Inductive Principles

Robert C. Williamson* Australian National University

Canberra, 0200 ACT, Australia



(Bowdlerised Edition)

* Joint work with **Ralf Herbrich**, Microsoft Research Cambridge



- Induction (what's "inductive"?)
- Inductive Principles (what's the "principle"?)
- Empirical Risk Minimization
- Key Theorem of Learning Theory
- Conditioning on the Data

After the break, we will move on to the more technical part of the talk ...

- "Conditioning on the data" in a Frequentist (PAC) setting The Luckiness Framework
- A new approach Algorithmic Luckiness

Induction

Hume's problem is how to justify Induction the inference interest of divinity or school (discovery of laws) from empirical datastract reasoning concerning quantity or number? No. Does it contain any experimental reasoning containing matter of fact and existence? No. Commit it then to the flames, for it can

Impossible "for all is but a woven web of guesses". contain nothing but sophistry and illusion.

Popper's key insight: scientific theories do not lead to certain knowledge; merely approximations to the truth. Thus no "justification"

We can, however, reason logically about the process of scientific discovery. Doing so shows one should prefer a more refutable theory over a less refutable one.





- David Hume



[W]e can always construct our machine so that it starts issuing probabilistic predictions only after the 1000th event, say, or after any other number *n* which we may choose, bearing in mind the Based on work by Menger (1924) Popperear gittee to condet for our 'world'. (The problem is so trivial that it is not worth making any effort to solve it ally consider the "dimension" of a the opperational that it is not worth making any effort to solve it Although it is impossible to build a general fearing machine and being able to probabilistically reason about its performance. We will study learning machines, and not induction in general.

Learning Problem

Given:

The players ... threw these abstract formulas at one another displaying the sequences and possibilities of their science.

- Herman Hesse: The Glass Bead Game



• A deterministic learning algorithm $\mathcal{A} : \mathcal{Z}^{(\infty)} \to \mathcal{Y}^{\mathcal{X}}$.

 $(\mathfrak{X} \times \mathfrak{Y})^m = \mathfrak{Z}^m$ drawn iid from \mathbf{P}_{Z} (unknown).

• A training sample $\boldsymbol{z} = (\boldsymbol{x}, \boldsymbol{y}) = (z_1, \dots, z_m)$

• A loss function $l : \mathcal{Y} \times \mathcal{Y} \rightarrow [0, 1]$.

Question: How can one tell whether \mathcal{A} is good or not?







Find a (probabilistic) bound on $R_l[\mathcal{A}(\boldsymbol{z})] := \mathbf{E}_{XY}[l(\mathcal{A}(\boldsymbol{z})(X), Y)]$, that is, a function ψ such that

$$\mathbf{P}_{\mathbf{Z}^{m}}\left(R_{l}\left[\mathcal{A}\left(\mathbf{Z}\right)\right] \leq \psi\left(\mathcal{A},\mathbf{Z},\delta\right)\right) \geq 1-\delta.$$



A bound such as

 $\mathbf{P}_{\mathbf{Z}^{m}}\left(R_{l}\left[\mathcal{A}\left(\mathbf{Z}\right)\right] \leq \psi\left(\mathcal{A},\mathbf{Z},\delta\right)\right) \geq 1{-}\delta$

is not an end in itself; it suggests how to adjust the parameters (or knobs) of the learning algorithm \mathcal{A} .



Thus the *closer* the analysis is to the algorithm the more insightful we would hope it to be.

Difficulty: Given $z \in \mathbb{Z}^m$ how can the algorithm \mathcal{A} choose an hypothesis that achieves a small value of $R_l[\mathcal{A}(z)]$?

Key point: Given $z \in \mathbb{Z}^m$. No chance of computing $R_l[\mathcal{A}(z)]$ even in principle because we do not know P_Z .

A Recipe for Generalisation Error Bounds

1. Relate the prediction error $R_l[h]$ to some empirical quantity, e.g. training error

$$\widehat{R}_{\boldsymbol{l}}\left[h,\boldsymbol{z}\right] := \frac{1}{|\boldsymbol{z}|} \sum_{(\boldsymbol{x},\boldsymbol{y}) \in \boldsymbol{z}} \boldsymbol{l}\left(h\left(\boldsymbol{x}\right),\boldsymbol{y}\right),$$

that converges exponentially to $R_l[h]$ for any h.

