Lecture 6. PAC Learning Theory

COMP90051 Statistical Machine Learning

Lecturer: Feng Liu

THE UNIVERSITY OF MELBOURNE

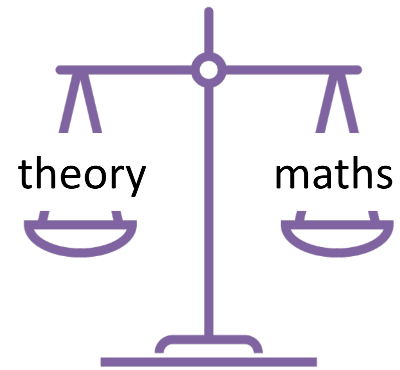
This lecture

- Excess risk
  - Decomposition: Estimation vs approximation
  - Bayes risk – irreducible error

Turing Award Inside

- 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

Problem we consider here: Supervised binary classification of

- data in $\mathcal{X}$ into label set $\mathcal{Y} = \{-1,1\}$

What we have:

- iid data $D^{\text{train}} = \{(x_i, y_i)\}_{i=1}^{m} \sim D$ *some* fixed unknown distribution. The D^{train} is called training data.

- Training error of a function f on D^{train} can be expressed by $\hat{R}[f] = \frac{1}{m}\sum_{i=1}^{m} \ell\big(y_i, f(x_i)\big)$.

What we will do in supervised binary classification:

- Learn a function f_m from a class of function $\mathcal{F}$ mapping (classifying) $\mathcal{X}$ into $\mathcal{Y}$ such that $f_m = \operatorname{argmin}_{f\in\mathcal{F}} \hat{R}[f]$.

Standard setup

Now, we have

- $f_m = \text{argmin}_{f\in\mathcal{F}} \hat{R}[f] = \text{argmin}_{f\in\mathcal{F}} \frac{1}{m}\sum_{i=1}^{m} \ell(y_i, f(x_i))$

and **want to**

analyse the performance of f_m on new data from the fixed distribution D.

Can you write down the test error based on f_m and D?

Standard setup

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- $f_m = \operatorname{argmin}_{f \in \mathcal{F}} \hat{R}[f] = \operatorname{argmin}_{f \in \mathcal{F}} \frac{1}{m} \sum_{i=1}^{m} \ell(y_i, f(x_i))$

and **want to**

analyse the performance of f_m on new data from the fixed distribution D.

Can you write down the test error based on f_m and D?

A lower $R[f_m]$ is better.

$R[f_m] = \mathbb{E}_{(X,Y)\sim D}[\ell(Y, f_m(X))]$ to represent the risk (or test error) of f_m on D.

Standard setup

Now, we have

- $f_m = \text{argmin}_{f \in \mathcal{F}} \hat{R}[f] = \text{argmin}_{f \in \mathcal{F}} \frac{1}{m} \sum_{i=1}^{m} \ell(y_i, f(x_i))$

and **want to (The Theoretical AIM)**

analyse $R[f_m] = \mathbb{E}_{(X,Y)\sim D}[\ell(Y, f_m(X))]$

- 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)

The Bayes Risk: One thing we cannot ignore

- We usually cannot even hope for perfection!
  - $R^* \in \inf_f R[f]$ called the Bayes risk;
  - cannot expect zero $R[f]$ and a clear decision boundary.
- Thus, we care about the following risk more:

