

CSCI B609:

“Foundations of Data Science”

Lecture 11/12: VC-Dimension and VC-Theorem

Slides at <http://grigory.us/data-science-class.html>

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Intro to ML

- Classification problem
 - Instance space $X: \{0,1\}^n$ or $\mathbb{R}^n$ (feature vectors)
 - Classification: come up with a mapping $f: X \rightarrow \{0,1\}$
- Formalization:
 - Assume there is a probability distribution D over X
 - $C^* =$ “target concept” (set $C^* \subseteq X$ of positive instances)
 - Given labeled i.i.d. samples from D produce $f \subseteq X \rightarrow \{0,1\}$
 - **Goal:** have f agree with C^* over distribution D
 - Minimize: $\Delta(f, C^*) = \Pr [f(x) \neq C^*(x)]$

Intro to ML

- Training error

- $\mathcal{S}$ = labeled sampled (pairs (x_i, y_i) , $x_i \in \mathcal{X}$, $y_i \in \{0,1\}$)

- Training error:
$$E_{\mathcal{S}}(h) = \frac{|\{ (x_i, y_i) \in \mathcal{S} : h(x_i) \neq y_i \}|}{|\mathcal{S}|}$$

- “Overfitting”: low training error, high true error

- Hypothesis classes:

- H : collection of subsets of $\mathcal{X}$ called hypotheses

- If $\mathcal{X} = \mathbb{R}$ could be all intervals $\{[a, b], a \leq b\}$

- If $\mathcal{X} = \mathbb{R}$ could be linear separators:

$$\{ \{ x \in \mathbb{R} \mid a \cdot x \geq b \} \mid a \in \mathbb{R}, b \in \mathbb{R} \}$$

- If n is large enough (compared to some property of H) then overfitting doesn't occur

Overfitting and Uniform Convergence

- **PAC learning (agnostic):** For $\epsilon, \delta > 0$ if $|S| \geq 1/\epsilon^2 (\ln |H| + \ln 2/\delta)$

then with probability $1 - \delta$:

$$\forall h \in H: \left| \frac{1}{|S|} \sum_{(x,y) \in S} h(x) - \mathbb{E}_{(x,y) \sim D} [h(x)] \right| \leq \epsilon$$

- Size of the class of hypotheses can be very large
- Can also be infinite, how to give a bound then?
- We will see ways around this today

VC-dimension

- $\text{VC-dim}(\mathcal{H}) \leq \ln \left| \mathcal{H} \right|$
- Consider database age vs. salary
- Query: fraction of the overall population with ages 35 – 45 and salary \$(50 – 70)K
- How big a database can answer with $\pm \epsilon$ error
- 100 ages $\times$ 1000 salaries $\Rightarrow 10^{10}$ rectangles
- $1 / 2^{\epsilon^2} (10 \ln 10 + \ln 2 / \epsilon^2)$ samples suffice
- What if we don't want to discretize?

VC-dimension

- **Def.** Concept class **shatters** a set A if $\forall \text{ labeling } h$ there is $h \in \mathcal{H}$ labeling A positive and $A \setminus A$ negative
- **Def.** $\text{VC-dim}(\mathcal{H})$ = size of the largest shattered set
- Example: axis-parallel rectangles on the plane
 - 4-point diamond is shattered
 - No 5-point set can be shattered
 - $\text{VC-dim}(\text{axis-parallel rectangles}) = 4$
- **Def.** $[\mathcal{H}]_A = \{h \cap A : h \in \mathcal{H}\}$ = set of labelings of the points in A by functions in $\mathcal{H}$
- **Def. Growth function** $\Pi_{\mathcal{H}}(n) = \max_{|A|=n} |\mathcal{H}|_A|$

