COMP5212: Machine Learning

Lecture 8

Minhao Cheng

Logistics

- Programming Homework 1 is out
  - Due on Oct 18
- Term project proposal
  - Due on this Friday

Theory of Generalization

A simple solution

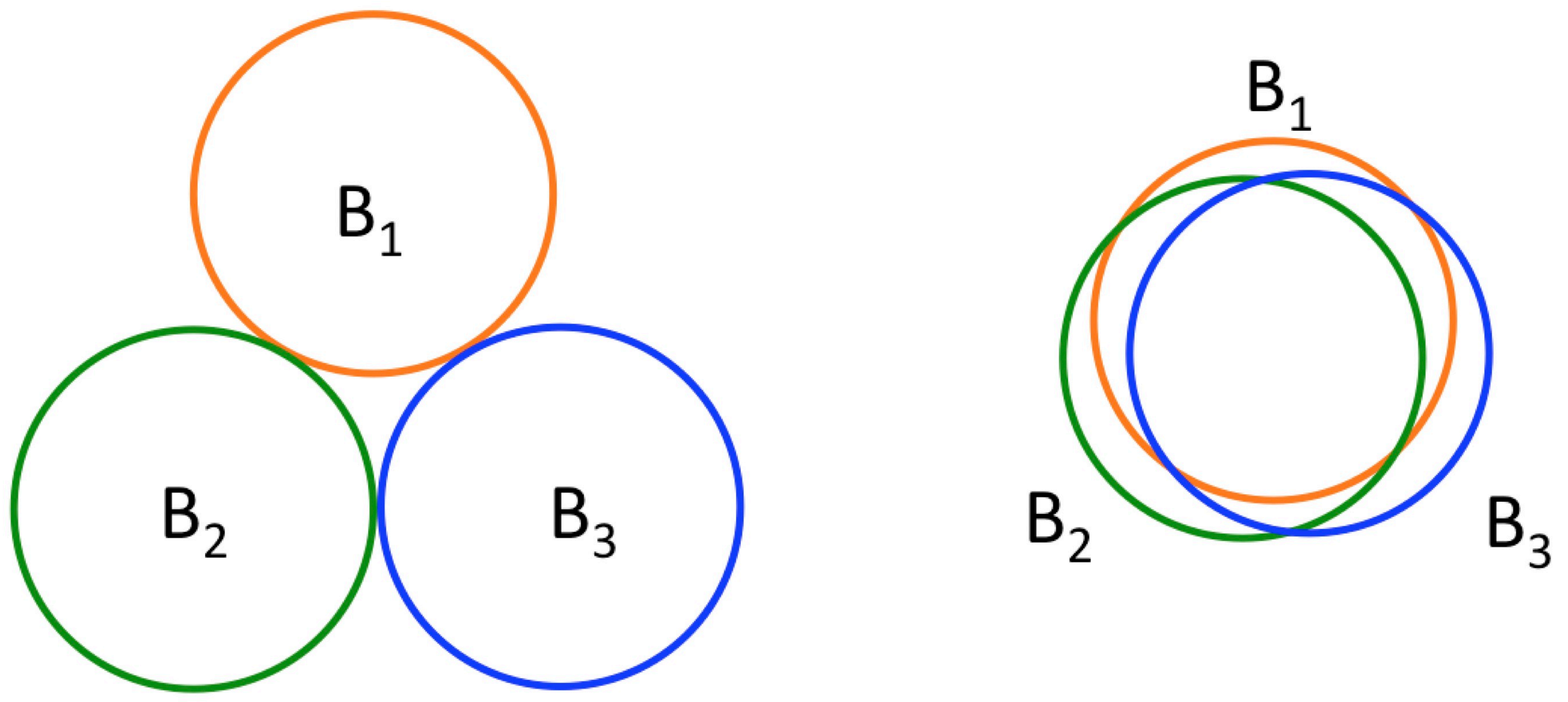
- For each particular h,
    - $P[\,|E_{tr}(h) - E(h)| > \epsilon] \leq 2e^{-2\epsilon^2 N}$
- If we have a hypothesis set $\mathscr{H}$,we want to derive the bound for $P[\text{sup}_{h\in\mathscr{H}}|E_{tr}(h) - E(h)| > \epsilon]$

Where did the $|\mathscr{H}|$ come from?

- The Bad events $\mathscr{B}_m$:
  - $|E_{\text{tr}}(h_m) - E(h_m)| > \epsilon$ with probability $\leq 2e^{-2\epsilon^2 N}$

Where did the $|\mathscr{H}|$ come from?

- The Bad events $\mathscr{B}_m$:
  - $|E_{\text{tr}}(h_m) - E(h_m)| > \epsilon$ with probability $\leq 2e^{-2\epsilon^2 N}$
- The union bound:
  - $\mathbb{P}[\mathscr{B}_1 \text{ or } \mathscr{B}_2 \text{ or } \ldots \text{ or } \mathscr{B}_M] \leq \underbrace{\mathbb{P}[\mathscr{B}_1] + \mathbb{P}[\mathscr{B}_2] + \ldots + \mathbb{P}[\mathscr{B}_M]}_{\text{consider worst case: no overlaps}} \leq 2|\mathscr{H}|e^{-2\epsilon^2 N}$



No overlap: bound is tight

Large overlap

Theory of Generalization

A simple solution

- For each particular h,
  - $P[\,|E_{tr}(h) - E(h)| > \epsilon] \leq 2e^{-2\epsilon^2 N}$
- If we have a hypothesis set $\mathscr{H}$,we want to derive the bound for $P[\text{sup}_{h\in\mathscr{H}}|E_{tr}(h) - E(h)| > \epsilon]$
  - $P[\,|E_{tr}(h_1) - E(h_1)| > \epsilon]$ or … or $P[\,|E_{tr}(h_{|\mathscr{H}|}) - E(h_{|\mathscr{H}|})| > \epsilon]$
  - $\leq \sum_{m=1}^{\mathscr{H}} P[\,|E_{tr}(h_m) - E(h_m)| > \epsilon] \leq 2|\mathscr{H}|e^{-2\epsilon^2 N}$
    - Because of union bound inequality $P(\bigcup_{i=1}^{\infty} A_i) \leq \sum_{i=1}^{\infty} P(A_i)$

Uniform convergence

- When our learning algorithm $\mathscr{A}$ picks the hypothesis g:
  - $P[\exists h \in \mathscr{H} \,|\, E_{tr}(h) - E(h) \,| > \epsilon] \leq 2 \,|\, \mathscr{H} \,|\, e^{-2\epsilon^2 N}$
- Subtract both sides from 1
  - $$P[\neg \exists h \in \mathscr{H} \,|\, E_{tr}(h) - E(h) \,| > \epsilon] = P[\forall h \in \mathscr{H} \,|\, E_{tr}(h) - E(h) \,| \leq \epsilon] \geq 1 - 2 \,|\, \mathscr{H} \,|\, e^{-2\epsilon^2 N}$$

What uniform convergence tell us?

- $$P[\neg \exists h \in \mathscr{H} \,|\, E_{tr}(h) - E(h) \,|\, > \epsilon] = P[\forall h \in \mathscr{H} \,|\, E_{tr}(h) - E(h) \,|\, \leq \epsilon] \\ \geq 1 - 2 \,|\, \mathscr{H} \,|\, e^{-2\epsilon^2 N}$$
- Given ϵ and some $\delta > 0$, how large must N be before we can guarantee that with probability at least $1 - \delta$, training error will be within ϵ of generalization error?
  - Set $\delta = 2 \,|\, \mathscr{H} \,|\, e^{-2\epsilon^2 N}$, solve N
  - $N \geq \frac{1}{2\epsilon^2} \log \frac{2 \,|\, \mathscr{H} \,|}{\delta}$
  - The training set size N that a certain method or algorithm requires in order to achieve a certain level of performance is also called the algorithm's **sample complexity**

What uniform convergence tell us?

- $$\begin{aligned} P[\neg \exists h \in \mathscr{H} \,|\, E_{tr}(h) - E(h) \,|\, > \epsilon] &= P[\forall h \in \mathscr{H} \,|\, E_{tr}(h) - E(h) \,|\, \leq \epsilon] \\ &\geq 1 - 2 \,|\, \mathscr{H} \,|\, e^{-2\epsilon^2 N} \end{aligned}$$
- Given N and some δ, we have
  - $$|\, E_{tr}(h) - E(h) \,| \leq \sqrt{\frac{1}{2N} \log \frac{2 \,|\, \mathscr{H} \,|}{\delta}}$$
  - i.e $|\, E_{tr}(h) - E(h) \,| \leq \gamma$ for all $h \in \mathscr{H}$

What uniform convergence tell us?

- $$P[\neg \exists h \in \mathcal{H} \, |E_{tr}(h) - E(h)| > \epsilon] = P[\forall h \in \mathcal{H} \, |E_{tr}(h) - E(h)| \leq \epsilon] \geq 1 - 2|\mathcal{H}|e^{-2\epsilon^2 N}$$
- Given N and some δ, we have
    - $|E_{tr}(h) - E(h)| \leq \sqrt{\frac{1}{2N} \log \frac{2|\mathcal{H}|}{\delta}}$
    - i.e $|E_{tr}(h) - E(h)| \leq \gamma$ for all $h \in \mathcal{H}$
    - What about the best hypothesis in training data?

What uniform convergence tell us?

