Lecture 7. Generalisation with Finite VC Dimension

COMP90051 Statistical Machine Learning

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This lecture

- Motivation
- Growth function
  - Considering patterns of labels possible on a data set
  - Gives good generalisation bounds provided possible patterns don't grow too fast in the data set size
- Vapnik-Chervonenkis (VC) dimension
  - Max number of points that can be labelled in all ways
  - Beyond this point, growth function is polynomial in data set size
  - Leads to famous VC generalisation theorem

Motivation

...from last lecture

A Countably Finite Model Class

- Consider we have 2 features and a countably finite set $\mathcal{F}$ of classifiers, containing:

$$f(x) = \operatorname{sgn}(x_1 + x_2) = \begin{cases} +1, \text{if } x_1 + x_2 > 0 \\ -1, \text{if } x_1 + x_2 \leq 0 \end{cases}$$

$$f(x) = \operatorname{sgn}(x_1 - x_2)$$
$$f(x) = \operatorname{sgn}(-x_1 + x_2)$$
$$f(x) = \operatorname{sgn}(-x_1 - x_2)$$
$$f(x) = \operatorname{sgn}(x_1)$$
$$f(x) = \operatorname{sgn}(-x_1)$$
$$f(x) = \operatorname{sgn}(x_2)$$
$$f(x) = \operatorname{sgn}(-x_2)$$

- Here $|\mathcal{F}| = 8$

Empirical Risk Minimisation

- Training data $\boldsymbol{D} = \{\boldsymbol{x}_1, y_1, \dots, \boldsymbol{x}_n, y_n\}$ is a random variable!
  - $(\boldsymbol{x}_i, y_i)$ i.i.d. with distribution P (unknown)
- The empirical risk of a classifier f for loss l is

$$\hat{R}_{\boldsymbol{D}}[f] = \frac{1}{n}\sum_{i=1}^{n} l\big(y_i, f(\boldsymbol{x}_i)\big)$$

- ERM: $\hat{f}_{\boldsymbol{D}}$ minimises the empirical risk

$$\hat{f}_{\boldsymbol{D}} = \operatorname{argmin}_{f\in\mathcal{F}} \hat{R}_{\boldsymbol{D}}[f]$$

Go trough all the $|\mathcal{F}| = 8$ classifiers and choose the best for data D

- Given f and n samples in $\boldsymbol{D}$, we can compute $\hat{R}_{\boldsymbol{D}}[f]$

True Risk

- The true risk is the expected value of the loss l
  - Intuitively speaking, the true risk is the empirical risk when using an infinite number of samples
- The true risk of a classifier f for loss l is

$$R[f] = \mathbb{E}\, l\big(Y, f(X)\big) = \int l\big(Y, f(X)\big) P(X, Y)\, dX dY$$

aka generalisation error (expected test error) for $l(y, y') = \begin{cases} 1, \text{if } y \neq y' \\ 0, \text{if } y = y' \end{cases}$

- Given f, we cannot compute $R[f]$ because the data distribution P is unknown

Generalisation Theorem

- For a finite model class $\mathcal{F}$, without knowing the data distribution P, with probability $\geq 1 - \delta$ over the choice of the training set D of n i.i.d. samples

$$R[\hat{f}_D] \leq \hat{R}_D[\hat{f}_D] + \sqrt{\frac{\log|\mathcal{F}| + \log(1/\delta)}{2n}}$$

We cannot compute $R[f]$, but we can bound it!

- The proof-sketch required upper bounding

$$\max_{f\in\mathcal{F}} \varphi_D[f] = \max_{f\in\mathcal{F}} (R[f] - \hat{R}_D[f])$$

Non-(Countably Finite) Model Class?

