Generalization and Overfitting

Sample Complexity Results for Supervised Classification

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Two Core Aspects of Machine Learning

Algorithm Design. How to optimize?

Computation

Automatically generate rules that do well on observed data.

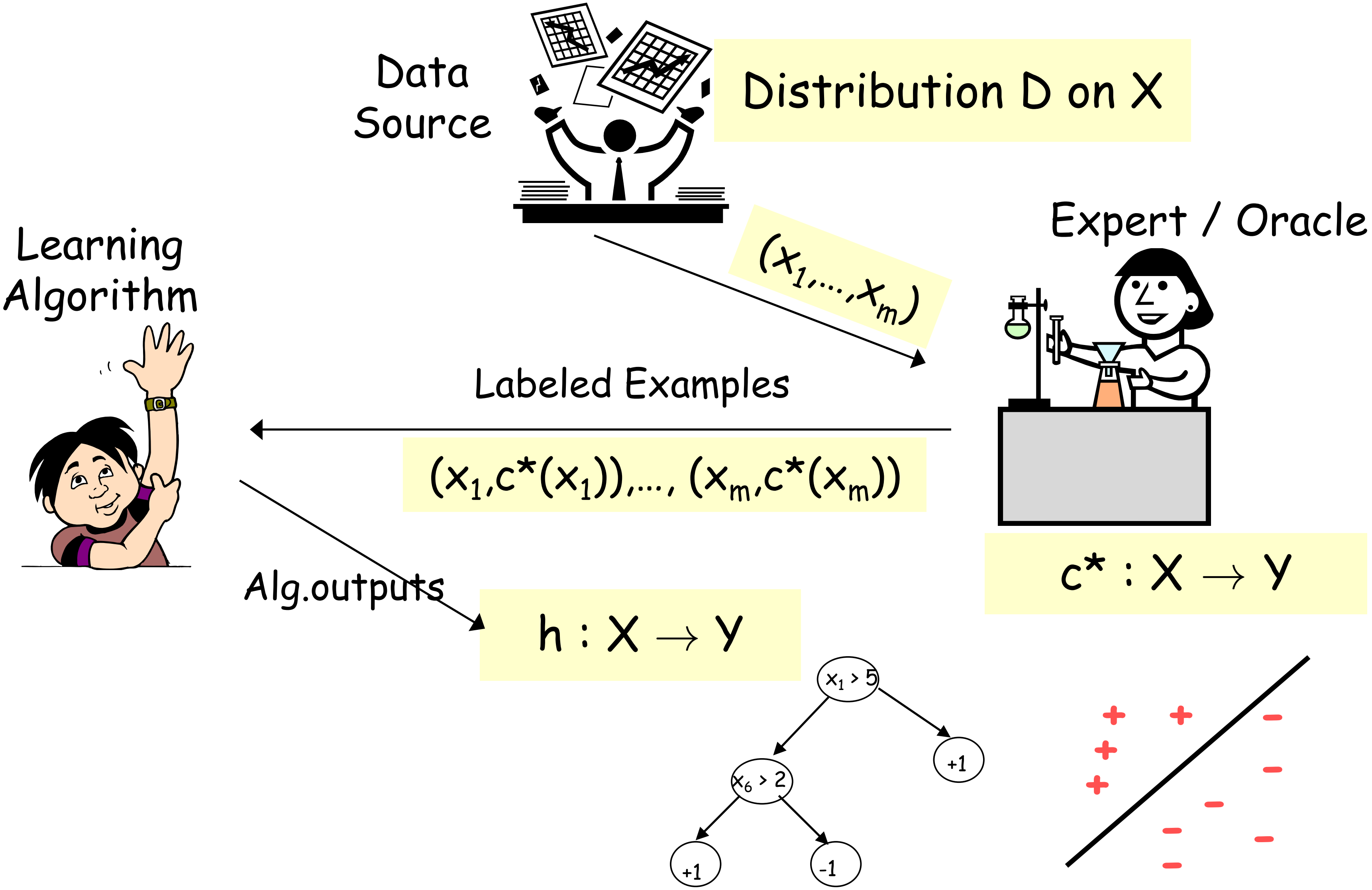
- E.g.: logistic regression, SVM, Adaboost, etc.

