Lecture 6. PAC Learning Theory

COMP90051 Statistical Machine Learning

Semester 2, 2020
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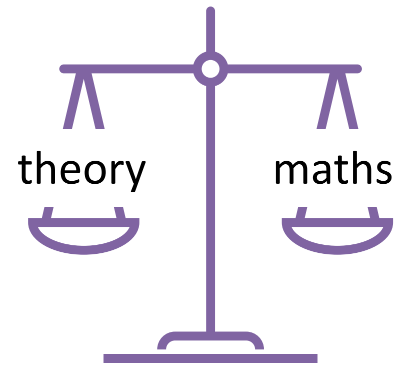
This lecture

- Excess risk
  - Decomposition: Estimation vs approximation
  - Bayes risk – irreducible error
- Probably approximation correct learning
- Bounding generalisation error with high probability
  - Single model: Hoeffding's inequality
  - Finite model class: Also use the union bound
- Importance & limitations of uniform deviation bounds

Generalisation and Model Complexity



- Theory we've seen so far (mostly statistics)
  - Asymptotic notions (consistency, efficiency)
  - Convergence could be really slow
  - Model complexity undefined
- Want: finite sample theory; convergence *rates,* trade-offs
- Want: define model complexity and relate it to test error
  - Test error can't be measured in real life, but it can be provably bounded!
  - Growth function, VC dimension
- Want: distribution-independent, learner-independent theory
  - A fundamental theory applicable *throughout ML*
  - Unlike bias-variance: distribution dependent, no model complexity,

Probably Approximately Correct Learning

The bedrock of machine learning theory in computer science.

Standard setup

- Supervised binary classification of
  - data in $\mathcal{X}$ into label set $\mathcal{Y} = \{-1,1\}$
- iid data $\{(x_i, y_i)\}_{i=1}^{m} \sim D$ *some* fixed unknown distribution
- Single test example independent from same D when representing generalisation performance (risk)
- Learning from a class of function $\mathcal{F}$ mapping (classifying) $\mathcal{X}$ into $\mathcal{Y}$
- What parts depend on the sample of data
  - Empirical risk $\hat{R}[f]$ that averages loss over the sample
  - $f_m \in \mathcal{F}$ the learned model (it could be same sample or different; theory is actually fully general here)

If the empirical risk is evaluated on the same data, then it is training set error. If it evaluated on different data, then its called test set error. The theory can generalise to both case.

