Lecture 7. VC Theory

COMP90051 Statistical Machine Learning

Semester 2, 2020
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This lecture

- PAC learning bounds:
  * Countably infinite case works as we've done so far
  * General infinite case? Needs new ideas!
- Growth functions for the general PAC case
  * Considering patterns of labels possible on a data set
  * Gives good PAC 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, general PAC bound from VC theory
- Optional proofs at end (just for fun)

Countably infinite $\mathcal{F}$?

Josh Staiger (CCA2.0)

- Hoeffding gave us for a single $f \in \mathcal{F}$

$$\Pr\left(R[f] - \hat{R}[f] \geq \sqrt{\frac{\log\left(\frac{1}{\delta(f)}\right)}{2m}}\right) \leq \delta(f)$$

…where we're free to choose (varying) $\delta(f)$ in $[0,1]$.

- Union bound "works" (sort of) for this case

$$\Pr\left(\exists f \in \mathcal{F}, R[f] - \hat{R}[f] \geq \sqrt{\frac{\log\left(\frac{1}{\delta(f)}\right)}{2m}}\right) \leq \sum_{f\in\mathcal{F}} \delta(f)$$

- Choose confidences to sum to constant δ, then this works
  * E.g. $\delta(f) = \delta \cdot p(f)$ where $1 = \sum_{f\in\mathcal{F}} p(f)$

Try this for finite $\mathcal{F}$ with uniform $p(f)$

- By inversion: w.h.p $1-\delta$, for all f, $R[f] \leq \hat{R}[f] + \sqrt{\frac{\log\left(\frac{1}{p(f)}\right) + \log\left(\frac{1}{\delta}\right)}{2m}}$

Ok fine, but general case?

- Much of ML has continuous parameters
  - Countably infinite covers only discrete parameters ☹
- Our argument fails! ☹ ☹
  - $p(f)$ becomes a density
  - Its zero for all f. No divide by zero!
  - Need a new argument!

$$\sqrt{\frac{\log\left(\frac{1}{p(f)}\right) + \log\left(\frac{1}{\delta}\right)}{2m}}$$

- Idea introduced by VC theory: intuition
  - Don't focus on whole class $\mathcal{F}$ as if each f is different
  - Focus on differences over sample $Z_1, \dots, Z_m$

Mini Summary

- Can eek out PAC bounds on countably infinite families using Hoeffding bound + union bound
- No good for general (uncountably infinite) cases
- Need another fundamentally new idea

Next: Organising analysis around patterns of labels possible on a data set, to avoid wort-case bad events

Growth Function

Focusing on the size of model families on data samples

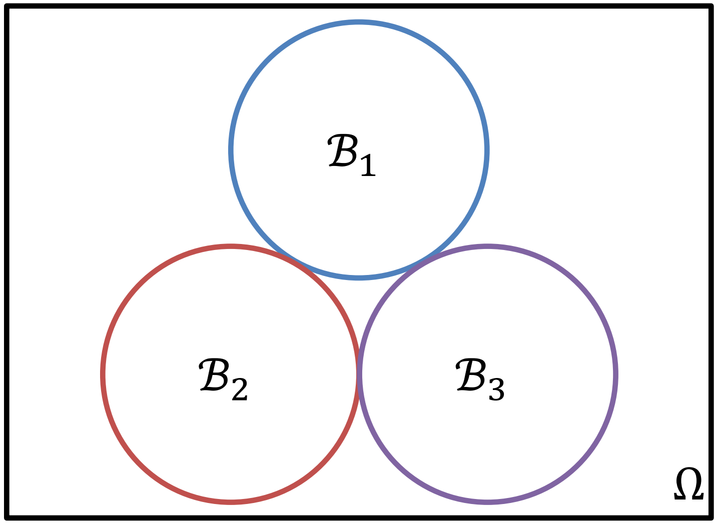
Bad events: Unreasonably worst case?

- Bad event $\mathcal{B}_i$ for model f_i

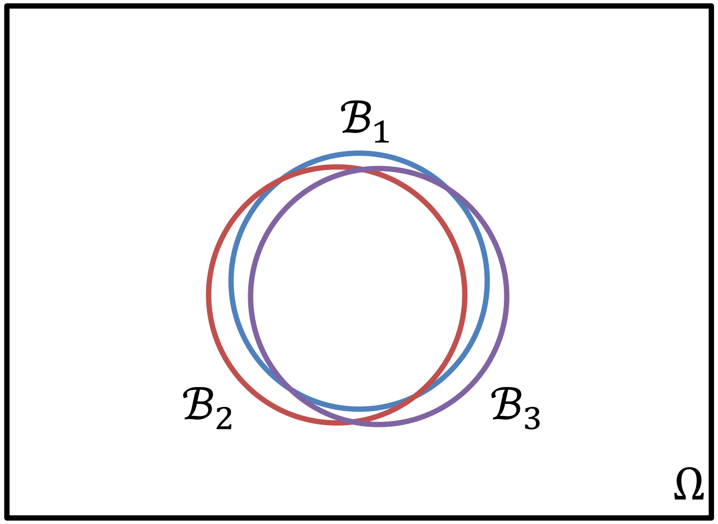
  $R[f_i] - \hat{R}[f_i] \geq \varepsilon$ with probability $\leq 2\exp(-2m\varepsilon^2)$

- Union bound: bad events don't overlap!?