Confidence Bounds, Generalization

(Labeled) Data

Confidence for rule effectiveness on future data.

PAC/SLT models for Supervised Learning



Data Source

Distribution D on X

$(x_1,\ldots,x_m)$

Expert / Oracle

Learning Algorithm

Labeled Examples

$(x_1,c^*(x_1)),\ldots, (x_m,c^*(x_m))$

$c^* : X \to Y$

Alg.outputs

$h : X \to Y$

PAC/SLT models for Supervised Learning

- X – feature/instance space; distribution D over X

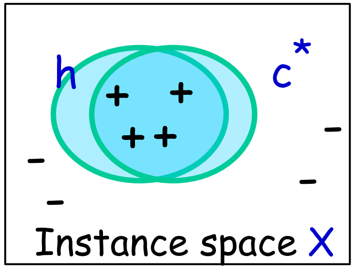
  e.g., $X = R^d$ or $X = \{0,1\}^d$

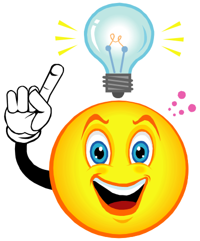
- Algo sees training sample S: $(x_1,c^*(x_1)),\ldots, (x_m,c^*(x_m))$, x_i i.i.d. from D
  - labeled examples - drawn i.i.d. from D and labeled by target c^*
  - labels $\in \{-1,1\}$ - binary classification

- Algo does optimization over S, find hypothesis h.

- Goal: h has small error over D.

$$err_D(h) = \Pr_{x \sim D}(h(x) \neq c^*(x))$$





Bias: fix hypothesis space H [whose complexity is not too large]

- Realizable: $c^* \in H$.
- Agnostic: c^* "close to" H.

PAC/SLT models for Supervised Learning

- Algo sees training sample S: $(x_1,c^*(x_1)),\ldots,(x_m,c^*(x_m))$, x_i i.i.d. from D
- Does optimization over S, find hypothesis $h \in H$.
- Goal: h has small error over D.

True error: $\mathrm{err}_D(h) = \Pr_{x\sim D}(h(x) \neq c^*(x))$

How often $h(x) \neq c^*(x)$ over future instances drawn at random from D

- But, can only measure:

Training error: $\mathrm{err}_S(h) = \frac{1}{m}\sum_i I\left(h(x_i) \neq c^*(x_i)\right)$

How often $h(x) \neq c^*(x)$ over training instances

Sample complexity: bound $err_D(h)$ in terms of $err_S(h)$

Sample Complexity for Supervised Learning

Consistent Learner

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

Bound only logarithmic in |H|, linear in $1/\epsilon$

Theorem

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

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

Probability over different samples of m training examples

So, if $c^* \in H$ and can find consistent fns, then only need this many examples to get generalization error $\leq \epsilon$ with prob. $\geq 1-\delta$

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 $\mathrm{err}_S(\mathrm{h})$

Theorem

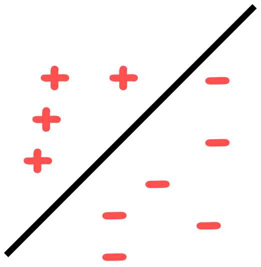
$$m \geq \frac{1}{2\varepsilon^2}\left[\ln(|H|) + \ln\left(\frac{2}{\delta}\right)\right]$$

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

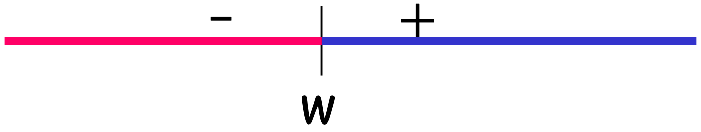
$1/\epsilon^2$ dependence [as opposed to$1/\epsilon$ for realizable]

What if H is infinite?

