Machine Learning Theory II

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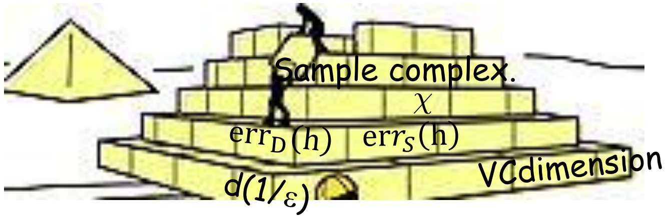
Today's focus

1. SLT for infinite H
2. Model selection



Machine Learning Theory

1. Binary classification
2. Noise-free labeling

$$err_D(h) \le err_S(h) + \varepsilon$$

?

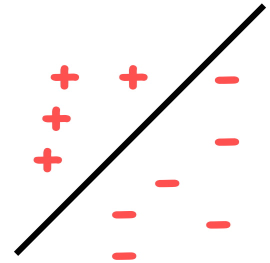
- Finite H
  - Realizable $c^* \in H$
    $$err_D(h) \le \frac{1}{m}\left(\ln|H| + \ln\frac{1}{\delta}\right)$$
  - Agnostic $c^* \notin H$
    $$err_D(h) \le err_S(h) + \sqrt{\frac{1}{2m}\ln\frac{2|H|}{\delta}}$$
- Infinite H
  - Realizable $c^* \in H$
    $$err_D(h) \le \mathcal{O}\left(\frac{1}{m}\left(d\ln\frac{m}{d} + \ln\frac{1}{\delta}\right)\right)$$
  - Agnostic $c^* \notin H$
    $$err_D(h) \le err_S(h) + \mathcal{O}\left(\sqrt{\frac{1}{m}\left(d\ln\frac{m}{d} + \ln\frac{1}{\delta}\right)}\right)$$

Some concepts:

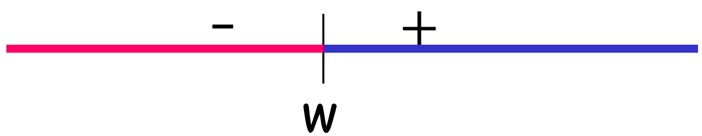
1. Consistent learner
2. Version space (VS)
3. ε-exhausted VS
4. PAC-learnable
5. Hoeffding inequality
6. Dichotomy
7. Shattering
8. Shattering coefficient (growth function)
9. VC-dimension
10. Sauer's lemma

What if H is infinite?

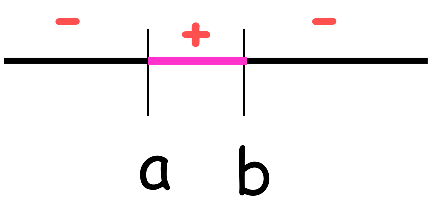
E.g., linear separators in $\mathbb{R}^d$



