Lecture 2: VC Dimension

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Advanced Machine Learning
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Representational capacity

PAC learning guarantee

Let $\mathcal{H}$ be a hypothesis class, $\delta, \epsilon > 0$ and S a training set of size $n \geq \frac{1}{\epsilon}(\ln |\mathcal{H}| + \ln(1/\delta))$ drawn using D. With probability $\geq 1 - \delta$, every $h \in \mathcal{H}$ with true error $\text{err}_D > \epsilon$ has training error $\text{err}_S > 0$.

hypothesis $\mathcal{H}$

Sample error 0

$\Rightarrow$ True error $< \epsilon$

train error $\neq 0$ $\Rightarrow$ true error $\not< \epsilon$

$= 0$ $\geq \epsilon$

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Uniform convergence

Let $\mathcal{H}$ be a hypothesis class, $\delta, \epsilon > 0$. If a training set S of size $n \geq \frac{1}{2\epsilon^2}(\ln|\mathcal{H}| + \ln(2/\delta))$ is drawn using D, then with probability $\geq 1 - \delta$, every $h \in \mathcal{H}$ satisfies $|\text{err}_S(h) - \text{err}_D(h)| \leq \epsilon$.

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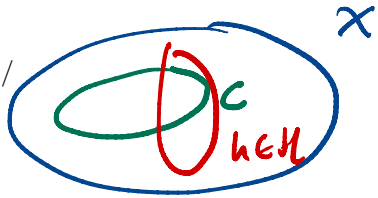
- $|\mathcal{H}|$ is representational capacity, when $\mathcal{H}$ is finite
- How do we adapt and apply these bounds when $\mathcal{H}$ is infinite?

Shattering

- Set system: $(X, \mathcal{H})$
  - X is a set — instance space
  - $\mathcal{H}$, set of subsets of X — set of possible classifiers / hypotheses



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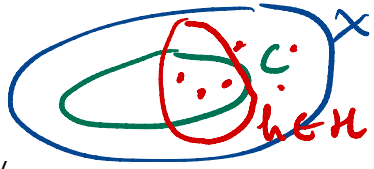
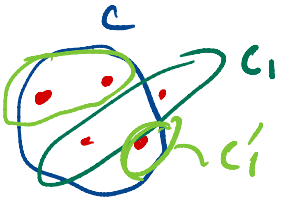


$2^{|A|}$ $A =$



$C_1 = \bar{C}_1'$

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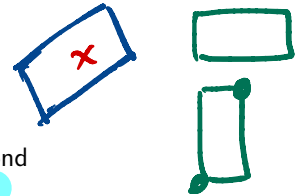
- Example:
  - $X = \mathbb{R} \times \mathbb{R}$
  - $\mathcal{H}$: Axis-parallel rectangles
  - A : Four points forming a diamond



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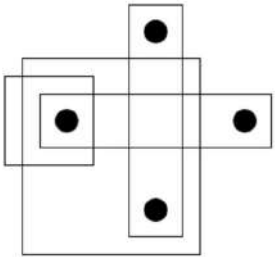
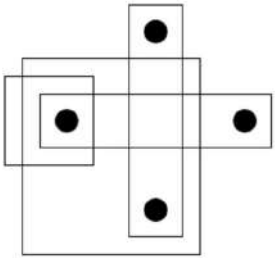


VC-Dimension [Vapnik-Chervonenkis]

- VC-Dimension of $\mathcal{H}$ — size of the largest subset of X shattered by $\mathcal{H}$
  - For axis-parallel rectangles, VC-dimension is at least 4



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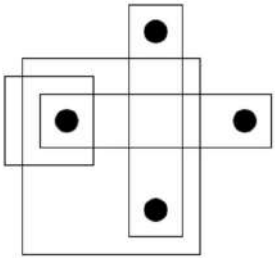
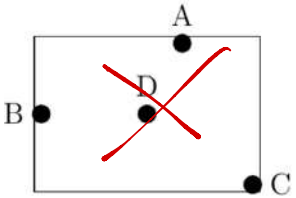