- **2.** Apply the basic lemma to the difference of the prediction error and the empirical quantity (training error). This introduces a ghost sample.
- error). This introduces a ghost sample. **3.** Fully exploit the independence assumption of *z* by using a technique known as symmetrisation by permutation: (probability is over double sample Z^{2m})

$$\mathbf{P}_{\mathbf{Z}^{2m}}\left(\Upsilon\left(\mathbf{Z}\right)\right) = \mathbf{E}_{\mathbf{I}}\left[\mathbf{P}_{\mathbf{Z}^{2m}|\mathbf{I}=\mathbf{i}}\left(\Pi_{\mathbf{i}}\left(\Upsilon\left(\mathbf{Z}\right)\right)\right)\right] = \mathbf{E}_{\mathbf{Z}^{2m}}\left[\mathbf{P}_{\mathbf{I}|\mathbf{Z}^{2m}=\boldsymbol{z}}\left(\Pi_{\mathbf{I}}\left(\Upsilon\left(\boldsymbol{z}\right)\right)\right)\right] \,.$$

4. Since $z \in \mathbb{Z}^{2m}$ is fixed, we can construct a cover w.r.t. the loss l and apply the union bound.





Possibility of computing such bounds motivates: Empirical Risk Minimization Algorithm

$$\begin{aligned} \mathcal{A}_{\mathrm{erm}}^{\mathcal{H}} &: \quad \mathcal{Z}^{(\infty)} \to \mathcal{H} \subseteq \mathcal{Y}^{\mathcal{X}} \\ \mathcal{A}_{\mathrm{erm}}^{\mathcal{H}} &: \quad \boldsymbol{z} \mapsto \arg\min_{h \in \mathcal{H}} \widehat{R}_{l} \left[h, \boldsymbol{z} \right] . \end{aligned}$$

This is a great algorithm to analyse.

-Ralf Herbrich



The "principle" is to minimize the empirical surrogate $\widehat{R}_{\text{Huls}}$, $\widehat{d}_{\text{ependin}} \stackrel{\text{bls}}{=} \widehat{d}_{\text{pendin}} \stackrel{\text$

Note that the algorithm $\mathcal{A}_{erm}^{\mathcal{H}}$ has one "knob": the class of functions \mathcal{H} .

How to choose \mathcal{H} ? Want \mathcal{H} as large as possible to ensure a good approximation of the underlying data generating process. Pay a price . . .



Question: Does $\mathcal{A}_{erm}^{\mathcal{H}}$ "work"? **More precise question:** Is $\mathcal{A}_{erm}^{\mathcal{H}}$ consistent?

Assume that \mathcal{H} and l are such that for any $\boldsymbol{z} \in \mathcal{Z}^m$

$$\widehat{R}_{l}\left[\mathcal{A}_{\mathrm{erm}}^{\mathcal{H}}(\boldsymbol{z}), \boldsymbol{z}\right] = \inf_{\boldsymbol{h}\in\mathcal{H}} \widehat{R}_{l}\left[\boldsymbol{h}(\boldsymbol{z}), \boldsymbol{z}\right]$$

and that for all $h \in \mathcal{H}$, $A \leq R_l[h] \leq B$. Let

 $\mathcal{H}(c) := \{h \in \mathcal{H} \colon R_l[h] \ge c\}.$

Say that $\mathcal{A}_{erm}^{\mathcal{H}}$ is *strictly (nontrivially) consistent* if for all $c \geq 0$, for all $\varepsilon > 0$,

$$\lim_{m\to\infty} \mathbf{P}_{\mathbf{Z}^m} \left(\left| \widehat{R}_l \left[\mathcal{A}_{emp}^{\mathcal{H}(c)}(\boldsymbol{z}), \boldsymbol{z} \right] - c \right| > \varepsilon \right) = 0.$$

Need a definition like this to rule out "coding" the identity of a function into one observation: can construct such artificial function classes of arbitrary complexity which can be learned using $\mathcal{A}_{erm}^{\mathcal{H}}$ with only one observation.