E.g., thresholds on the real line

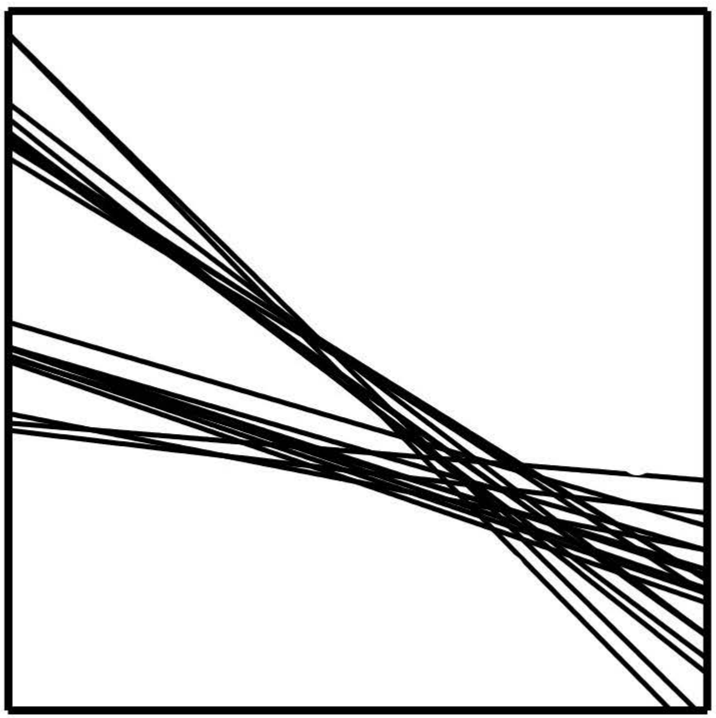


E.g., intervals on the real line

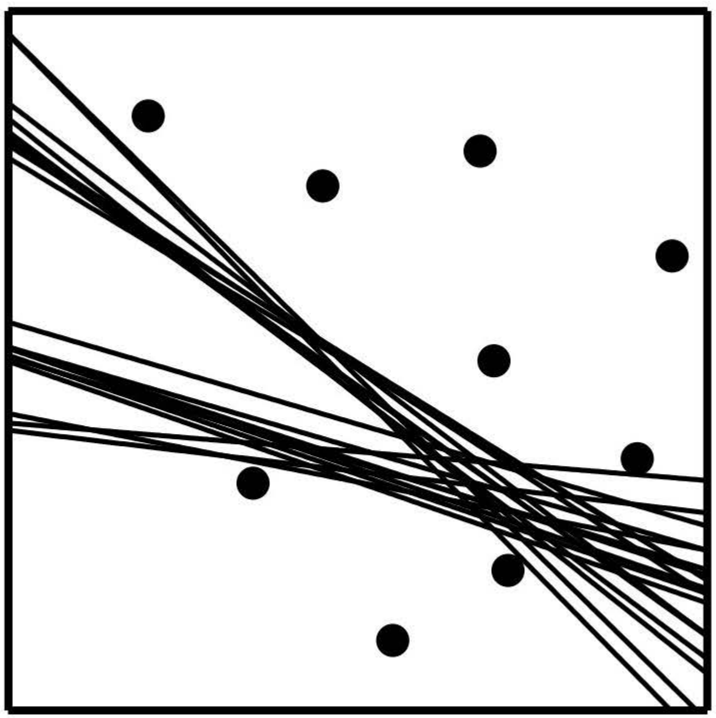


An Effective Number of Hypotheses

|H| only measures the maximum possible diversity of H



$\mathcal{H}$



$\mathcal{H}$ through the eyes of the $\mathcal{D}$

An Effective Number of Hypotheses

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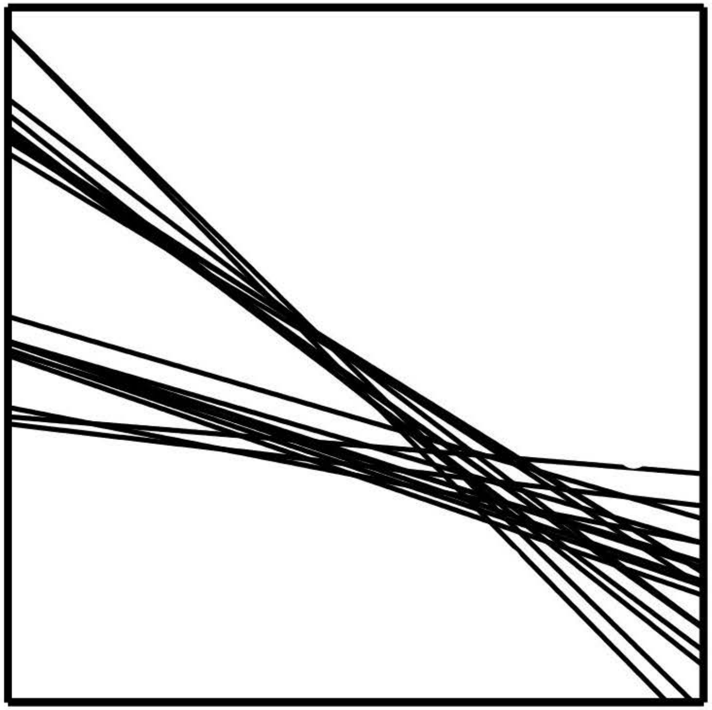
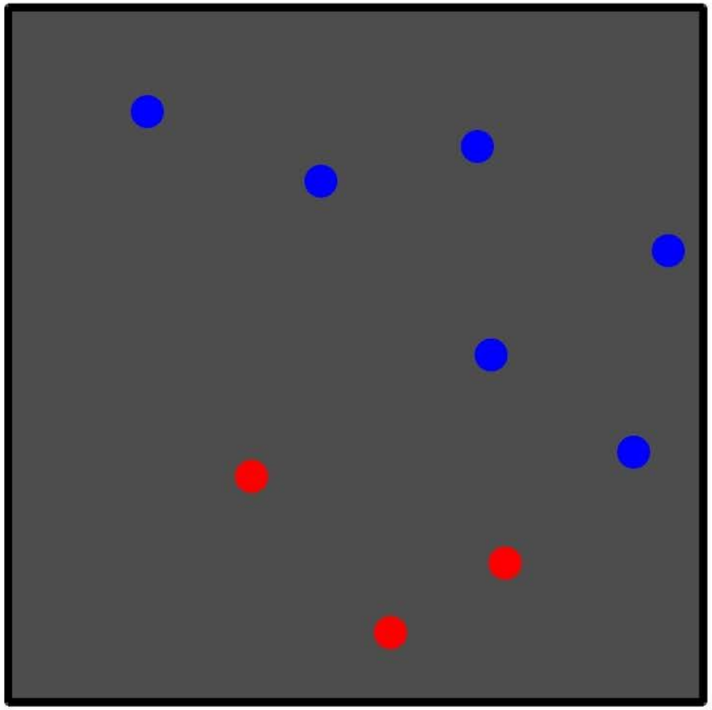




From the viewpoint of S, the entire H is just one dichotomy

An Effective Number of Hypotheses

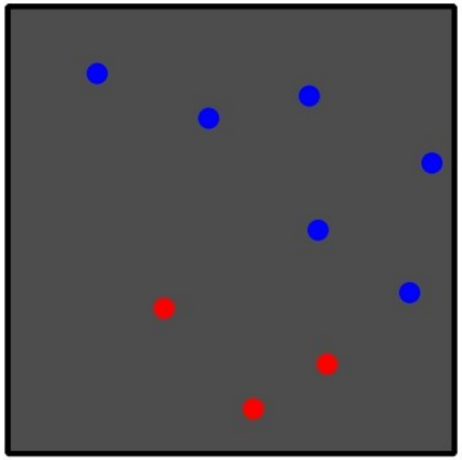
|H| only measures the maximum possible diversity of H

Given a dataset $S=\{x_1,\ldots,x_m\}$,

$(h(x_1),\ldots,h(x_m))$

A dichotomy of S

1. *If H is diverse, we get many different dichotomies.*
2. *If H contains many similar function, we only get a few dichotomies.*



dichotomy

*The **shattering coefficient** quantifies this.*

Sample Complexity: Infinite Hypothesis Spaces

- H[m] - maximum number of ways to split m points using concepts in H; i.e. $H[m] = \max_{|S|=m} |H[S]|$

Theorem For any class H, distrib. D, if the number of labeled examples seen m satisfies

$$m \geq \frac{2}{\varepsilon}\left[\log_2(2H[2m]) + \log_2\left(\frac{1}{\delta}\right)\right]$$

then with probab. $1-\delta$, all $h \in H$ with $err_D(h) \geq \varepsilon$ have $err_S(h) > 0$.

Sauer's Lemma: $\mathrm{H[m]} = \mathrm{O}\left(\mathrm{m}^{\mathrm{VCdim(H)}}\right)$

Theorem

$$m = O\left(\frac{1}{\varepsilon}\left[VCdim(H)\log\left(\frac{1}{\varepsilon}\right) + \log\left(\frac{1}{\delta}\right)\right]\right)$$

labeled examples are sufficient so that with probab. $1-\delta$, all $h \in H$ with $err_D(h) \geq \varepsilon$ have $err_S(h) > 0$.

