# Introduction to Machine Learning 

Foundations and Applications

Paul J. Atzberger<br>University of California Santa<br>Barbara

## Hypothesis Class Complexity

## Motivations

Hypothesis classes are typically infinite $|\mathscr{H}|=\infty$.
Can we still efficiently learn concepts $\mathbf{c}$ ?
Yes, recall interval problem and axis-aligned rectangle problem was infinite but PAC-Learnable.

We need a notion of complexity for hypothesis class $\mathscr{H}$ beyond cardinality $|\mathscr{H}|$.

Ultimately, we aim to obtain bounds on the generalization error in terms of the empirical risk.

Obstacle Navigation


Google Maps: UCSB South Hall
Picture Annotation, Facial Recognition


## Rademacher Complexity

## Notation and definitions:

$\mathcal{X}$ input space, $\mathscr{y}$ output space
$\mathcal{C}$ concept class, concept c(x): $\boldsymbol{X} \rightarrow \boldsymbol{y}$
 $\mathscr{H}$ hypothesis class, hypothesis $\mathrm{h}(\mathrm{x}): \mathcal{X} \rightarrow \boldsymbol{y}$.

Issue: Hypothesis classes are typically infinite $|\mathscr{H}|=\infty$. Can we still efficiently learn concepts c?
Recall: Axis-aligned rectangle problem has infinite $|\mathscr{H}|=\infty$ but proved is PAC-Learnable.
Need a notion of complexity for hypothesis class $\mathscr{H}$ beyond cardinality $|\mathscr{H}| . \quad h \in \mathcal{H}, \quad g(x, y)=L(h(x), y)$
Let loss function be denoted $\mathrm{L}: \mathcal{Y} \times \mathscr{Y} \rightarrow \mathbb{R}$ and let $G$ be family of loss functions associated with $\mathscr{H}$.
Definition: The empirical Rademacher complexity of a family of functions $G$ with $g(z): Z \rightarrow[a, b] \subset \mathbb{R}$ and $m$ fixed samples $S=\left(z_{1}, z_{2}, \ldots, z_{m}\right)$ is given by

$$
\hat{\mathcal{R}}_{S}(G)=E_{\sigma}\left[\sup _{g \in G} \frac{1}{m} \sum_{i=1}^{m} \sigma_{i} g\left(z_{i}\right)\right] \text {, where } \boldsymbol{\sigma}=\left(\sigma_{1}, \sigma_{2}, \ldots, \sigma_{\mathrm{m}}\right) \text { are uniform random variables in }\{-1,+1\} .
$$

## Rademacher Complexity

## Notation and definitions:

$\mathcal{X}$ input space, $\mathscr{y}$ output space
$\mathcal{C}$ concept class, concept c(x): $\boldsymbol{X} \rightarrow \boldsymbol{y}$

$\mathscr{H}$ hypothesis class, hypothesis $\mathrm{h}(\mathrm{x}): \mathcal{X} \rightarrow \boldsymbol{\mathcal { Y }}$.


Definition: The empirical Rademacher complexity of a family of functions $G$ with $g(z): Z \rightarrow[a, b] \subset \mathbb{R}$ and $m$ fixed samples $S=\left(z_{1}, z_{2}, \ldots, z_{m}\right)$ is given by

$$
\hat{\mathcal{R}}_{S}(G)=E_{\sigma}\left[\sup _{g \in G} \frac{1}{m} \sum_{i=1}^{m} \sigma_{i} g\left(z_{i}\right)\right], \text { where } \boldsymbol{\sigma}=\left(\sigma_{1}, \sigma_{2}, \ldots, \sigma_{m}\right) \text { are uniform random variables in }\{-1,+1\} .
$$

Definition: The Rademacher complexity of a family of functions $G$ on $m$ samples is

$$
\mathcal{R}_{m}(G)=E_{S \sim D^{m}}\left[\hat{\mathcal{R}}_{S}(G)\right]
$$

- Averaged sum term can be viewed as an inner-product: $\sum \sigma_{i} \cdot g\left(z_{i}\right)=\boldsymbol{\sigma} \cdot \mathbf{g}_{\mathrm{s}}$.
- Rademacher complexity gives a measure of the "richness" of family G in approximating random functions. $\mathcal{R}_{m}(G)=E_{S \sim D^{m}, \sigma}\left[\sup _{g \in G} \frac{1}{m} \sigma \cdot \mathbf{g}_{S}\right]$. Gives a measure of the "correlation" between $\boldsymbol{g}_{\mathrm{S}}$ and $\boldsymbol{\sigma}$.