- Given N and some δ, we have
  - $|E_{tr}(h) - E(h)| \leq \sqrt{\frac{1}{2N} \log \frac{2|\mathscr{H}|}{\delta}}$
  - i.e $|E_{tr}(h) - E(h)| \leq \gamma$ for all $h \in \mathscr{H}$
  - What about the best hypothesis in training data? $\hat{h} = \arg\min_{h \in \mathscr{H}} E_{tr}(h)$
  - Define the best hypothesis as $h^* = \arg\min_{h \in \mathscr{H}} E(h)$
  - We have $E(\hat{h}) \leq E_{tr}(\hat{h}) + \gamma \leq E_{tr}(h^*) + \gamma \leq E(h^*) + 2\gamma$

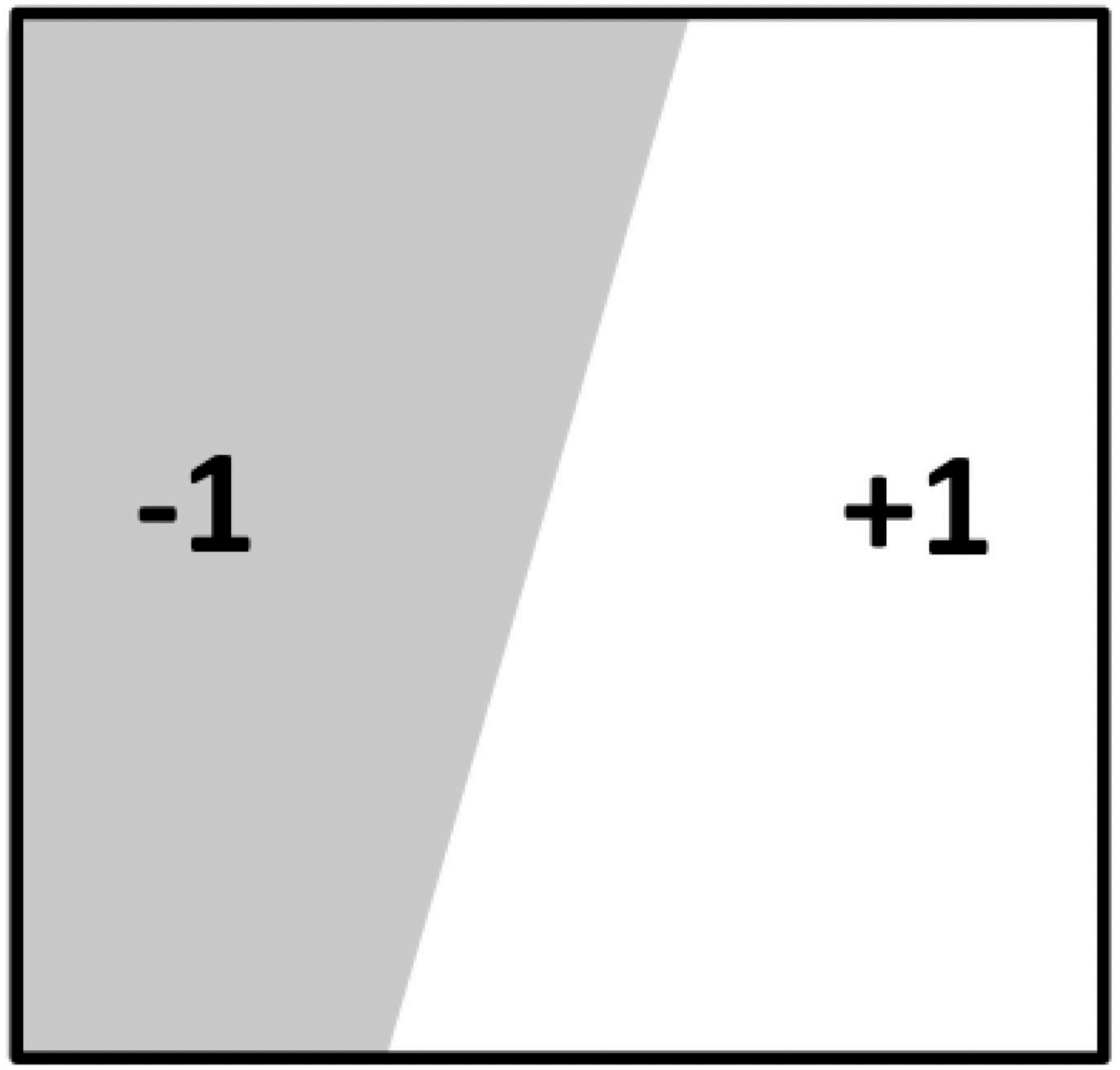
What uniform convergence tell us?

- What about the best hypothesis in training data? $\hat{h} = \arg\min_{h \in \mathcal{H}} E_{tr}(h)$
  - Define the best hypothesis as $h* = \arg\min_{h \in \mathcal{H}} E(h)$
    - We have $E(\hat{h}) \le E_{tr}(\hat{h}) + \gamma \le E_{tr}(h*) + \gamma \le E(h*) + 2\gamma$
  - So we have
    - $E(\hat{h}) \le (\min_{h \in \mathcal{H}} E(h)) + 2\sqrt{\frac{1}{2N} \log \frac{2|\mathcal{H}|}{\delta}}$
    - Connection with bias/variance tradeoff

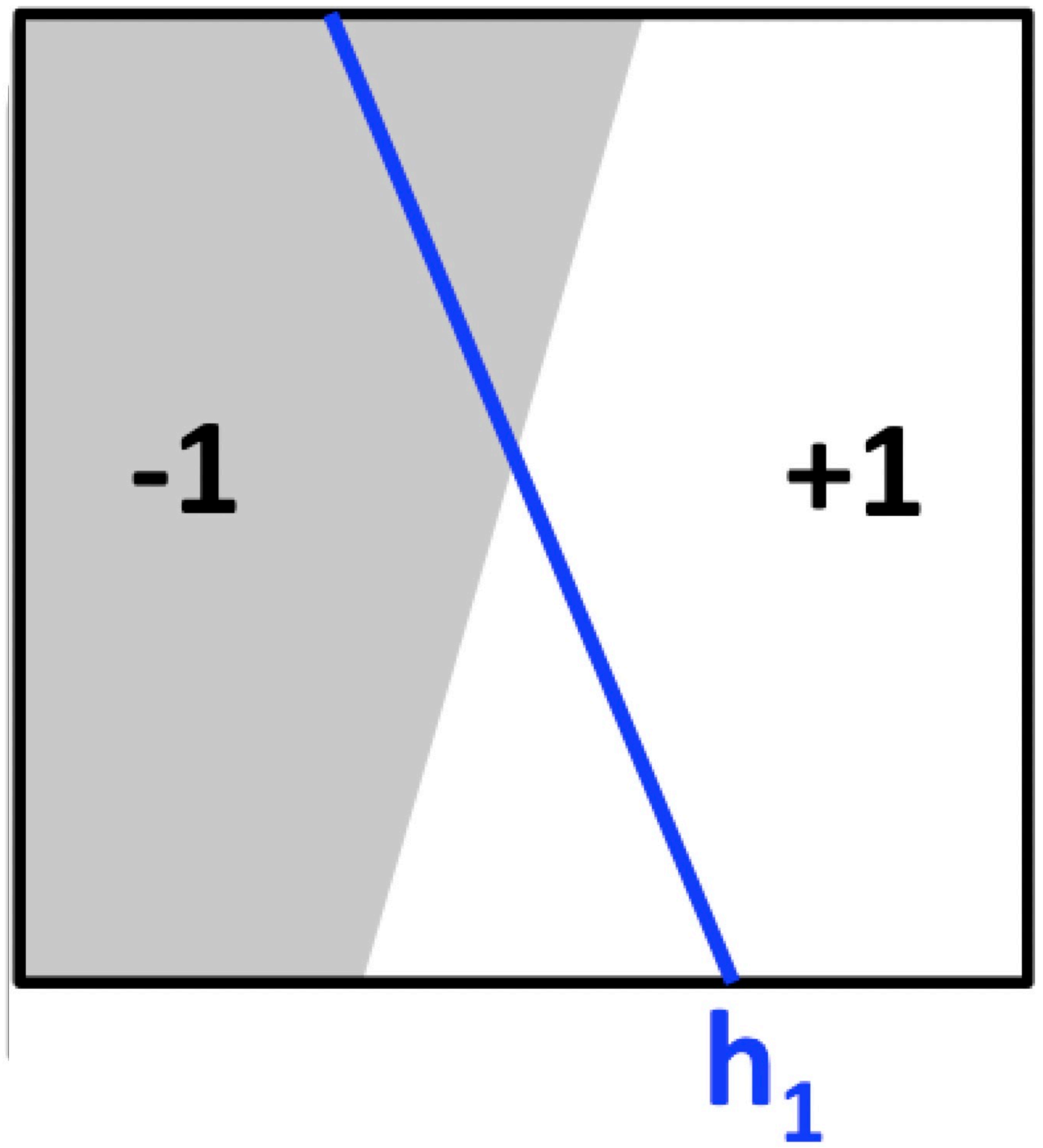
What uniform convergence tell us?

- What about the best hypothesis in training data? $\hat{h} = \arg\min_{h \in \mathscr{H}} E_{tr}(h)$
  - Define the best hypothesis as $h^* = \arg\min_{h \in \mathscr{H}} E(h)$
    - We have $E(\hat{h}) \leq E_{tr}(\hat{h}) + \gamma \leq E_{tr}(h^*) + \gamma \leq E(h^*) + 2\gamma$
  - So we have
    - $E(\hat{h}) \leq (\min_{h \in \mathscr{H}} E(h)) + 2\sqrt{\frac{1}{2N} \log \frac{2|\mathscr{H}|}{\delta}}$
    - Connection with bias/variance tradeoff
  - Further, given ϵ and some $\delta > 0$, is suffices that
    - $N \geq \frac{1}{2\epsilon^2} \log \frac{2|\mathscr{H}|}{\delta} = O(\frac{1}{\epsilon^2} \log \frac{|\mathscr{H}|}{\delta})$

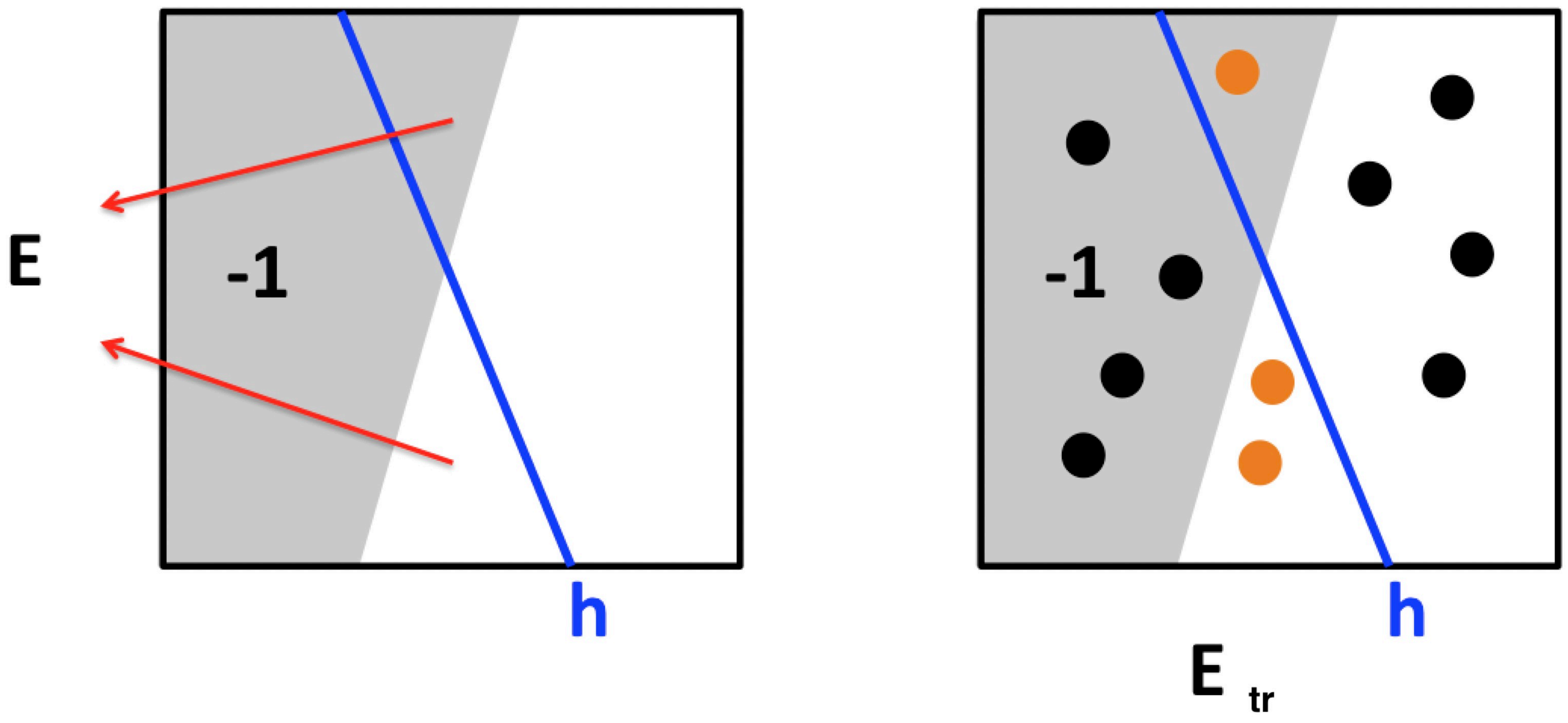
Can we improve on $|\mathscr{H}|$?