Effective number of hypotheses

- $H[S]$ – the set of splittings of dataset S using concepts from H.
- $H[m]$ - max number of ways to split m points using concepts in H

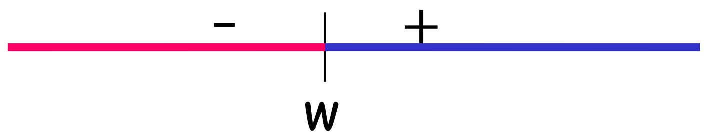
$$H[m] = \max_{|S|=m} |H[S]|$$

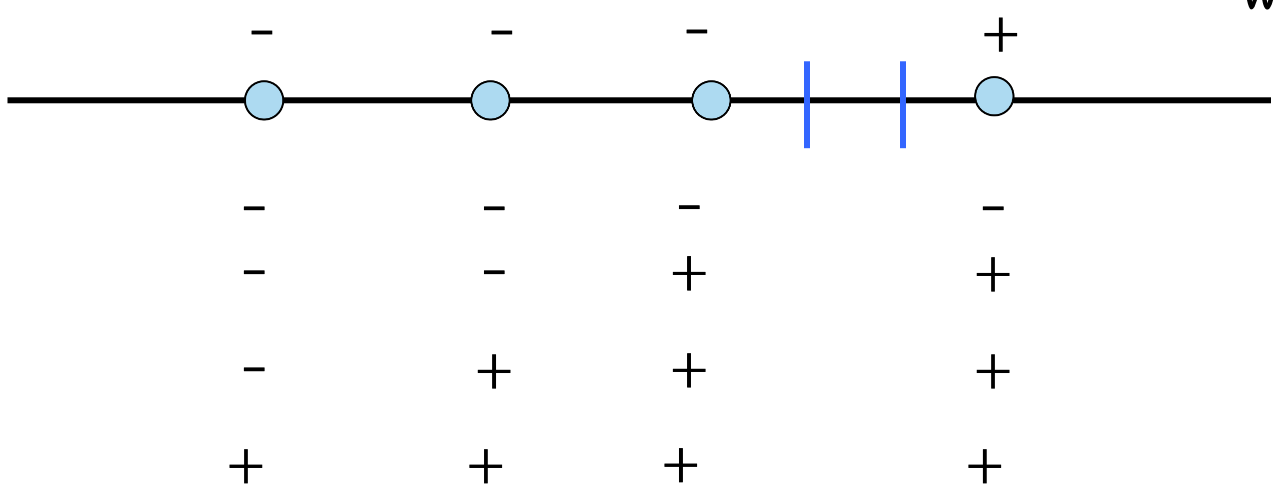
Effective number of hypotheses

- H[S] – the set of splittings of dataset S using concepts from H.
- H[m] - max number of ways to split m points using concepts in H

$$H[m] = \max_{|S|=m} |H[S]| \qquad H[m] \leq 2^m$$

E.g., H= Thresholds on the real line





$|H[S]| = 5$

In general, if |S|=m (all distinct), $|H[S]| = m + 1 \ll 2^m$

Effective number of hypotheses

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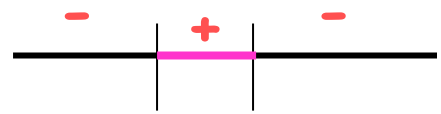
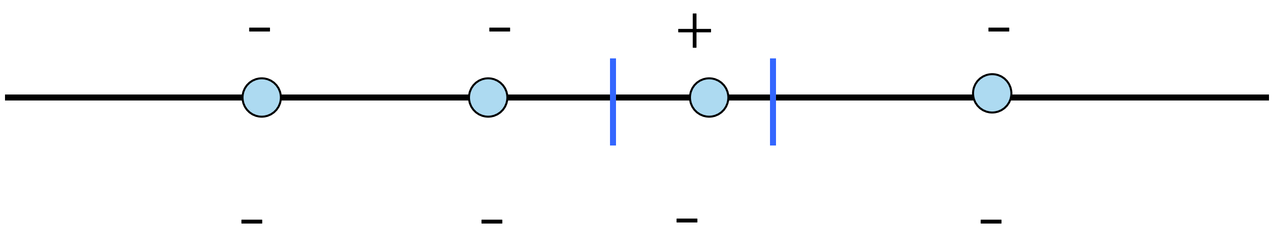
$$H[m] = \max_{|S|=m} |H[S]| \qquad H[m] \le 2^m$$

E.g., H= Intervals on the real line





In general, |S|=m (all distinct), $H[m] = \frac{m(m+1)}{2} + 1 = O(m^2) \ll 2^m$

There are m+1 possible options for the first part, m left for the second part, the order does not matter, so (m choose 2) + 1 (for empty interval).

Effective number of hypotheses

- H[S] – the set of splittings of dataset S using concepts from H.
- H[m] - max number of ways to split m points using concepts in H

$$\mathrm{H[m]} = \max_{|\mathrm{S}|=\mathrm{m}} |\mathrm{H[S]}| \qquad \mathrm{H[m]} \leq 2^{\mathrm{m}}$$

Definition: H shatters S if $|\mathrm{H[S]}| = 2^{|S|}$.

Sample Complexity: Infinite Hypothesis Spaces Realizable Case

H[m] - max number of ways to split m points using concepts in H

Theorem For any class H, distrib. D, if the number of labeled examples seen m satisfies

$$m \geq \frac{2}{\varepsilon}\left[\log_2(2H[2m]) + \log_2\left(\frac{1}{\delta}\right)\right]$$

then with probab. $1-\delta$, all $h \in H$ with $err_D(h) \geq \varepsilon$ have $err_S(h) > 0$.