$$R[f_m] - R^*$$

Excess risk

Decomposed Risk: The good, bad and ugly

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

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

Decomposed Risk: The good, bad and ugly

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

- **Good**: what we'd aim for in our class, with infinite data
  - $R[f^*]$ true risk of best in class $f^* \in \operatorname{argmin}_{f\in\mathcal{F}} R[f]$
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- **Ugly**: we usually cannot even hope for perfection!
  - $R^* \in \inf_f R[f]$ called the Bayes risk;
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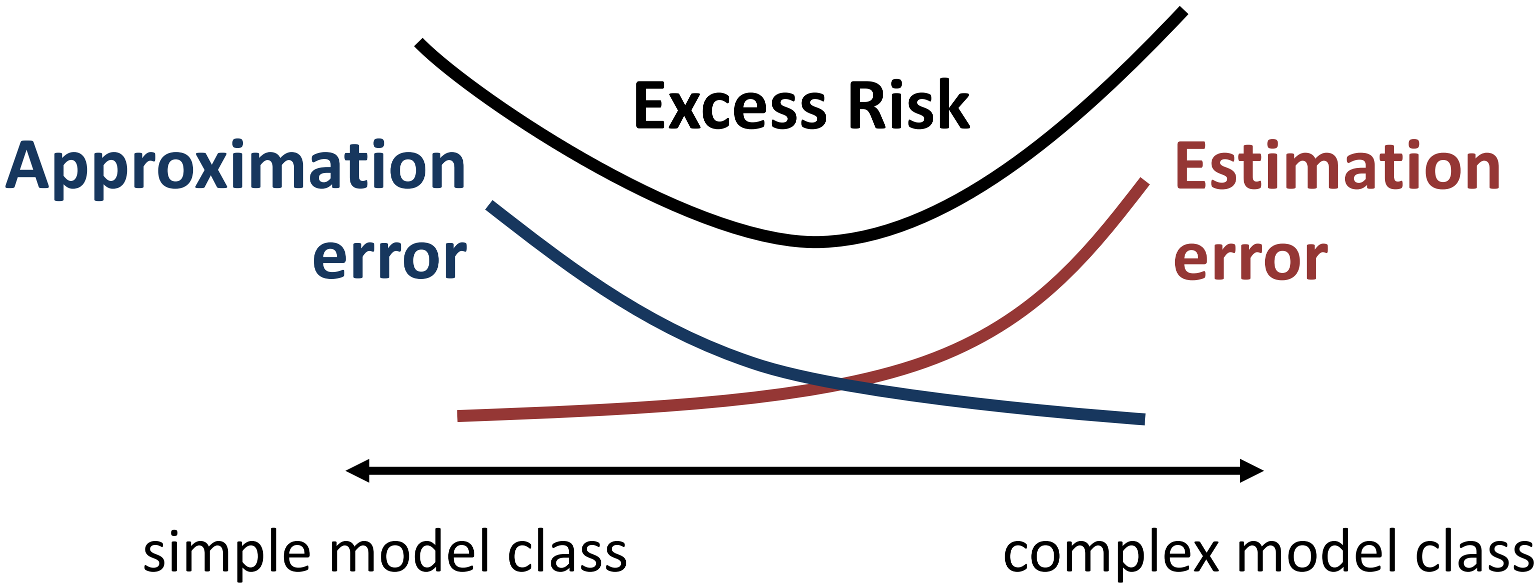
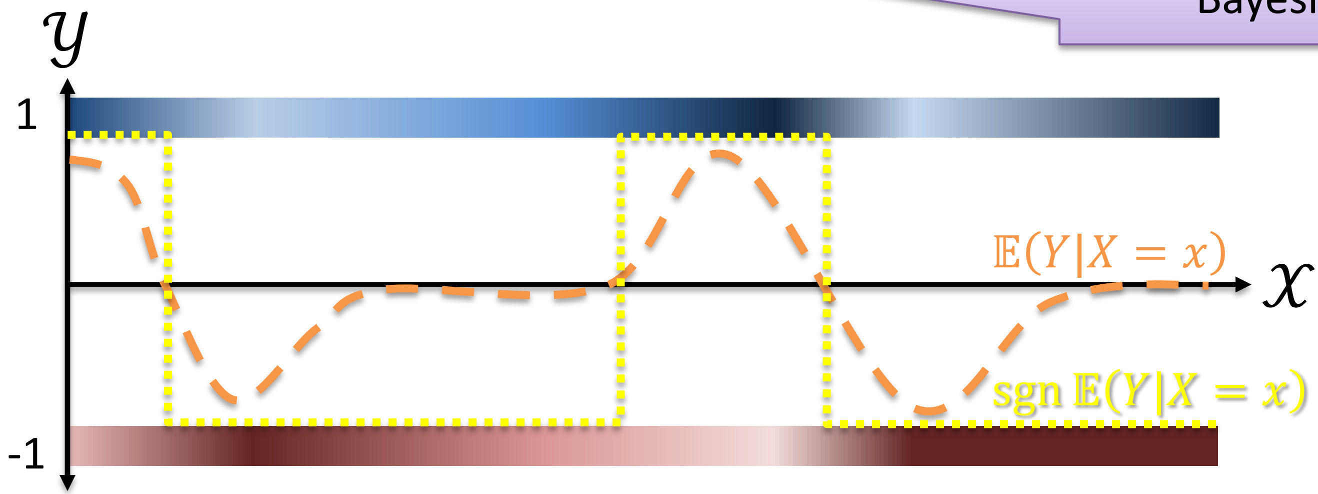
A familiar trade-off: More intuition