  $\Pr(\mathcal{B}_1 \text{ or} \dots \text{or } \mathcal{B}_{|\mathcal{F}|}) \leq \Pr(\mathcal{B}_1) + \cdots + \Pr(\mathcal{B}_{|\mathcal{F}|}) \leq 2|\mathcal{F}|\exp(-2m\varepsilon^2)$

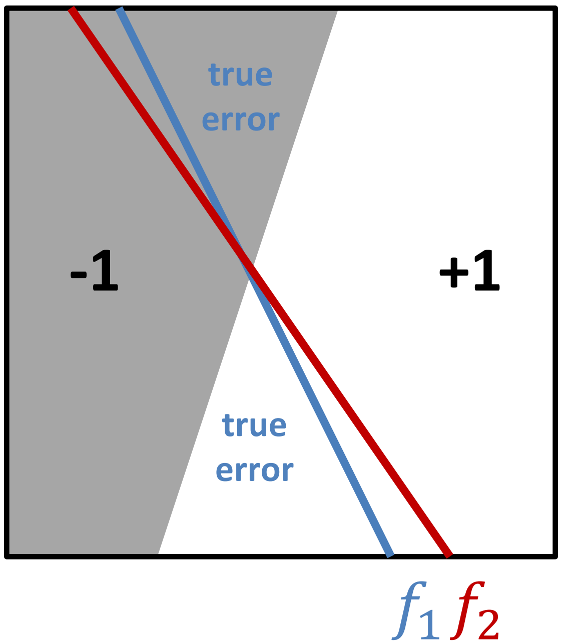


Tight bound: No overlaps

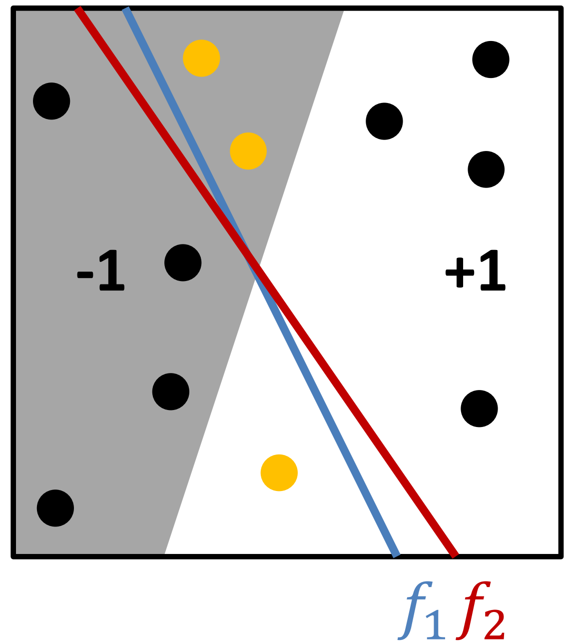


Loose bound: Overlaps

How do overlaps arise?