## Rademacher Complexity

Definition: The empirical Rademacher complexity of a family of functions $G$ with $g(z): Z \rightarrow[a, b] \subset \mathbb{R}$ and $m$ fixed samples $S=\left(z_{1}, z_{2}, \ldots, z_{m}\right)$ is given by
$\hat{\mathcal{R}}_{S}(G)=E_{\sigma}\left[\sup _{g \in G} \frac{1}{m} \sum_{i=1}^{m} \sigma_{i} g\left(z_{i}\right)\right]$, where $\boldsymbol{\sigma}=\left(\sigma_{1}, \sigma_{2}, \ldots, \sigma_{m}\right)$ are random in set $\{-1,+1\}$.


Example: Rademacher Complexity for family of functions $\mathrm{G}=\left\{\mathrm{g}(\mathrm{z})=g_{0} \in[-\mathrm{c}, \mathrm{c}]\right\}$ (constants).

$$
\begin{aligned}
\tilde{\mathcal{R}}_{s}(\mathcal{G}) & =E_{\sigma}\left[\sup _{g \in \mathcal{G}} \frac{1}{m} \sum_{i=1}^{m} \sigma_{i} g\left(z_{i}\right)\right]=E_{\sigma}\left[\max \left\{\frac{1}{m} \sum_{i=1}^{m} c \sigma_{i},-\frac{1}{m} \sum_{i=1}^{m} c \sigma_{i}\right\}\right] \\
& =E_{\sigma}\left[\frac{1}{m} c\left|\#\left\{\sigma_{i}=+1\right\}-\#\left\{\sigma_{i}=-1\right\}\right|\right]=\frac{c}{m} E_{\sigma}\left[\left|\sum_{i=1}^{m} \sigma_{i}\right|\right] \leq \frac{c \sqrt{m}}{m}=\frac{c}{\sqrt{m}}
\end{aligned}
$$

Jensen Inequality ( $\phi$ convex): $\phi(E[X]) \leq E[\phi(X)]$ $(E[|X|])^{2} \leq E\left[|X|^{2}\right]$

$$
\begin{aligned}
E\left[\left|\sum_{i=1}^{m} \sigma_{i}\right|\right] & \leq E\left[\left|\sum_{i=1}^{m} \sigma_{i}\right|^{2}\right]^{1 / 2} \\
& =E\left[\sum_{i, i=1}^{m} \sigma_{i} \sigma_{j}\right]^{1 / 2}=\sqrt{m}
\end{aligned}
$$

## Rademacher Complexity

## Notation and definitions:

$\mathcal{X}$ input space, $\mathscr{y}$ output space
e concept class, concept c(x): $\boldsymbol{x} \rightarrow \boldsymbol{y}$
$\mathscr{H}$ hypothesis class, hypothesis $\mathrm{h}(\mathrm{x}): \mathcal{X} \rightarrow \mathcal{Y}$.


Hans Rademacher 1892-1969

Theorem: (expectation bounds $\mathrm{g}: \mathrm{Z} \rightarrow[0,1]$ ) For family of loss functions G into $[0,1]$ and any $\delta>0$ we have with probability $1-\delta$ that the following bounds hold uniformly for any $g \in G$,

$$
\begin{aligned}
& E[g(z)] \leq \frac{1}{m} \sum_{i=1}^{m} g\left(z_{i}\right)+2 \mathcal{R}_{m}(G)+\sqrt{\frac{\log \left(\frac{1}{\delta}\right)}{2 m}} \text {, (Rademacher bound) } \\
& E[g(z)] \leq \underbrace{\frac{1}{m} \sum_{i=1}^{m} g\left(z_{i}\right)}_{\begin{array}{c}
\text { empirical } \\
\text { estimate }
\end{array}}+\underbrace{2 \hat{\mathcal{R}}_{S}(G)}_{\begin{array}{c}
\text { model } \\
\text { complexity }
\end{array}}+\underbrace{3 \sqrt{\frac{\log \left(\frac{2}{\delta}\right)}{2 m}}}_{\begin{array}{c}
\text { sampling } \\
\text { confidence }
\end{array}} \text {, (Empirical Rademacher bound) }
\end{aligned}
$$

Significance: The expected value E[g] can be bounded by the observed empirical average. This differs at most by the Rademacher Complexity plus a term vanishing as $\mathrm{m} \rightarrow \infty$.

We shall use for bound on the generalization error by the empirical risk.

## Rademacher Complexity

## Notation and definitions:

$x$ input space, $\mathscr{y}$ output space
e concept class, concept c(x): $\boldsymbol{x} \rightarrow \boldsymbol{y}$
$\mathscr{H}$ hypothesis class, hypothesis $\mathrm{h}(\mathrm{x}): \mathcal{X} \rightarrow \mathcal{Y}$.


