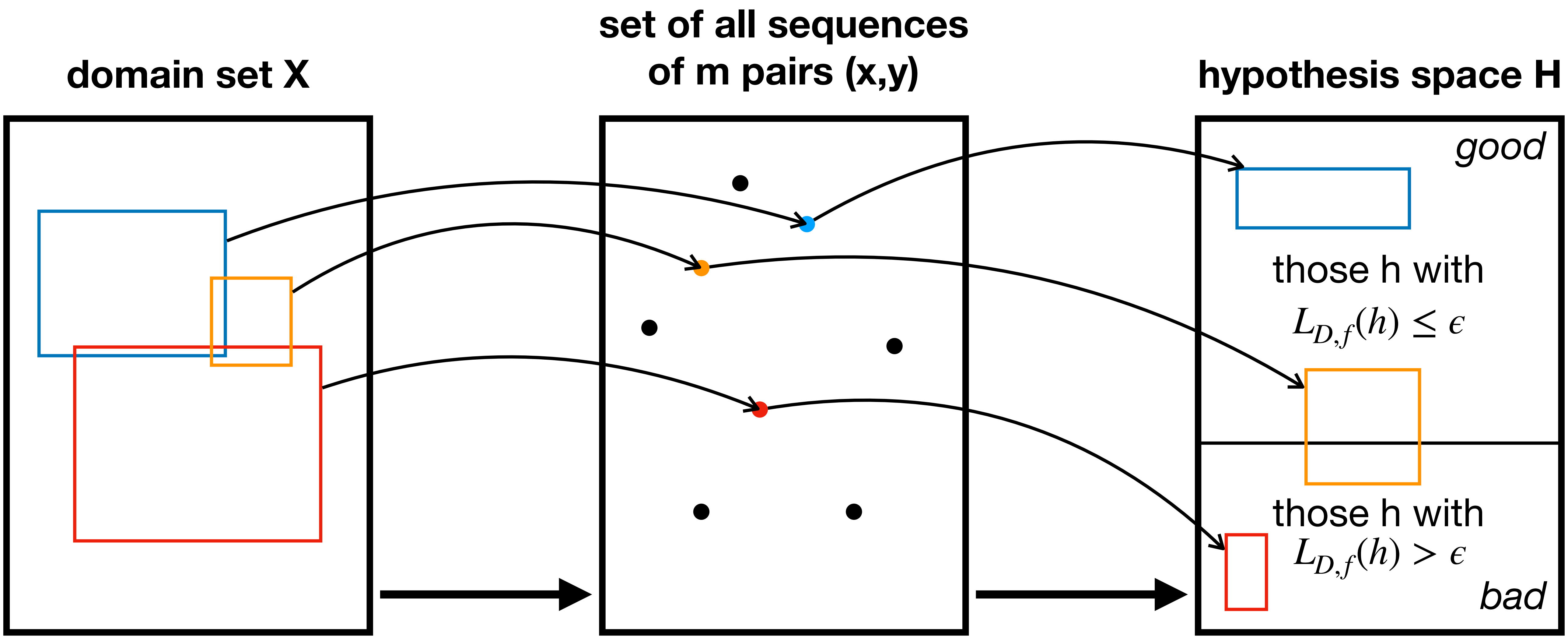
m=5

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),…,(x_m,y_m))

ERM$_H$ selects

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

what is the probability that the true error of h_S is small?



unknown probability distribution D generating samples

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

ERM_H selects

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

unknown tie-breaking mechanism selecting one of the hypotheses consistent with S

good news: *bad* is defined using $L_{D,f}(h)$, the probability of h making an error on x drawn from D

goal: upper-bound the probability that ERM_H selects a bad hypothesis

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 $P(L_{D,f}(h_S) > \epsilon) \leq \delta$?