$$\begin{aligned} & \mathcal{A}_{\text{erm}}^{\mathcal{H}} \text{ is strictly consistent} \\ \Leftrightarrow \\ & \forall \varepsilon > 0 \quad \lim_{m \to \infty} \mathbf{P}_{\mathbf{Z}^m} \left\{ \sup_{h \in \mathcal{H}} \left(R[h] - \widehat{R}_l[h, \mathbf{z}] \right) > \varepsilon \right\} = 0 \\ & \star \\ & \forall \varepsilon > 0 \quad \lim_{m \to \infty} \mathbf{P}_{\mathbf{Z}^m} \left\{ \sup_{h \in \mathcal{H}} \left| R_l[h] - \widehat{R}_l[h, \mathbf{z}] \right| > \varepsilon \right\} = 0 \\ & \leftrightarrow \\ & \forall \varepsilon > 0 \quad \lim_{m \to \infty} \frac{1}{m} \mathbf{E}_{\mathbf{Z}^m} \log \underbrace{\mathcal{N}(\varepsilon, \mathcal{H}, \ell_1(\mathbf{z}))}_{\substack{\text{Covering number of } \mathcal{H} \text{ at scale } \varepsilon}_{\substack{\text{w.r.t. ot bh } \ell_1(\mathbf{z}) \text{ metric: for } h \in \\ \mathcal{H}, \|h\|_{\ell_1(\mathbf{z})} := \frac{1}{m} \sum_{z \in \mathbf{z}} |h(z)|. \end{aligned}$$

The effective gap in the reasoning implicit in the difference between \star and $\star\star$ can be plugged using a more complex notion of cover — a one sided bracket cover. I am unaware of any results on the relative sizes of such covering numbers compared to $\mathcal{N}(\varepsilon, \mathcal{H}, \ell_1(\boldsymbol{z}))$.



The big deal is that (modulo the small gap mentioned)

 $\mathbf{E}_{\mathbf{Z}^m} \log \mathcal{N}\left(\varepsilon, \mathcal{H}, \ell_1(\boldsymbol{z})\right)$

is the "right" quantity to study for understanding the effect of the \mathcal{H} knob on $\mathcal{A}_{erm}^{\mathcal{H}}$. (Why it is worth fussing with strict consistency.)

Thus we know how to understand the effect of the "knob" \mathcal{H} .

Note it is impossible to compute (even in principle) since we do not know P_{Z^m} (the distribution from which z is drawn).

Can upper bound by $\sup_{\boldsymbol{z} \in \mathbb{Z}^m} \log \mathcal{N}(\varepsilon, \mathcal{H}, \ell_1(\boldsymbol{z}))$ which can be effectively bounded.

Leads to "generalization bounds" of the form: for $\boldsymbol{z} \in \mathbb{Z}^m$

$$\mathbf{P}_{\mathbf{Z}^{m}}\left(R_{l}\left[\mathcal{A}_{\mathrm{erm}}^{\mathcal{H}}\left(\mathbf{Z}\right)\right] \leq \psi_{l}\left(\mathcal{H},\mathbf{Z},\delta\right)\right) \geq 1-\delta\,.$$



"ERM is strictly consistent iff covering numbers behave nicely"

Observe that whilst we set out to understand the behaviour of $\mathcal{A}_{erm}^{\mathcal{H}}$ our bounds are in fact for

$$\mathcal{A}_{\text{worst}}^{\mathcal{H}} := \boldsymbol{z} \mapsto \arg \max_{h \in S(\mathcal{H}, \boldsymbol{z})} R_l[h]$$

where

$$S(\mathcal{H}, \boldsymbol{z}) = \left\{ h \in \mathcal{H} \colon \widehat{R}_{l}[h, \boldsymbol{z}] = \widehat{R}_{l}[\mathcal{A}_{\mathrm{erm}}^{\mathcal{H}}, \boldsymbol{z}] \right\}.$$

Consequently the bounds are very loose.