Whole of population

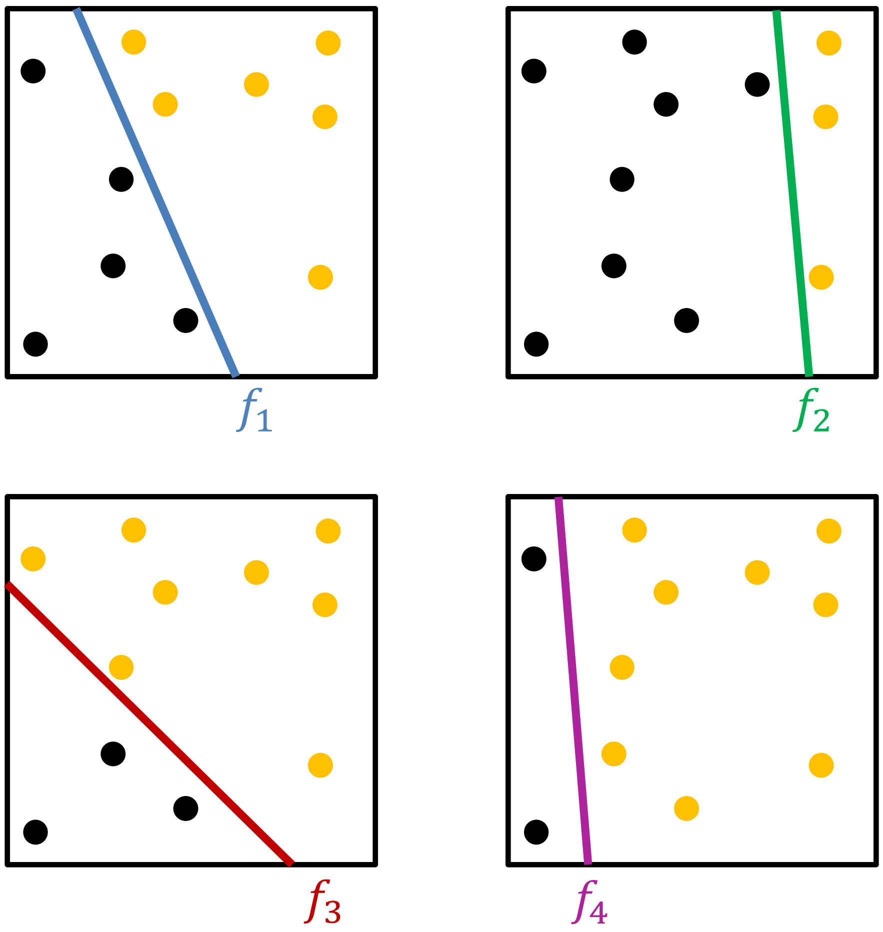


On a sample

Significantly overlapping events $\mathcal{B}_1$ and $\mathcal{B}_2$

How do overlaps arise?

VC theory focuses on the pattern of labels any $f \in \mathcal{F}$ could make



Dichotomies and Growth Function

- Definition: Given sample $x_1, \dots, x_m$ and family $\mathcal{F}$, a **dichotomy** is a $\left(f(x_1), \dots, f(x_m)\right) \in \{-1, +1\}^m$ for some $f \in \mathcal{F}$.

- Unique dichotomies $\mathcal{F}(\mathbf{x}) = \left\{\left(f(x_1), \dots, f(x_m)\right) : f \in \mathcal{F}\right\}$, patterns of labels possible with the family

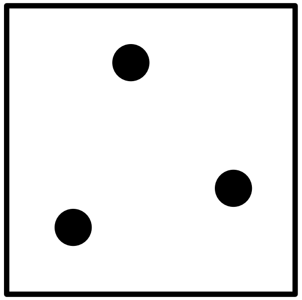
- Even when $\mathcal{F}$ infinite, $|\mathcal{F}(\mathbf{x})| \leq 2^m$ (why?)

- And also (relevant for $\mathcal{F}$ finite, tiny), $|\mathcal{F}(\mathbf{x})| \leq |\mathcal{F}|$ (why?)

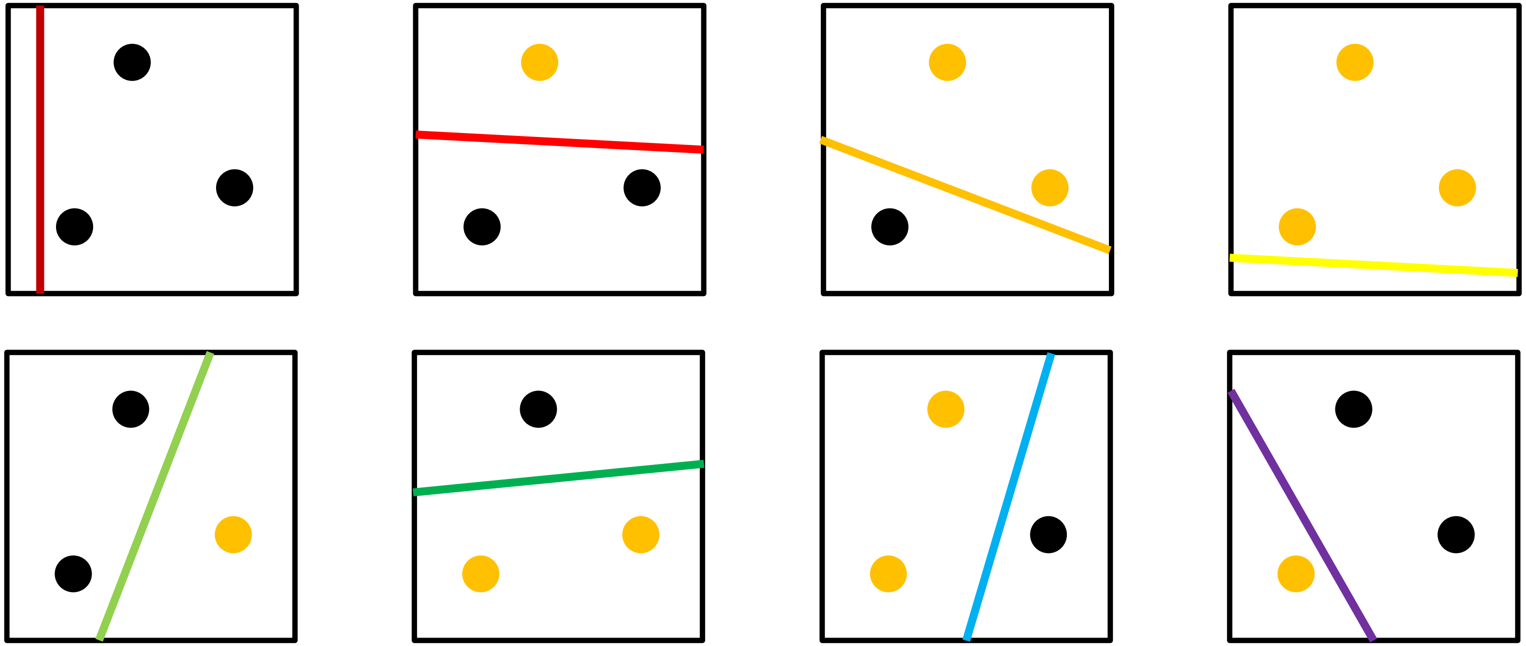
- *Intuition: $|\mathcal{F}(\boldsymbol{x})|$ might replace $|\mathcal{F}|$ in union bound? How remove* **x***?*