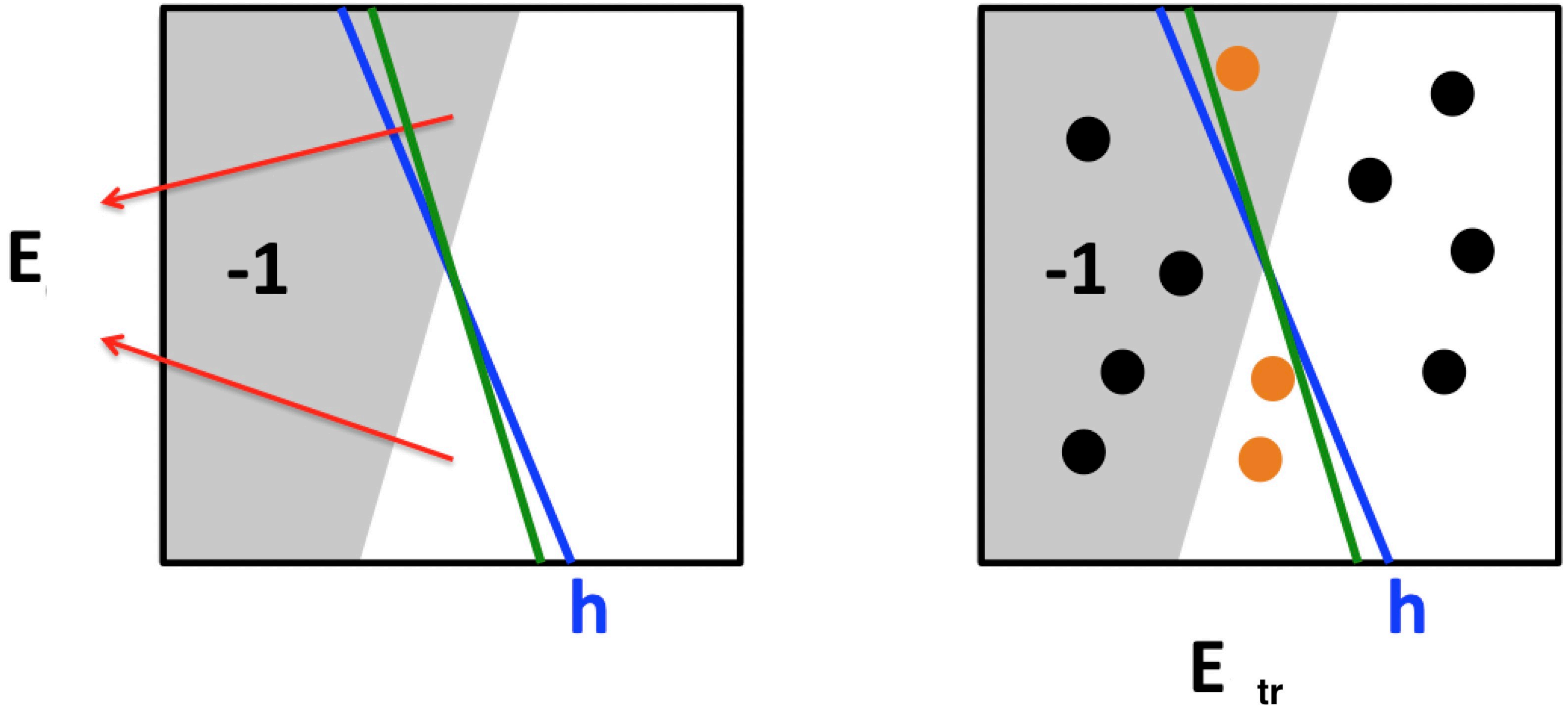
Can we improve on $|\mathscr{H}|$?



Can we improve on $|\mathscr{H}|$?



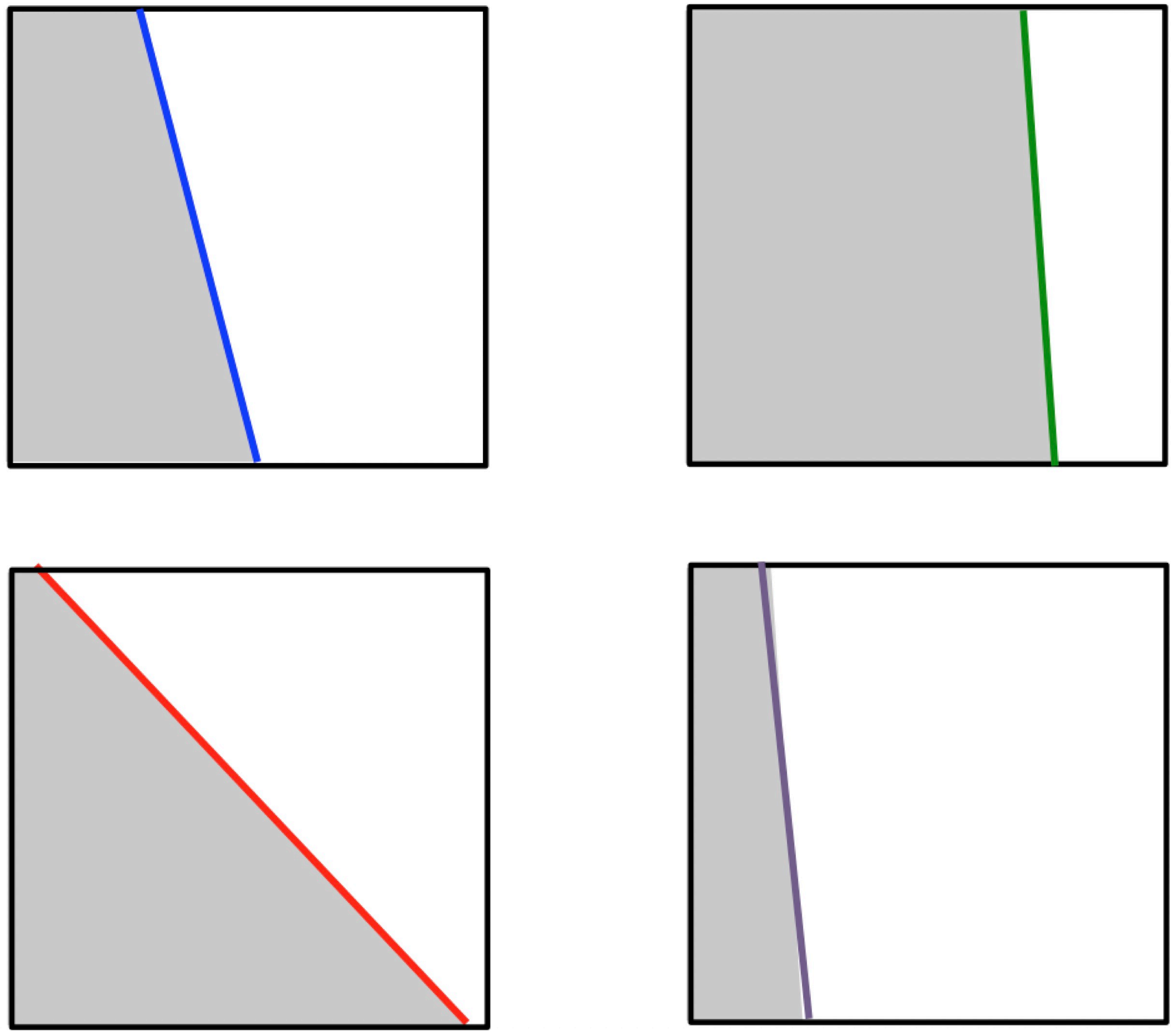
Can we improve on $|\mathscr{H}|$?



- The event that $|E_{\text{tr}}(h_1) - E(h_1)| > \epsilon$ and $|E_{\text{tr}}(h_2) - E(h_2)| > \epsilon$ are largely overlapped