Hans Rademacher 1892-1969

Definition: The Empirical Rademacher Complexity of a hypothesis class $\mathfrak{H}$ is

$$
\hat{\mathcal{R}}_{S^{\mathcal{X}}}(H)=E_{\sigma}\left[\sup _{h \in H} \frac{1}{m} \sum_{i=1}^{m} \sigma_{i} h\left(x_{i}\right)\right],(\text { note: we take } \mathrm{h} \in\{-1,1\})
$$

Definition: The Rademacher Complexity of a hypothesis class $\mathscr{H}$ is

$$
\mathcal{R}_{m}(H)=E_{S \sim D^{m}}\left[\hat{\mathcal{R}}_{S^{\mathcal{X}}}(H)\right] \quad,(\text { note: we take } \mathrm{h} \in\{-1,1\})
$$

Lemma: For the family of 0-1 loss functions $G=\left\{(x, y) \rightarrow 1_{h(x) \neq y} \mid h \in H\right\}$ we have

$$
\hat{\mathcal{R}}_{S}(G)=\frac{1}{2} \hat{\mathcal{R}}_{S^{\mathcal{X}}}(H)
$$

- Allows for working more directly with the hypothesis space in constructing bounds.


## Rademacher Complexity

## Notation and definitions:

$x$ input space, $\mathscr{y}$ output space
e concept class, concept c(x): $\boldsymbol{x} \rightarrow \boldsymbol{y}$
$\mathscr{H}$ hypothesis class, hypothesis $\mathrm{h}(\mathrm{x}): \mathcal{X} \rightarrow \mathcal{Y}$.


Hans Rademacher 1892-1969

Theorem: (bound on generalization error for 0-1 loss) For 0-1 loss $G=\left\{(x, y) \rightarrow 1_{h(x) \neq y} \mid h \in H\right\}$ and any $\delta>0$ we have with probability $1-\delta$ that the following bounds hold uniformly for any $g \in G$,

$$
\begin{aligned}
& R(h) \leq \hat{R}_{S}(h)+\mathcal{R}_{m}(H)+\underbrace{\sqrt{\frac{\log \left(\frac{1}{\delta}\right)}{2 m}},}_{\begin{array}{c}
\text { empirical } \\
\text { estimate }
\end{array}} \text {, (Rademacher bound) } \\
& R(h) \leq \underbrace{\hat{R}_{S}(h)}_{\begin{array}{c}
\text { model } \\
\text { complexity }
\end{array}}+\underbrace{\hat{\mathcal{R}}_{S^{\chi}}(H)}_{\begin{array}{c}
\text { sampling } \\
\text { confidence }
\end{array}}+3 \sqrt{\frac{\log \left(\frac{2}{\delta}\right)}{2 m}}, \text { (Empirical Rademacher bound) }
\end{aligned}
$$

Significance: The generalization error can be bounded by the observed empirical risk. This differs most by the Rademacher Complexity plus a term vanishing as $m \rightarrow \infty$.

- This shows we can use Rademacher complexity in place of $|\mathscr{H}|$ to obtain bounds on generalization error to obtain scaling in m .


## Rademacher Complexity

Theorem: (bound on generalization error for 0-1 loss) For 0-1 loss
$G=\left\{(x, y) \rightarrow 1_{h(x) \neq y} \mid h \in H\right\}$ and any $\delta>0$ we have with probability $1-\delta$ that the following bounds hold uniformly for any $g \in G$,

$$
R(h) \leq \hat{R}_{S}(h)+\hat{\mathcal{R}}_{S^{\mathcal{X}}}(H)+3 \sqrt{\frac{\log \left(\frac{2}{\delta}\right)}{2 m}}, \quad \text { (Empirical Rademacher bound) }
$$



Example: Rademacher Complexity for family of functions $\mathrm{H}=\left\{\mathrm{h}(\mathrm{x})=h_{0} \in[-\mathrm{c}, \mathrm{c}], c=1\right\}$ (constants).

$$
\begin{aligned}
& \tilde{\mathcal{R}}_{S}(\mathcal{G})=E_{\sigma}\left[\sup _{g \in \mathcal{G}} \frac{1}{m} \sum_{i=1}^{m} \sigma_{i} g\left(z_{i}\right)\right] \leq \frac{c \sqrt{m}}{m}=\frac{c}{\sqrt{m}} \quad \text { (from previous derivation) } \\
& \tilde{\mathcal{R}}_{S}(\mathcal{H})=2 \tilde{\mathcal{R}}(\mathcal{G})=\frac{2 c}{\sqrt{m}}
\end{aligned}
$$