- Definition: The **growth function** $S_{\mathcal{F}}(m) = \sup_{\mathbf{x} \in \mathcal{D}^m} |\mathcal{F}(\mathbf{x})|$ is the max number of label patterns achievable by $\mathcal{F}$ for any m sample.

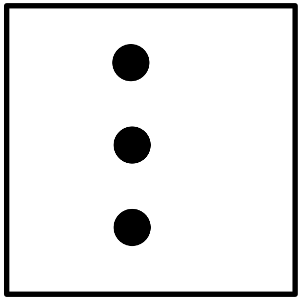
$S_{\mathcal{F}}(3)$ for $\mathcal{F}$ linear classifiers in 2D?



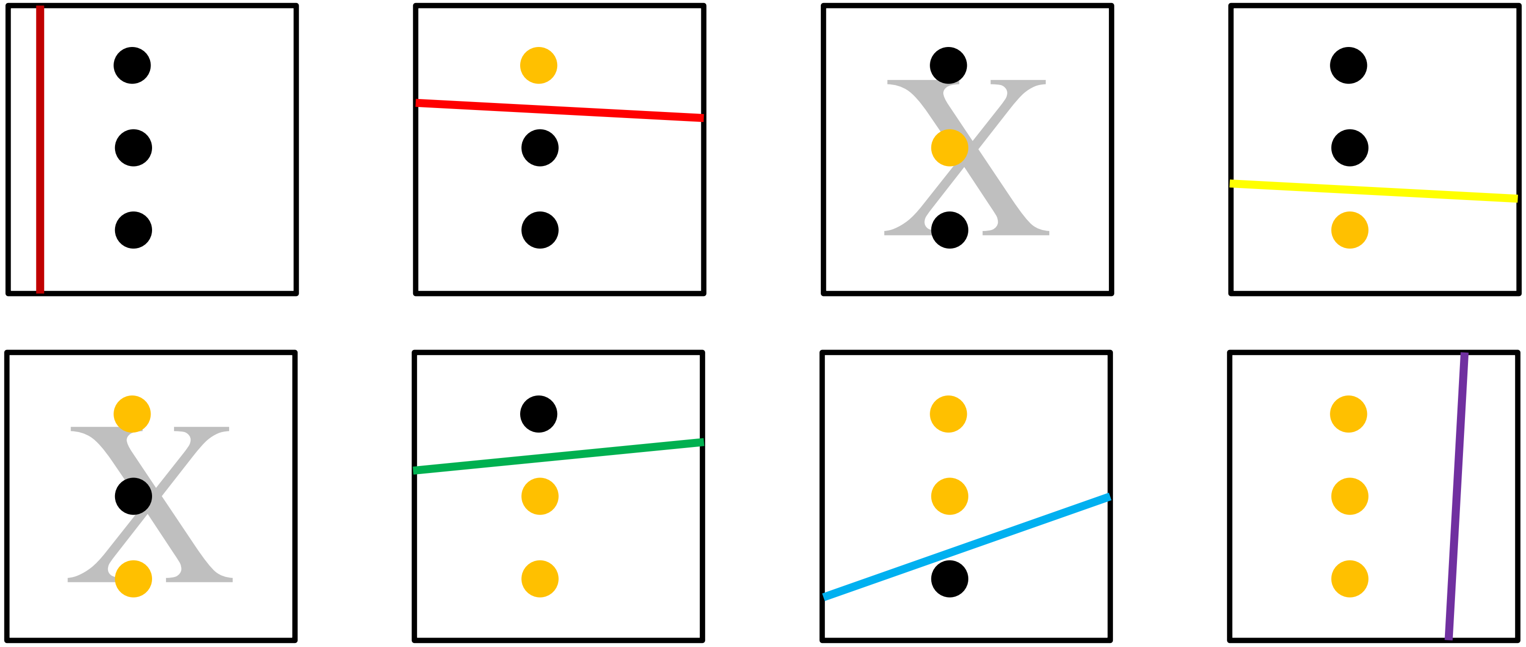
$S_{\mathcal{F}}(3) = 8$



$S_{\mathcal{F}}(3)$ for $\mathcal{F}$ linear classifiers in 2D?