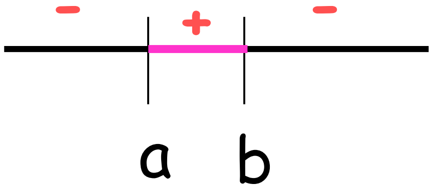
E.g., linear separators in R^d



E.g., thresholds on the real line



E.g., intervals on the real line



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

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

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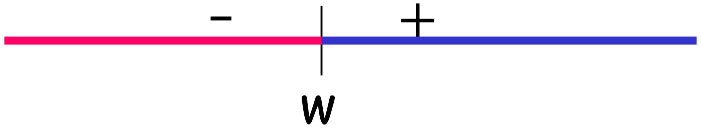
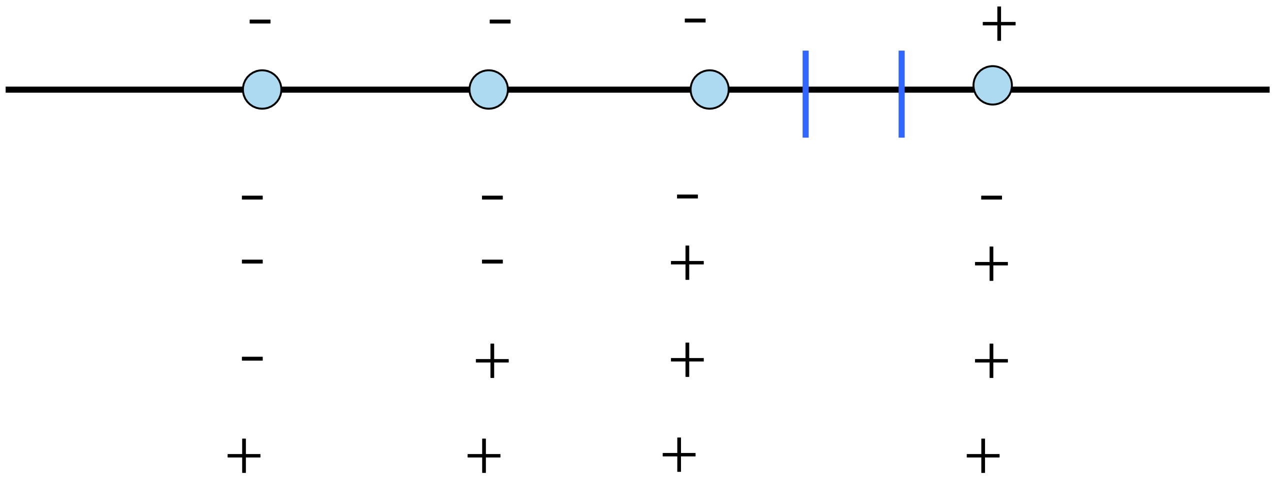
E.g., H= Thresholds on the real line





$|H[S]| = 5$

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

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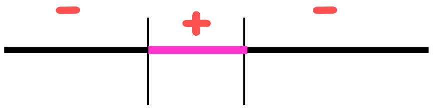
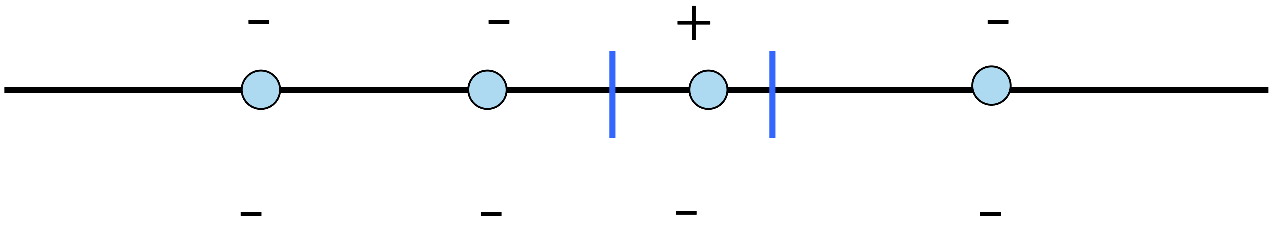