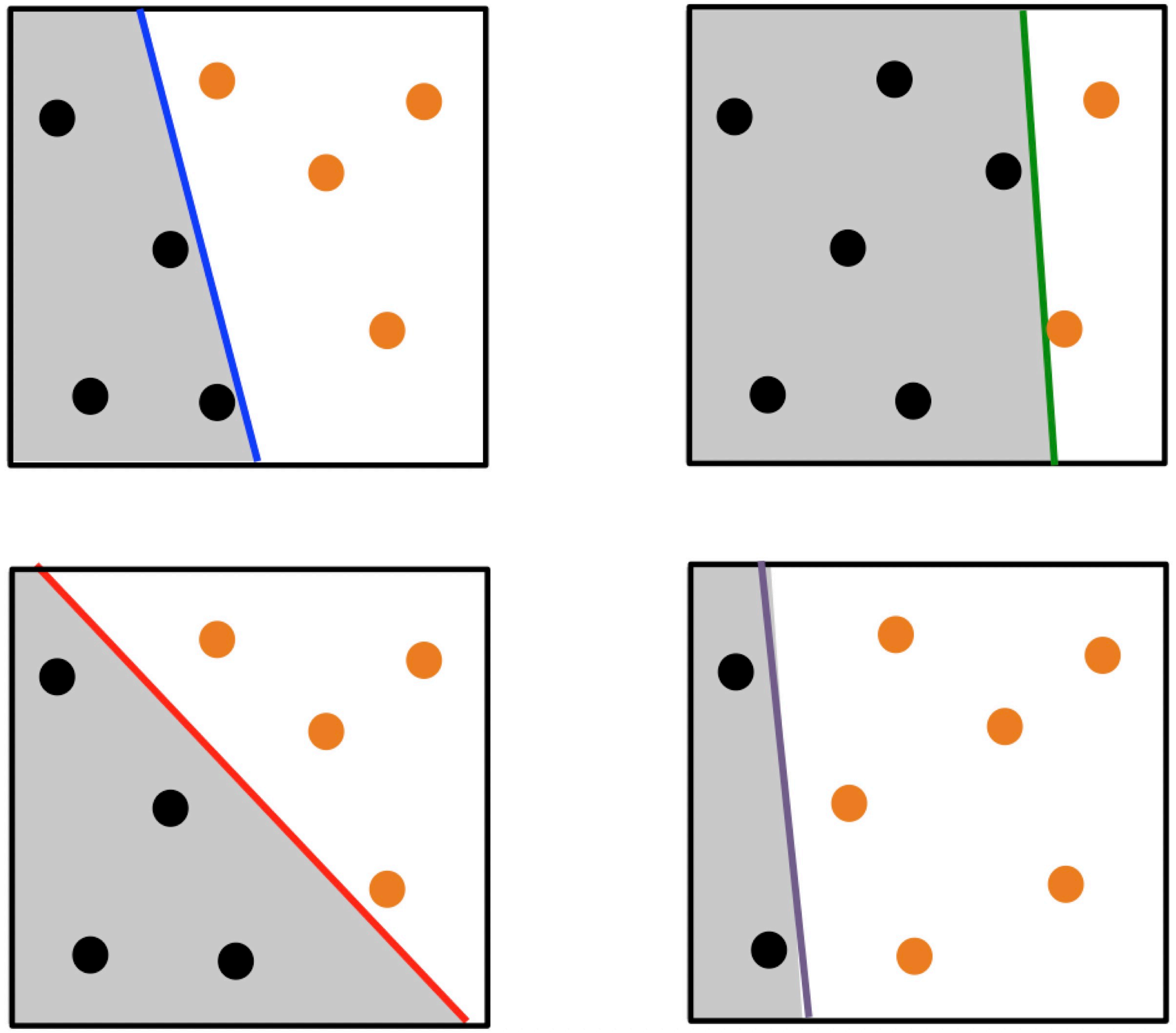
What can we replace $|\mathcal{H}|$ with?

- Instead of the whole input space



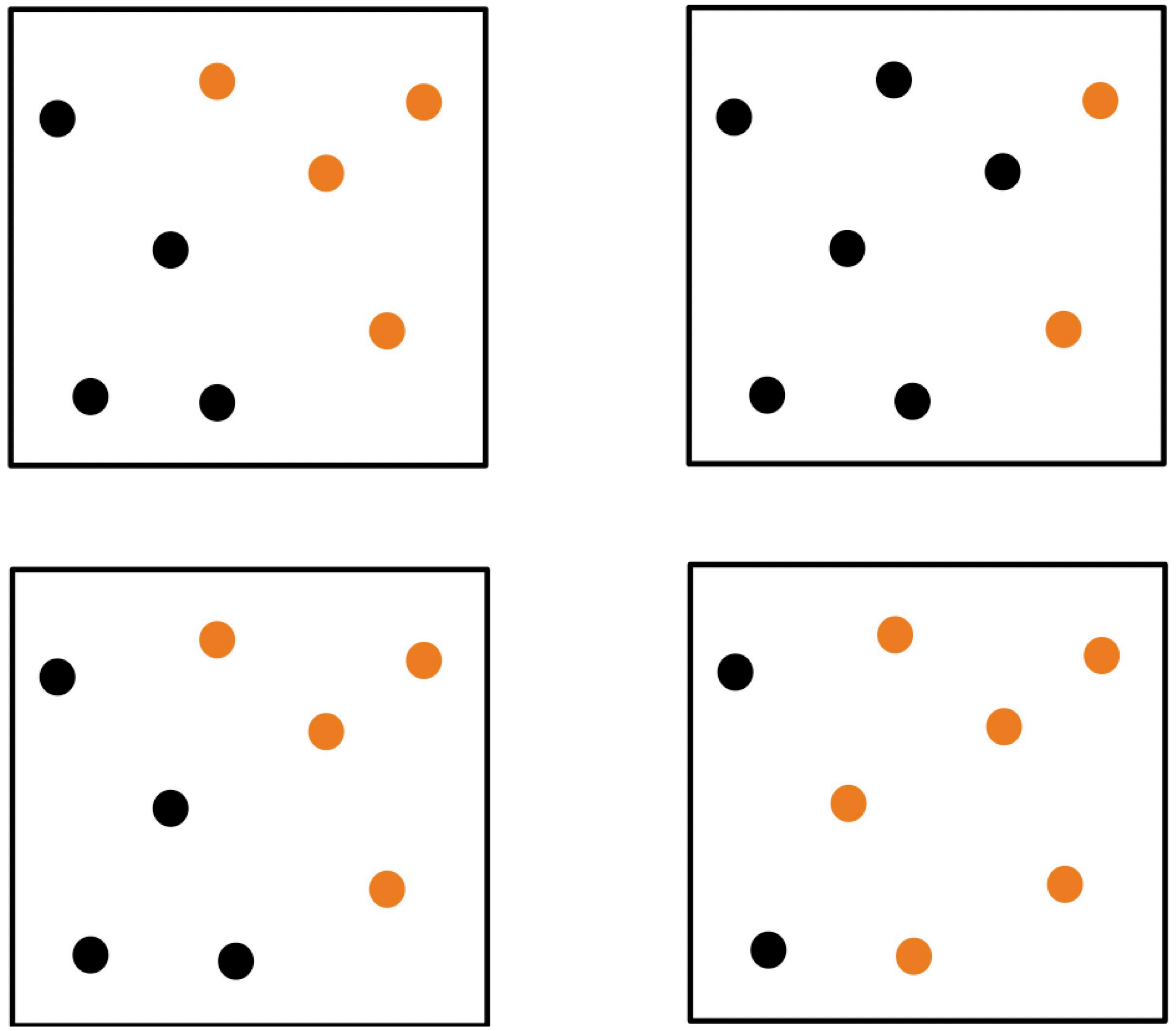
What can we replace $|\mathscr{H}|$ with?

- Instead of the whole input space
- Let's consider a finite set of input points



What can we replace $|\mathscr{H}|$ with?

- Instead of the whole input space
- Let's consider a finite set of input points
- How many patterns of colors can you get?



Dichotomies: mini-hypotheses

- A hypothesis: $h : \mathscr{X} \to \{-1, +1\}$
- A dichotomy: $h : \{x_1, x_2, \ldots, x_N\} \to \{-1, +1\}$

Dichotomies: mini-hypotheses

- A hypothesis: $h : \mathscr{X} \to \{-1, +1\}$
- A dichotomy: $h : \{x_1, x_2, \ldots, x_N\} \to \{-1, +1\}$
- Number of hypotheses $|\mathscr{H}|$ can be infinite
- Number of dichotomies $|\mathscr{H}(x_1, x_2, \ldots, x_N)|$ at most 2^N

Dichotomies: mini-hypotheses

- A hypothesis: $h : \mathscr{X} \to \{-1, +1\}$
- A dichotomy: $h : \{x_1, x_2, \ldots, x_N\} \to \{-1, +1\}$
- Number of hypotheses $|\mathscr{H}|$ can be infinite
- Number of dichotomies $|\mathscr{H}(x_1, x_2, \ldots, x_N)|$ at most 2^N
  - $\Rightarrow$ Candidate for replacing $|\mathscr{H}|$
  - Why?

Theory of Generalization

Symmetrization lemma

- Imagine we have the ghost dataset S' with also size N:
- $P[\text{SUP}_{h \in \mathcal{H}} |E_{tr}(h) - E(h)| > \epsilon] \le 2P[\text{SUP}_{h \in \mathcal{H}} |E_{tr}(h) - E'_{tr}(h)| > \frac{\epsilon}{2}]$

Theory of Generalization

Growth function

- Imagine we have the ghost dataset S' with also size N:
  - $P[\text{SUP}_{h \in \mathscr{H}} |E_{tr}(h) - E(h)| > \epsilon] \leq 2P[\text{SUP}_{h \in \mathscr{H}} |E_{tr}(h) - E'_{tr}(h)| > \frac{\epsilon}{2}]$
- By union bound:
  - $P[\text{SUP}_{h \in \mathscr{H}_{S \cup S'}} |E_{tr}(h) - E'_{tr}(h)| > \frac{\epsilon}{2}] \leq |\mathscr{H}_{S \cup S'}| P[|E_{tr}(h) - E'_{tr}(h)| > \frac{\epsilon}{2}]$