- Finite model class
  - Bounding uniform deviation with union bound and Hoeffding's inequality
- Consider we have 2 features and an uncountable set $\mathcal{F}$ of classifiers, containing for all $w_1 \in \mathbb{R}$, $w_2 \in \mathbb{R}$:

$$f(x) = \operatorname{sgn}(w_1 x_1 + w_2 x_2)$$

- As before, still requires upper bounding

$$\sup_{f \in \mathcal{F}} (R[f] - \hat{R}_D[f])$$

Mini Summary

- No good for general (countably infinite and uncountable) cases
- Need another fundamentally new idea

Next: Organising analysis around patterns of labels possible on any data set

Growth Function

Focusing on the size of model families on data samples

Example: Decision stumps

- Consider a dataset of 6 samples, each with a single continuous feature (x) and label (y)

x	y
0	+1
4	-1
-2	+1
1	+1
-3	-1
2	-1

- We would like to find a threshold β, and then classify all samples with feature value x above β as $+1$, and feature value x below β as -1 (or viceversa)

Example: Decision stumps

- Lets sort with respect to x

x	y
0	+1
4	-1
-2	+1
1	+1
-3	-1
2	-1

sort

x	y
-3	-1
-2	+1
0	+1
1	+1
2	-1
4	-1

- Lets use the classifier:

$$f(x) = \operatorname{sgn}(x - \beta) = \begin{cases} +1, \text{if } x > \beta \\ -1, \text{if } x \leq \beta \end{cases}$$

- How to find the threshold β? Try all midpoints of x

Example: Decision stumps

- Lets use the classifier:

$$f(x) = \mathrm{sgn}(x - \beta) = \begin{cases} +1, \text{if } x > \beta \\ -1, \text{if } x \leq \beta \end{cases}$$

- Count the number of mistakes for all thresholds β

x	y	$f(x)$				
		β=-2.5	β=-1	β=0.5	β=1.5	β=3
-3	-1	-1	-1	-1	-1	-1
-2	+1	+1	-1	-1	-1	-1
0	+1	+1	+1	-1	-1	-1
1	+1	+1	+1	+1	-1	-1
2	-1	+1	+1	+1	+1	-1
4	-1	+1	+1	+1	+1	+1
# mistakes		2	3	4	5	4

Example: Decision stumps

- Lets use the classifier:

$$f(x) = \mathrm{sgn}(\beta - x) = \begin{cases} +1, \text{if } x < \beta \\ -1, \text{if } x \geq \beta \end{cases}$$

- Count the number of mistakes for all thresholds β

x	y	$f(x)$				
		β=-2.5	β=-1	β=0.5	β=1.5	β=3
-3	-1	+1	+1	+1	+1	+1
-2	+1	-1	+1	+1	+1	+1
0	+1	-1	-1	+1	+1	+1
1	+1	-1	-1	-1	+1	+1
2	-1	-1	-1	-1	-1	+1
4	-1	-1	-1	-1	-1	-1
# mistakes		4	3	2	1	2

Example: Decision stumps

- Thus our best decision stump classifier is

$$f(x) = \mathrm{sgn}(1.5 - x) = \begin{cases} +1, \text{if } x < 1.5 \\ -1, \text{if } x \geq 1.5 \end{cases}$$

- We consider all classifiers of the form (for all $\beta \in \mathbb{R}$)

$$f(x) = \mathrm{sgn}(x - \beta) = \begin{cases} +1, \text{if } x > \beta \\ -1, \text{if } x \leq \beta \end{cases}$$

$$f(x) = \mathrm{sgn}(\beta - x) = \begin{cases} +1, \text{if } x < \beta \\ -1, \text{if } x \geq \beta \end{cases}$$

- Although these are simple classifiers, the set of decision stump classifiers $\mathcal{F}$ is uncountable (there are as “many” as real values)