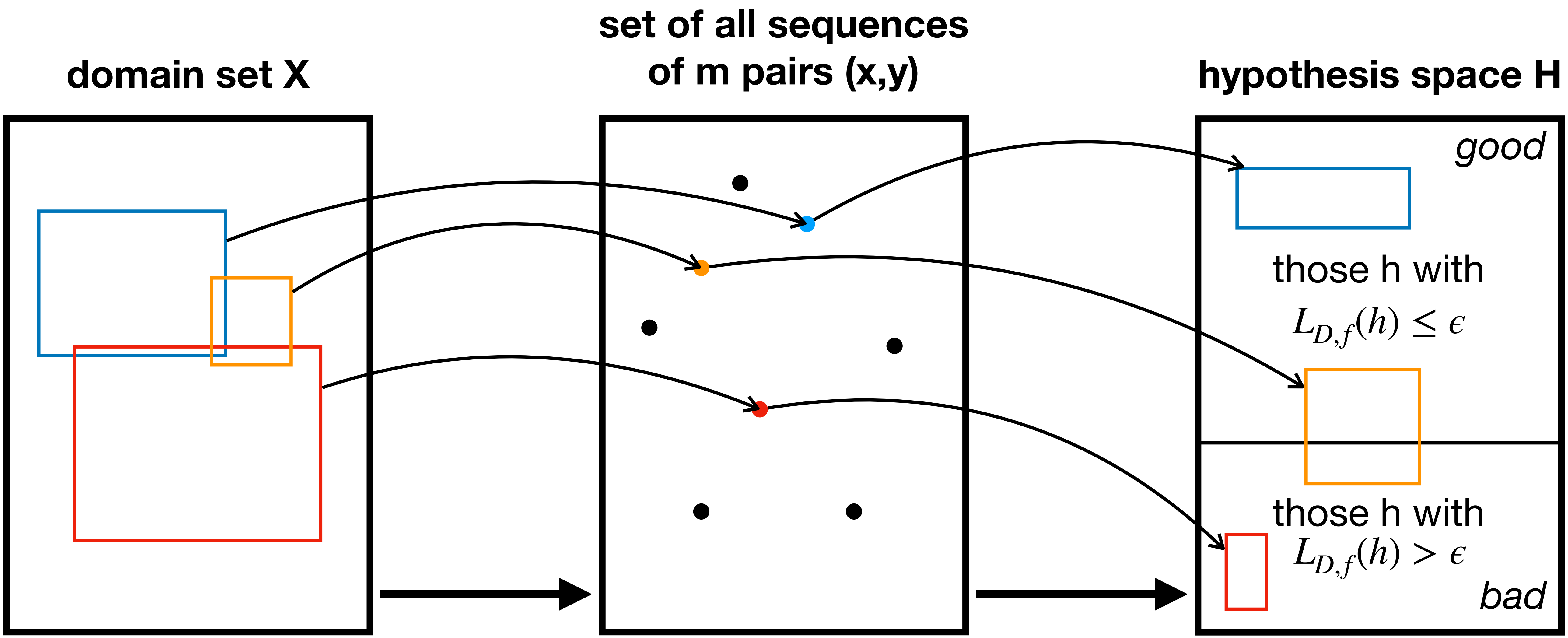
- We'll answer this question by

  - 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: $m \geq \dfrac{\log(|H|/\delta)}{\epsilon}$