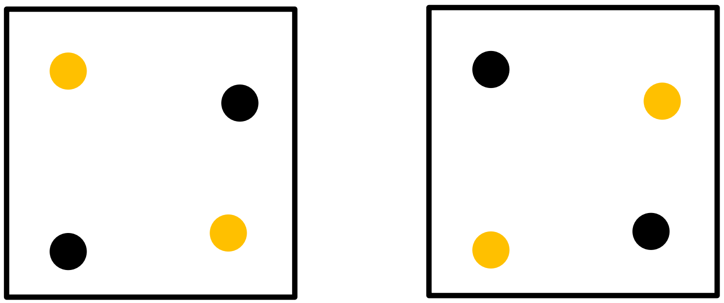


$|\mathcal{F}(\mathbf{x})| = 6$
but still have
$S_{\mathcal{F}}(3) = 8$



$S_{\mathcal{F}}(4)$ for $\mathcal{F}$ linear classifiers in 2D?

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



- In fact $S_{\mathcal{F}}(4) = 14 < 2^4$
- Guess/exercise: What about general m and dimension?

PAC Bound with Growth Function

- Theorem: Consider any $\delta > 0$ and any class $\mathcal{F}$. Then w.h.p. at least $1-\delta$: For all $f \in \mathcal{F}$

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

- Proof: out of scope ("only" 2-3pgs), optional reading.

- Compare to PAC bounds so far
  * A few negligible extra constants (the 2s, the 4)
  * $|\mathcal{F}|$ has become $S_{\mathcal{F}}(2m)$
  * $S_{\mathcal{F}}(m) \leq |\mathcal{F}|$, not "worse" than union bound for finite $\mathcal{F}$
  * $S_{\mathcal{F}}(m) \leq 2^m$, very bad for big family with exponential growth function gets $R[f] \leq \hat{R}[f] + Big\ Constant$. Even $R[f] \leq \hat{R}[f] + 1$ meaningless!!

Mini Summary

- The previous PAC bound approach that organises bad events by model and applies uniform bound is only tight if bad events are disjoint
- In reality some models generate overlapping bad events
- Better to organise families by possible patterns of labels on a data set: the dichotomies of the family
- Counting possible dichotomies gives the growth function
- PAC bound with growth function potentially tackles general (uncountably infinite) 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, general, PAC bound

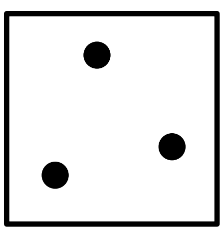
The VC dimension

Computable, bounds growth function

Vapnik-Chervonenkis dimension

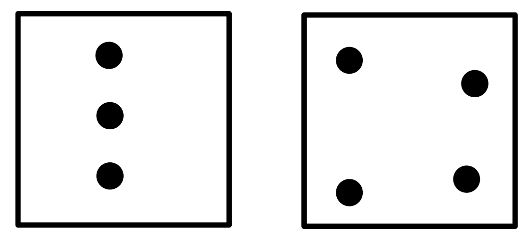
- Definition: The VC dimension $\mathrm{VC}(\mathcal{F})$ of a family $\mathcal{F}$ is the largest m such that $S_{\mathcal{F}}(m) = 2^m$.
  - Points $\mathbf{x} = (x_1, \dots, x_m)$ are shattered by $\mathcal{F}$ if $|\mathcal{F}(\mathbf{x})| = 2^m$
  - So $\mathrm{VC}(\mathcal{F})$ is the size of the largest set shattered by $\mathcal{F}$

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



Shattered

Not shattered



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

Example: VC($\mathcal{F}$) from $\mathcal{F}(\mathbf{x})$ 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 points $\mathbf{x}' \subseteq \{x_1, \dots, x_4\}$ by: drop columns, drop dupe rows
- $\mathcal{F}$ shatters $\mathbf{x}'$ if number of rows is $2^{|\mathbf{x}'|}$

x_1	x_2	x_4
0	0	0
0	1	0
1	0	1
1	1	1
$\cancel{0}$	$\cancel{1}$	$\cancel{0}$
1	0	0
$\cancel{1}$	$\cancel{1}$	$\cancel{1}$
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