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



About Bayes risk

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

- 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: $f(X_i, Y_i) = l(Y_i, f(X_i))$

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

- Unlucky training sets, no always-guarantees possible!
- With probability $\geq 1 - \delta$: $R[f_m] \leq \hat{R}[f_m] + \varepsilon(m, \mathcal{F}, \delta)$
- 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

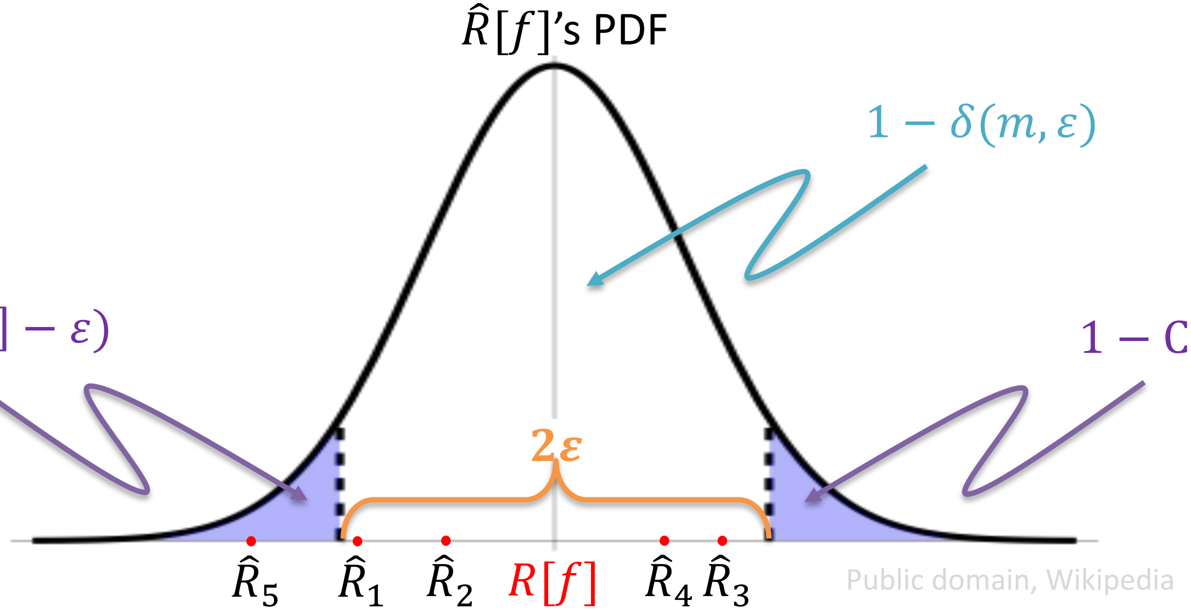
- Excess risk as the goal of ML
- Decomposition into approximation, estimation errors
- Probably Approximately Correct (PAC) learning
  - Like asymptotic theory in stats, but for finite sample size
  - Worst-case on distributions: We don’t want to assume something unrealistic about where the data comes 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

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*!!*

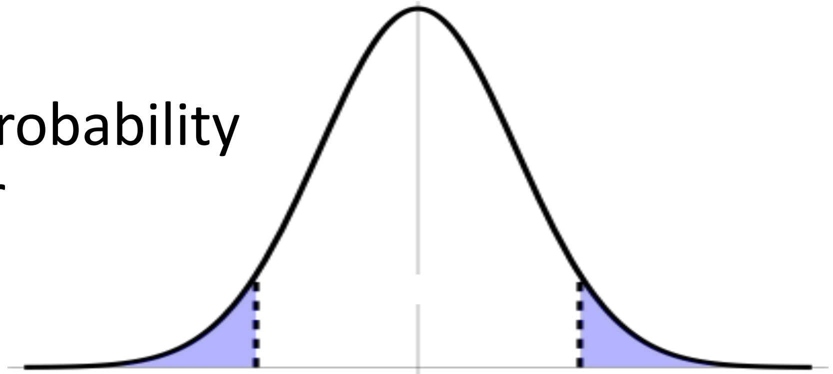
Hoeffding's inequality

- Many such concentration inequalities; a simplest one…
- **Theorem**: Let $Z_1, \dots, Z_m, Z$ 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

Et voila: A bound on true risk!