unknown probability distribution D generating samples

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

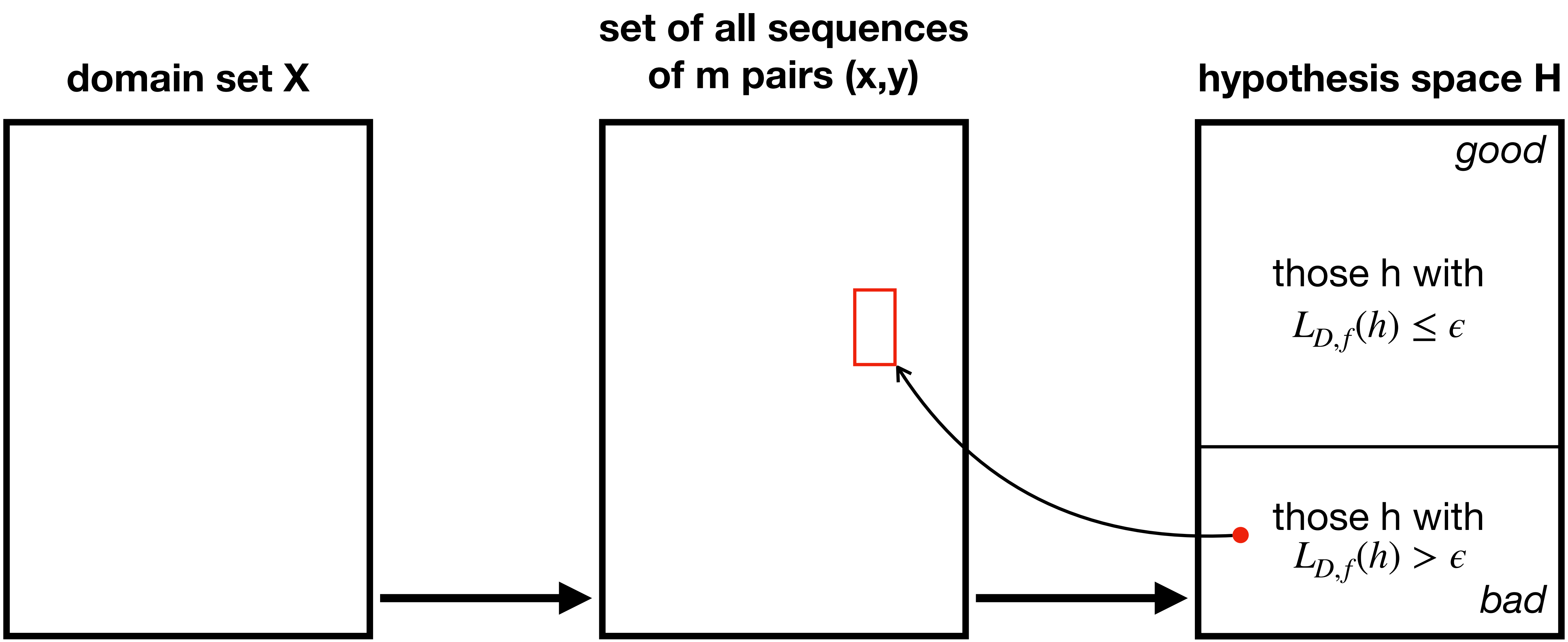
ERM_H selects

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

unknown tie-breaking mechanism selecting one of the hypotheses consistent with S

goal: upper-bound the probability that ERM_H selects a bad hypothesis

one such upper bound is the **probability** of getting a sequence $S=((x_1,y_1),\ldots,(x_m,y_m))$ such that **some bad h is consistent** with S