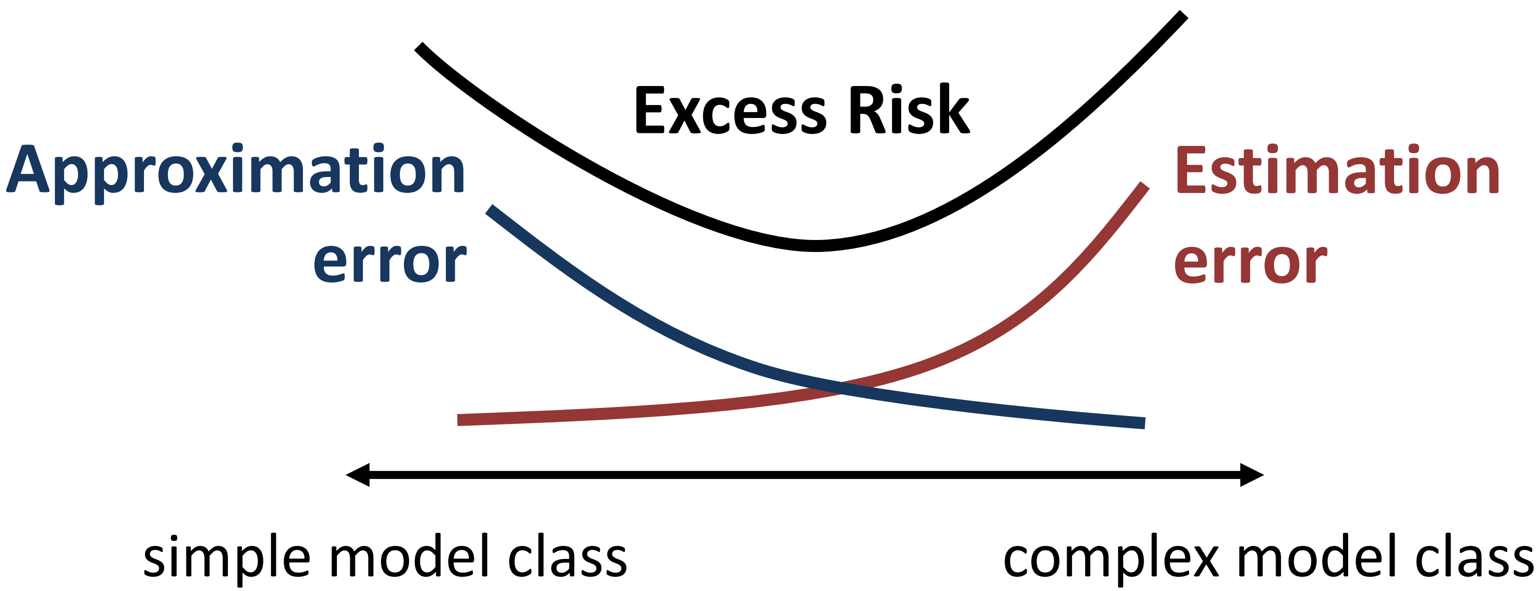
Risk: The good, bad and ugly

$$\underbrace{R[f_m] - R^*}_{\text{Excess risk}} = \underbrace{\left(R[f_m] - R[f^*]\right)}_{\text{Estimation error}} + \underbrace{\left(R[f^*] - R^*\right)}_{\text{Approximation error}}$$

- **Good**: what we'd aim for in our class, with infinite data
  * $R[f^*]$ true risk of best in class $f^* \in \operatorname{argmin}_{f \in \mathcal{F}} R[f]$
- **Bad**: we get what we get and don't get upset
  * $R[f_m]$ true risk of learned $f_m \in \arg\min_{f \in \mathcal{F}} \underbrace{\hat{R}[f] + C\|f\|^2}_{\text{Training risk + some regulariser}}$ (e.g.)
- **Ugly**: we usually cannot even hope for perfection!
  * $R^* \in \inf_f R[f]$ called the Bayes risk; noisy labels makes large

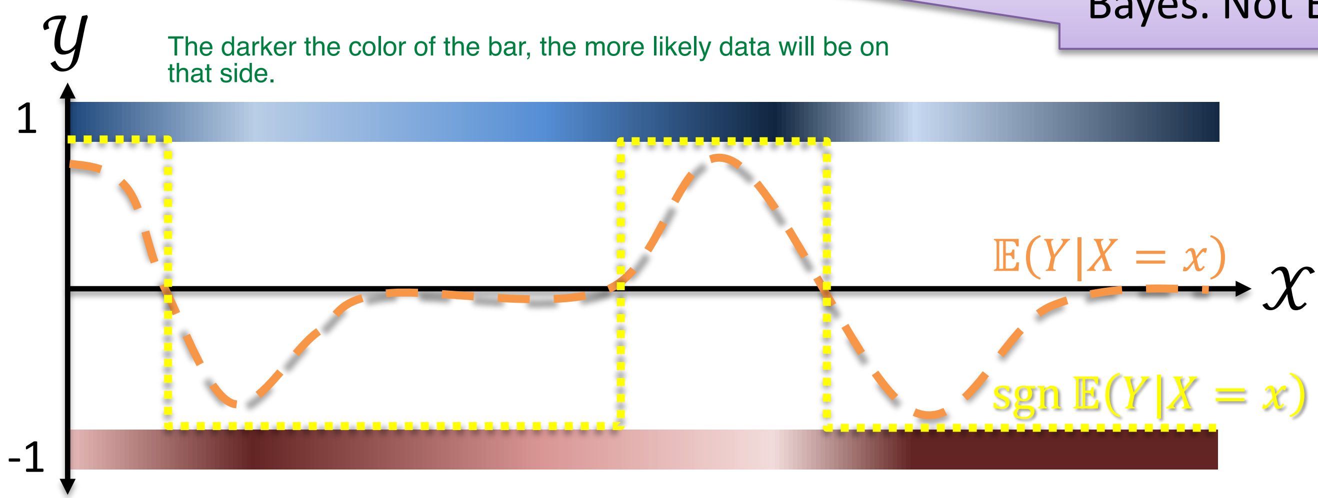
A familiar trade-off: More intuition

- simple family → may underfit due to approximation error
- complex family → may overfit due to estimation error



About Bayes risk

Once again, named after Bayes. Not Bayesian ML.