- Not too easy to interpret sometimes hard to calculate exactly, but can get a good bound using "VC-dimension

If $\mathrm{H[m]} = 2^{\mathrm{m}}$, then $\mathrm{m} \geq \frac{\mathrm{m}}{\epsilon}(\ldots.)$ ☹

- VC-dimension is roughly the point at which H stops looking like it contains all functions, so hope for solving for m.

Sample Complexity: Infinite Hypothesis Spaces

H[m] - max number of ways to split m points using concepts in H

Theorem For any class H, distrib. D, if the number of labeled examples seen m satisfies

$$m \geq \frac{2}{\varepsilon}\left[\log_2(2H[2m]) + \log_2\left(\frac{1}{\delta}\right)\right]$$

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Sauer's Lemma: $\mathrm{H[m]} = \mathrm{O}\left(\mathrm{m}^{\mathrm{VCdim(H)}}\right)$

Theorem

$$m = O\left(\frac{1}{\varepsilon}\left[VCdim(H)\log\left(\frac{1}{\varepsilon}\right) + \log\left(\frac{1}{\delta}\right)\right]\right)$$

labeled examples are sufficient so that with probab. $1-\delta$, all $h \in H$ with $err_D(h) \geq \varepsilon$ have $err_S(h) > 0$.

Shattering, VC-dimension

Definition: H shatters S if $|\mathrm{H}[\mathrm{S}]| = 2^{|S|}$.

A set of points S is shattered by H is there are hypotheses in H that split S in all of the $2^{|S|}$ possible ways, all possible ways of classifying points in S are achievable using concepts in H.

Definition: VC-dimension (Vapnik-Chervonenkis dimension)

The VC-dimension of a hypothesis space H is the cardinality of the largest set S that can be shattered by H.

If arbitrarily large finite sets can be shattered by H, then $\mathrm{VCdim}(\mathrm{H}) = \infty$

Shattering, VC-dimension

Definition: VC-dimension (Vapnik-Chervonenkis dimension)

The VC-dimension of a hypothesis space H is the cardinality of the largest set S that can be shattered by H.

If arbitrarily large finite sets can be shattered by H, then $\mathrm{VCdim}(H) = \infty$

To show that VC-dimension is d:

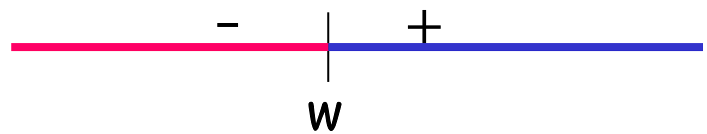
- there exists a set of d points that can be shattered
- there is no set of d+1 points that can be shattered.

Fact: If H is finite, then $\mathrm{VCdim}(H) \leq \log(|H|)$.

Shattering, VC-dimension

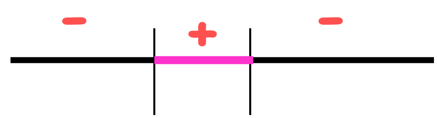
If the VC-dimension is d, that means there exists a set of d points that can be shattered, but there is no set of d+1 points that can be shattered.

E.g., H= Thresholds on the real line

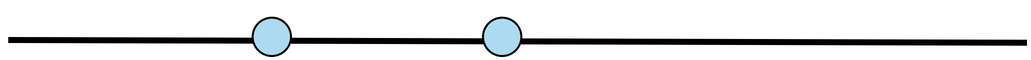


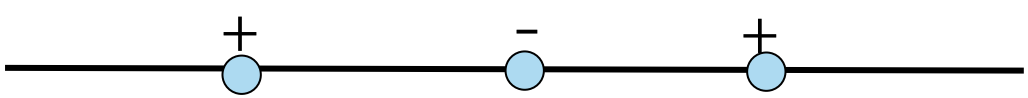
$\mathrm{VCdim}(\mathrm{H}) = 1$

E.g., H= Intervals on the real line



$\mathrm{VCdim}(\mathrm{H}) = 2$

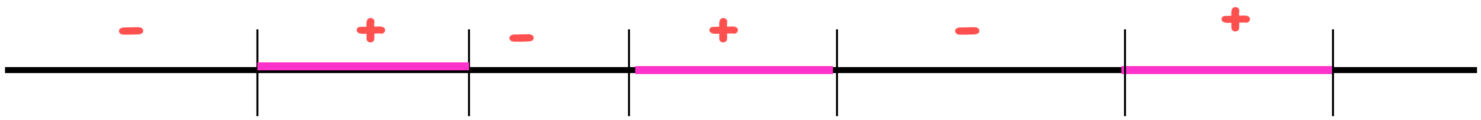




Shattering, VC-dimension

If the VC-dimension is d, that means there exists a set of d points that can be shattered, but there is no set of d+1 points that can be shattered.

E.g., H= Union of k intervals on the real line $\mathrm{VCdim}(\mathrm{H}) = 2\mathrm{k}$



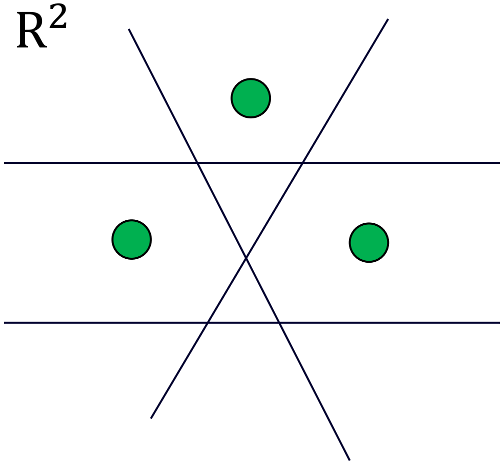
$\mathrm{VCdim}(\mathrm{H}) \geq 2\mathrm{k}$

A sample of size 2k shatters (treat each pair of points as a separate case of intervals)