Theory of Generalization

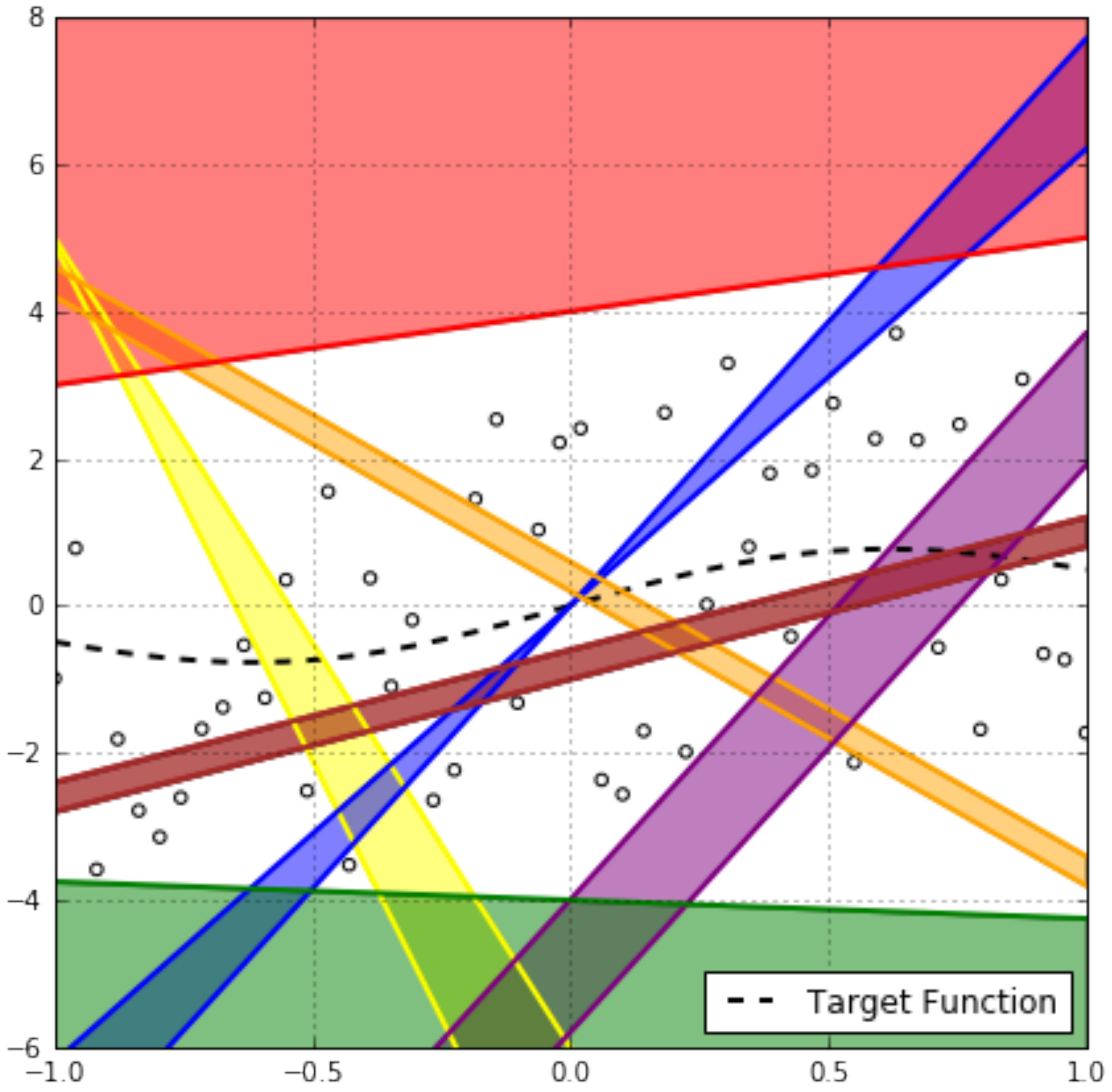
Growth function

- Imagine we have the ghost dataset S' with also size N:
  - $P[\text{SUP}_{h \in \mathcal{H}} |E_{tr}(h) - E(h)| > \epsilon] \leq 2P[\text{SUP}_{h \in \mathcal{H}} |E_{tr}(h) - E'_{tr}(h)| > \frac{\epsilon}{2}]$
- By union bound:
  - $P[\text{SUP}_{h \in \mathcal{H}_{S \cup S'}} |E_{tr}(h) - E'_{tr}(h)| > \frac{\epsilon}{2}] \leq |\mathcal{H}_{S \cup S'}| P[|E_{tr}(h) - E'_{tr}(h)| > \frac{\epsilon}{2}]$
- How to bound $|\mathcal{H}_{S \cup S'}|$

Theory of Generalization

Deduce the dimension

- Why do we need to consider every possible hypothesis?
    - $P[\text{SUP}_{h \in \mathscr{H}} | E_{tr}(h) - E(h) | > \epsilon]$
    - If we omit one hypothesis, we might miss the biggest gap
- However, are the events of each hypothesis having a big generalization gap are likely to be independent?
    - No



The growth function

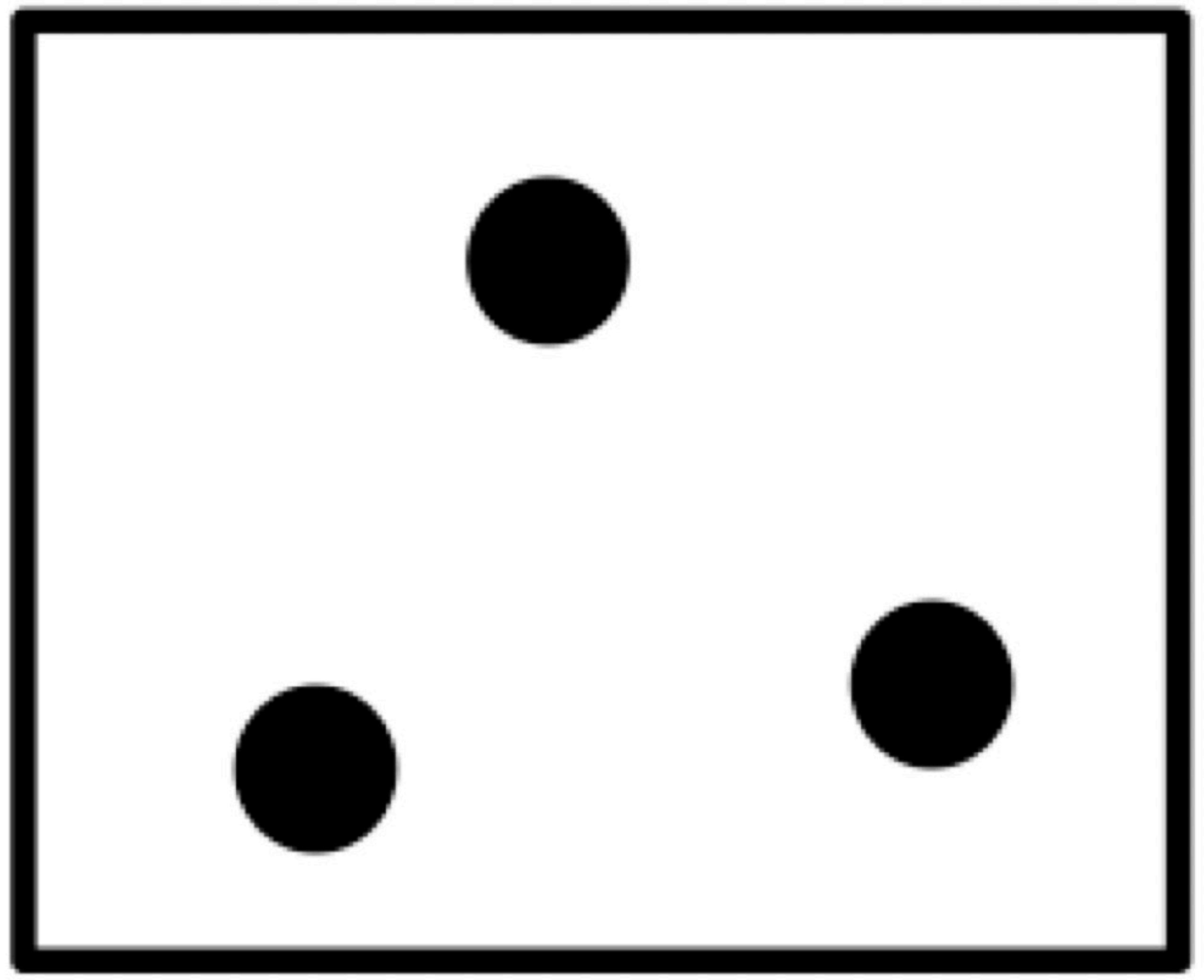
- The growth function counts the most dichotomies on any N points:
- $m_{\mathscr{H}}(N) = \max_{x_1,\ldots,x_N \in \mathscr{X}} |\mathscr{H}(x_1,\ldots,x_N)|$

The growth function

- The growth function counts the most dichotomies on any N points:
  - $m_{\mathscr{H}}(N) = \max_{x_1,\ldots,x_N \in \mathscr{X}} |\mathscr{H}(x_1,\ldots,x_N)|$
- The growth function satisfies:
  - $m_{\mathscr{H}}(N) \leq 2^N$

Growth function for linear classifiers

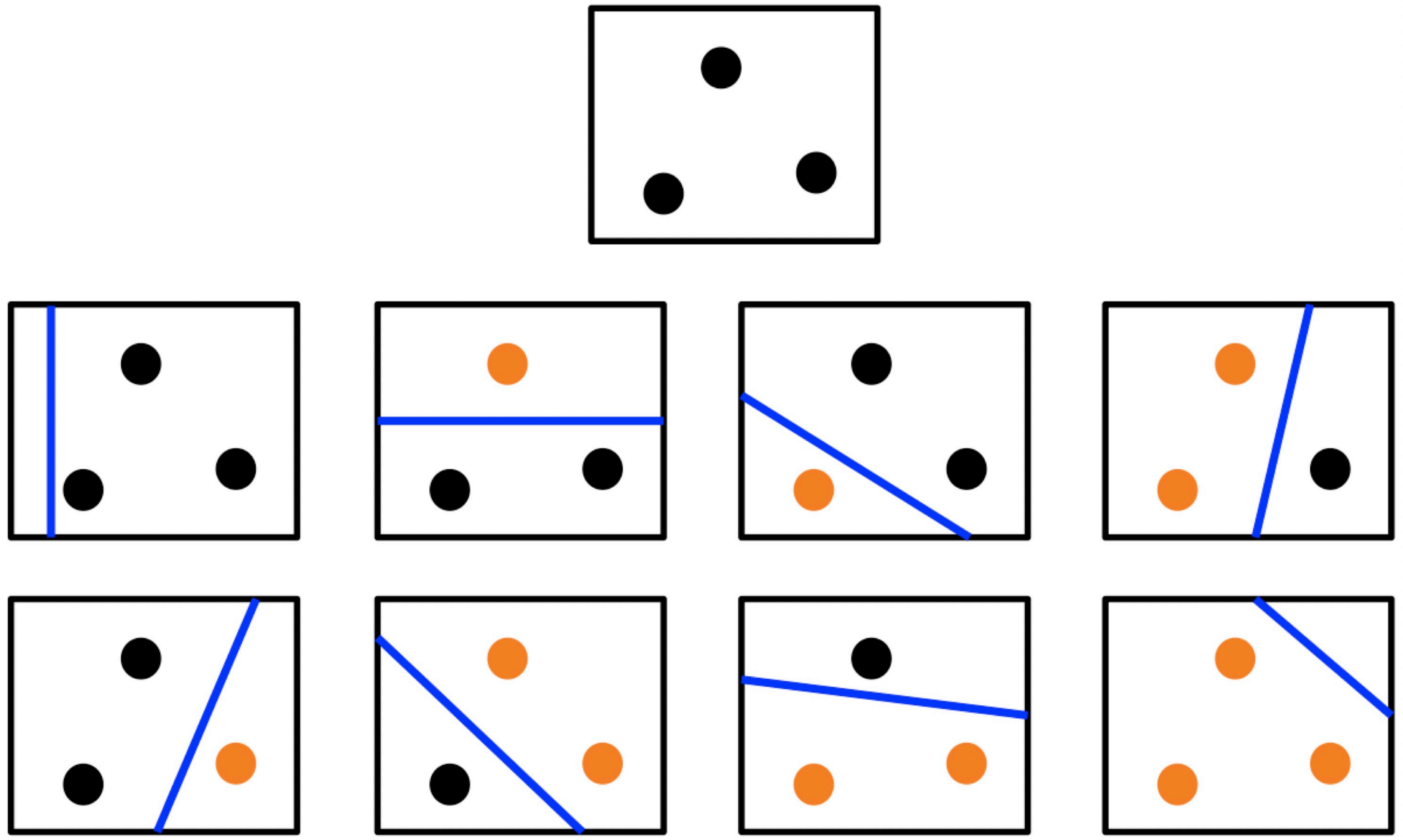
- Compute $m_{\mathscr{H}}(3)$ in 2-D space



- What's $|\mathscr{H}(x_1, x_2, x_3)|$?