$\{A, B, C\}$ cannot be captured



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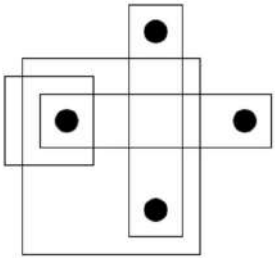
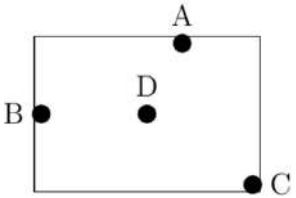
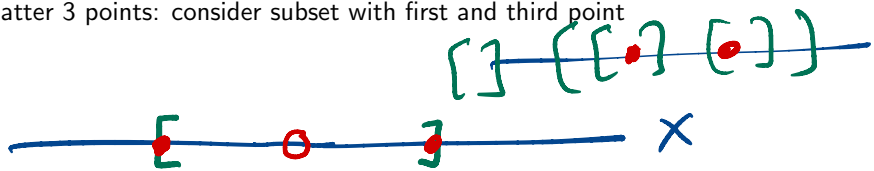
  - For axis-parallel rectangles, VC-dimension is at least 4
  - Not a universal requirement — some sets of size 4 may not be shattered
- No set of size 5 can be shattered by axis-parallel rectangles
  - Draw a bounding box rectangle — each edge touches a boundary point
  - At least one point lies inside the bounding box
  - Any set that includes the boundary points also includes the interior point





VC-Dimension, Examples

- Intervals of reals have VC-dimension 2
  - $X = \mathbb{R}$, $\mathcal{H} = \{[a, b] \mid a \leq b \in \mathbb{R}\}$
  - Cannot shatter 3 points: consider subset with first and third point



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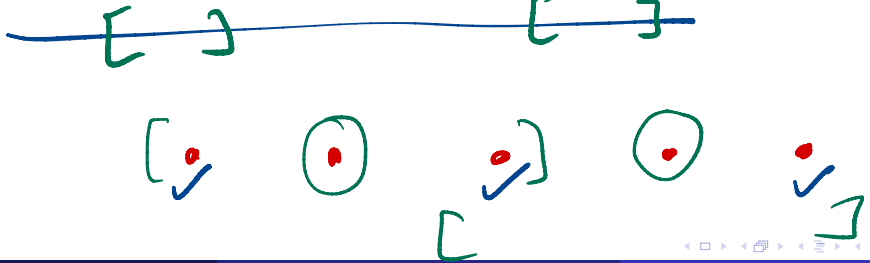
- Pairs of intervals of reals have VC-dimension 4
  - $X = \mathbb{R}$, $\mathcal{H} = \{[a, b] \cup [c, d] \mid a \leq b, c \leq d \in \mathbb{R}\}$
  - Cannot shatter 5 points: consider subset with first, third and fifth point



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- Finite sets of real numbers
  - $X = \mathbb{R}$, $\mathcal{H} = \{Z \mid Z \subseteq \mathbb{R}, |Z| < \infty\}$
  - Can shatter any finite set of reals — VC-dimension is infinite

$A \subseteq_{fin} \mathbb{R}$

$X \subseteq A$, $X \subseteq_{fin} \mathbb{R}$

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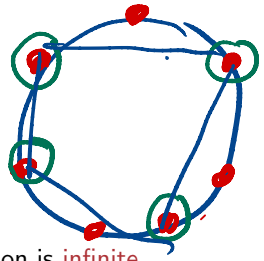
- Convex polygons, $X = \mathbb{R} \times \mathbb{R}$
  - For any n, place n points on unit circle
  - Each subset of these points is a convex polygon — VC-dimension is infinite

$|A| = 7$



VC-dimension and machine learning

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Let $\mathcal{H}$ be a hypothesis class, $\delta, \epsilon > 0$ and S a training set of size $n \geq \frac{1}{\epsilon}(\ln |\mathcal{H}| + \ln(1/\delta))$ drawn using D. With probability $\geq 1 - \delta$, every $h \in \mathcal{H}$ with true error $\text{err}_D > \epsilon$ has training error $\text{err}_S > 0$.