$\mathrm{VCdim}(\mathrm{H}) < 2\mathrm{k} + 1$

Shattering, VC-dimension

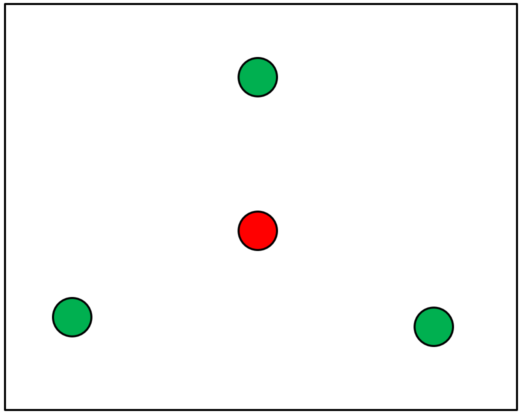
E.g., **H=** linear separators in R^2



$\mathrm{VCdim(H)} \geq 3$

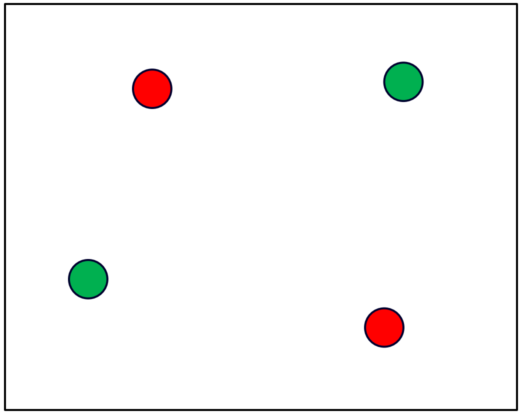
Shattering, VC-dimension

E.g., **H=** linear separators in R^2



$\mathrm{VCdim(H)} < 4$

Case 1: one point inside the triangle formed by the others. Cannot label inside point as positive and outside points as negative.



Case 2: all points on the boundary (convex hull). Cannot label two diagonally as positive and other two as negative.

Fact: VCdim of linear separators in R^d is d+1

Today's Quiz

Sauer's Lemma

Sauer's Lemma:

Let d = VCdim(H)

- $\mathrm{m} \leq \mathrm{d}$, then $\mathrm{H[m]} = 2^{\mathrm{m}}$
- m>d, then $\mathrm{H[m]} = O\left(\mathrm{m}^{d}\right)$

Proof: induction on m and d. Cool combinatorial argument!

Hint: try proving it for intervals…

Sample Complexity: Infinite Hypothesis Spaces
Realizable Case

Theorem For any class H, distrib. D, if the number of labeled examples seen m satisfies

$$m \geq \frac{2}{\varepsilon}\left[\log_2(2H[2m]) + \log_2\left(\frac{1}{\delta}\right)\right]$$

then with probab. $1-\delta$, all $h \in H$ with $err_D(h) \geq \varepsilon$ have $err_S(h) > 0$.

Sauer's Lemma: $H[m] = O\left(m^{VCdim(H)}\right)$

Theorem

$$m = O\left(\frac{1}{\varepsilon}\left[VCdim(H)\log\left(\frac{1}{\varepsilon}\right) + \log\left(\frac{1}{\delta}\right)\right]\right)$$

labeled examples are sufficient so that with probab. $1-\delta$, all $h \in H$ with $err_D(h) \geq \varepsilon$ have $err_S(h) > 0$.

Sample Complexity for Supervised Learning

Realizable Case

Consistent Learner

- Input: S: $(x_1,c^*(x_1)),\ldots,(x_m,c^*(x_m))$
- Output: Find h in H consistent with S (if one exits).

Theorem

$$m \geq \frac{1}{\varepsilon}\left[\ln(|H|) + \ln\left(\frac{1}{\delta}\right)\right]$$

Prob. over different samples of m training examples

labeled examples are sufficient so that with prob. $1-\delta$, all $h \in H$ with $err_D(h) \geq \varepsilon$ have $err_S(h) > 0$.

Linear in $1/\epsilon$

Theorem

$$m = O\left(\frac{1}{\varepsilon}\left[VCdim(H)\log\left(\frac{1}{\varepsilon}\right) + \log\left(\frac{1}{\delta}\right)\right]\right)$$

labeled examples are sufficient so that with probab. $1-\delta$, all $h \in H$ with $err_D(h) \geq \varepsilon$ have $err_S(h) > 0$.

Sample Complexity: Infinite Hypothesis Spaces

Realizable Case

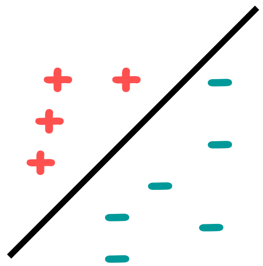
Theorem

$$m = O\left(\frac{1}{\varepsilon}\left[VCdim(H)\log\left(\frac{1}{\varepsilon}\right) + \log\left(\frac{1}{\delta}\right)\right]\right)$$

labeled examples are sufficient so that with probab. $1-\delta$, all $h \in H$ with $err_D(h) \geq \varepsilon$ have $err_S(h) > 0$.

E.g., H= linear separators in $\mathbb{R}^d$

VCdim(H)= d+1



$$m = O\left(\frac{1}{\varepsilon}\left[d\log\left(\frac{1}{\varepsilon}\right) + \log\left(\frac{1}{\delta}\right)\right]\right)$$

Sample complexity linear in d

So, if double the number of features, then I only need roughly twice the number of samples to do well.

Practical rule of thumb: *VCdim(H) ~ #free parameters of H*

What if $c^* \notin H$?

Sample Complexity: Uniform Convergence

Agnostic Case

Empirical Risk Minimization (ERM)

- Input: S: $(x_1,c^*(x_1)),\ldots,(x_m,c^*(x_m))$
- Output: Find h in H with smallest $err_S(h)$

Theorem

$$m \geq \frac{1}{2\varepsilon^2}\left[\ln(|H|) + \ln\left(\frac{2}{\delta}\right)\right]$$

labeled examples are sufficient s.t. with probab. $\geq 1-\delta$, all $h \in H$ have $|err_D(h) - err_S(h)| < \varepsilon$.