Furthermore $\mathcal{A}_{erm}^{\mathcal{H}}$ could perform as poorly as $\mathcal{A}_{worst}^{\mathcal{H}}$ (what is there to stop it?). **Conclusion:** behaviour of covering numbers is the crucial quantity for this inductive principle (algorithm). Suggests to make \mathcal{H} as small as possible.



An obvious difficulty with $\mathcal{A}_{erm}^{\mathcal{H}}$ is that if one chooses \mathcal{H} badly, the algorithm has no hope of approximating the data.

Suppose for $\boldsymbol{z} \in \mathbb{Z}^m$, we know

$$\mathbf{P}_{\mathbf{Z}^{m}}\left(R_{l}\left[\mathcal{A}_{\mathrm{erm}}^{\mathcal{H}}\left(\mathbf{Z}\right)\right] \leq \psi_{l}\left(\mathcal{H},\mathbf{Z},\delta\right)\right) \geq 1-\delta\,.$$

Given a sequence of nonnegative numbers $\delta = (\delta_i)_{i \in \mathbb{N}}$ such that $\sum_i \delta_i = \delta$ and a sequence of hypothesis classes $\mathcal{H} = (\mathcal{H}_i)_{i \in \mathbb{N}}$

$$egin{aligned} &i^* = i^*(oldsymbol{z},oldsymbol{\mathcal{H}},oldsymbol{\delta},\psi) \ := \ rg\min_{i\in\mathbb{N}}\psi_{oldsymbol{l}}(oldsymbol{\mathcal{H}}_i,oldsymbol{z},\delta_i) \ &\mathcal{A}^{oldsymbol{\mathcal{H}},oldsymbol{\delta}}_{\mathrm{srm}}(oldsymbol{z}) \ := \ \mathcal{A}^{oldsymbol{\mathcal{H}}_{i^*}}_{\mathrm{erm}}(oldsymbol{z}). \end{aligned}$$



By the definition of $\mathcal{A}_{\text{srm}}^{\mathcal{H},\delta}$ it comes with a performance bound already. For $i \in \mathbb{N}$, with probability at least $1 - \delta_i$ over a random draw of \boldsymbol{z} ,

$$R\left[\mathcal{A}_{\mathrm{erm}}^{\mathcal{H}_{i}}(\boldsymbol{z})\right] \leq \psi_{l}(\mathcal{H}_{i}, \boldsymbol{z}, \delta_{i})$$

Thus the union bound ensures that with probability at least $1 - \delta$ over a random draw of \boldsymbol{z} , for all $i \in \mathbb{N}$

$$R\left[\mathcal{A}_{\mathrm{erm}}^{\mathcal{H}_{i}}(\boldsymbol{z})\right] \leq \psi_{l}(\mathcal{H}_{i}, \boldsymbol{z}, \delta_{i})$$

and thus with probability at least $1 - \delta$ over a random draw of \boldsymbol{z} ,

$$R\left[\mathcal{A}_{\mathrm{srm}}^{\mathcal{H},\boldsymbol{\delta}}(\boldsymbol{z})\right] \leq \psi_{l}(\mathcal{H}_{i^{*}},\boldsymbol{z},\delta_{i^{*}}) \qquad \boldsymbol{\wedge}$$

Algorithm Independence of Bound

Classical bound takes form: with probability at least $1 - \delta$ over a random draw of $\boldsymbol{z} \in \mathbb{Z}^m$ according to $P_{\mathbb{Z}^m}$,

$$R_l[\mathcal{A}_{\mathrm{erm}}^{\mathcal{H}}(\boldsymbol{z})] \leq \psi(\mathcal{H}, \boldsymbol{z}, \delta).$$

Thus *any* algorithm

for which
$$\widehat{R}_{l}[\mathcal{A}_{any}^{\mathcal{H}}(\boldsymbol{z}), \boldsymbol{z}] = 0$$
 has the same bound on performance.

 $\mathcal{A}_{\mathrm{anv}}^{\mathcal{H}} \colon \mathcal{Z}^m \to \mathcal{H}$

This is good because one gets a general theory.

It is *bad* because the same bound holds for the *worst* algorithm.

Bayesians would say the problem is that we are not *conditioning on the data*.





"You must condition on the data!"