Example: Growth function of Decision stumps

- Consider all possible ways we can classify data

$$f(x) = \text{sgn}(x-\beta) = \begin{cases} +1, \text{if } x > \beta \\ -1, \text{if } x \leq \beta \end{cases} \qquad f(x) = \text{sgn}(\beta - x) = \begin{cases} +1, \text{if } x < \beta \\ -1, \text{if } x \geq \beta \end{cases}$$

x	$f(x)$					
	β=-2.5	β=-1	β=0.5	β=1.5	β=3	β=∞
-3	-1	-1	-1	-1	-1	-1
-2	+1	-1	-1	-1	-1	-1
0	+1	+1	-1	-1	-1	-1
1	+1	+1	+1	-1	-1	-1
2	+1	+1	+1	+1	-1	-1
4	+1	+1	+1	+1	+1	-1

x	$f(x)$					
	β=-2.5	β=-1	β=0.5	β=1.5	β=3	β=∞
-3	+1	+1	+1	+1	+1	+1
-2	-1	+1	+1	+1	+1	+1
0	-1	-1	+1	+1	+1	+1
1	-1	-1	-1	+1	+1	+1
2	-1	-1	-1	-1	+1	+1
4	-1	-1	-1	-1	-1	+1

- A dichotomy (in blue) is one way of classifying the 6 samples
- We have 12 unique dichotomies

Dichotomies

- Given dataset $\mathcal{X} = \{x_1, \dots, x_n\}$ of size $|\mathcal{X}| = n$ and a classifier $f \in \mathcal{F}$, a **dichotomy** is the pattern of labels (n-dimensional vector of labels) produced by f on $\mathcal{X}$

$$\left(f(x_1), \dots, f(x_n)\right) \in \{-1, +1\}^n.$$

- **Unique dichotomies:** unique patterns of labels possible with all classifiers in the model class $\mathcal{F}$

$$\mathcal{F}(\mathcal{X}) = \left\{\left(f(x_1), \dots, f(x_n)\right) : f \in \mathcal{F}\right\}$$

  - Even when $\mathcal{F}$ infinite, $|\mathcal{F}(\mathcal{X})| \leq 2^n$ (why?)
  - For $\mathcal{F}$ countably finite, $|\mathcal{F}(\mathcal{X})| \leq |\mathcal{F}|$ (why?)

Growth Function

- The **growth function**

$$S_{\mathcal{F}}(n) = \sup_{|\boldsymbol{x}|=n} |\mathcal{F}(\boldsymbol{x})|$$

- is the maximum number of label patterns achievable by classifiers in the model class $\mathcal{F}$ for any set of n samples.
  * Even when $\mathcal{F}$ infinite, $S_{\mathcal{F}}(n) \leq 2^n$ (why?)
  * For $\mathcal{F}$ countably finite, $S_{\mathcal{F}}(n) \leq |\mathcal{F}|$ (why?)

Example: Growth function of Decision stumps

- In general, the set of decision stump classifiers lead to $2n$ unique dichotomies for n samples
  - We classify the n samples as -1's followed by +1's
  - We also classify the n samples as +1's followed by -1's
- Thus, $S_{\mathcal{F}}(n) = 2n$
- More complex classifiers would lead to more than $2n$ unique dichotomies for n samples

Growth-Function Generalisation Theorem

- For a model class $\mathcal{F}$ with growth function $S_{\mathcal{F}}(n)$, without knowing the data distribution P, with probability $\geq 1 - \delta$ over the choice of the training set D of n i.i.d. samples

$$R[\hat{f}_D] \leq \hat{R}_D[\hat{f}_D] + \sqrt{8\frac{\log S_{\mathcal{F}}(2n) + \log(4/\delta)}{n}}$$

(Proof outside scope of COMP90051)

- $|\mathcal{F}|$ becomes $S_{\mathcal{F}}(2n)$, and few negligible extra constants
- If $S_{\mathcal{F}}(n)$ grows exponentially in n, e.g., $S_{\mathcal{F}}(n) = 2^n$ then $\frac{\log S_{\mathcal{F}}(2n)}{n} = 2\log 2$, the bound does not decay with more samples n

Mini Summary

- Better to organise families by possible patterns of labels on a data set: the dichotomies of the model class
- Counting possible dichotomies gives the growth function
- Generalisation bound with growth function potentially tackles general (countably infinite and uncountable) families provided growth function is sub-exponential in data size

Next: VC dimension for a computable bound on growth functions, with the polynomial behaviour we need! Gives our final VC generalisation bound