## Rademacher Complexity

Theorem: (bound on generalization error for 0-1 loss) For 0-1 loss
$G=\left\{(x, y) \rightarrow 1_{h(x) \neq y} \mid h \in H\right\}$ and any $\delta>0$ we have with probability $1-\delta$ that the following bounds hold uniformly for any $g \in G$,

$$
R(h) \leq \hat{R}_{S}(h)+\hat{\mathcal{R}}_{S^{\mathcal{X}}}(H)+3 \sqrt{\frac{\log \left(\frac{2}{\delta}\right)}{2 m}}, \quad \text { (Empirical Rademacher bound) }
$$

Theorem (Massert's lemma): Let $A \subseteq \mathbb{R}^{n}$ be a finite set of vectors with $r=\max _{a \in A}\|a\|_{2}$ then

$$
\hat{\mathcal{R}}_{S}(A)=E_{\sigma}\left[\sup _{\mathrm{a} \in A} \frac{1}{m} \sum_{i=1}^{m} \sigma_{i} a_{i}\right] \leq \frac{r \sqrt{2 \log |A|}}{m}
$$

Hypothesis class $\mathscr{H}$ and $\mathbf{m}$ samples consider the set $\mathrm{A}=\left\{\left(h\left(x_{1}\right), h\left(x_{2}\right), \ldots, h\left(x_{m}\right)\right): h \in \mathscr{H}\right\}$.
Finite hypothesis class we have $|A| \leq|\mathscr{H}|$.
Note: Result similar to prior complexity bound for finite consistent case

$$
R\left(h_{S}\right) \leq \frac{1}{m}\left(\log |H|+\log \frac{1}{\delta}\right)
$$

Massert's Lemma significantly generalizes this result since $|A|$ is now allowed to grow with $m$ for $|\mathscr{H}|=\infty$.
Alternatively, combinatorial measures like complexity $|A|$ may be easier to estimate than Rademacher complexity.

## Growth Function

Definition: The growth function $\Pi_{H}: \mathbb{N} \rightarrow \mathbb{N}$ for a hypothesis class $\mathscr{H}$ is defined as

$$
\Pi_{H}(m)=\max _{\left\{x_{1}, x_{2}, \ldots, x m\right\} \subseteq X}\left|\left\{\left(h\left(x_{1}\right), h\left(x_{2}\right), \ldots, h\left(x_{m}\right)\right): h \in \mathscr{H}\right\}\right|
$$

Counts maximum number of distinct m-vectors $\left(h\left(x_{1}\right), h\left(x_{2}\right), \ldots, h\left(x_{m}\right)\right)$ that can be generated by the hypothesis class $\mathfrak{H}$.

Upper bound on the number of distinct ways m points can be classified by $\mathscr{H}$.
Example: $\boldsymbol{X}=\{-2,-1,1\}, \boldsymbol{y}=\{-1,1\}, \mathscr{H}=\left\{h_{1}(x)=\operatorname{sign}(x), h_{2}(x)=\operatorname{sign}(x-1.5)\right\}, h_{1}:-1,-1,1 ; h_{2}:-1,-1,-1$. For $m=2$, most variation for $\mathrm{x}_{1}=-1, \mathrm{x}_{2}=1$, with $\Pi_{H}(2)=|\{(-1,+1),(-1,-1)\}|=2$. In general, we have $\Pi_{H}(m)=2$.

Remark: For finite hypothesis class always have $\Pi_{H}(m) \leq|\mathscr{H}|$.
Example: $\boldsymbol{X}=\mathbb{R}, \boldsymbol{y}=\{-1,1\}, \mathscr{H}=\{\mathrm{h}(\mathrm{x})=\operatorname{sign}(\mathrm{p}(\mathrm{x}))$ with $\mathrm{p}(\mathrm{x})$ polynomial degree n$\}$. Now $|\mathscr{H}|=\infty$ and we have $\Pi_{H}(m) \leq r(m) 2^{n+1}, r=$ poly. Follows from Lagrange interpolation.


Example: $\mathcal{X}=\mathbb{R}, \boldsymbol{y}=\{-1,1\}, \mathscr{H}=\{\mathrm{h}(\mathrm{x})=\operatorname{sign}(\mathrm{x}-\mathrm{a})$ with $\mathrm{a} \in \mathbb{R}\}$ half-space classifiers. Now $|\mathscr{H}|=\infty$ and we have $\Pi_{H}(m)=m+1 . \quad \#\left\{h\left(\mathrm{x}_{i}\right)=-1\right\}, \quad i \in\{1, \ldots, m\}$


## Growth Function

Definition: The growth function $\Pi_{H}: \mathbb{N} \rightarrow \mathbb{N}$ for a hypothesis class $\mathscr{H}$ is defined as

$$
\Pi_{H}(m)=\max _{\left\{x_{1}, x_{2}, \ldots, x m\right\} \subseteq X}\left|\left\{\left(h\left(x_{1}\right), h\left(x_{2}\right), \ldots, h\left(x_{m}\right)\right): h \in \mathscr{H}\right\}\right|
$$

- Counts maximum number of distinct m-vectors $\left(h\left(x_{1}\right), h\left(x_{2}\right), \ldots, h\left(x_{m}\right)\right)$ that can be generated by the hypothesis class $\mathfrak{H}$.
- Upper bound on the number of distinct ways m points can be classified by $\mathscr{H}$.