- Bayes risk $R^* \in \inf_f R[f]$
  - Best risk possible, ever; but can be large
  - Depends on distribution and loss function
- Bayes classifier achieves Bayes risk
  - $f_{Bayes}(x) = \operatorname{sgn}\mathbb{E}(Y|X=x)$

Let's focus on $R[f_m]$

Leslie Valiant
CCA2.0 Renate Schmid

- Since we don't know data distribution, we need to bound generalisation to be small
  - Bound by test error $\hat{R}[f_m] = \frac{1}{m}\sum_{i=1}^{m} f(X_i, Y_i)$
  - Abusing notation: $f(X_i, Y_i) = l(Y_i, f(X_i))$

$$R[f_m] \le \hat{R}[f_m] + \varepsilon(m, \mathcal{F})$$

- Unlucky training sets, no always-guarantees possible!
- With probability $\ge 1 - \delta$: $R[f_m] \le \hat{R}[f_m] + \varepsilon(m, \mathcal{F}, \delta)$
- Called Probably Approximately Correct (PAC) learning
  - $\mathcal{F}$ called PAC learnable if $m = O(\text{poly}(1/\varepsilon, 1/\delta))$ to learn f_m for any ε, δ
  - Won Leslie Valiant (Harvard) the 2010 Turing Award
- Later: Why this bounds estimation error.

Don't require exponential growth in training size m

Mini Summary

- Excess risk as the goal of ML
- Decomposition into approximation, estimation errors
- Probably Approximately Correct (PAC) learning
  * Like asymptotic theory in stats, but for finite sample size
  * Worst-case on distributions: We don't want to assume something unrealistic about where the data comes from
  * Worst-case on models: We don't want a theory that applies to narrow set of learners, but to ML in general
  * We want it to produce a useful measure of model complexity

Next: First step to PAC theory – bounding single model risk

Bounding true risk of one function

One step at a time

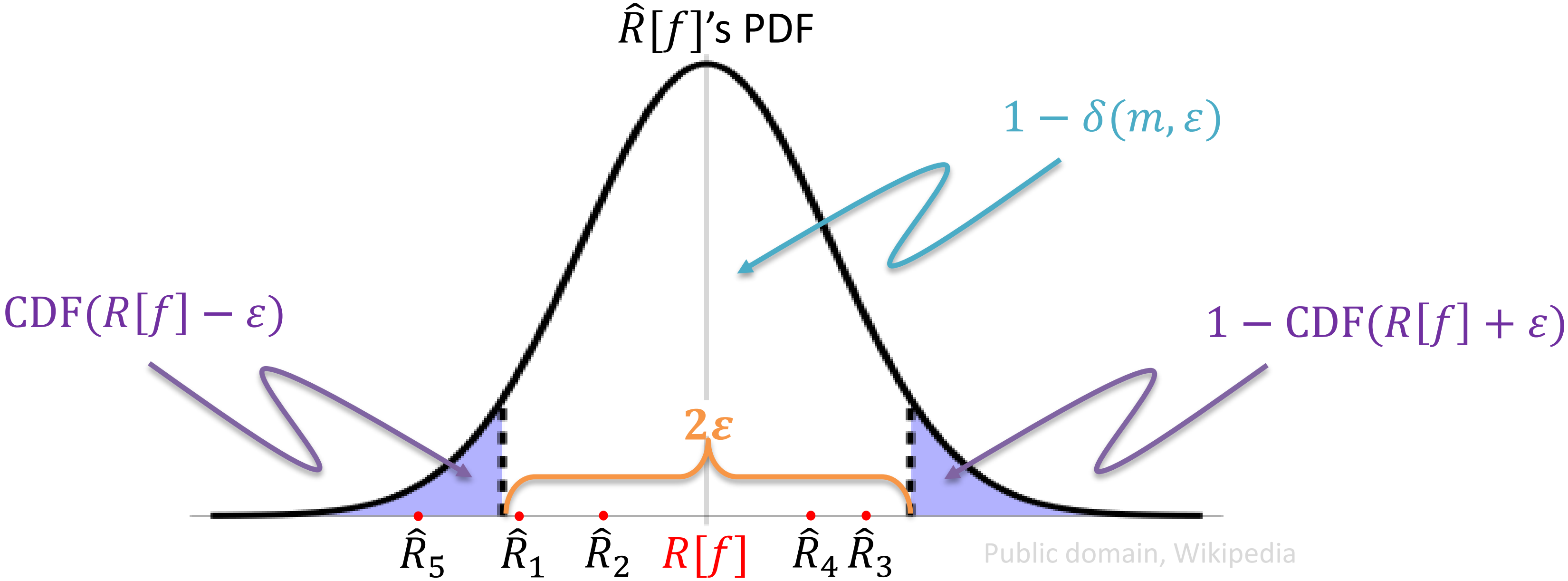
This is my understanding:

$R[f]$ - the loss you get for a particular f in the family F based on the true distribution. You can think about this as the true error for f.