The VC dimension

Computable, bounds growth function

Vapnik-Chervonenkis dimension

- The **VC dimension** $\mathrm{VC}(\mathcal{F})$ of a model class $\mathcal{F}$ is the largest n such that $S_{\mathcal{F}}(n) = 2^n$.
- Set of samples $\boldsymbol{\mathcal{X}} = \{x_1, \dots, x_n\}$ are shattered by $\mathcal{F}$ if $|\mathcal{F}(\boldsymbol{\mathcal{X}})| = 2^n$, that is, if $\boldsymbol{\mathcal{X}}$ can be classified in all possible ways
- $\mathrm{VC}(\mathcal{F})$ is the size of the largest set of samples shattered by $\mathcal{F}$

Example: VC Dimension of Decision Stumps

- Recall that for decision stump classifiers $S_{\mathcal{F}}(n) = 2n$
- Find the maximum n for which $2n = 2^n$
- The VC dimension is $VC(\mathcal{F}) = 2$

n	$2n$	2^n
1	2	2
2	4	4
3	6	8

- For more intuition, see the $2n$ ways of classifying n samples

n=1

+1	-1

n=2

+1	+1	-1	-1
+1	-1	+1	-1

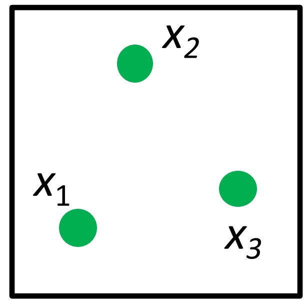
n=3

+1	+1	+1	+1	-1	-1	-1	-1
+1	+1	-1	-1	+1	+1	-1	-1
+1	-1	+1	-1	+1	-1	+1	-1

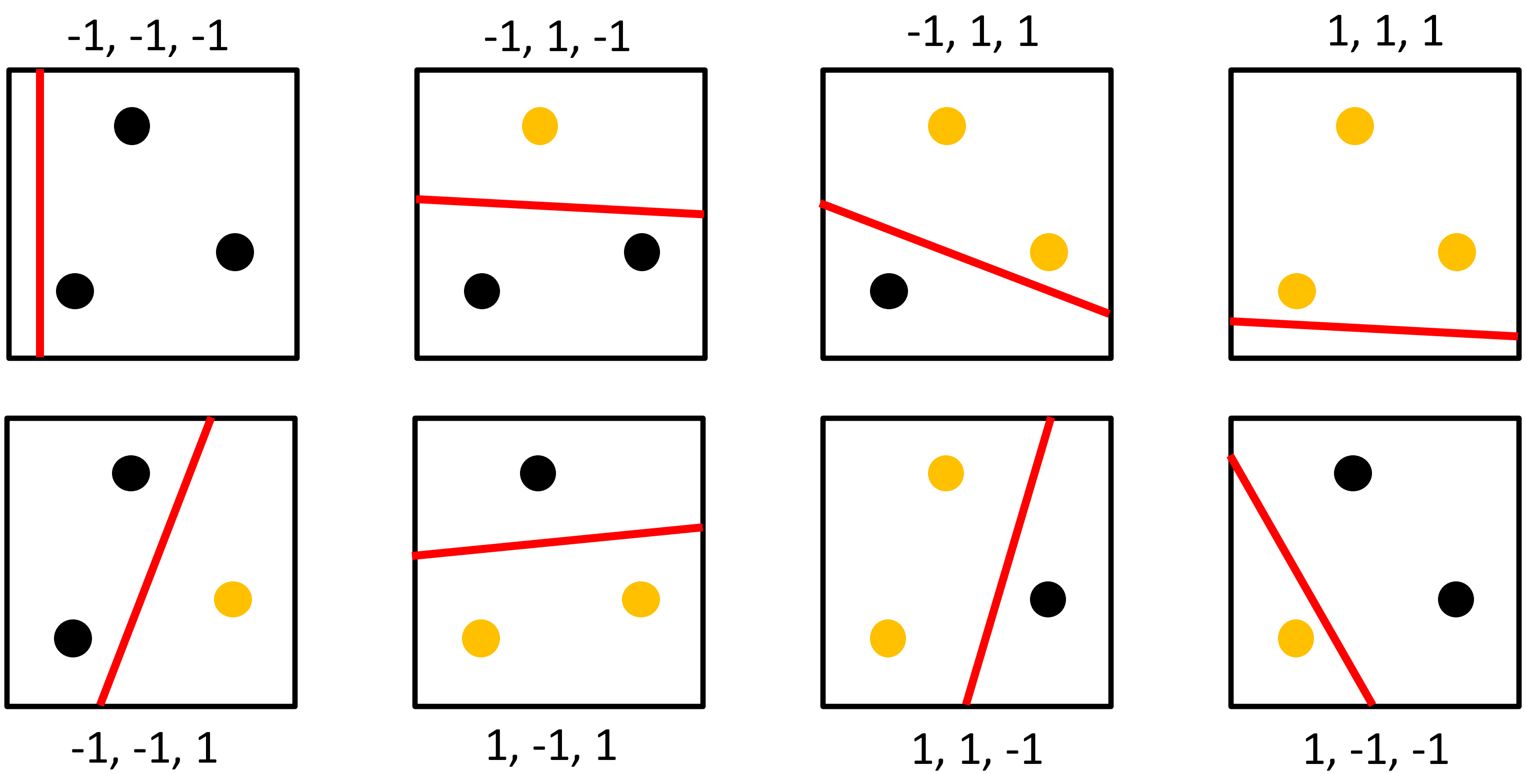
2 ways (2^3-2*3 = 2) of classifying (in red) are not -1's followed by +1's, neither +1's followed by -1's