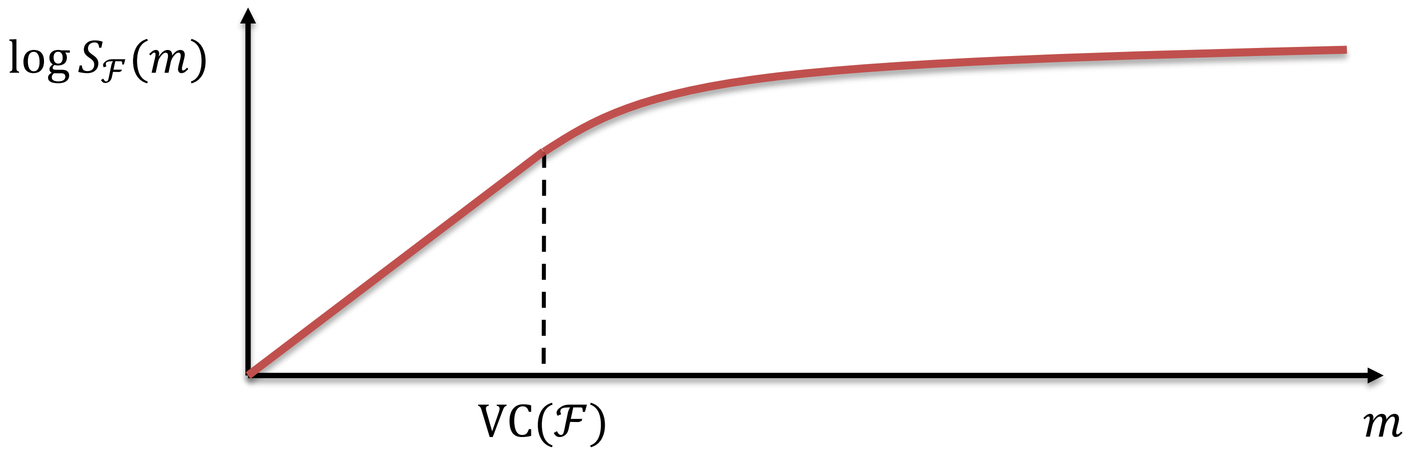
- Lemma (Sauer-Shelah): Consider any $\mathcal{F}$ with finite $\mathrm{VC}(\mathcal{F}) = k$, any sample size m. Then $S_{\mathcal{F}}(m) \leq \sum_{i=0}^{k} \binom{m}{i}$.

- From basic facts of Binomial coefficients
  - Bound is $O(m^k)$: finite VC ⇒ eventually polynomial growth!
  - For $m \geq k$, it is bounded by $\left(\frac{em}{k}\right)^k$

- Theorem (VC bound): Consider any $\delta > 0$ and any VC-k class $\mathcal{F}$. Then w.h.p. at least $1 - \delta$: For all $f \in \mathcal{F}$

$$R[f] \leq \hat{R}[f] + 2\sqrt{2\frac{k \log \frac{2em}{k} + \log \frac{4}{\delta}}{m}}$$

VC bound big picture



- (Uniform) difference between $R[f], \hat{R}[f]$ is $O\left(\sqrt{\frac{k \log m}{m}}\right)$ down from ∞
- Limiting complexity of $\mathcal{F}$ leads to better generalisation
- VC dim, growth function measure "effective" size of $\mathcal{F}$
- VC dim doesn't count functions, but uses geometry of family: projections of family members onto possible samples
- Example: linear "gap-tolerant" classifiers (like SVMs) with "margin" Δ have VC $= O(1/\Delta^2)$. Maximising "margin" reduces VC-dimension.

Mini Summary

- VC-dim is the largest set size shattered by a family
  - It is $d+1$ for linear classifiers in $\mathbb{R}^d$
  - Can calculate it on entire-domain dichotomies of a family by dropping columns and counting unique rows
- Sauer-Shelah: The growth function grows only polynomially in the set size beyond the VC-dim
- As a result, VC PAC bounds uniform risk and empirical risk deviation by $O\left(\sqrt{(\mathrm{VC}(\mathcal{F}) \log m)/m}\right)$

Next: Two selected proofs. Optional but beautiful.

Two Selected Proofs

Green slides: Not examinable.

Food for thought. Soul food.