Theorem (Massert's Lemma): The Rademacher complexity is bounded by the growth function as

$$
\mathcal{R}_{m}(\mathcal{H}) \leq \sqrt{\frac{2 \log \left(\Pi_{\mathcal{H}}(m)\right)}{m}}
$$

Theorem (bound on generalization error for $0-1$ loss): For any $\delta>0$ we have with probability $1-\delta$ that the following bounds hold uniformly for any $\mathrm{h} \in \mathscr{H}$,

$$
R(h) \leq \hat{R}_{S}(h)+\sqrt{\frac{2 \log \left(\Pi_{\mathcal{H}}(m)\right)}{m}}+\sqrt{\frac{\log \left(\frac{1}{\delta}\right)}{2 m}}
$$

Note: Bound is now distribution $D$ independent depending only on combinatorial features of $\mathscr{H}$.

## VC-Dimension

Definition: For a sample set $S=\left(x_{1}, x_{2}, \ldots, x_{m}\right)$ of size $m$, a dichotomy is one of the possible ways to label the set $\left(y_{1}, y_{2}, \ldots, y_{m}\right)$.

Definition: A set $S$ of size $m$ is said to be shattered by the hypothesis class $\mathscr{H}$


Vladimir Vapnik


Alexey Chervonenkis if for each dichotomy $\boldsymbol{y}$ there is an $h \in \mathscr{H}$ so that $\left(h\left(x_{1}\right)=y_{1}, h\left(x_{2}\right)=y_{2}, \ldots, h\left(x_{m}\right)=y_{m}\right)$.

Example: $\mathcal{X}=\{-2,-1,1\}, \boldsymbol{y}=\{-1,1\}, \mathrm{H}=\left\{\mathrm{h}_{1}(\mathrm{x})=\operatorname{sign}(\mathrm{x}), \mathrm{h}_{2}(\mathrm{x})=\operatorname{sign}(\mathrm{x}-1.5)\right\}$.
$h_{1}:-1,-1,1 ; h_{2}:-1,-1,-1$. Now for $x_{1}=-2$ with dichotomy $y_{1}=1$ can not be obtained from either $h_{1}$ or $h_{2}$ this hypothesis class fails to shatter even $\mathscr{X}^{\mathrm{m}}$ for $\mathrm{m}=1$.

Example: $\mathcal{X}=\mathbb{R}, \boldsymbol{Y}=\{-1,1\}, \mathscr{H}=\{\mathrm{h}: \mathrm{h}(\mathrm{x})=\operatorname{sign}(x-a) \cdot \operatorname{sign}(b-x)$ for some $\mathrm{a}, b \in \mathbb{R}\}$ the set of intervals $[\mathrm{a}, \mathrm{b}]$. Now for $m=2$ for any two points $\mathrm{x} 1, \mathrm{x} 2 \in \mathbb{R}$ we have $\mathscr{H}$ shatters $X^{2}$ by taking [a,b] to contain points with $\mathrm{y}_{i}=1$ and exclude any point with $\mathrm{y}_{i}=-1$.

However, for $\mathrm{m} \geq 3$ we can not match all dichotomies. Take for example $x_{1}<x_{2}<x_{3}$ with the labels $\mathrm{y}_{1}=+1, \mathrm{y}_{2}=-1, \mathrm{y}_{3}=+1$ then there is no interval containing both $\mathrm{x}_{1}$ and $\mathrm{x}_{3}$ but excluding $\mathrm{x}_{2}$. Therefore, there exists dichotomies when $\mathrm{m}=3$ that no $h \in \mathscr{H}$ can classify correctly.

## VC-Dimension

Definition: The Vapnik-Chervonenkis dimension is defined as $V C \operatorname{dim}(\mathscr{H})=\max \left\{m: \Pi_{H}(m)=2^{m}\right\}$

- The VC-dimension measures the size of the largest set that can be shattered by the hypothesis class $\mathscr{H}$.


Vladimir Vapnik


Alexey Chervonenkis

- When $V \operatorname{Cdim}(\mathscr{H})=d$ this means all sets of size $d$ can be fully shattered by $\mathscr{H}$.
- For finite $|\mathscr{H}|<\infty$ hypothesis space we have VCdim $(\mathscr{H}) \leq \log (|\mathscr{H}|)$.