Why Conditioning on the Data is Important

That bayesians and frequentists are willing to discuss these matters is an important first step toward developing a theory that synthesizes both unconditional and conditional inference.

— George Casella (1988)





Why condition — a simple example. Suppose $X = (X_1, X_2), X_1, X_2$ iid according to

$$\mathbf{P}_{\boldsymbol{\theta}}(X_i = \boldsymbol{\theta} - 1) = \mathbf{P}_{\boldsymbol{\theta}}(X_i = \boldsymbol{\theta} + 1) = \frac{1}{2}$$

for $-\infty < \theta < \infty$

Consider the "confidence procedure"

$$C(x) := \begin{cases} \frac{x_1 + x_2}{2} & \text{if } |x_1 - x_2| = 2\\ x_1 - 1 & \text{if } |x_1 - x_2| = 0 \end{cases}$$

where $x = (x_1, x_2)$. Can check that

 $\mathbf{P}_{\boldsymbol{\theta}}(C(X) \text{ contains } \boldsymbol{\theta}) = 0.75 \quad \forall \boldsymbol{\theta}$

so we would be happy using C(X) according to standard frequentist notions of acceptability.





But after one sees the data:

If
$$|x_1 - x_2| = 2$$
 know *for certain* that $\theta \in C(X)$

If $|x_1 - x_2| = 0$, equally unsure whether $\theta = x_1 - 1$ or $x_1 + 1$.

Statisticians have expended considerable effort to develop procedures that have frequentist guarantees of performance *and* which can condition on the data to exploit a lucky observation.

Bayesian methods intrinsically condition on the data, but offer no frequentist guarantees of performance (most Bayesians would say this is no problem because such guarantees are neither necessary nor useful).

Many subtleties. To date really only for simple parameter estimation.

Something like this is needed in order to provide frequentist guarantees of performance for learning algorithms that do more than merely minimize and empirical risk functional. If there exists one separating hyperplane then there exist many Maximum Margin Classifier: $\mathcal{H}_i(\boldsymbol{z})$ comprises on type two not choose the optimal one? planes $h_{\mathbf{w}}$ achieving margin $\gamma_{\boldsymbol{z}}(h_{\mathbf{w}}) = \gamma_i$ on \boldsymbol{z} . Here -Vladimir Vapnik

$$\gamma_{\boldsymbol{z}}(h_{\mathbf{w}}) := \max_{(x_i, y_i) \in \boldsymbol{z}} y_i \langle \mathbf{w}, x_i \rangle / \| \mathbf{w} \|.$$

For linear hyperplanes, the risk bound is of the form

$$\psi(i) \le \frac{c}{\gamma_i^2} \log^2(m) + c \log(1/\delta).$$

Maximum Margin algorithm: For \mathcal{H} the set of linear hyperplanes.

 $\mathcal{A}_{\mathrm{MM}} := \boldsymbol{z} \mapsto \arg \max_{h \in \mathcal{H}} \gamma_{\boldsymbol{z}}(h)$

("Optimal" only in the sense that it optimizes the particular ψ function used.) Try to understand \mathcal{A}_{MM} as an instance of $\mathcal{A}_{srm}^{\mathcal{H},\delta}$.









New algorithm: *Penalize complexity of* $\mathcal{H}(\boldsymbol{z})$ *as if independent of* \boldsymbol{z} . Consider $\mathcal{H}(\boldsymbol{z}) = (\mathcal{H}_i(\boldsymbol{z}))_i$. Suppose for data-independent \mathcal{H}_i and $h_{emp}^i = \mathcal{A}_{erm}^{\mathcal{H}_i}(\boldsymbol{z})$ have a bound

$$R_l[h_{ ext{emp}}^i] \le \psi(\mathcal{H}, \boldsymbol{z}, \delta_i) =: \chi(i)$$

Let

$$i^* := rg\min_i \chi(i)$$
 $\mathcal{A}_{\mathrm{dsrm}}^{\mathcal{H}(\boldsymbol{z}), \boldsymbol{\delta}}(\boldsymbol{z}) := \mathcal{A}_{\mathrm{erm}}^{\mathcal{H}_{i^*}(\boldsymbol{z})}(\boldsymbol{z})$

Gist: penalize complexity ignoring data-dependence; apply SRM.