Linear classifiers in d-dim: $\mathrm{VC}(\mathcal{F}) \geq d + 1$

- Goal: construct $m = d + 1$ specific points in $\mathbb{R}^d$ that are shattered by the linear classifier family
- Data in rows of $\mathbf{X} = \begin{pmatrix} 1 & 0 & 0 & \dots & 0 \\ 1 & 1 & 0 & \dots & 0 \\ 1 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & 0 & \cdots & 1 \end{pmatrix}$ is invertible!
- Any dichotomy $y \in \{-1,1\}^{d+1}$, need $\mathbf{w}$ with $\mathrm{sign}(\mathbf{Xw}) = \mathbf{y}$
- $\mathbf{w} = \mathbf{X}^{-1}\mathbf{y}$ works*!!* $\mathrm{sign}(\mathbf{Xw}) = \mathrm{sign}(\mathbf{XX}^{-1}\mathbf{y}) = \mathrm{sign}(\mathbf{y}) = \mathbf{y}$
- We've shown that $\mathcal{F}$ can shatter $d + 1$ points: $\mathrm{VC}(\mathcal{F}) \geq d + 1$

Linear classifiers in d-dim: $\mathrm{VC}(\mathcal{F}) \leq d+1$

- Goal: cannot shatter any set of $d+2$ points
- Any $\mathbf{x}_1, \ldots, \mathbf{x}_{d+2}$, have more pts than dims: linear dependent

  $\mathbf{x}_j = \sum_{i \neq j} a_i \mathbf{x}_i$, for some j, where not all a_i's are zero

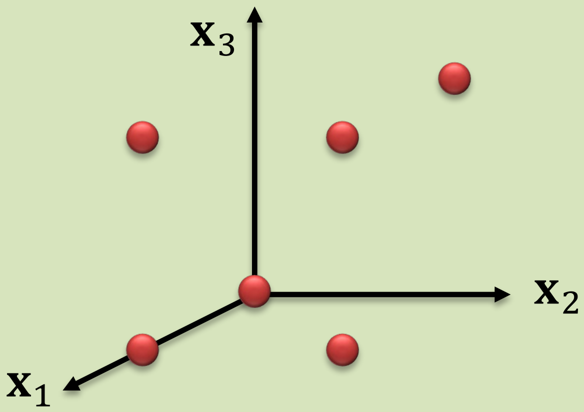
- Possible dichotomy $\mathbf{y}$? $\quad y_i = \begin{cases} \mathrm{sign}(a_i), & \text{if } i \neq j \\ -1, & \text{if } i = j \end{cases}$
  * Suppose $\mathbf{w}$ generated $i \neq j$: $\mathrm{sign}(a_i) = \mathrm{sign}(\mathbf{w}'\mathbf{x}_i)$ so $a_i \mathbf{w}'\mathbf{x}_i > 0$
  * Can $\mathbf{w}$ generate $i = j$??
  * $\mathbf{w}'\mathbf{x}_j = \mathbf{w}' \sum_{i \neq j} a_i \mathbf{x}_i = \sum_{i \neq j} a_i \mathbf{w}'\mathbf{x}_i > 0$ so $\mathrm{sign}(\mathbf{w}'\mathbf{x}_j) \neq y_i$
- We've shown $\mathrm{VC}(\mathcal{F}) < d+2$, in other words $\mathrm{VC}(\mathcal{F}) = d+1$

Proof of Sauer-Shelah Lemma (by Haussler '95)

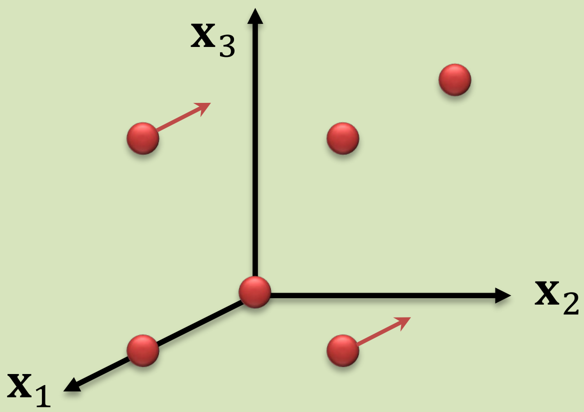
- To show that growth function $S_{\mathcal{F}}(m) \leq \sum_{i=0}^{k} \binom{m}{i}$ we prove the bound for any dichotomies $|\mathcal{F}(x_1, \ldots, x_m)|$ since $|\mathcal{F}(x_1, \ldots, x_m)| \leq S_{\mathcal{F}}(m)$
- Write $\mathbf{Y} = \mathcal{F}(x_1, \ldots, x_m) \subseteq \{0,1\}^m$, where $-1 \to 0$.
- Definition: Consider any column $1 \leq i \leq m$ and dichotomy $\mathbf{y} \in \mathbf{Y}$. The shift operator $H_i(\mathbf{y}; \mathbf{Y})$ returns $\mathbf{y}$ if there exists some $\mathbf{y}' \in \mathbf{Y}$ differing to $\mathbf{y}$ only in the i^{th} coordinate; otherwise it returns $\mathbf{y}$ with $y_i = 0$. Define $H_i(\mathbf{Y}) = \{H_i(\mathbf{y}; \mathbf{Y}) : \mathbf{y} \in \mathbf{Y}\}$ the shifting all dichotomies.
  - Intuition: Shifting along a column drops a +1 to 0 in that column so long as now other row would become duplicated.
- Definition: A set of dichotomies $\mathbf{V} \subseteq \{0,1\}^m$ is called closed below if for all $1 \leq i \leq m$, shifting does nothing $H_i(\mathbf{V}) = \mathbf{V}$.
  - Intuition: Every $\mathbf{v} \in \mathbf{V}$ has, for every $1 \leq i \leq m$ for which $v_i = 1$, some $\mathbf{u} \in \mathbf{V}$ the same as $\mathbf{v}$ except with $u_i = 1$.