In general, |S|=m (all distinct), $H[m] = \frac{m(m+1)}{2} + 1 = O(m^2) \ll 2^m$

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

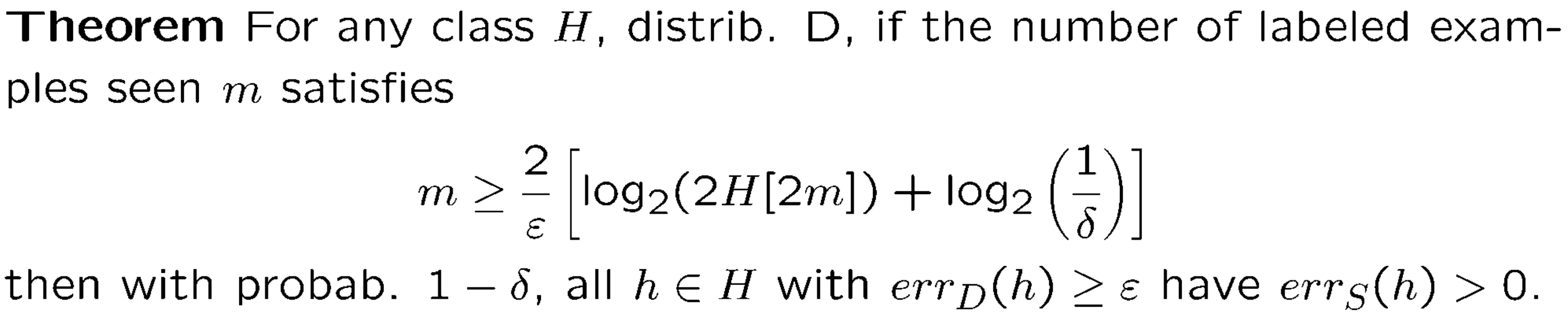
- H[S] – the set of splittings of dataset S using concepts from H.
- H[m] - max number of ways to split m points using concepts in H

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

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

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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 $err_S(h) > 0$.

Shattering, VC-dimension

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

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

Shattering, VC-dimension

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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:

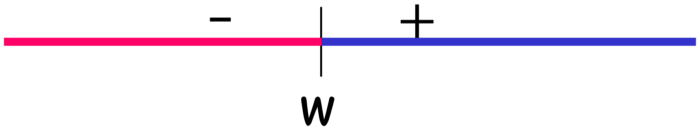
- there exists a set of d points that can be shattered
- there is no set of d+1 points that can be shattered.

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

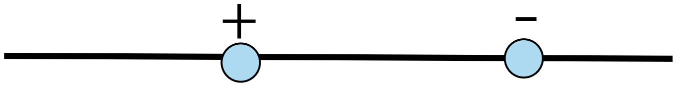
Shattering, VC-dimension

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.

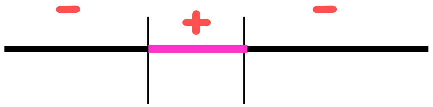
E.g., H= Thresholds on the real line



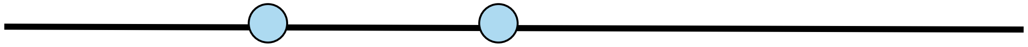
$\mathrm{VCdim}(H) = 1$

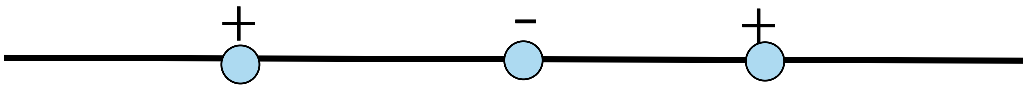


E.g., H= Intervals on the real line



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

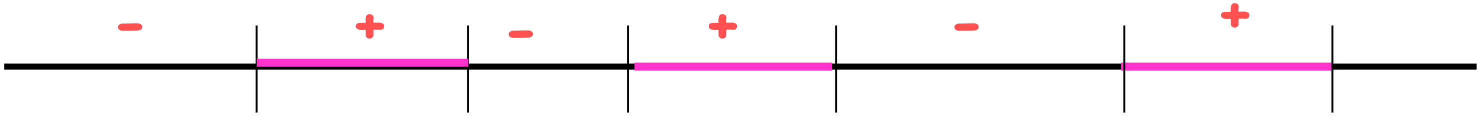




Shattering, VC-dimension

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.