Problem: how to rigorously justify?

How to conceptualize what's going on?



Can not strictly justify the algorithm as an unapplications "Of make more conclusive sounding statements than they would for "unlucky outcomes". — Jack Kieffer: Conditional Confidence Statements ... 1977

If as well as $\widehat{R}_{l}[h, \mathbf{z}] = 0$ we have $\gamma_{\mathbf{z}}(h) = \gamma \gg 0$, then $R_{l}[h]$ is small.



We are *lucky* if our data is like this.

We want to condition on the data like Bayesians do.

Would like to capture this notion in a general formal way.

BREAK

Have covered

- Induction (what's "inductive"?)
- Inductive Principles (what's the "principle"?)
- Empirical Risk Minimization
- Key Theorem of Learning Theory
- Conditioning on the Data

Yet to come:

- "Conditioning on the data" in a Frequentist (PAC) setting The Luckiness Framework
- A new approach Algorithmic Luckiness

Robert C Williamson: Inductive Principles — Machine Learning Summer School, Canberra. February 2002

Luckiness

I should be so lucky; lucky, lucky, lucky, I should be so lucky in love.



The margin $\gamma_{\boldsymbol{z}}(h_{\mathbf{w}})$ measures how *lucky* $h_{\mathbf{w}}$ is on \boldsymbol{z} . In general $L: \mathfrak{H} \times \mathfrak{Z}^m \to \mathbb{R}$. Would like a bound that says with probability at least $1 - \delta$ over a random draw of \boldsymbol{z} according to $\mathbf{P}_{\mathbf{Z}^m}$ if $\widehat{R}_l[h, \boldsymbol{z}] = 0$ and $\omega(L(h, \boldsymbol{z}), \delta) \leq 2^d$ then

 $R_{l}[h] \le \psi(m, \mathbf{d})$

The parameter *d* is an *effective complexity*.

There needs to be some restrictions on L: if we "use up" all of the information in the sample estimating its luckiness there is "none left" to estimate $R_l[h]$. A bound like \diamondsuit is a bound for the algorithm

$$\mathcal{A}_{\text{lucky}}^{L,\mathcal{H}} := \boldsymbol{z} \mapsto \arg\min_{h \in \mathcal{H}} \psi(m, \log \omega(L(h, \boldsymbol{z}), \delta))$$



Luckiness (continued)

Given a *luckiness function* $L \colon \mathcal{H} \times \mathcal{Z}^m \to \mathbb{R}$, the *level* is

 $\ell_L(h, \mathbf{z}) := |\{ (l(g(x_i), y_i))_{i=1}^m : L(g, \mathbf{z}) \ge L(h, \mathbf{z}) \} |,$

the number of dichotomies induced on z by functions at least as lucky as h. Require L to be well behaved:

L is *probably smooth* w.r.t. $\omega \colon \mathbb{R} \times (0, 1] \to \mathbb{N}$ if for all $m \in \mathbb{N}$ all distributions $\mathbf{P}_{\mathbf{Z}}$ and all $\delta \in (0, 1]$

 $\mathbf{P}_{\mathbf{Z}^{2m}}(\exists h \in \mathfrak{H} \colon \ell_L(h, \mathbf{Z}_{[1:2m]}) > \omega(L(h, \mathbf{Z}_{[1:m]})), \delta)) \leq \delta \; .$

If *L* is probably smooth w.r.t. ω , $\delta = (\delta_i)_i$, $\sum_i \delta_i = \delta$, with probability at least $1 - \delta$ over a random draw of \boldsymbol{z} , if $\widehat{R}_l[h, \boldsymbol{z}] = 0$ and $\omega(L(h, \boldsymbol{z}), \delta_d/4) \leq 2^d$ then

 $R_{l}[h] \leq \frac{2}{m} \left(d + \log_2(4/\delta_d) \right) \qquad \heartsuit$

Effectively $\mathcal{H}(\boldsymbol{z}) = (\mathcal{H}_i(\boldsymbol{z}))_i$ with $\mathcal{H}_i(\boldsymbol{z}) = \{h \in \mathcal{H} : \omega(L(h, \boldsymbol{z}), \delta_i/4) \le 2^i\}.$