Proof of Sauer-Shelah Lemma (by Haussler '95)

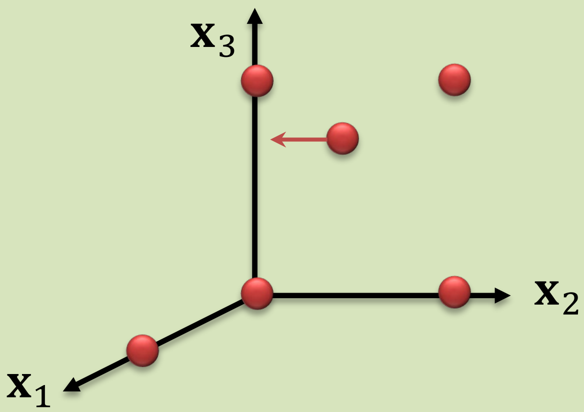
x_1	x_2	x_3
0	0	0
0	1	1
1	0	0
1	1	0
1	0	1
1	1	1



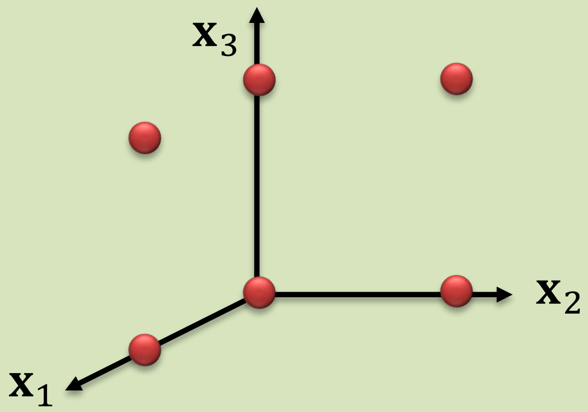
- Example set of 6 unique dichotomies on $m = 3$ pts with VC=2



Shift down along $i = 1$



Shift down along $i = 2$



Closed below

Proof of Sauer-Shelah Lemma (by Haussler '95)

- Goal: show that (1) shifting almost maintains VC dimension and cardinality all the way to a closed-below end, (2) closed-below sets have the desired Sauer-Shelah bound

- Shifting property 1: $|H_i(\mathbf{Y})| = |\mathbf{Y}|$ for any $\mathbf{Y}$.
  - Proof: no two dichotomies in $\mathbf{Y}$ shift to the same dichotomy

- Shifting property 2: $\mathrm{VC}(H_i(\mathbf{Y})) \leq \mathrm{VC}(\mathbf{Y})$ for any $i, \mathbf{Y}$.
  - Proof sketch: If $H_i(\mathbf{Y})$ shatters a subset of points, then so too does $\mathbf{Y}$

- Shifting property 3: if $\mathbf{Y}$ is closed below, then all dichotomies $\mathbf{y} \in \mathbf{Y}$ have at most $\mathrm{VC}(\mathbf{Y})$-many $y_i = 1$ (the rest 0).
  - Therefore: $|\mathbf{Y}| \leq \binom{m}{0} + \binom{m}{1} + \cdots + \binom{m}{\mathrm{VC}(\mathbf{Y})}$ by counting
  - Proof sketch: if a $\mathbf{y} \in \mathbf{Y}$ had more 1s, all combinations would exist "below"

- Together: exists a shift sequence $i_1, \ldots, i_N$ to a closed below $H_{i_N}(\mathbf{Y})$:

$$|\mathbf{Y}| = \left|H_{i_1}(\mathbf{Y})\right| = \cdots = \left|H_{i_N}(\mathbf{Y})\right| \leq \sum_{i=0}^{\mathrm{VC}\left(H_{i_N}(\mathbf{Y})\right)} \binom{m}{i} \leq \cdots \leq \sum_{i=0}^{\mathrm{VC}(\mathbf{Y})} \binom{m}{i}$$

Mini Summary

- Linear classifiers in $\mathbb{R}^d$ have VC dimension $d + 1$
  - Lower bound VC-dim with specific points that are shattered
  - Upper bound VC-dim by lin. dependence of any $d + 2$ points
- Sauer-Shelah lemma bounds a family's growth function by a polynomial in VC dimension.
  - Ingenious shifting operator transforms sets of dichotomies into boundable closed-below sets
  - Along the way keeps cardinality and VC-dim controlled

Next time: Support vector machines