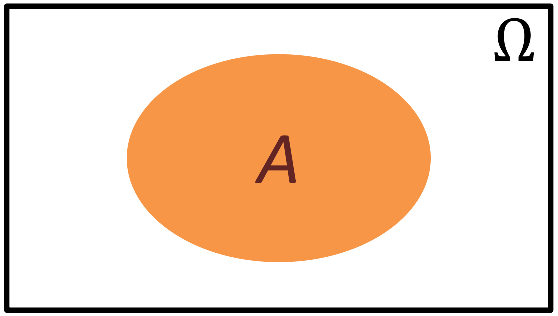
Result! $R[f] \leq \hat{R}[f] + \sqrt{\frac{\log(1/\delta)}{2m}}$ with high probability (w.h.p.) $\geq 1 - \delta$

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: $\Pr\left(R[f] - \hat{R}[f] \geq \varepsilon\right) \leq \exp(-2m\varepsilon^2)$
- Then, substitute $\varepsilon = \sqrt{\frac{\log(1/\delta)}{2m}}$ into the above inequality, we have
- $\Pr\left(R[f] - \hat{R}[f] \geq \sqrt{\frac{\log(1/\delta)}{2m}}\right) \leq \delta$, i.e., $\Pr\left(R[f] - \hat{R}[f] \leq \sqrt{\frac{\log(1/\delta)}{2m}}\right) \geq 1 - \delta$

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

Try to derive the bound on your own!

Mini Summary

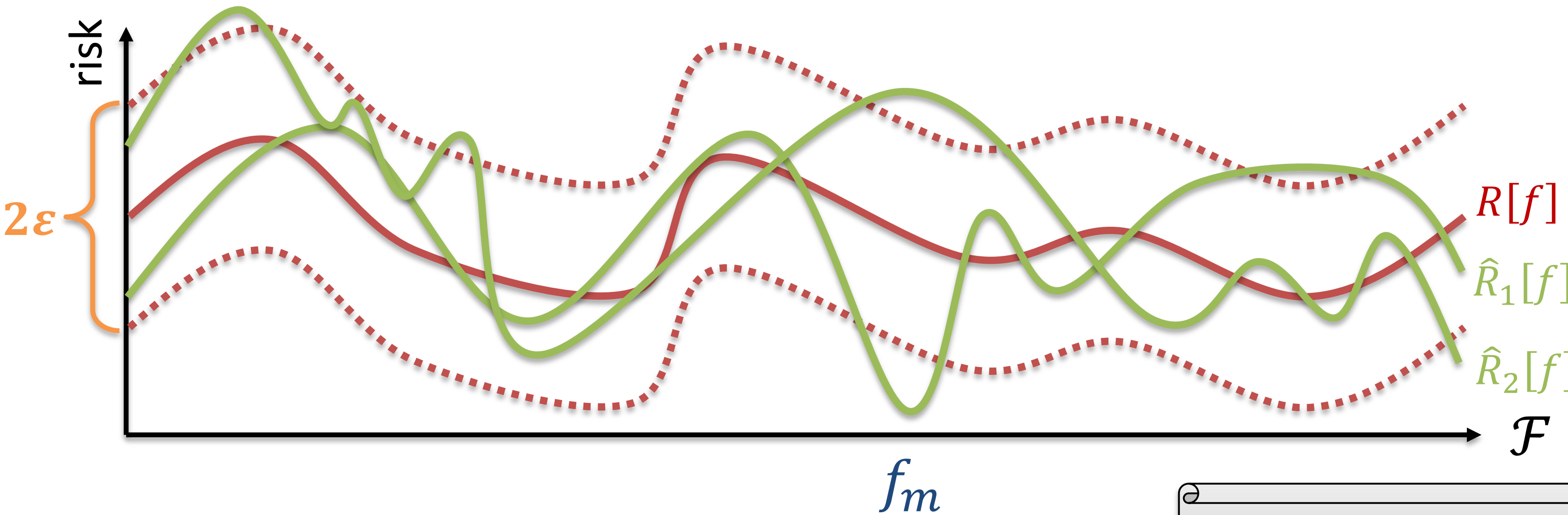
- Goal: Bound true risk of a classifier based on its empirical risk plus “stuff”
- Caveat: Bound is “with high probability” since we could be unlucky with the data
- Approach: Hoeffding’s inequality which bounds how far a mean is likely to be from an expectation