Comments on Luckiness

- Can put \mathcal{A}_{MM} into this framework.
- The luckiness function L is how we *encode our prior knowledge*. We weight with δ_i the *i*th data-dependent hypothesis class

 $\mathcal{H}_{i}(\boldsymbol{z}) = \left\{ \boldsymbol{h} \in \mathcal{H} \colon \omega(L(\boldsymbol{h}, \boldsymbol{z}), \delta_{i}/4) \leq 2^{i} \right\}$

- Key practical difficulty is showing L is probably smooth w.r.t. a "good" ω the smaller the ω the tighter \heartsuit is.
- **Problem:** Still do not pay enough attention to the algorithm, which motivates . . .





Algorithmic Luckiness — Foundation



It is possible to prove a basic lemma for algorithms which means that the symmetrisation by permutation step only considers all hypotheses that can be learned using \mathcal{A} . Basic lemma says:

$$\mathbf{P}_{\mathbf{Z}^{m}}\left(R_{l}\left[\mathcal{A}\left(\mathbf{Z}\right)\right]-\widehat{R}_{l}\left[\mathcal{A}\left(\mathbf{Z}\right),\mathbf{Z}\right]>\varepsilon\right)<$$



$$2 \cdot \mathbf{P}_{\mathbf{Z}^{2m}} \left(\widehat{R}_l \left[\mathcal{A} \left(\mathbf{Z}_{[1:m]} \right), \mathbf{Z}_{[(m+1):2m]} \right] - \widehat{R}_l \left[\mathcal{A} \left(\mathbf{Z}_{[1:m]} \right), \mathbf{Z}_{[1:m]} \right] > \frac{\varepsilon}{2} \right)$$

Again, we introduce an ordering between the at most (2m)! hypotheses using an algorithmic luckiness $L(\mathcal{A}, \mathbf{z})$. This gives

$$egin{aligned} &\mathcal{H}\left(\mathcal{A},L,oldsymbol{z}
ight) \, := \, \left\{ oldsymbol{\mathcal{A}}\left(\Pi_{\mathbf{i}}\left(oldsymbol{z}
ight)_{[1:m]}
ight) \, \mid \mathbf{i}\in \mathbb{J}\left(\mathcal{A},L,oldsymbol{z}
ight)
ight\} \,, \ &\mathcal{J}\left(\mathcal{A},L,oldsymbol{z}
ight) \, := \, \left\{ \mathbf{i} \, \left| \, L\left(oldsymbol{\mathcal{A}},\Pi_{\mathbf{i}}\left(oldsymbol{z}
ight)_{[1:m]}
ight) \geq L\left(oldsymbol{\mathcal{A}},oldsymbol{z}_{[1:m]}
ight)
ight\} \,. \end{aligned}$$





Consider the simple case of m = 2. Consider all the hypotheses generated by \mathcal{A} and take $\mathcal{H}(\mathcal{A}, L, \mathbf{z})$ to be those so generated that are at least as lucky as $\mathcal{A}((z_1, z_2))$ where the luckiness is measured on (z_1, z_2) .



Need to be able to bound the covering number \mathcal{N} of hypotheses $h \in \mathcal{H}(\mathcal{A}, L, \mathbf{z})$ on the double sample \mathbf{z} only using the luckiness on the first half, i.e. the training sample.

 $\begin{array}{l} \omega - \text{smallness of } L: \ Given \ an \ algorithm \ \mathcal{A} \ and \ a \\ loss \ l, \ the \ algorithmic \ luckiness \ L \ is \ \omega - small \ at \\ \mathsf{Scale} \ \tau, \ \mathsf{If for \ all'} \delta \end{array} \right) < \delta \ . \end{array}$

To prove this property we can only exploit that $P_{Z^{2m}}$ is a product measure.