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- We can rewrite this using VC-dimension.

Sample bound using VC-dimension

For any class $\mathcal{H}$ and distribution D, if a training sample S is drawn using D of size $O\left(\frac{1}{\epsilon}\left[\text{VC-dim}(\mathcal{H})\ln\frac{1}{\epsilon} + \ln\frac{1}{\delta}\right]\right)$, then with probability $\geq 1 - \delta$,

- every $h \in \mathcal{H}$ with true error $\text{err}_D(h) \geq \epsilon$ has training error $\text{err}_S(h) > 0$,
- i.e., every $h \in \mathcal{H}$ with training error $\text{err}_S(h) = 0$. has true error $\text{err}_D(h) < \epsilon$

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- We can rewrite this using VC-dimension. Can similarly restate uniform convergence.

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Summary

- PAC learning and uniform convergence use size of finite hypothesis set as measure of representational capacity
- VC-dimension provides a way of measuring capacity for infinite hypothesis sets
- VC-dimension may be finite or infinite
- For finite VC-dimension, we have analogues of PAC learning guarantee and uniform convergence
- Note that these theoretical bounds are hard to use in practice
- Difficult, if not impossible, to compute VC-dimension for complex models

Lecture 3: Loss functions

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Gradient descent

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- Parameter estimate is through gradient descent
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- How do arrive at these loss functions?

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- Likelihood is $\prod_{i=1}^{n} P_{\text{model}}(y_i \mid x_i, \theta)$
- Find M that maximizes the likelihood

Log likelihood

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- Rewrite log likelihood as a sum

$$\log\left(\prod_{i=1}^{n} P_{\text{model}}(y_i \mid x_i, \theta)\right) = \sum_{i=1}^{n} \log(P_{\text{model}}(y_i \mid x_i, \theta))$$

Maximizing Log likelihood

- Define $P_{\text{data}}(y \mid x_i)$ as follows: $P_{\text{data}}(y \mid x_i) = \begin{cases} 1 & \text{if } y = y_i \\ 0 & \text{otherwise} \end{cases}$

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$$\sum_{i=1}^{n} \log(P_{\text{model}}(y_i \mid x_i, \theta)) = \sum_{i=1}^{n} P_{\text{data}}(y_i \mid x_i) \cdot \log(P_{\text{model}}(y_i \mid x_i, \theta))$$

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- To maximize, find an optimum value of θ: $\dfrac{\partial \mathcal{L}(\theta)}{\partial \theta} = 0$

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- Note that cross entropy is not symmetric: $H(P, Q) \neq H(Q, P)$

Cross entropy and MLE

- Maximum likelihood estimator (MLE) — maximize

$$\mathcal{L}(\theta) = \sum_{i=1}^{n} P_{\text{data}}(y_i \mid x_i) \log(P_{\text{model}}(y_i \mid x_i, \theta))$$

P( ) log (a( ))

Cross entropy and MLE

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- P_{model} is an estimate for the true distribution P_{data}

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- $H(P_{\text{data}}, P_{\text{model}}) = -\sum_{i=1}^{k} P_{\text{data}}(y \mid x_i) \log(P_{\text{model}}(y \mid x_i, \theta))$

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- The "cross entropy loss function" is a special form of this generic observation

Regression and MSE loss

- Training input is $\{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\}$
  - Noisy outputs from a linear function
  - $y_i = w^T x_i + \epsilon$
  - $\epsilon \sim \mathcal{N}(0, \sigma^2)$: Gaussian noise, mean 0, fixed variance σ^2
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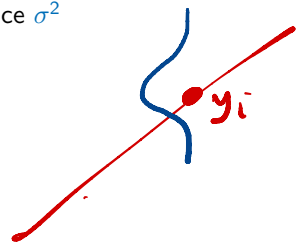

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- Assuming data points are generated by linear function and then perturbed by Gaussian noise, MSE is the "correct" loss function to maximize likelihood (and minimize cross entropy)

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- Recommended loss function, directly minimizes cross entropy

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