Growth function & uniform convergence

- **PAC learning via growth function:** For $\epsilon, \delta > 0$ if $|S| \geq \frac{8}{\epsilon^2} (\ln |H| + \ln 1/\delta)$

then with probability $1 - \delta$:

$$\forall h \in H: \left| \frac{1}{|S|} \sum_{S} h(x_i) - \int h(x) dP(x) \right| \leq \epsilon$$

- **Thm (Sauer's lemma).** If $\text{VC-dim}(H) = d$ then:

$$|H(S)| \leq \sum_{i=0}^d \binom{|S|}{i} \leq \left(\frac{e|S|}{d} \right)^d$$

- For half-planes, $\text{VC-dim} = 3$, $|H(S)| = O(|S|^3)$

Sauer's Lemma Proof

- Let $n = \dim(V)$ we'll show that if $|F| \leq 2^n$:

$$| \{ [A] \mid A \in F \} | \leq \sum_{i=0}^n \binom{n}{i}$$

- $\binom{n}{i} = \binom{n-1}{i} + \binom{n-1}{i-1}$

Proof (induction by set size):

- $F \setminus \{A\}$: by induction $| \{ [A] \mid A \in F \setminus \{A\} \} | \leq \binom{n-1}{i}$

- $| \{ [A] \mid A \in F \} | = | \{ [A] \mid A \in F \setminus \{A\} \} | + 1 \leq \binom{n-1}{i} + 1$

$$| [] | - | [\setminus \{ \}] | \leq \begin{pmatrix} -1 \\ \leq -1 \end{pmatrix}$$

- If $[] > [\setminus \{ \}]$ then it is because of the sets that differ only on $\{ \}$ so let's pair them up
- For $h \in []$ containing $\{ \}$ let $\begin{pmatrix} () \\ () \end{pmatrix} = h \setminus \{ \}$
 $= \{ h \in [] : \{ \} \in h \}$
- Note: $| [] | - | [\setminus \{ \}] | = | \begin{pmatrix} () \\ () \end{pmatrix} |$
- What is the VC-dimension of $\begin{pmatrix} () \\ () \end{pmatrix}$?
 - If $\text{VC-dim}(\begin{pmatrix} () \\ () \end{pmatrix}) = d'$ then $\begin{pmatrix} () \\ () \end{pmatrix} \subseteq [] \setminus \{ \}$ of $[]$ is shattered
 - All $2^{d'}$ subsets of $\begin{pmatrix} () \\ () \end{pmatrix}$ are 0/1 extendable on $\{ \}$
 - $d \geq d' + 1 \Rightarrow \text{VC-dim}(\begin{pmatrix} () \\ () \end{pmatrix}) \leq d - 1 \Rightarrow$ apply induction

Examples

- Intervals of the reals:
 - Shatter 2 points, don't shatter 3 $\Rightarrow$ $\text{-dim} = 2$
- Pairs of intervals of the reals:
 - Shatter 4 points, don't shatter 5 $\Rightarrow$ $\text{-dim} = 4$
- Convex polygons
 - Shatter any n points on a circle $\Rightarrow$ $\text{-dim} = \infty$
- Linear separators in d dimensions:
 - Shatter $d + 1$ points (unit vectors + origin)
 - Take subset S and set $\text{separator} = 0$ if $\sum_{x \in S} \langle x, w \rangle \leq 0$:

VC-dimension of linear separators

No set of $n + 2$ points can be shattered

- **Thm (Radon).** Any set $S \subseteq \mathbb{R}^d$ with $|S| = n + 2$ can be partitioned into two subsets S_1, S_2 s.t.:

$$\text{Convex}(S_1) \cap \text{Convex}(S_2) \neq \emptyset$$

- Form $n \times (n + 2)$ matrix A, columns = points in S
- Add extra all-1 row $\Rightarrow$ matrix B
- $v = \begin{pmatrix} x_1, x_2, \dots, x_{n+2} \end{pmatrix}$, non-zero vector: $Bv = 0$
- Reordering: $x_1, x_2, \dots, x_{n+1} \geq 0, x_{n+2} < 0$

$$\sum_{i=1}^{n+1} x_i \geq 0, \quad x_{n+2} < 0$$

Radon's Theorem (cont.)