$1/\epsilon^2$ dependence [as opposed to $1/\epsilon$ for realizable]

Theorem

$$m = O\left(\frac{1}{\varepsilon^2}\left[VCdim(H) + \log\left(\frac{1}{\delta}\right)\right]\right)$$

labeled examples are sufficient so that with probab. $1-\delta$, all $h \in H$ with $|err_D(h) - err_S(h)| \leq \epsilon$.

Sample Complexity: Finite Hypothesis Spaces Agnostic Case

1) How many examples suffice to get UC whp (so success for ERM).

$1/\epsilon^2$ dependence [as opposed to $1/\epsilon$ for realizable], but get for something stronger.

Theorem

$$m \geq \frac{1}{2\varepsilon^2}\left[\ln(|H|) + \ln\left(\frac{2}{\delta}\right)\right]$$

labeled examples are sufficient s.t. with probab. $\geq 1-\delta$, all $h \in H$ have $|err_D(h) - err_S(h)| < \varepsilon$.

2) Statistical Learning Theory style:

$\sqrt{\frac{1}{m}}$ as opposed to $\frac{1}{m}$ for realizable

With prob. at least $1-\delta$, for all $h \in H$:

$$\mathrm{err}_D(h) \leq \mathrm{err}_S(h) + \sqrt{\frac{1}{2m}\left(\ln\left(2|H|\right) + \ln\left(\frac{1}{\delta}\right)\right)}.$$

Sample Complexity: Infinite Hypothesis Spaces

Agnostic Case

1) How many examples suffice to get UC whp (so success for ERM).

Theorem

$$m = O\left(\frac{1}{\varepsilon^2}\left[VCdim(H) + \log\left(\frac{1}{\delta}\right)\right]\right)$$

labeled examples are sufficient so that with probab. $1-\delta$, all $h \in H$ with $|err_D(h) - err_S(h)| \leq \epsilon$.

2) Statistical Learning Theory style:

With prob. at least $1-\delta$, for all $\mathrm{h} \in \mathrm{H}$:

$$\mathrm{err_D(h)} \leq \mathrm{err_S(h)} + O\left(\sqrt{\frac{1}{2m}\left(\mathrm{VCdim(H)} \ln\left(\frac{em}{\mathrm{VCdim(H)}}\right) + \ln\left(\frac{1}{\delta}\right)\right)}\right).$$

VCdimension Generalization Bounds

E.g., $\mathrm{err}_D(h) \le \mathrm{err}_S(h) + O\left(\sqrt{\frac{1}{2m}\left(\mathrm{VCdim}(H)\ln\left(\frac{em}{\mathrm{VCdim}(H)}\right) + \ln\left(\frac{1}{\delta}\right)\right)}\right)$.

VC bounds: distribution independent bounds

- Generic: hold for any concept class and any distribution.

  [nearly tight in the WC over choice of D]

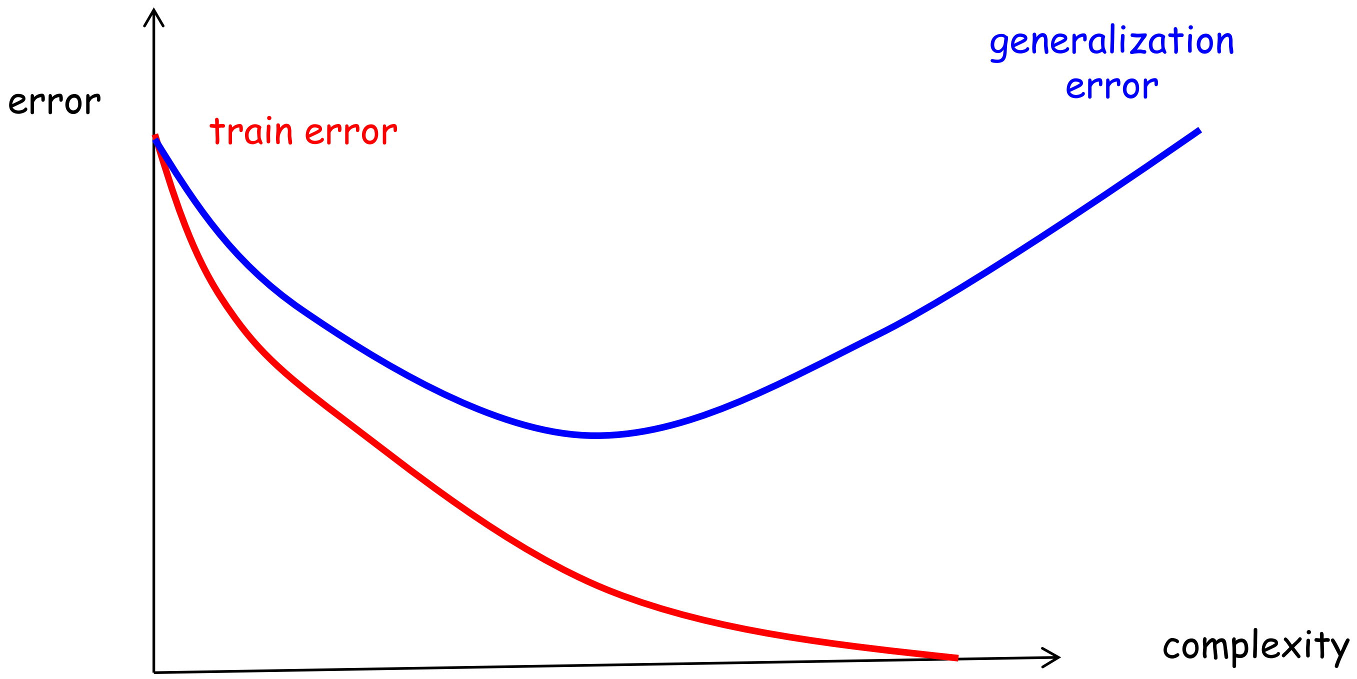
- Might be very loose specific distr. that are more benign than the worst case….
- Hold only for binary classification; we want bounds for fns approximation in general (e.g., multiclass classification and regression).

Can we use our bounds for model selection?