Example: $\mathcal{X}=\mathbb{R}, \mathscr{Y}=\{-1,1\}, \mathscr{H}=\{\mathrm{h}: \mathrm{h}(\mathrm{x})=\operatorname{sign}(x-a) \cdot \operatorname{sign}(b-x)$ for some $\mathrm{a}, b \in \mathbb{R}\}$ the set of intervals $[\mathrm{a}, \mathrm{b}]$. For $m=2$ for any two points $x_{1}, x_{2} \in \mathbb{R}$ we have $\mathscr{H}$ shatters $X^{2}$ by taking [a,b] to contain points with $y_{i}$ $=1$ and exclude any point with $y_{i}=-1$.

However, for $\mathrm{m} \geq 3$ we can not match all dichotomies. Take for example $x_{1}<x_{2}<x_{3}$ with the labels $\mathrm{y}_{1}=+1, \mathrm{y}_{2}=-1, \mathrm{y}_{3}=+1$ then there is no interval containing both $\mathrm{x}_{1}$ and $\mathrm{x}_{3}$ but excluding $\mathrm{x}_{2}$. Therefore, $\operatorname{VCdim}(\mathscr{H})=2$.

Example: $\mathcal{X}=\mathbb{R}, \mathscr{Y}=\{-1,1\}, \mathscr{H}=\{\mathrm{h}: \mathrm{h}(\mathrm{x})=\operatorname{sign}(\mathrm{p}(\mathrm{x}))$ polynomial $\mathrm{p}(\mathrm{x})$ of degree n$\}$. We have $\mathscr{H}$ shatters $\mathcal{X}^{\mathrm{m}}$ for $m=n+1$. This follows from Lagrange interpolation. However, can not shatter for $m>n+1$, so $\mathrm{d}=V \operatorname{Cdim}(\mathscr{H})=n+1$.

## VC-Dimension

Definition: The Vapnik-Chervonenkis dimension is defined as
$\operatorname{VCdim}(\mathscr{H})=\max \left\{m: \Pi_{H}(m)=2^{m}\right\}$

- The VC-dimension measures the size of the largest set that can be shattered by the


Vladimir Vapnik


Alexey Chervonenkis hypothesis class $\mathscr{H}$.

- When $V C \operatorname{dim}(\mathscr{H})=d$ this means all sets of size $d$ can be fully shattered by $\mathscr{H}$.

Theorem (bound on generalization error for 0-1 loss): When $V C \operatorname{dim}(\mathscr{H})=d$, for any $\delta>0$ we have with probability $1-\delta$ that the following bounds hold uniformly for any $\mathrm{h} \in \mathscr{H}$,

$$
R(h) \leq \hat{R}_{S}(h)+\sqrt{\frac{2 d \log \left(\frac{e m}{d}\right)}{m}}+\sqrt{\frac{\log \left(\frac{1}{\delta}\right)}{2 m}}
$$

- Note the ratio of $m / d$ governs the bound. This corresponds to the overall form

$$
R(h) \leq \hat{R}_{S}(h)+O\left(\sqrt{\frac{\log (m / d)}{(m / d)}}\right) "
$$

- This shows we need sample size $m \gg d$ to obtain small bound. Provides useful complexity when $|\mathscr{H}|=\infty$.


## VC Dimension

Example: VCdim( $\mathcal{H})$ axis-aligned rectangles.
Claim: VCdim $(\mathscr{H})=4$.
Two steps:
(i) lower bound $V C \operatorname{dim}(\mathcal{H}) \geq 4$
(ii) upper bound $V \operatorname{Cdim}(\mathscr{H})<5$



Google Maps: UCSB South Hall
Picture Annotation, Facial Recognition

usplash

Lower bound: Place 4 points into a diamond configuration.
All cases can clearly be handled.
Upper bound: Place 5 points with 4 on rectangle and the $5^{\text {th }}$ point in the interior. No axis-aligned rectangle that can correctly classify these points for all labels. Hence, VCdim $(\mathscr{H})<5$.


## VC-Dimension: Hyperplanes

Example: Learning separating hyperplane in $\mathbb{R}^{N}$ (related to SVM).

## Hypothesis class:

$\mathscr{H}=\left\{h: h(\mathbf{x})=\operatorname{sign}\left(\mathbf{w}^{\mathrm{T}} \mathbf{x}+\mathrm{b}\right)\right.$ with $\left.\boldsymbol{w} \in \mathbb{R}^{\mathrm{N}}, \mathrm{b} \in \mathbb{R}\right\}$.