- , = i-th columns of and

- $$\sum_{i=1}^n |v_i| |w_i| = \sum_{i=1}^{n+2} |v_i| |w_i|$$

$$- \sum_{i=1}^n |v_i| |w_i| = \sum_{i=1}^{n+2} |v_i| |w_i|$$

$$- \sum_{i=1}^n |v_i| |w_i| = \sum_{i=1}^{n+2} |v_i| |w_i| = 1$$

- Convex combinations of two subjects intersect

Growth function & uniform convergence

- **PAC learning via growth function:** For $\epsilon, \delta > 0$ if
$$|S| \geq \frac{8}{\epsilon^2} (\ln |H| + \ln \frac{1}{\delta})$$

then with probability $1 - \delta$:

$$\forall h \in H: \left| \frac{1}{|S|} \sum_{i=1}^{|S|} h(x_i) - \mathbb{E}_{x \sim D} h(x) \right| \leq \epsilon$$

- Assume **event A**:

$$\exists h \in H: \left| \frac{1}{|S|} \sum_{i=1}^{|S|} h(x_i) - \mathbb{E}_{x \sim D} h(x) \right| > \epsilon$$

- Draw S' of size $|S|/2$, **event B**:

$$\begin{aligned} \exists h \in H: & \left| \frac{1}{|S'|} \sum_{i=1}^{|S'|} h(x_i) - \mathbb{E}_{x \sim D} h(x) \right| > \epsilon \\ & \left| \frac{1}{|S|} \sum_{i=1}^{|S|} h(x_i) - \mathbb{E}_{x \sim D} h(x) \right| < \epsilon/2 \end{aligned}$$

$$[] \geq \Pr[f_0] / 2$$

- **Lem.** If $\epsilon = \Omega(1/n^2)$ then $[] \geq \Pr[f_0] / 2$.

- **Proof:**

$$[] \geq \Pr[,] = \Pr[] \Pr[f_0] / n$$

- Suppose occurs:

$$\exists \epsilon \in H: | \langle \cdot \rangle - \langle \cdot \rangle | >$$

- When we draw ϵ' :

$$[\langle \cdot \rangle] = \langle \cdot \rangle$$

- By Chernoff:

$$\Pr[| \langle \cdot \rangle - \langle \cdot \rangle | < \epsilon / 2] \geq \frac{1}{2}$$

VC-theorem Proof

- Suffices to show that $\left[\frac{n}{2} \right] \leq \frac{n}{2}$
- Consider drawing 2 samples S and then randomly partitioning into S' and S''
- χ^2 : same as χ^2 for such $(S', S'') \Rightarrow \Pr[\chi^2 \geq t] = \Pr[\chi^2 \geq t]$
- **Will show:** $\forall$ fixed S'' , $\Pr[\chi^2 \geq t / |S''|]$ is small
- **Key observation:** once S'' is fixed there are only $|S'| \leq (2^d)$ events to care about
- Suffices: for every fixed $h \in S''$:

VC-theorem Proof (cont.)

- Randomly pair points in S into (x_i, y_i) pairs
- With prob. $1/2$: $x_i \rightarrow x'_i$ or $y_i \rightarrow y'_i$
- Diff. between $f(x_i)$ and $f(y_i)$ for $i = 1, \dots, n$
- Only changes if mistake on only one of (x_i, y_i)
 - With prob. $1/2$ difference changes by ± 1
 - By Chernoff:
$$\Pr\left[\left| \sum_{i=1}^n (f(x_i) - f(y_i)) \right| > \frac{n}{4}\right] = e^{-\Omega(n^2)}$$
- $e^{-\Omega(n^2)} \leq \frac{1}{n^2}$ for $n \geq 4$ from the Thm. statement