$\hat{R}[f]$ - the loss you get for a particular f in the family F for a particular data set S (empirical error). f is assumed to be data independent here. The same f will be chosen for any data set S used.

But f_m is data dependent. f_m is found based on a particular data set S. Hence, with a different data set S, you will find a different f_m. Thus, we try to find a bound not for one f, but a bound for any f (we use $sup_{f \in \mathcal{F}}$) that f_m may possibly be found depending on the data set S used.

We need a concentration inequality



- $\hat{R}[f]$ is an unbiased estimate of $R[f]$ for any fixed f (*why?*)
- That means on average $\hat{R}[f]$ lands on $R[f]$
- What's the likelihood $1-\delta$ that $\hat{R}[f]$ lands within ε of $R[f]$? Or more precisely, what $1-\delta(m,\varepsilon)$ achieves a given $\varepsilon > 0$?
- Intuition: Just bounding CDF of $\hat{R}[f]$, independent of distribution*!!*

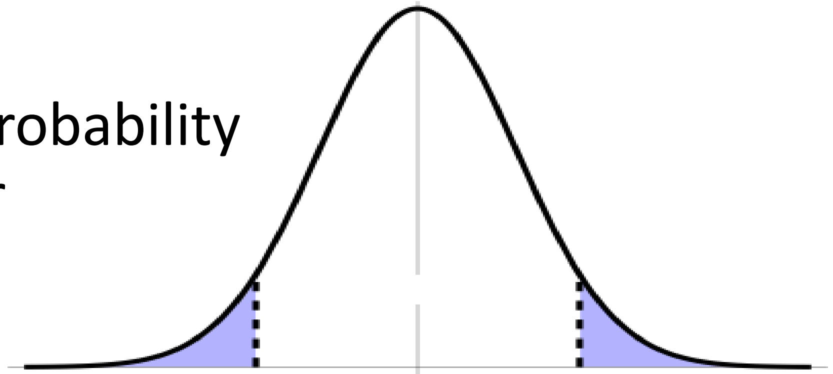
Hoeffding's inequality

- Many such concentration inequalities; a simplest one…
- **Theorem**: Let $Z_1, \ldots, Z_m, Z$ be iid random variables and $h(z) \in [a, b]$ be a bounded function. For all $\varepsilon > 0$

$$\Pr\left(\left|\mathbb{E}[h(Z)] - \frac{1}{m}\sum_{i=1}^{m} h(Z_i)\right| \geq \varepsilon\right) \leq 2\exp\left(-\frac{2m\varepsilon^2}{(b-a)^2}\right)$$

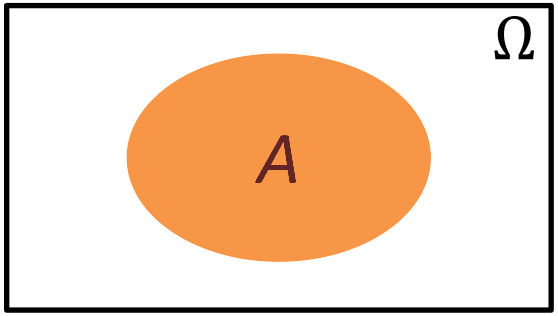
$$\Pr\left(\mathbb{E}[h(Z)] - \frac{1}{m}\sum_{i=1}^{m} h(Z_i) \geq \varepsilon\right) \leq \exp\left(-\frac{2m\varepsilon^2}{(b-a)^2}\right)$$

- Two-sided case in words: The probability that the empirical average is far from the expectation is small.



Public domain, Wikipedia

Common probability 'tricks'



- Inversion:
  - For any event A, $\Pr(\bar{A}) = 1 - \Pr(A)$
  - Application: $\Pr(X > \varepsilon) \leq \delta$ implies $\Pr(X \leq \varepsilon) \geq 1 - \delta$
- Solving for, in high-probability bounds:
  - For given ε with $\delta(\varepsilon)$ function ε: $\Pr(X > \varepsilon) \leq \delta(\varepsilon)$
  - Given δ' can write $\varepsilon = \delta^{-1}(\delta')$: $\Pr(X > \delta^{-1}(\delta')) \leq \delta'$
  - Let's you specify either parameter
  - Sometimes sample size m a variable we can solve for too

Et voila: A bound on true risk!