## What is the VCdim $(\mathscr{H})$ ?

Claim: $\operatorname{VCdim}(\mathscr{H})=\mathrm{N}+1$

## Two steps:

(i) lower bound $V C \operatorname{dim}(\mathscr{H}) \geq \mathrm{N}+1$.
(ii) upper bound $V C \operatorname{dim}(\mathscr{H})<\mathrm{N}+2$.

Linear Classifier


Lower bound: For $N+1$ points, let $\mathbf{x}_{0}=(0,0, \ldots, 0)$ origin, $\mathbf{x}_{i}=(0, \ldots 1, \ldots 0,0)=\mathbf{e}_{\mathrm{i}}$, with $\mathrm{i}^{\text {th }}$ component one. For any labels $y_{i} \in\{-1,1\}$, let $\mathbf{w}=\left(\mathrm{y}_{1}, \mathrm{y}_{2}, \ldots, \mathrm{y}_{N}\right)$ and $b=\frac{y 0}{2}$ which defines the classifier $\mathrm{h}\left(\mathbf{x}_{\mathrm{i}}\right)=\operatorname{sign}\left(\mathbf{w}^{\mathrm{T}} \mathbf{x}_{\mathbf{i}}+\mathrm{b}\right)=\operatorname{sign}\left(y_{i}+\frac{y 0}{2}\right)=y_{i}$. This verifies any $\mathrm{N}+1$ labels can be classified correctly.

Hyperplanes $\mathscr{H}$ shatters this $\mathrm{N}+1$ point-set so $\operatorname{VCdim}(\mathrm{H}) \geq \mathrm{N}+1$.

## VC-Dimension: Hyperplanes

Example: Learning separating hyperplane in $\mathbb{R}^{\mathrm{N}}$ (related to SVM). For data $\left\{\left(\mathrm{x}_{\mathrm{i}}, \mathrm{y}_{\mathrm{i}}\right)\right\}$ with $\mathrm{x}_{\mathrm{i}} \in \mathbb{R}^{N}$ and $\mathrm{y}_{\mathrm{i}} \in\{-1,1\}$. Ideally, find $\mathbf{w}, \mathrm{b}$ so

Linear Classifier that $\operatorname{sign}\left(\boldsymbol{w}^{T} \boldsymbol{x}_{i}+b\right)=y_{i}$.

Upper bound: $V C \operatorname{dim}(\mathscr{H})<\mathrm{N}+2$. Must show for any $\mathrm{N}+2$ points for some labels there is no hyperplane classifier.

Theorem (Radon): In $\mathbb{R}^{N}$ a set of $N+2$ points always can be partitioned into two disjoint subsets $x_{1}$ and $x_{2}$ that have intersecting convex hulls $C\left(x_{1}\right) \bigcap \mathrm{C}\left(x_{2}\right) \neq \varnothing$.

Implication: Let labels of $X_{1}$ be say +1 and $x_{2}$ be -1 then there is no separating hyperplane (it would separate the convex hulls).


Proof (Radon): Consider the set of $\mathrm{N}+1$ linear equations in $\mathrm{N}+2$ unknowns: $\sum_{i=1}^{N+2} \alpha_{i} \mathbf{x}_{i}=\mathbf{0}$ and $\sum_{i=1}^{N+2} \alpha_{i}=0$ Non-trivial null-space so equations have non-zero solution $\beta_{\mathrm{i}}, \ldots, \beta_{\mathrm{d}+2}$ with $\sum_{i=1}^{N+2} \beta_{i}=0$. Let $I_{1}=\left\{\mathrm{i}: \beta_{\mathrm{i}}>0\right\}$ and $I_{2}=\left\{\mathrm{i}: \beta_{\mathrm{i}} \leq 0\right\}$, then both non-empty. Let $\mathrm{x}^{*}=\sum_{i_{1} \in I_{1}} \frac{\beta_{i_{1}}}{\beta} \mathbf{x}_{i_{1}}=\sum_{i_{2} \in I_{2}} \frac{-\beta_{i_{2}}}{\beta} \mathbf{x}_{i_{2}}$ with $\beta=\sum_{i_{1} \in I_{1}} \beta_{i_{1}}$.
We have $\sum_{i_{1} \in I_{1}} \frac{\beta_{i_{1}}}{\beta}=\sum_{i_{2} \in I_{2}} \frac{-\beta_{i_{2}}}{\beta}=1$ and $\frac{\beta_{\mathrm{i1}}}{\beta} \geq 0, \frac{-\beta_{\mathrm{i} 2}}{\beta} \geq 0$, so $x^{*} \in C\left(X_{1}\right) \bigcap \mathrm{C}\left(X_{2}\right) \neq \emptyset$ so convex hulls intersect.