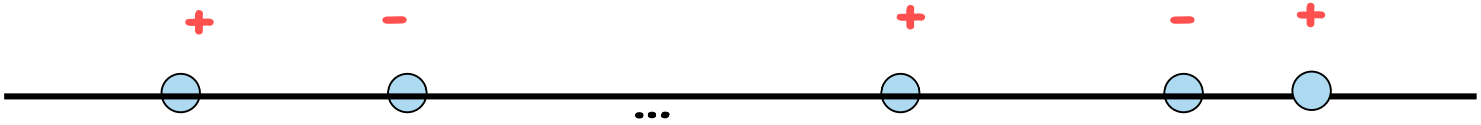
E.g., H= Union of k intervals on the real line $\mathrm{VCdim}(\mathrm{H}) = 2\mathrm{k}$



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

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

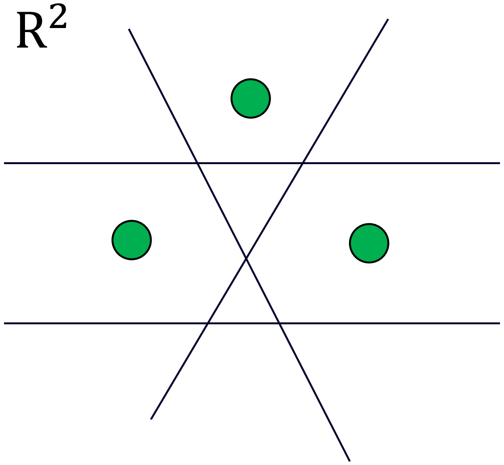
$\mathrm{VCdim}(\mathrm{H}) < 2\mathrm{k} + 1$



Shattering, VC-dimension

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

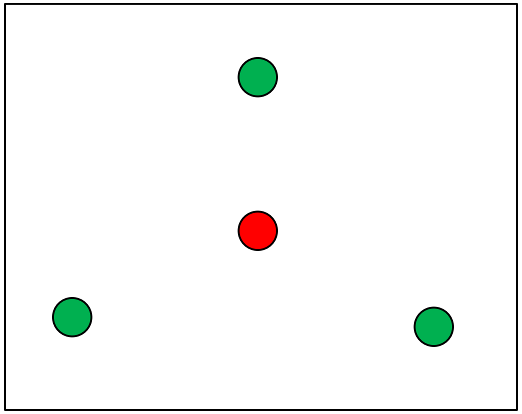
$\mathrm{VCdim(H)} \geq 3$



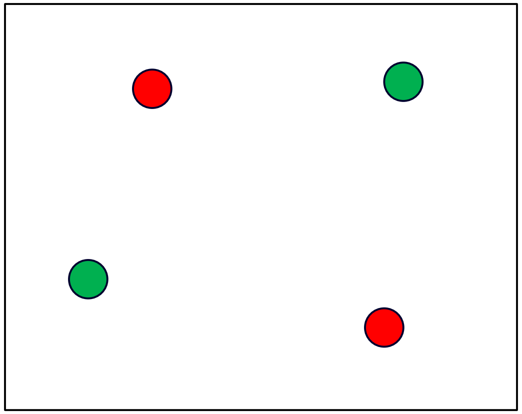
Shattering, VC-dimension

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

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 $\mathrm{H[m]} = O\left(\mathrm{m}^{d}\right)$

Sample Complexity: Infinite Hypothesis Spaces

Realizable Case

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

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Theorem

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

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E.g., H= linear separators in R^d

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

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.

Sample Complexity: Infinite Hypothesis Spaces Realizable Case

Theorem

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

Statistical Learning Theory Style

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

What you should know

- Notion of sample complexity.
- Shattering, VC dimension as measure of complexity, Sauer's lemma, form of the VC bounds.