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

ERM_H selects

$$h_S \in \underset{h \in H}{\arg\min}\, L_S(h)$$

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

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

for each x_i, $h(x_i)=y_i$

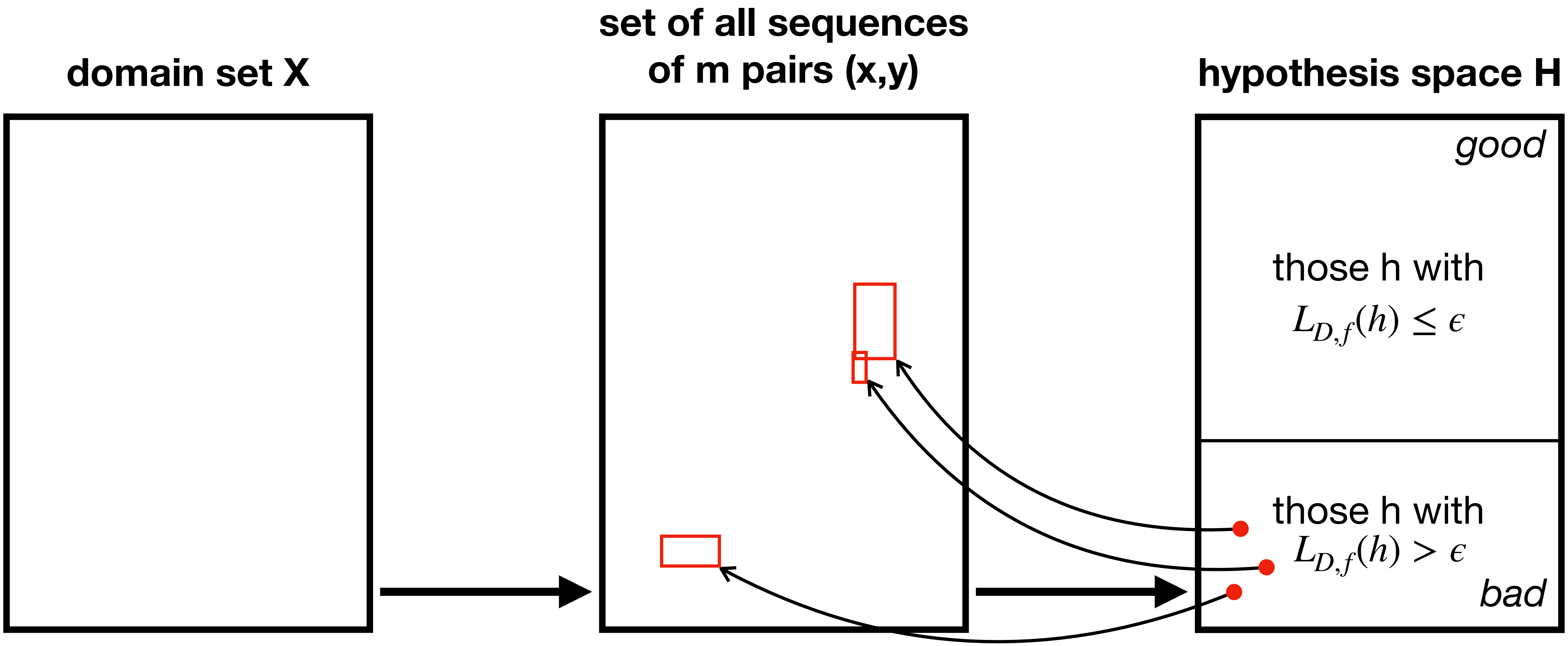
for each x_i, $h(x_i)=f(x_i)$

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



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

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 $S=((x_1,y_1),\ldots,(x_m,y_m))$ such that this h is consistent with S? $\leq (1-\epsilon)^m$

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

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

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

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

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

days described by

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

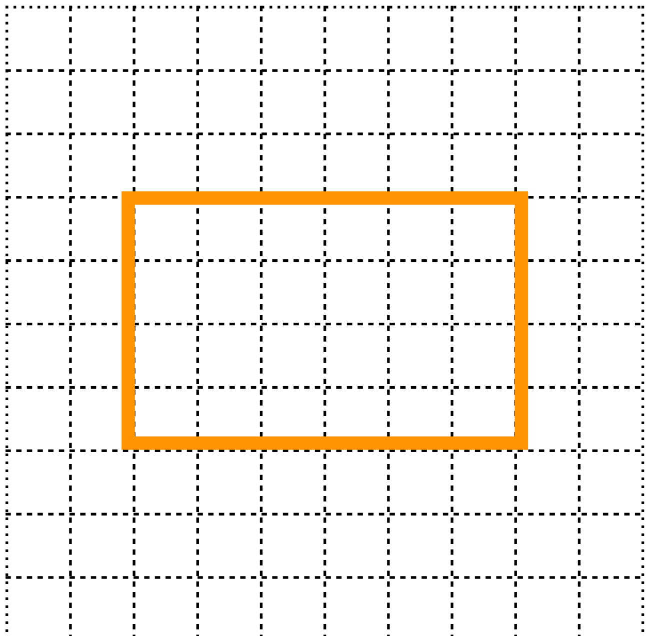
- *Sky*: Sunny / Cloudy / Rainy
- *AirTemp*: Warm / Cold
- *Humidity*: Normal / High
- *Wind*: Strong / Weak
- *Water*: Warm / Cool
- *Forecast*: Same / Change