Result! $R[f] \leq \hat{R}[f] + \sqrt{\frac{\log(1/\delta)}{2m}}$ with high probability (w.h.p.) $\geq 1 - \delta$

Proof

- Take the Z_i as labelled examples (X_i, Y_i)
- Take $h(X, Y) = l(Y, f(X))$ zero-one loss for some fixed $f \in \mathcal{F}$ then $h(X, Y) \in [0,1]$
- Apply one-sided Hoeffding: $\Pr\left(R[f] - \hat{R}[f] \geq \varepsilon\right) \leq \exp(-2m\varepsilon^2)$

$$\Pr(R - \hat{R} \leq \varepsilon) \geq 1 - \delta$$

$$\delta = \exp(-2m\varepsilon^2)$$

$$\Rightarrow \varepsilon = \sqrt{\frac{\log(1/\delta)}{2m}}$$

Mini Summary

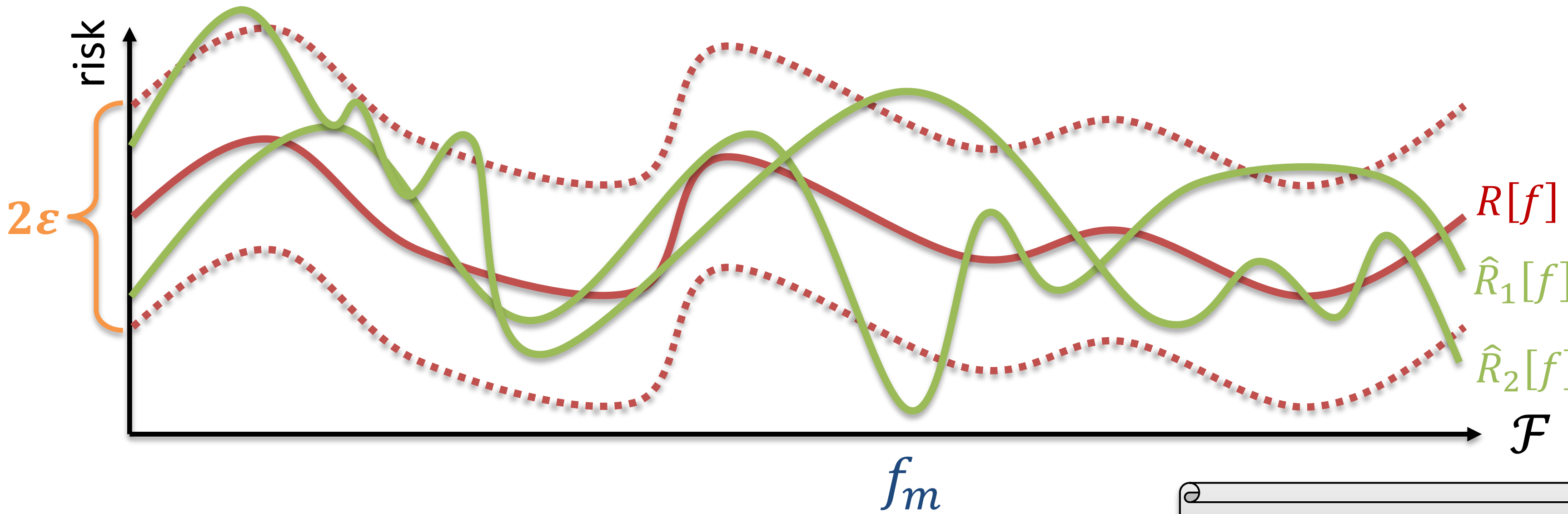
- Goal: Bound true risk of a classifier based on its empirical risk plus “stuff”
- Caveat: Bound is “with high probability” since we could be unlucky with the data
- Approach: Hoeffding’s inequality which bounds how far a mean is likely to be from an expectation

Next: PAC learning as uniform deviation bounds

Uniform deviation bounds

*Why we need our bound to **simultaneously** (or uniformly) hold over a family of functions.*