Example 2: Growth function for linear classifiers in 2D

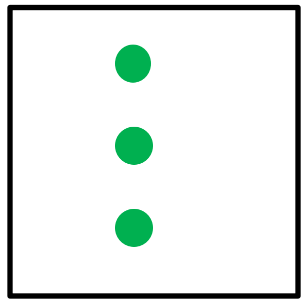
- Black means f(x)=-1
- Yellow means f(x)=1



$$S_{\mathcal{F}}(3) = 8$$



Example 2: Growth function for linear classifiers in 2D

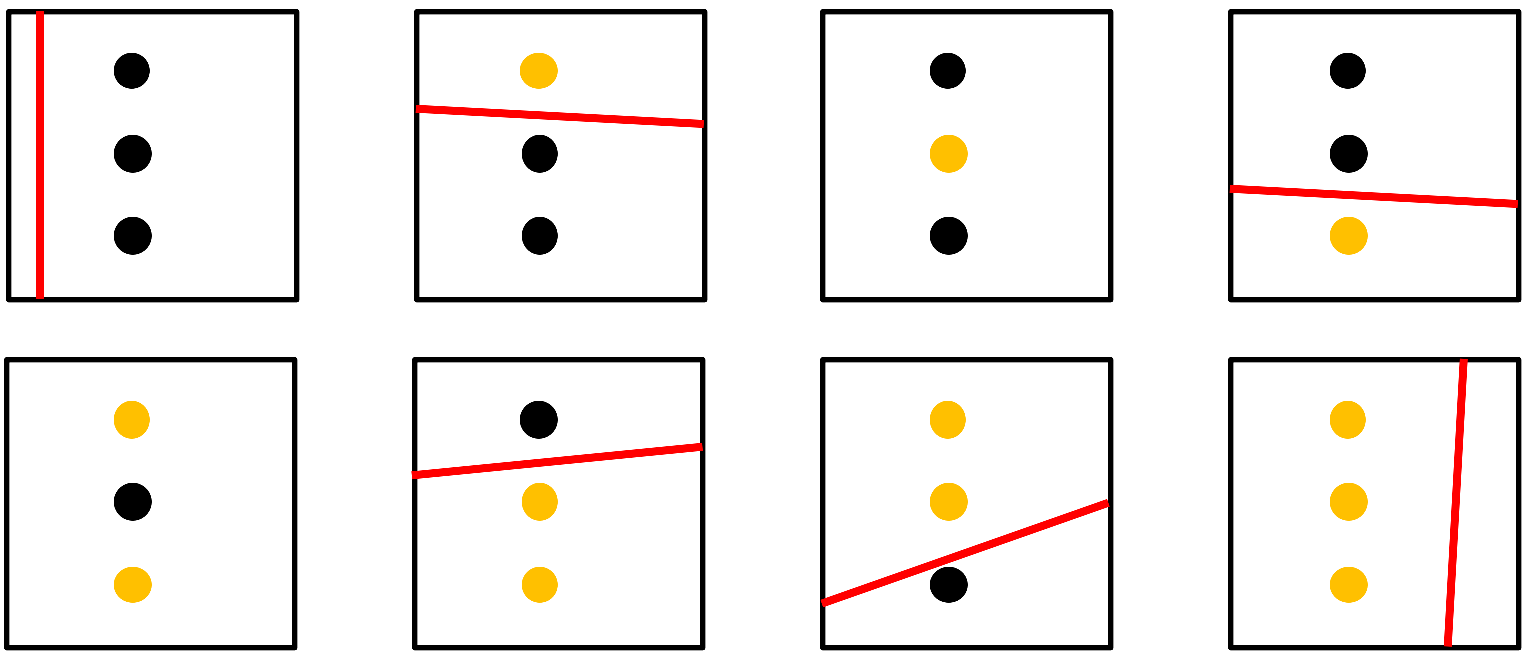


$|\mathcal{F}(\mathcal{X})| = 6$

but still have

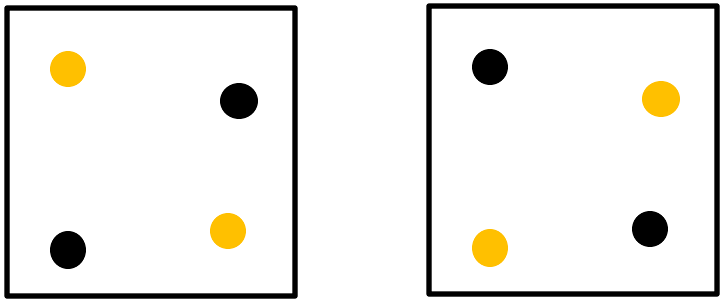
$S_{\mathcal{F}}(3) = 8$

The possible patterns should be



Example 2: Growth function for linear classifiers in 2D

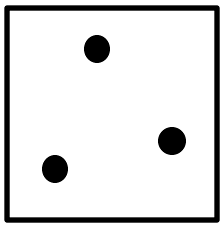
- What about $n = 4$ points?
- Can never produce the criss-cross (XOR) dichotomy



- In fact $S_{\mathcal{F}}(4) = 14 < 2^4$

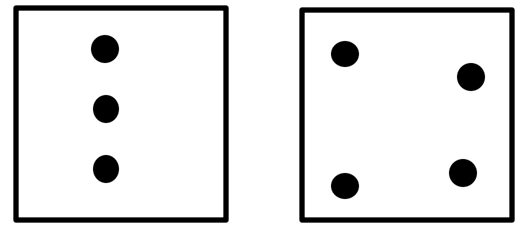
Example 2: VC dimension for linear classifiers in 2D

- Example: linear classifiers in $\mathbb{R}^2$, $\mathrm{VC}(\mathcal{F}) = 3$



Shattered

Not shattered



- Guess: VC dimension of linear classifiers in $\mathbb{R}^d$?

Example 3: VC dimension from dichotomies on whole domain?

x_1	x_2	x_3	x_4
0	0	0	0
0	1	1	0
1	0	0	1
1	1	0	1
0	1	0	0
1	0	1	0
1	1	1	1
0	0	1	1
0	1	0	1
1	1	1	0

Note we're using labels {0,1} instead of {-1,+1}. Why OK?