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.*

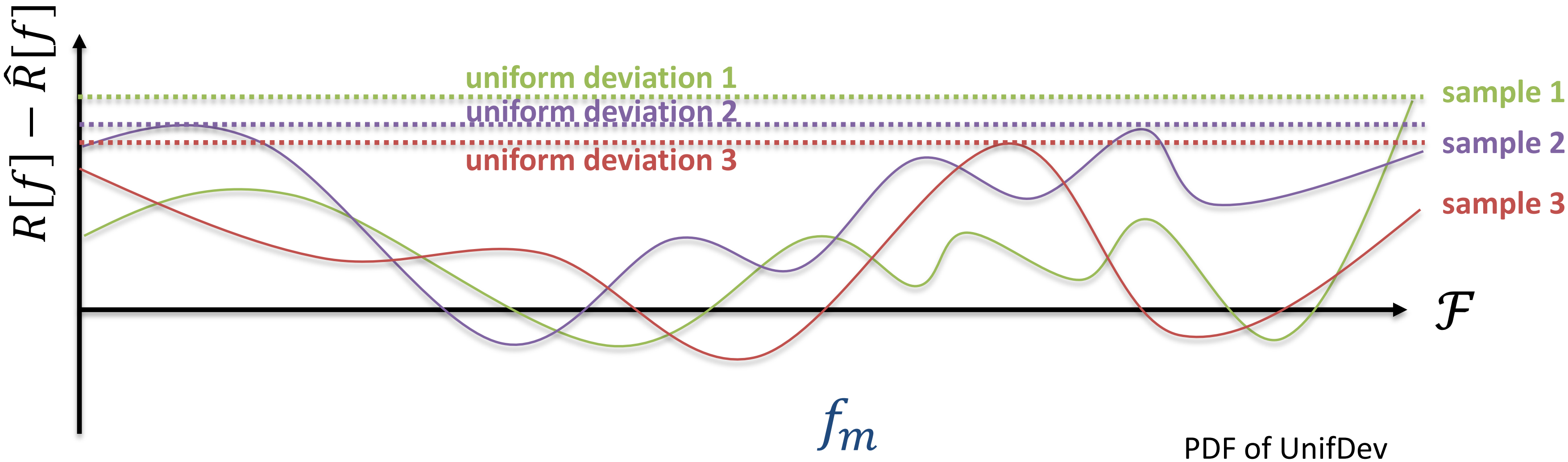
Our bound doesn't hold for $f = f_m$

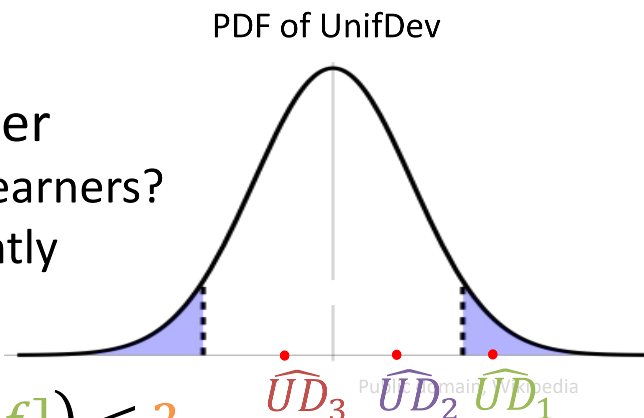


Problematic that f_m depends on data

- 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

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 $\mathcal{F}$

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

  - 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!

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

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 ...

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

Proof:

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

1. We know: $\bigcup_i B_i = \bigcup_i A_i$ (could prove by induction)
2. The B_i are disjoint (empty intersections)
3. We know: $B_i \subseteq A_i$ so $\Pr(B_i) \le \Pr(A_i)$ by monotonicity
4. $\Pr(\bigcup_i A_i) = \Pr(\bigcup_i \mathrm{B}_i) = \sum_i \Pr(B_i) \le \sum_i \Pr(A_i)$

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!