Our bound doesn't hold for $f = f_m$

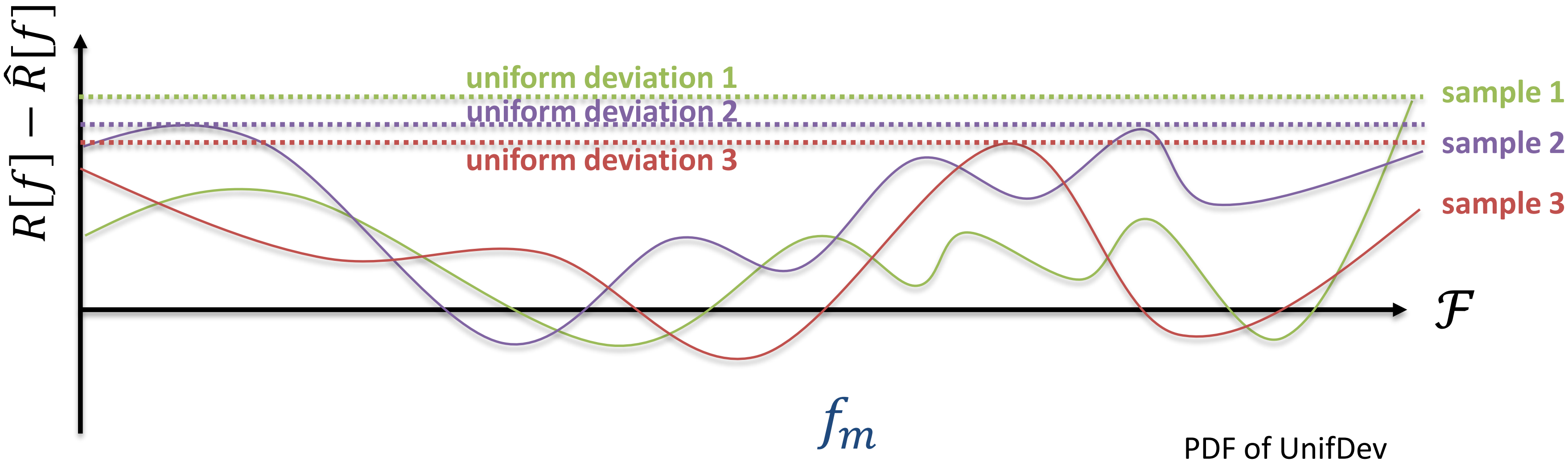


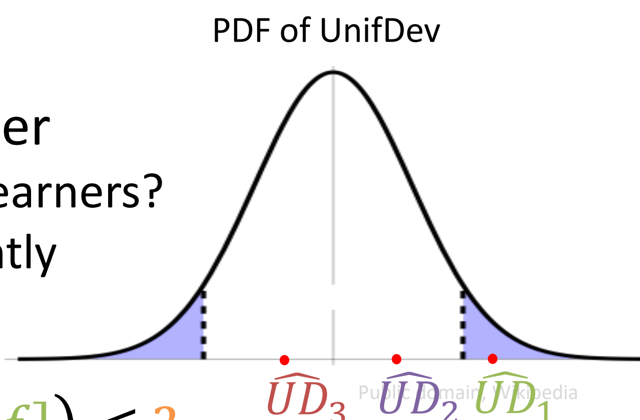
Problematic that f_m depends on data

- Result says there's set S of good samples for which $R[f] \leq \hat{R}[f] + \sqrt{\frac{\log(1/\delta)}{2m}}$ and $\Pr(\mathbf{Z} \in S) \geq 1 - \delta$
- But for different functions $f_1, f_2, \ldots$ we might get very different sets $S_1, S_2, \ldots$
- S observed may be bad for f_m. Learning minimises $\hat{R}[f_m]$, exacerbating this

  The data that we are trying to train on is bad

Uniform deviation bounds





- We could analyse risks of f_m from specific learner
  - But repeating for new learners? How to compare learners?
  - Note there are ways to do this, and data-dependently
- Bound uniform deviations across whole class $\mathcal{F}$

$$R[f_m] - \hat{R}[f_m] \le \sup_{f\in\mathcal{F}}\left(R[f] - \hat{R}[f]\right) \le ?$$

  - Worst deviation over an entire class bounds learned risk!
  - Convenient, but could be much worse than the actual gap for f_m

Relation to estimation error?