Growth function for linear classifiers

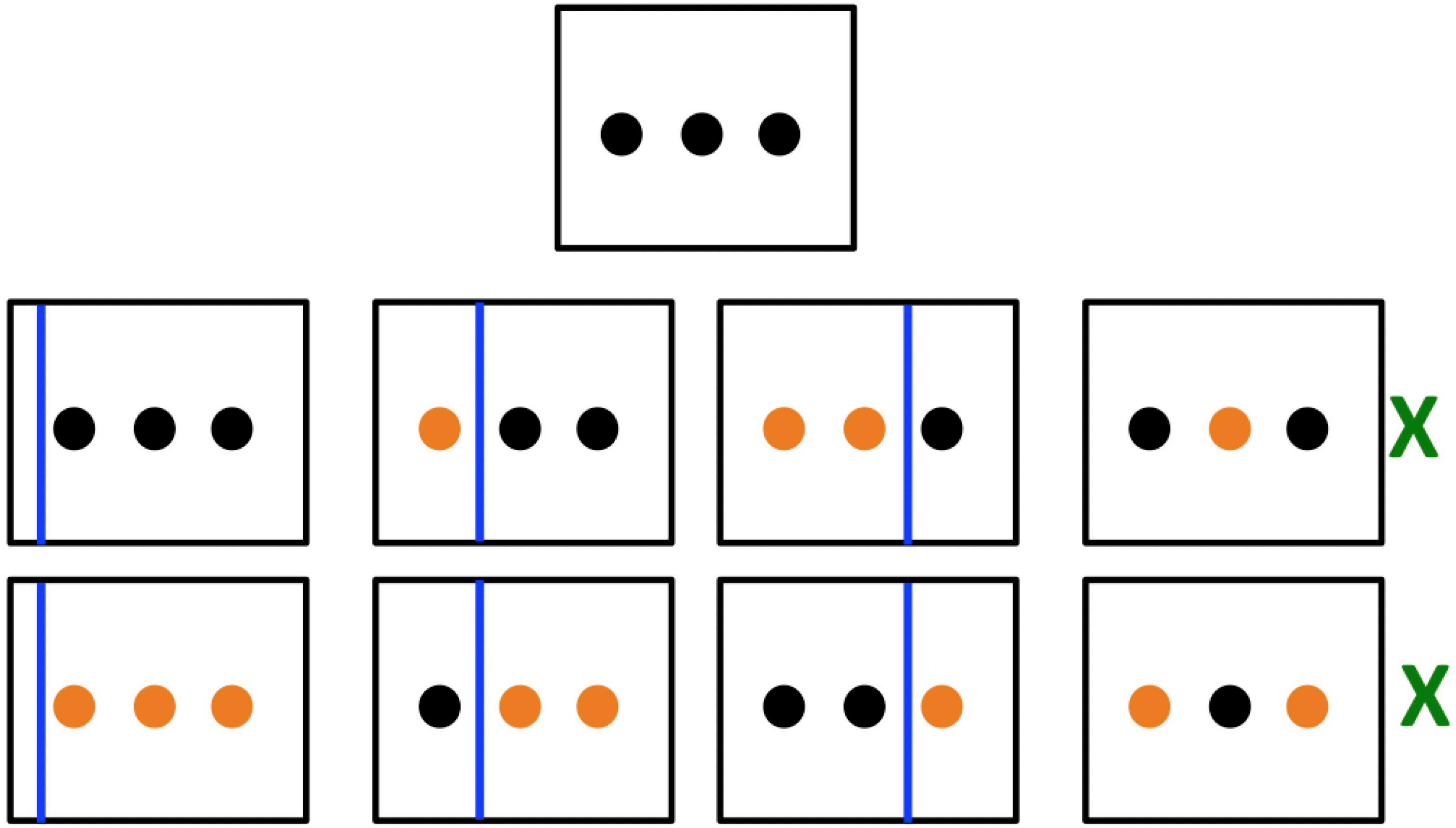
- Compute $m_{\mathscr{H}}(3)$ in 2-D space when $\mathscr{H}$ is perceptron (linear hyperplanes)



$$m_{\mathscr{H}}(3) = 8$$

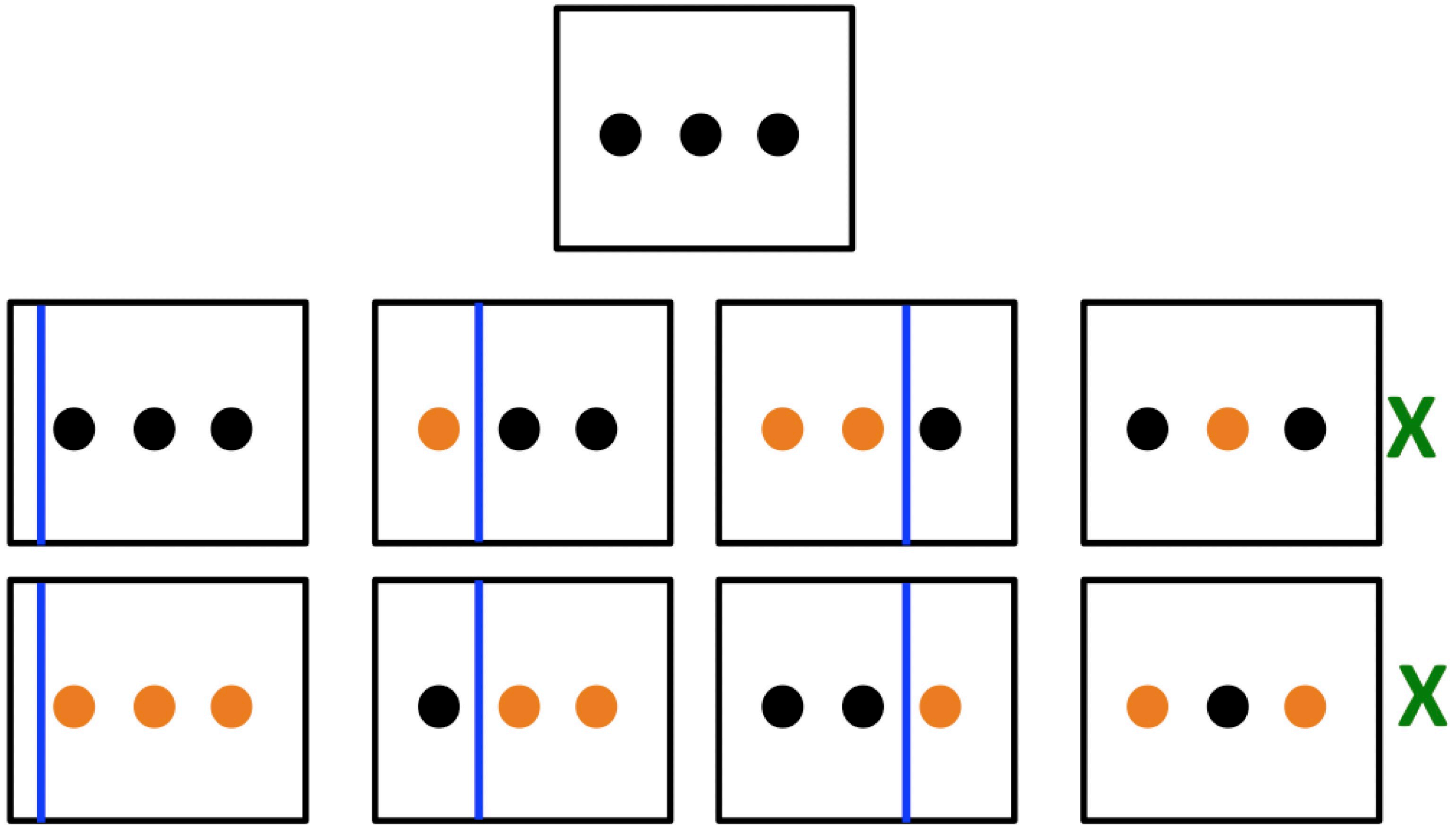
Growth function for linear classifiers

- Compute $m_{\mathscr{H}}(3)$ in 2-D space when $\mathscr{H}$ is perceptron (linear hyperplanes)



Growth function for linear classifiers

- Compute $m_{\mathscr{H}}(3)$ in 2-D space when $\mathscr{H}$ is perceptron (linear hyperplanes)



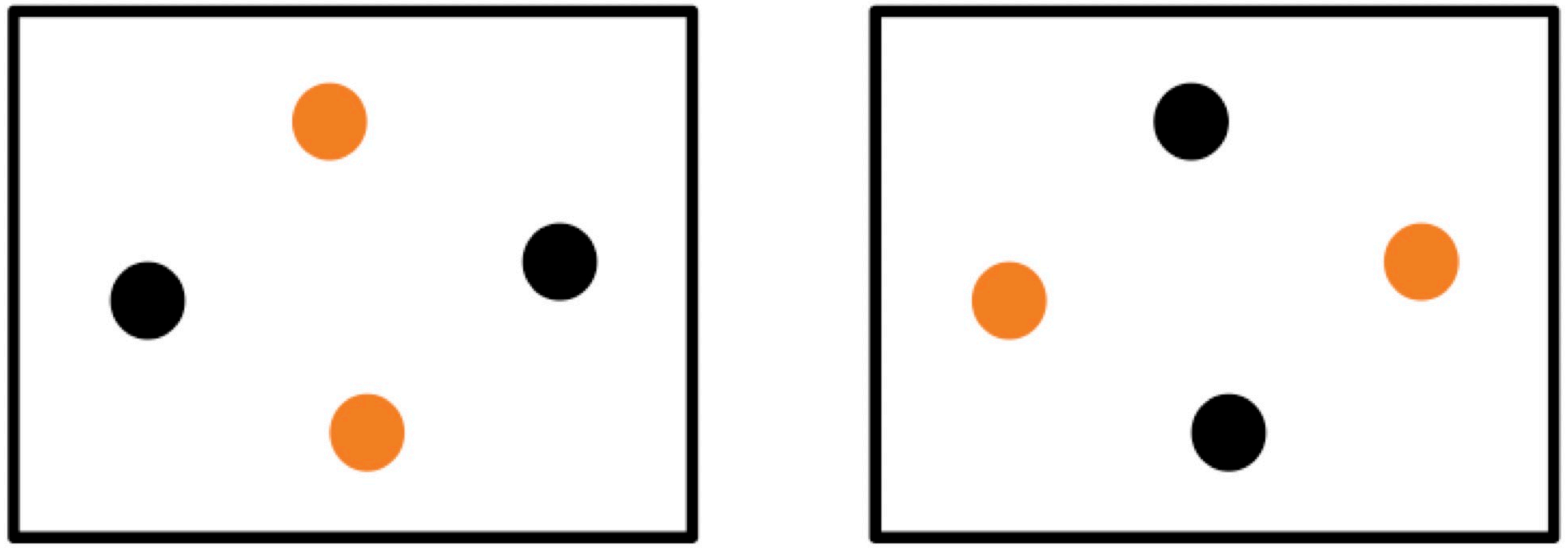
- Doesn't matter because we only counts the most dichotomies

Growth function for linear classifier

- What's $m_{\mathscr{H}}(4)$?