$$|H| = 1 + 4 \cdot 3 \cdot 3 \cdot 3 \cdot 3 \cdot 3 = 973$$

δ \ ϵ	**0.05**	**0.01**
0.05	$m \geq \frac{\log(973/0.05)}{0.05} = 197.5$	$m \geq \frac{\log(973/0.05)}{0.01} = 987.6$
0.01	$m \geq \frac{\log(973/0.01)}{0.05} = 229.7$	$m \geq \frac{\log(973/0.01)}{0.01} = 1148.6$

Example

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



$$|H| = 1 + \sum_{j=1}^{11} \sum_{i=1}^{11} ij = 4357$$

very loose bounds!
note there are only 121 points…

δ \ ϵ	**0.05**	**0.01**
0.05	$m \geq \frac{\log(4357/0.05)}{0.05} = 227.5$	$m \geq \frac{\log(4357/0.05)}{0.01} = 1137.5$
0.01	$m \geq \frac{\log(4357/0.01)}{0.05} = 259.7$	$m \geq \frac{\log(4357/0.01)}{0.01} = 1298.5$

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 A 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 A 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

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

hypothesis h

conjunction of attribute constraints

ERM Learning

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

the set of objects we want to label

domain set X

{0,1}

label set Y

the possible hypotheses

hypothesis space H

training data S

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

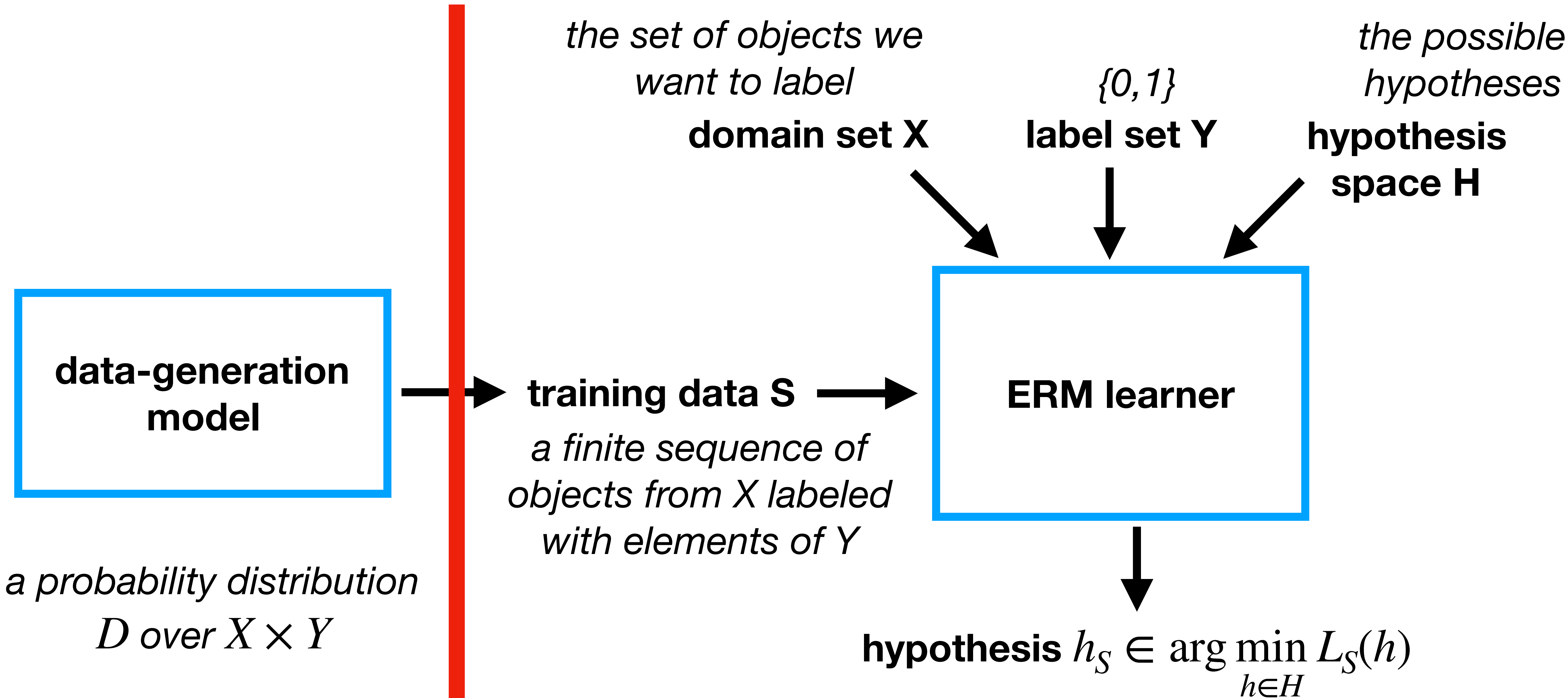
ERM learner

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

i.i.d. assumption, $S \sim D^m$ **:** S contains m examples that are independently and identically distributed according to D and labeled using f

ERM Learning

with randomly labeled examples



the learner does not know D

i.i.d. assumption, $S \sim D^m$: S contains m examples that are independently and identically distributed according to D

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

- best = no other $g : X \to \{0,1\}$ has lower true 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 $m_H : (0,1)^2 \to \mathbb{N}$ and a learning algorithm A 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 A 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.
- Finite hypothesis classes are agnostic PAC learnable using ERM *(see the book if interested)*
- 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)*