True Error, Training Error, Overfitting

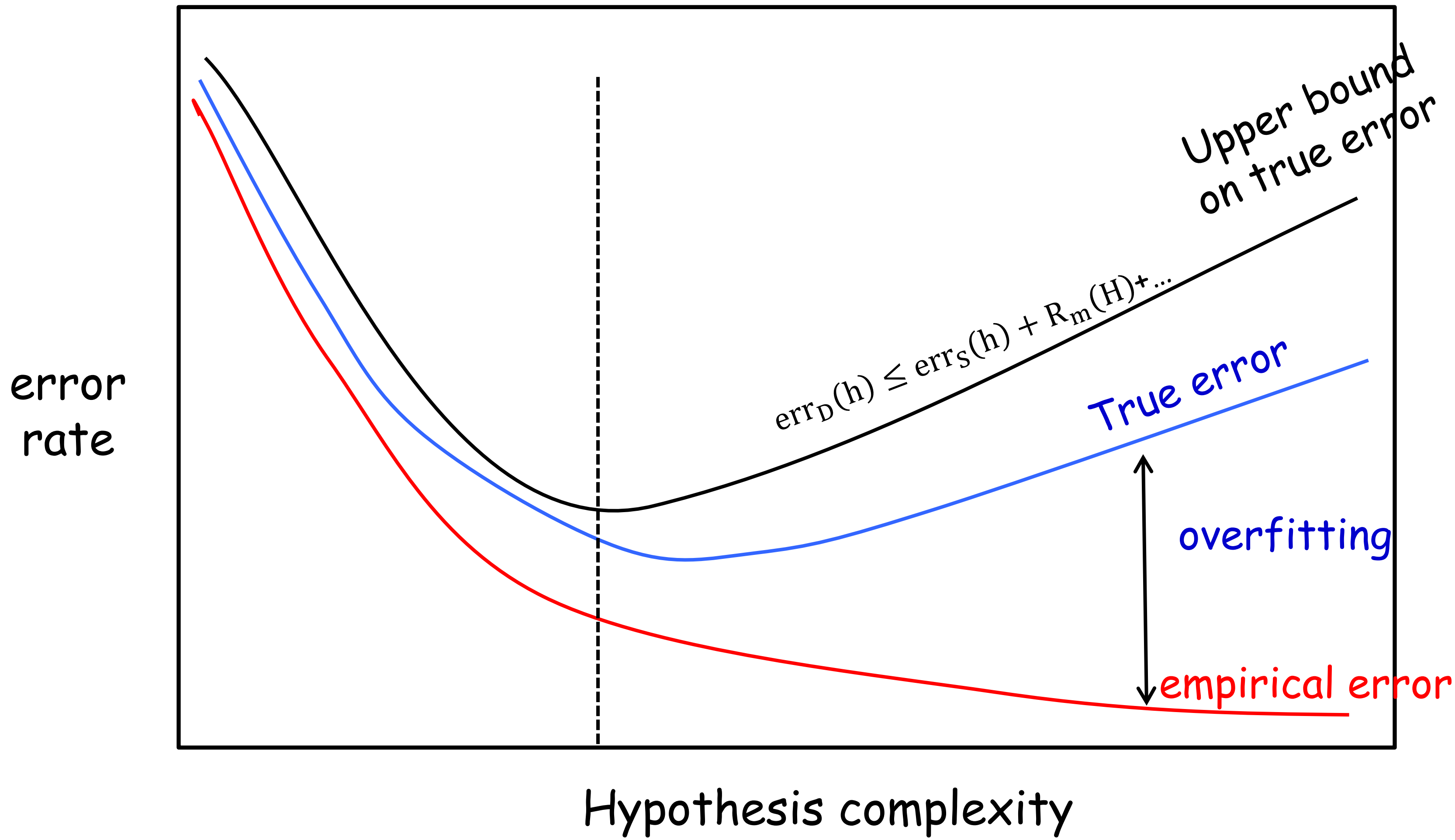
Model selection: trade-off between decreasing training error and keeping H simple.

$$\mathrm{err}_D(h) \leq \mathrm{err}_S(h) + R_m(H) + \ldots$$



Structural Risk Minimization (SRM)

$H_1 \subseteq H_2 \subseteq H_3 \subseteq \cdots \subseteq H_i \subseteq \ldots$