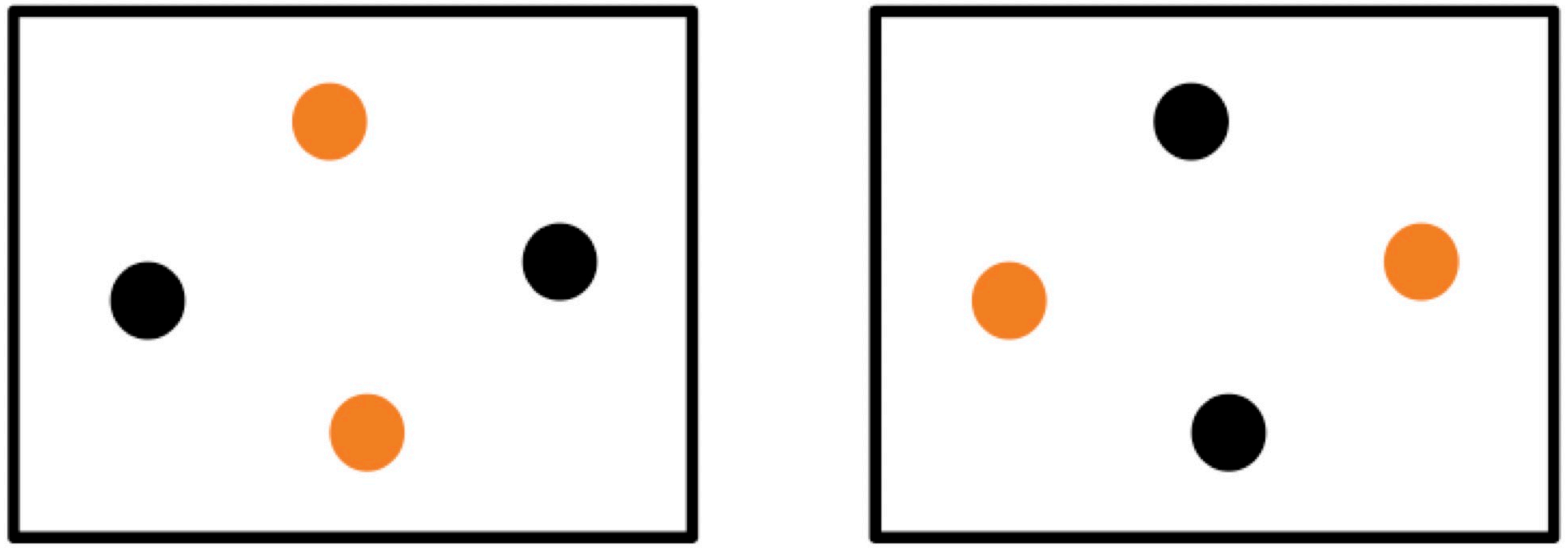
Growth function for linear classifier

- What's $m_{\mathscr{H}}(4)$?
- (At least) missing two dichotomies:



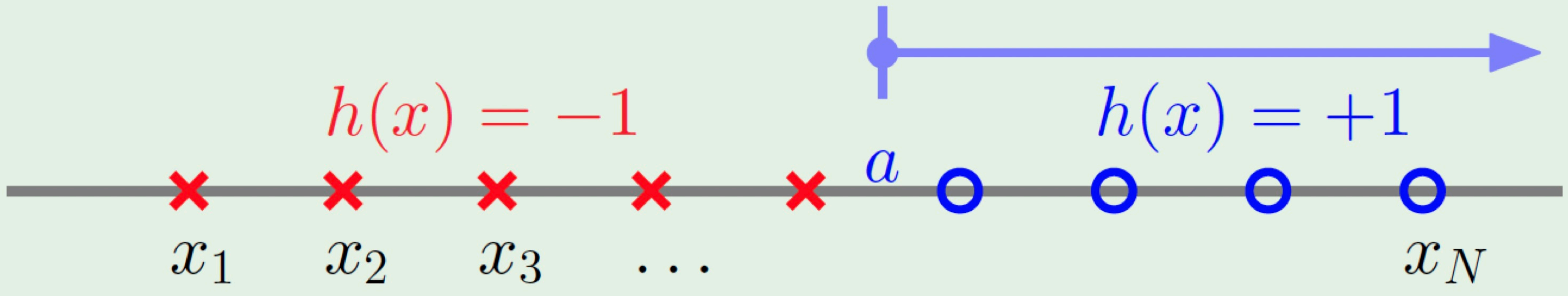
Growth function for linear classifier

- What's $m_{\mathscr{H}}(4)$?
- (At least) missing two dichotomies:



- $m_{\mathscr{H}}(4) = 14 < 2^4$

Example I: positive rays

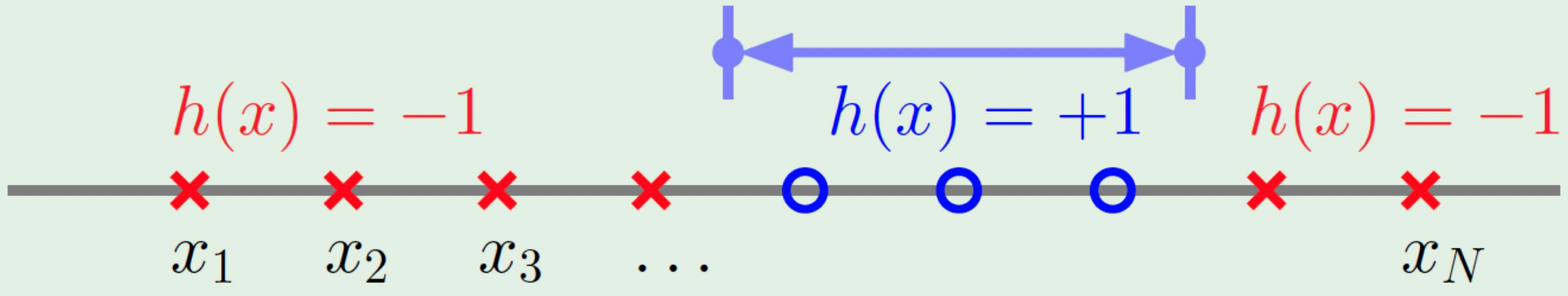


$$\mathcal{H} \text{ is set of } h : \mathbb{R} \to \{-1, +1\}$$

$$h(x) = \text{sign}(x - a)$$

$$m_{\mathcal{H}}(N) = N + 1$$

Example II: positive intervals



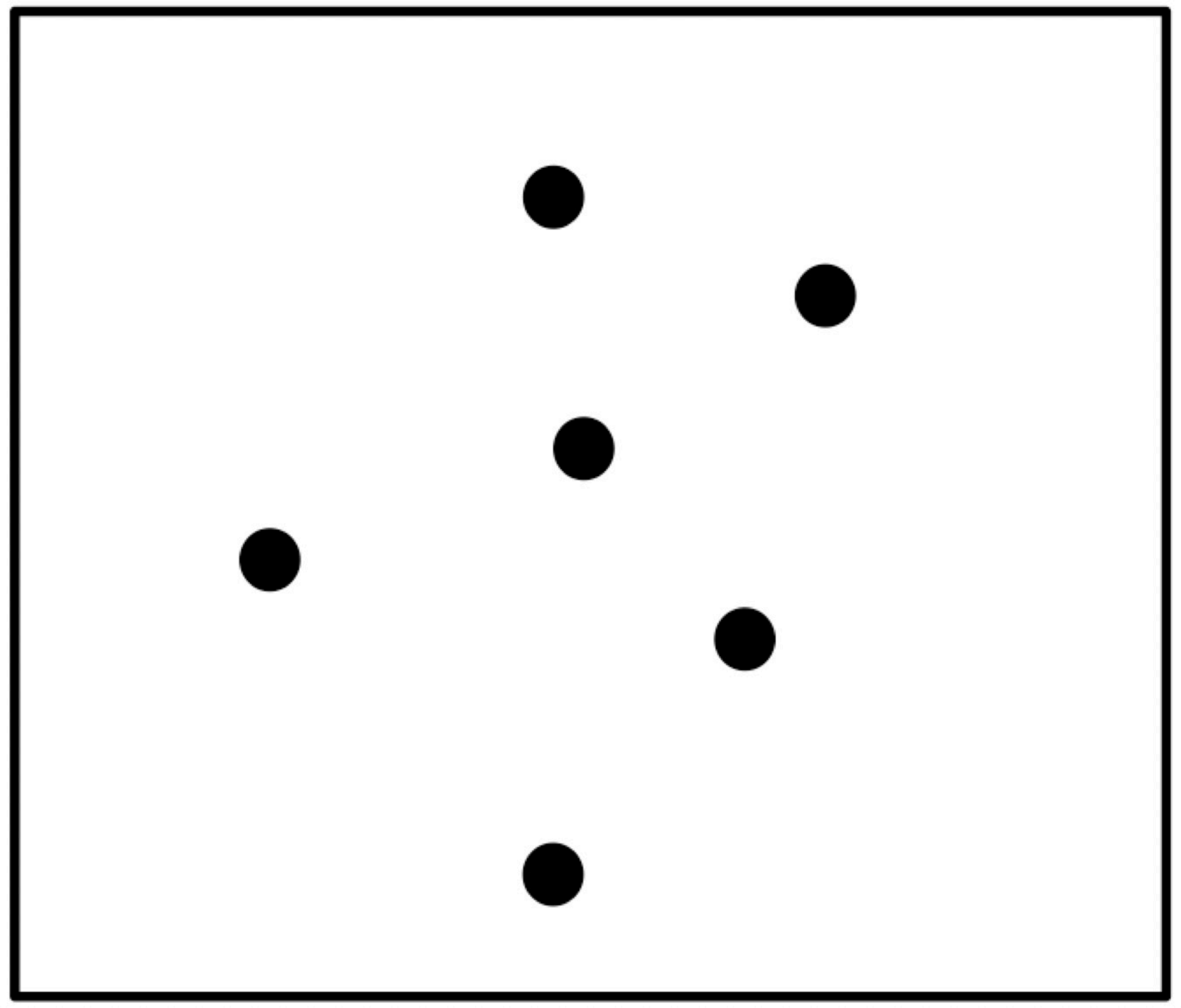
$\mathcal{H}$ is set of $h\colon \mathbb{R} \to \{-1, +1\}$