- Both PAC learning and agnostic PAC learning first fix H, and then choose an algorithm A — is there an algorithm that would work for any H?

No-Free-Lunch Theorem

training data contains less than half of all possible elements

Let A be any learning algorithm for Boolean concept learning over domain set X. Let $m < |X|/2$. Then there exists a distribution D over $X \times \{0,1\}$ such that

there is a function with true error zero

- There exists a function $f : X \to \{0,1\}$ with $L_D(f) = 0$.
- With probability of at least $1/7$ over the choice of $S \sim D^m$ we have that $L_D(A(S)) \geq 1/8$.

algorithm A is likely to return a bad hypothesis

No-Free-Lunch

- In other words, no Boolean concept learner can succeed on all learnable tasks — every learner will fail on some tasks where other learners succeed

- Key idea behind proof: every learner that sees less than half of all possible instances during training cannot be sure about the labels of the unseen instances, and may get all of them wrong

- We will not study the formal proof *(if interested, see the book or Shai Ben-Davis' video lecture)*

Prior Knowledge

- Successful learning needs to incorporate prior knowledge about the distribution D to avoid distributions causing failure, e.g.,
    - D comes from a specific parametric family of distributions *(we'll see examples in the second part of the module)*
    - Some h in a predefined class H has $L_D(h) = 0$ *(realisability)*
    - $\min_{h \in H} L_D(h)$ is small for predefined class H

Bias-Complexity Tradeoff

- For a given learning task, we'd like to choose H that allows for small error, but if we make H too large, learning fails.

approximation error: the error due to choosing this H (inductive bias)

- Let h_S be an ERM$_H$ hypothesis, set $\epsilon_{app} = \min_{h \in H} L_D(h)$ and

$$\epsilon_{est} = L_D(h_S) - \epsilon_{app}$$

estimation error: difference between true error achieved by ERM and best possible error in H

Which classes H provide a good balance?

* we’ll see later that any PAC-learnable class is PAC-learnable by ERM

Which H are PAC-learnable*?