## VC-Dimension: Hyperplanes

Example: Learning separating hyperplane in $\mathbb{R}^{N}$ (related to SVM).
For data $\left\{\left(\mathrm{x}_{\mathrm{i}} \mathrm{y}_{\mathrm{i}}\right)\right\}$ with $\mathrm{x}_{\mathrm{i}} \in \mathbb{R}^{\mathrm{N}}$ and $\mathrm{y}_{\mathrm{i}} \in\{-1,1\}$. Ideally, find $\mathbf{w}, \mathrm{b}$ so that $\operatorname{sign}\left(\boldsymbol{w}^{T} \boldsymbol{x}_{i}+b\right)=y_{i}$.

## Hypothesis class:

$$
\mathscr{H}=\left\{\mathrm{h}: \mathrm{h}(\mathrm{x})=\operatorname{sign}\left(\mathbf{w}^{\mathrm{T}} \mathbf{x}+\mathrm{b}\right) \text { with } \boldsymbol{w} \in \mathbb{R}^{\mathrm{N}}, \mathrm{~b} \in \mathbb{R}\right\} .
$$

## What is the $V \operatorname{Cdim}(\mathscr{H})$ ?

Claim: $\operatorname{VCdim}(\mathscr{H})=\mathrm{N}+1$
Shows in separable case that we have bound on generalization error


$$
R(h) \leq \widehat{R}(h)+\sqrt{\frac{2(N+1) \log \frac{e m}{N+1}}{m}}+\sqrt{\frac{\log \frac{1}{\delta}}{2 m}}
$$

Turns out we can do even better in bounding sampling complexity for SVM. Want independent of feature dimension N , for bounded features (future lectures).

Will discuss further these results later when we cover Support Vector Machines.

## VC Dimension: Lower Bounds

Lower Bounds: Given assumptions of PAC-Learning and $V C \operatorname{dim}(\mathscr{H})$. What is lower bound on generalization error given $m$ samples?

Theorem: Under assumptions of PAC for $\mathrm{d}=\operatorname{VC\operatorname {dim}}(\mathscr{H})>1$ given any learning algorithm of there always exists a distribution $\mathbf{D}$ and concept $f \in \mathcal{C}$ so that for m samples

$$
\operatorname{Pr}_{S \sim D^{m}}\left[R_{D}\left(h_{S}, f\right)>\frac{d-1}{32 m}\right] \geq 1 / 100
$$

Shows that at least $1 \%$ of the time you will always have generalization error bigger than $\frac{d-1}{32 m}$.

Characterizes the worse-case generalization errors given complexity of $\mathscr{H}$.


Google Maps: UCSB South Hall

Picture Annotation, Facial Recognition

usplash

Consequence: If $V \operatorname{Cdim}(\mathscr{H})=\infty$ then task is not PAC-Learnable.

## VC Dimension: Lower Bounds

Example: Consider hypothesis class of all polynomials
$\mathscr{H}=\{\mathrm{h}: \mathrm{h}(\mathrm{x})=\operatorname{sign}(\mathrm{p}(\mathrm{x}))$ any polynomial of finite degree $\}$.
Complexity: VCdim $(\mathscr{H})=\infty($ recall for $n$ degree polynomial VCdim $=\mathrm{n}+1)$.
Consequence: Concepts from $\mathscr{H}$ are not PAC-Learnable.
Why? At least $1 \%$ of the time you will always have generalization error
bigger than $\frac{d-1}{32 m}$ so make $d=\lceil 31.7 m+1\rceil$ (since $\operatorname{VCdim}(\mathscr{H})=\infty$ can take any $\mathrm{d}>1$ ) then we have
$\operatorname{Pr}_{S \sim D^{m}}\left[R_{D}\left(h_{S}, f\right)>\frac{d-1}{32 m}\right] \geq 1 / 100 \longrightarrow \operatorname{Pr}_{S \sim D^{m}}\left\{R_{D}\left(h_{S}, f\right)>0.99\right\} \geq 1 / 100$
Shows no matter how many samples m used, $1 \%$ of the time the generalization error is greater than $99 \%$.
Not enough information from finite data alone to distinguish unknown function in $\mathscr{H}$ without further assumptions (i.e. could miss local variations). Need other approaches (i.e. regularization, level of smoothness).

Consequence, if $\operatorname{VCdim}(\mathscr{H})=\infty$ then task is not PAC-Learnable.

## Complexity: Rademacher, Growth Functions, VC-Dimension

## Complexity Bounds Theory and Practice

Significance: Complexity measures give some guarantees to assess generalization errors based on observed empirical risk.

In practice, often challenging since models have large complexity and we want to avoid ${ }_{\text {tuec }}^{\text {silip }}$ overfitting data by only minimizing empirical risk. Training methods often also have

Robotics and Control


MIT and Boston Dynamics


Manifold Learning


Forecasting

washingtonpost.com