Place interval ends in two of $N+1$ spots

$$m_{\mathcal{H}}(N) = \binom{N+1}{2} + 1 = \tfrac{1}{2}N^2 + \tfrac{1}{2}N + 1$$

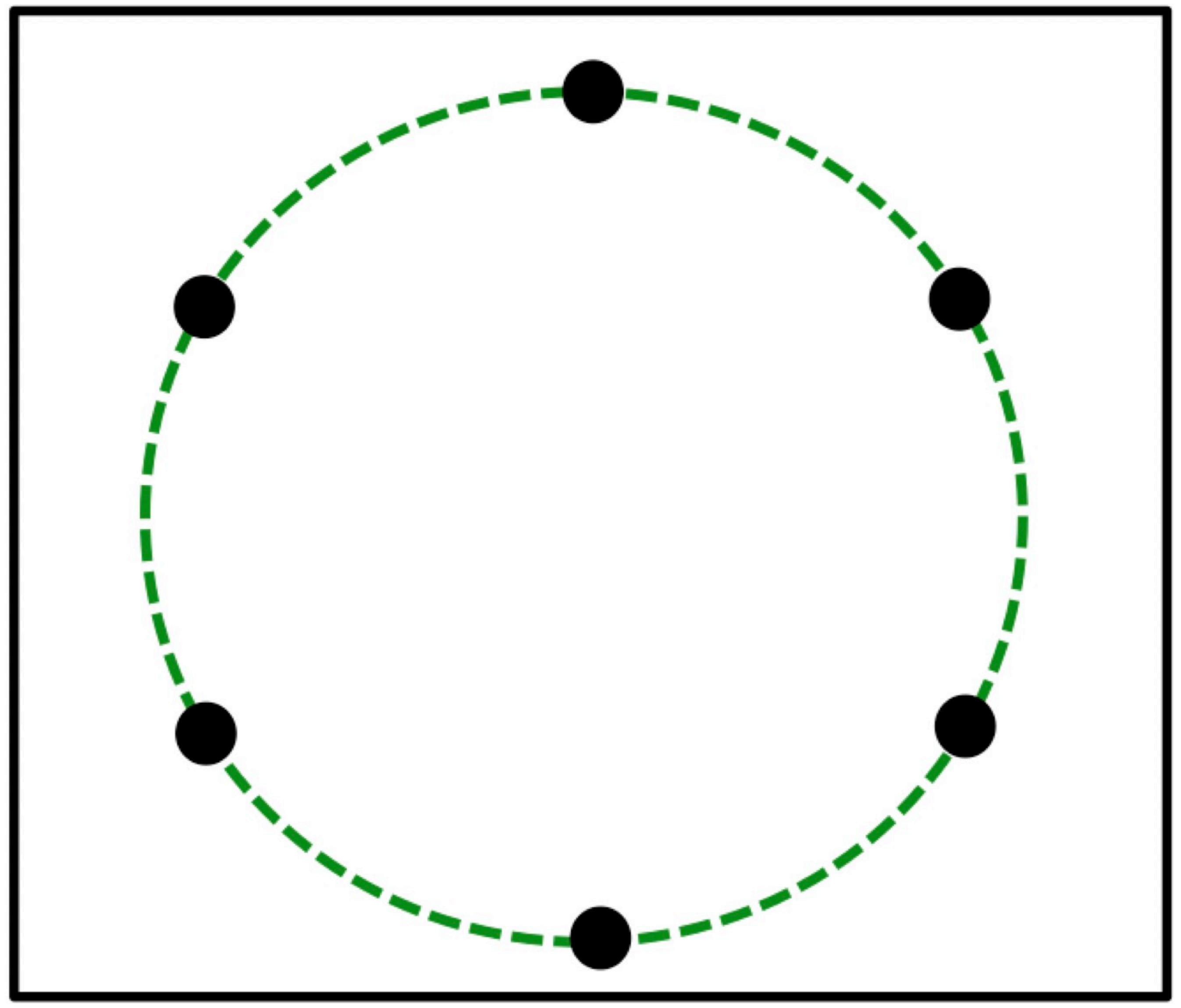
Example III: convex sets

- $\mathscr{H}$ is set of $h : \mathbb{R}^2 \to \{-1, +1\}$
  - $h(x) = +1$ is convex
- How many dichotomies can we generate?



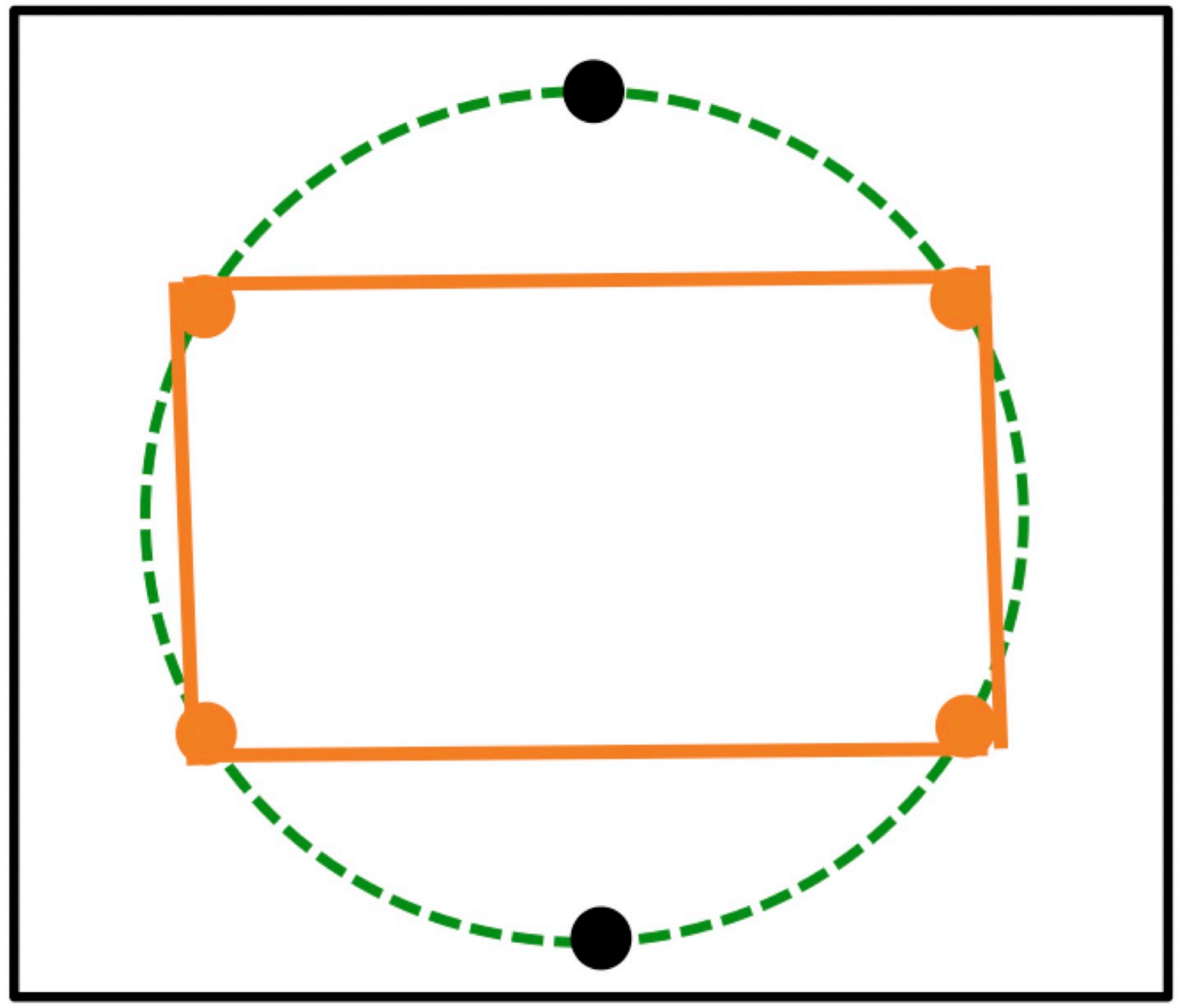
Example III: convex sets

- $\mathscr{H}$ is set of $h : \mathbb{R}^2 \to \{-1, +1\}$
    - $h(x) = +1$ is convex
- How many dichotomies can we generate?



Example III: convex sets

- $\mathscr{H}$ is set of $h : \mathbb{R}^2 \rightarrow \{-1, +1\}$
    - $h(x) = +1$ is convex
- How many dichotomies can we generate?



Example III: convex sets

- $\mathscr{H}$ is set of $h : \mathbb{R}^2 \to \{-1, +1\}$
  - $h(x) = +1$ is convex
- $m_{\mathscr{H}}(N) = 2^N$ for any $N \Rightarrow$ We say the N points are "shattered" by h

Shattered

- Given a set $S = \{x^{(i)}, \ldots, x^{(d)}\}$ (no relation to the training set) of points $x^{(i)} \in \mathscr{X}$, we say that $\mathscr{H}$ shatters S if $\mathscr{H}$ can realize any labeling on S. I.e, if for any set of labels $\{y^{(i)}, \ldots, y^{(d)}\}$, there exist some $h \in \mathscr{H}$ so that $h(x^{(i)}) = y^{(i)}$ for all $i = 1, \ldots, d$

The 3 growth functions

- $\mathscr{H}$ is positive rays:
  - $m_{\mathscr{H}}(N) = N + 1$
- $\mathscr{H}$ is positive intervals:
  - $m_{\mathscr{H}}(N) = \frac{1}{2}N^2 + \frac{1}{2}N + 1$
- $\mathscr{H}$ is convex sets:
  - $m_{\mathscr{H}}(N) = 2^N$

What's next?

- Remember the inequality
  - $\mathbb{P}[\,|E_{\text{in}} - E_{\text{out}}| > \epsilon] \leq 2|\mathcal{H}|e^{-2\epsilon^2 N}$
- What happens if we replace $|\mathcal{H}|$ by $m_{\mathcal{H}}(N)$
  - $m_{\mathcal{H}}(N)$ polynomial $\Rightarrow$ Good!

What's next?

- Remember the inequality
  - $\mathbb{P}[\,|E_{\text{tr}} - E| > \epsilon] \leq 2\,|\mathcal{H}|\,e^{-2\epsilon^2 N}$
- What happens if we replace $|\mathcal{H}|$ by $m_{\mathcal{H}}(N)$
  - $m_{\mathcal{H}}(N)$ polynomial $\Rightarrow$ Good!
  - Why?
- How to show $m_{\mathcal{H}}(N)$ is polynomial?