- Columns are *all* points in domain
- Each row is a dichotomy on entire input domain
- Obtain dichotomies on a subset of samples $\mathcal{X}' \subseteq \{x_1, \ldots, x_4\}$ by: drop columns, drop dupe rows
- $\mathcal{F}$ shatters $\mathcal{X}'$ if number of rows is $2^{|\mathcal{X}'|}$

x_1	x_2	x_4
0	0	0
0	1	0
1	0	1
1	1	1
~~0~~	~~1~~	~~0~~
1	0	0
~~1~~	~~1~~	~~1~~
0	0	1
0	1	1
1	1	0

This example:

- Dropping column 3 leaves 8 rows behind: $\mathcal{F}$ shatters $\{x_1, x_2, x_4\}$
- Original table has $< 2^4$ rows: $\mathcal{F}$ doesn't shatter more than 3
- $\mathrm{VC}(\mathcal{F}) = 3$

Sauer-Shelah Lemma

- Consider any model class $\mathcal{F}$ with finite $\mathrm{VC}(\mathcal{F})$, and any sample size n. Then

$$S_{\mathcal{F}}(n) \leq \sum_{i=0}^{\mathrm{VC}(\mathcal{F})} \binom{n}{i}$$

(Proof outside scope of COMP90051)

- Since $\sum_{i=0}^{k} \binom{n}{i} \leq (n+1)^k$, the above implies

$$\log S_{\mathcal{F}}(n) \leq \mathrm{VC}(\mathcal{F}) \log(n+1)$$

VC Generalisation Theorem

- For a model class $\mathcal{F}$ with VC dimension $\mathrm{VC}(\mathcal{F})$, without knowing the data distribution P, with probability $\geq 1-\delta$ over the choice of the training set D of n i.i.d. samples

$$R[\hat{f}_D] \leq \hat{R}_D[\hat{f}_D] + \sqrt{8\frac{\mathrm{VC}(\mathcal{F})\log(2n+1)+\log(4/\delta)}{n}}$$

  - Proof-sketch: From the growth-function generalization theorem and since

$$\log S_{\mathcal{F}}(2n) \leq \mathrm{VC}(\mathcal{F})\log(2n+1)$$

Structural Risk Minimisation

- Choose the model class $\mathcal{F}$ with best guarantee of generalisation:

$$\underbrace{\hat{R}_{\boldsymbol{D}}\left[\hat{f}_{\boldsymbol{D}}\right]}_{\text{Large for simple classifiers, small for complex classifiers}} + \underbrace{\sqrt{8\frac{\mathrm{VC}(\mathcal{F})\log(2n+1)+\log(4/\delta)}{n}}}_{\text{Small for simple classifiers (small } \mathrm{VC}(\mathcal{F})\text{), large for complex classifiers (large } \mathrm{VC}(\mathcal{F})\text{)}}$$

Large for simple classifiers,
small for complex classifiers

Small for simple classifiers (small $\mathrm{VC}(\mathcal{F})$),
large for complex classifiers (large $\mathrm{VC}(\mathcal{F})$)

Large for small n (few samples),
small for large n (many samples)

Mini Summary

- VC dimension is the size of the largest set of samples shattered by a model class
  - It is $d + 1$ for linear classifiers in $\mathbb{R}^d$
- Sauer-Shelah: The growth function grows only polynomially in the set size beyond the VC dimension
- As a result, VC generalisation bounds true risk and empirical risk deviation by $\mathrm{O}\left(\sqrt{(\mathrm{VC}(\mathcal{F}) \log n)/n}\right)$

Much more…

- Finite VC dimension equivalent to Provably approximately correct (PAC) learning
- VC dimension is not the only tool in learning theory
  - Some problems might have infinite VC dimension
  - Other problems beyond classification
- The generalization of some methods require different complexity measures or analysis frameworks, such as:
  - Fat shattering dimension
  - Provably approximately correct (PAC) Bayes bounds
  - Rademacher complexity