- Recall estimation error? *Learning* part of excess risk!

$$R[f_m] - R^* = (R[f_m] - R[f^*]) - (R[f^*] - R^*)$$

Theorem: ERM's estimation error is at most twice the uniform divergence

- Proof: a bunch of algebra!

$$\begin{aligned} R[f_m] &\leq \overbrace{\left(\hat{R}[f^*] - \hat{R}[f_m]\right)}^{\text{Non-negative}} + R[f_m] \overbrace{- R[f^*] + R[f^*]}^{=0} \\ &= \hat{R}[f^*] - R[f^*] + R[f_m] - \hat{R}[f_m] + R[f^*] \\ &\leq \left|R[f^*] - \hat{R}[f^*]\right| + \left|R[f_m] - \hat{R}[f_m]\right| + R[f^*] \\ &\leq 2 \sup_{f \in \mathcal{F}} \left|R[f] - \hat{R}[f]\right| + R[f^*] \end{aligned}$$

Mini Summary

- Why Hoeffding doesn't cover a model f_m learned from data, only a fixed data-independent f
- Uniform deviation idea: Cover the worst case deviation between risk and empirical risk, across $\mathcal{F}$
- Advantages: works for any learner, data distribution
- Connection back to bounding estimation error

Next: Next step for PAC learning – finite classes

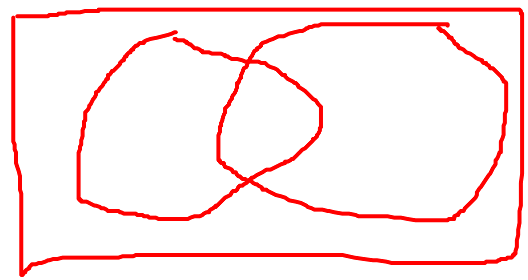
Error bound for finite function classes

Our first uniform deviation bound

The Union Bound

- If each model f having large risk deviation is a "bad event", we need a tool to bound the probability that any bad event happens. I.e. the union of bad events!
- **Union bound**: for a sequence of events A_1, A_2 ...

$$\Pr\left(\bigcup_i A_i\right) \leq \sum_i \Pr(A_i)$$



Proof:

Define $B_i = A_i \setminus \cup_{j=1}^{i-1} A_j$ with $B_1 = A_1$.

1. We know: $\cup_i B_i = \cup_i A_i$ (could prove by induction)
2. The B_i are disjoint (empty intersections)
3. We know: $B_i \subseteq A_i$ so $\Pr(B_i) \leq \Pr(A_i)$ by monotonicity

$$\Pr\left(\cup A_i\right) = \Pr\left(\cup B_i\right) = \sum_i \Pr(B_i) \leq \sum_i \Pr(A_i)$$

Bound for finite classes $\mathcal{F}$

- A uniform deviation bound over *any* finite class or distribution

Theorem: Consider any $\delta > 0$ and finite class $\mathcal{F}$. Then w.h.p at least $1 - \delta$: For all $f \in \mathcal{F}$, $R[f] \leq \hat{R}[f] + \sqrt{\frac{\log|\mathcal{F}| + \log(1/\delta)}{2m}}$

Proof:

- If each model f having large risk deviation is a "bad event", we bound the probability that any bad event happens.
- $\Pr\left(\exists f \in \mathcal{F}, R[f] - \hat{R}[f] \geq \varepsilon\right) \leq \sum_{f \in \mathcal{F}} \Pr\left(R[f] - \hat{R}[f] \geq \varepsilon\right)$
- $\leq |\mathcal{F}| \exp(-2m\varepsilon^2)$ by the union bound
- Followed by inversion, setting $\delta = |\mathcal{F}| \exp(-2m\varepsilon^2)$

Discussion

- Hoeffding's inequality only uses boundedness of the loss, not the variance of the loss random variables
  - Fancier concentration inequalities leverage variance
- Uniform deviation is worst-case, ERM on a very large over-parametrised $\mathcal{F}$ may approach the worst-case, but learners generally may not
  - Custom analysis, data-dependent bounds, PAC-Bayes, etc.
- Dependent data?
  - Martingale theory
- Union bound is in general loose, as bad is if all the bad events were independent (not necessarily the case even though underlying data modelled as independent); and **finite $\boldsymbol{\mathcal{F}}$**
  - VC theory coming up next!

Mini Summary

- More on uniform deviation bounds
- The union bound (generic tool in probability theory)
- Finite classes: Bounding uniform deviation with union+Hoeffding

Next time: PAC learning with infinite function classes!