- All finite classes are PAC-learnable
- What about infinite classes?
  - $H_{thr} = \{h_{\leq i} \,|\, i \in \mathbb{R}\}$ with $h_{\leq i}(x) = 1$ if $x \leq i$ and 0 otherwise **is PAC-learnable** using ERM
  - $H_{fin} = \{h_M \,|\, (M \subseteq \mathbb{R} \wedge |M| < \infty) \vee M = \mathbb{R}\}$ with $h_M(x) = 1$ if $x \in M$ and 0 otherwise **is not PAC-learnable** using ERM

Key difference

- Intuitively, for every finite sample, H_{fin} contains a hypothesis that overfits to that sample, while this is not the case for H_{thr}
- This is formalised by the VC-dimension (named after Vapnik and Chervonenkis)

VC-Dimension

- Let H be a class of functions from X to {0,1} and $C = \{c_1, \ldots, c_m\}$ a finite subset of X. The **restriction** H_C of H to C contains exactly those functions from C to {0,1} that agree with some h in H on C.

- A hypothesis class H **shatters** a finite subset C of X if the restriction of H to C contains all functions from C to {0,1}.

- The **VC-dimension** VCdim(H) of a hypothesis class H is the maximal size of a set C that can be shattered by H. VCdim(H) is infinite if H can shatter arbitrarily large sets.

VC-Dimension

- To show that the VC-dimension of class H is d, we need to show that

  providing an example and showing it is shattered is enough

  - there is a set C of size d that is shattered by H
  - every set C of size d+1 is **not** shattered by H

  requires proving that whatever C of size d+1 we choose, it is not shattered

Example

- $H_{thr} = \{h_{\leq i} \,|\, i \in \mathbb{R}\}$ with $h_{\leq i}(x) = 1$ if $x \leq i$ and 0 otherwise

- If C contains a single point c, there are two functions from C to {0,1}, and both agree with some h in H_{thr} (why?). Thus H_{thr} shatters C and $VCdim(H_{thr}) \geq 1$.

- If C contains two different points c_1 and c_2, there are four functions from C to {0,1}, but only three of them agree with some h in H_{thr} (why?). Thus no set of size two is shattered by H_{thr} and $VCdim(H_{thr}) = 1$.

Example

- $H_{fin} = \{h_M \mid (M \subseteq \mathbb{R} \land |M| < \infty) \lor M = \mathbb{R}\}$ with $h_M(x) = 1$ if $x \in M$ and 0 otherwise

- Consider $C = \{c_1, \ldots, c_m\}$ for some finite m. There are 2^m functions from C to {0,1}, and all agree with some H in H_{fin} (why?).

- Thus H_{fin} shatters arbitrarily large sets, and $VCdim(H_{fin}) = \infty$

VC-Dimension

- If H is finite, $VCdim(H) \leq \log_2(|H|)$ *(why?)*
- If H shatters some set C of size 2m then we cannot learn H using m examples.
- If H has infinite VC-dimension, then H is not PAC-learnable.

Example

days described by

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

- Sky: *Sunny / Cloudy / Rainy*
- AirTemp: *Warm / Cold*
- Humidity: *Normal / High*
- Wind: *Strong / Weak*
- Water: *Warm / Cool*
- Forecast: *Same / Change*

- Let H be our earlier hypothesis space for this setting.

- $VCdim(H) \leq \log_2(|H|) = \log_2(973) = 9.93$

- $VCdim(H) \geq 6$ because H shatters the following set of six examples:

< cloudy, warm, normal, strong, warm, same >
< sunny, cold, normal, strong, warm, same >
< sunny, warm, high, strong, warm, same >
< sunny, warm, normal, weak, warm, same >
< sunny, warm, normal, strong, cool, same >
< sunny, warm, normal, strong, warm, change >

Fundamental Theorem of Statistical Learning

Let H be a class of functions from X to {0,1}. Then, the following are equivalent:

- H has finite VC-dimension.
- H is PAC-learnable.
- Any ERM learner is a successful PAC learner for H.
- H is agnostic PAC-learnable.
- Any ERM learner is a successful agnostic PAC learner for H.