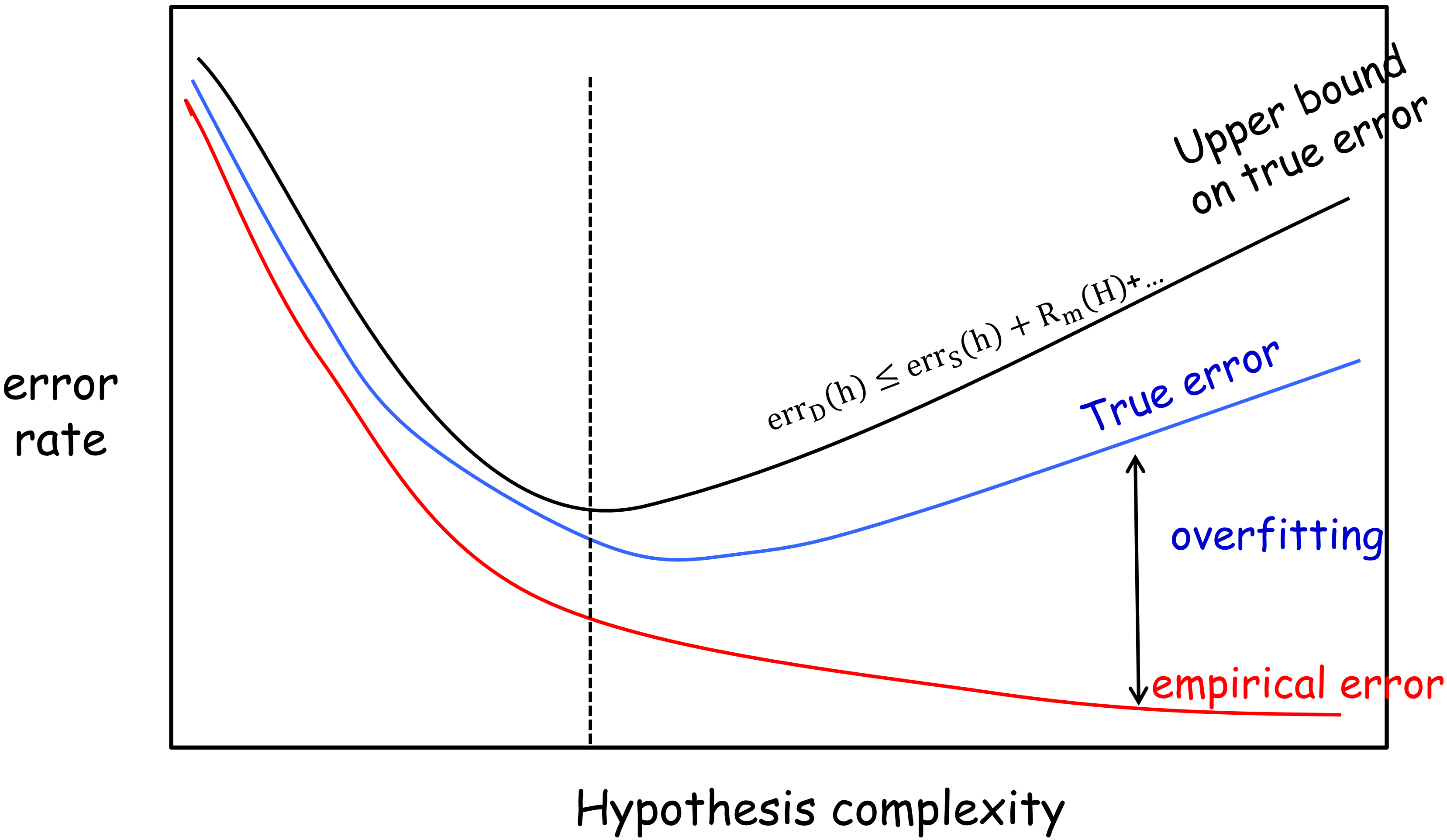


What happens if we increase m?

Black curve will stay close to the red curve for longer, everything shifts to the right…

Structural Risk Minimization (SRM)

$H_1 \subseteq H_2 \subseteq H_3 \subseteq \cdots \subseteq H_i \subseteq \ldots$



Structural Risk Minimization (SRM)

- $H_1 \subseteq H_2 \subseteq H_3 \subseteq \cdots \subseteq H_i \subseteq \ldots$
- $\hat{\mathrm{h}}_{\mathrm{k}} = \mathrm{argmin}_{\mathrm{h} \in \mathrm{H}_{\mathrm{k}}}\{\mathrm{err}_{\mathrm{S}}(\mathrm{h})\}$

  As k increases, $\mathrm{err}_{\mathrm{S}}(\hat{\mathrm{h}}_{\mathrm{k}})$ goes down but complex. term goes up.

- $\hat{k} = \mathrm{argmin}_{\mathrm{k} \geq 1}\{\mathrm{err}_{\mathrm{S}}(\hat{\mathrm{h}}_{\mathrm{k}}) + \mathrm{complexity}(\mathrm{H}_{\mathrm{k}})\}$

  Output $\hat{h} = \hat{h}_{\hat{k}}$

Claim: W.h.p., $\mathrm{err}_{\mathrm{D}}(\hat{\mathrm{h}}) \leq \min_{\mathrm{k}^*} \min_{\mathrm{h}^* \in \mathrm{H}_{\mathrm{k}^*}} [\mathrm{err}_{\mathrm{D}}(\mathrm{h}^*) + 2\mathrm{complexity}(\mathrm{H}_{\mathrm{k}^*})]$

Proof:

- We chose $\hat{\mathrm{h}}$ s.t. $\mathrm{err}_{\mathrm{s}}(\hat{\mathrm{h}}) + \mathrm{complexity}(\mathrm{H}_{\hat{\mathrm{k}}}) \leq \mathrm{err}_{\mathrm{S}}(\mathrm{h}^*) + \mathrm{complexity}(\mathrm{H}_{\mathrm{k}^*})$.
- Whp, $\mathrm{err}_{\mathrm{D}}(\hat{\mathrm{h}}) \leq \mathrm{err}_{\mathrm{s}}(\hat{\mathrm{h}}) + \mathrm{complexity}(\mathrm{H}_{\hat{\mathrm{k}}})$.
- Whp, $\mathrm{err}_{\mathrm{S}}(\mathrm{h}^*) \leq \mathrm{err}_{\mathrm{D}}(\mathrm{h}^*) + \mathrm{complexity}(\mathrm{H}_{\mathrm{k}^*})$.

Techniques to Handle Overfitting

- **Structural Risk Minimization (SRM).** $H_1 \subseteq H_2 \subseteq \cdots \subseteq H_i \subseteq \ldots$

  Minimize gener. bound: $\hat{h} = \mathrm{argmin}_{k \geq 1}\{\mathrm{err}_S(\hat{h}_k) + \mathrm{complexity}(H_k)\}$

  - Often computationally hard….
  - Nice case where it is possible: M. Kearns, Y. Mansour, ICML'98, "A Fast, Bottom-Up Decision Tree Pruning Algorithm with Near-Optimal Generalization"

- **Regularization:** general family closely related to SRM
  - E.g., SVM, regularized logistic regression, etc.
  - minimizes expressions of the form: $\mathrm{err}_S(h) + \lambda ||h||^2$

    Some norm when H is a vector space; e.g., L_2 norm

    Picked through cross validation

- **Cross Validation:**
  - Hold out part of the training data and use it as a proxy for the generalization error

What you should know

- Notion of sample complexity.
- Understand reasoning behind the simple sample complexity bound for finite H.
- Shattering, VC dimension as measure of complexity, Sauer's lemma, form of the VC bounds.
- Model Selection, Structural Risk Minimization.