Fundamental Theorem of Statistical Learning

- There is a quantitative version of this theorem for classes with finite VC-dimension that provides both lower and upper bounds on the sample complexity.

- For finite H, the lower bound on the sample complexity for PAC learning grows linearly in VCdim(H) compared to logarithmically in the size of H.

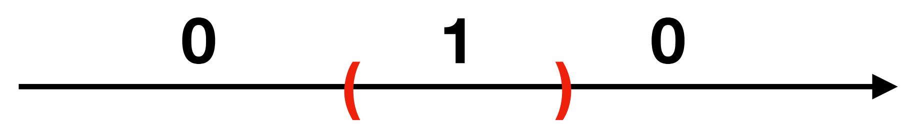
e.g., for (integer) threshold functions on $X=\{1,\ldots,k\}$, VCDim(H)=1 but $|H|=k$

Exercise: determine the VC-dimension for each of these classes

- $H_{int} = \{h_{a,b} \mid a, b \in \mathbb{R}, a < b\}$ where

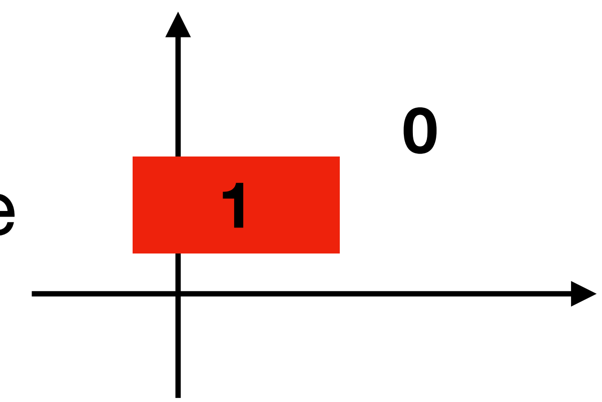
$$h_{a,b}(x) = \begin{cases} 1 & \text{if } x \in (a, b) \\ 0 & \text{otherwise} \end{cases}$$

open intervals on the real line



- $H_{rect} = \{h_{(a,b,c,d)} \mid a, b, c, d \in \mathbb{R}, a \leq b, c \leq d\}$ where

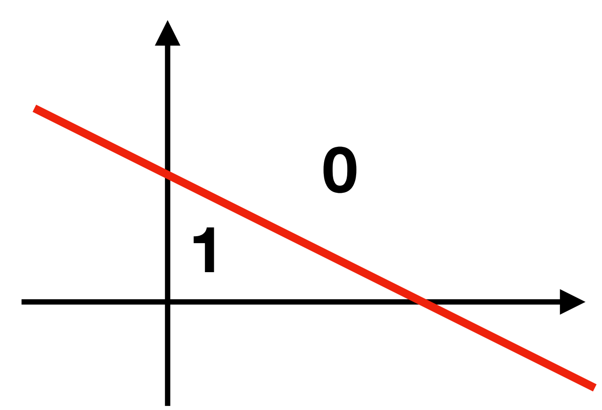
$$h_{(a,b,c,d)}(x, y) = \begin{cases} 1 & \text{if } a \leq x \leq b \text{ and } c \leq y \leq d \\ 0 & \text{otherwise} \end{cases}$$



axis-aligned rectangles on the real plane

- $H_{lin} = \{h_{(a,b,\theta)} \mid a, b \in \mathbb{R}, \theta \in \{ \leq , \geq \}\}$ where

$$h_{(a,b,\theta)}(x, y) = \begin{cases} 1 & \text{if } (ax + b)\theta y \\ 0 & \text{otherwise} \end{cases}$$



separating lines on the real plane

Reading material

- Understanding machine learning: parts of
  - chapter 2 for ERM & finite H
  - chapter 3 for PAC & agnostic PAC
  - chapter 5 for no-free-lunch
  - chapter 6 for VC-dimension & fundamental theorem
- next time (in two weeks!) we'll discuss the **computational** complexity of learning (chapter 8)