Algorithmic Luckiness — Main Result



Algorithmic Luckiness Bound: For all [0, 1]-valued loss functions l, for all ω -small algorithmic luckiness functions L w.r.t. \mathcal{A} , for all τ , with probability at least $1 - \delta$ over $\boldsymbol{z} \in \mathbb{Z}^m$,

And the winner is ... Lucky! — Britney Spears

) +
$$4\tau$$

$$R_{l}\left[\mathcal{A}\left(\boldsymbol{z}\right)\right] \leq \widehat{R}_{l}\left[\mathcal{A}\left(\boldsymbol{z}\right),\boldsymbol{z}\right] + \sqrt{\frac{8}{m}}\left(\left\lceil d \right\rceil + \log_{2}\left(\frac{4m}{\delta}\right)\right) + 4\tau$$

where $d = \log \left(\omega \left(L(\mathcal{A}, \boldsymbol{z}), \frac{\delta}{4m}, \tau \right) \right)$. If l is $\{0, 1\}$ -valued, then whenever $\mathcal{A}(\boldsymbol{z})$ has zero training error, $\widehat{R}_l \left[\mathcal{A}(\boldsymbol{z}), \boldsymbol{z} \right] = 0$, for $\tau = 1/2m$

$$R_{l}\left[\mathcal{A}\left(\boldsymbol{z}\right)\right] \leq \frac{2}{m}\left(\left\lceil d \right\rceil + \log_{2}\left(\frac{4m}{\delta}\right)\right).$$

Application — Classical VC Setting



If $\mathcal{A} : \mathcal{Z}^{(\infty)} \to \mathcal{Y}^{\mathcal{X}}$ maps to a hypothesis space $\mathcal{H} \subseteq \mathcal{Y}^{\mathcal{X}}$, we know that \mathcal{V}^{C} -dimension is not most important quantity. - Vladimir Vapnik: Dagstuhl, Germany (July 2001)

$$\mathcal{H}(\mathcal{A}, L, \boldsymbol{z}) \subseteq \mathcal{H}$$

regardless of \boldsymbol{z} and L.



Thus, for the zero-one loss $l(\hat{y}, y) = \mathbb{I}_{\hat{y}\neq y}$ the growth function is an upper bound on $\mathcal{N}\left(|\boldsymbol{z}|^{-1}, \mathcal{H}(\mathcal{A}, L, \boldsymbol{z}), \ell_{l,1}(\boldsymbol{z})\right)$ and can thus serve as a ω function.

Neither the serendipity of the sample nor the properties of the algorithm \mathcal{A} have been exploited!

As is widely known, this results in bounds which are quite loose.



I used to be God... — Manfred Warmuth: Dagstuhl, Germany (2001)

Sparsity luckiness: If $\mathcal{A} : \mathbb{Z}^{(\infty)} \to \mathcal{Y}^{\mathfrak{X}}$ is a compression scheme, that is, $\mathcal{A}(\mathbf{z}) = \mathcal{R}(\mathfrak{C}(\mathbf{z}))$, then

 $L_{ ext{sparse}}\left(\mathcal{A}, \boldsymbol{z}
ight) := -\left|\mathfrak{C}\left(\boldsymbol{z}
ight)
ight|$

is ω -small at any scale τ , where

$$\omega\left(\boldsymbol{L},\boldsymbol{\delta},\tau\right) = \left(\frac{2em}{-L}\right)^{-L}$$

Plugging this result into \clubsuit gives a new compression result for regression as well as resembling the original result of Littlestone and Warmuth (1986).





Since we only have to consider permutations $\Pi_{\mathbf{i}}$ where

$$\left| \mathcal{C} \left(\Pi_{\mathbf{i}} \left(\boldsymbol{z} \right)_{[1:m]} \right) \right| \leq \left| \mathcal{C} \left(\boldsymbol{z}_{[1:m]} \right) \right| =: -L_0$$

we know that the permutation invariant reconstruction function \mathcal{R} never uses more than $-L_0$ examples.

The number of different choices of no more than $-L_0$ examples out of 2m (double sample size) is given by

$$\sum_{i=0}^{-L_0} \binom{2m}{i} \le \left(\frac{2em}{-L_0}\right)^{-L_0}$$

You must be my lucky star ... But I'm the luckiest by far. — Madonna





Robert C Williamson: Inductive Principles — Machine Learning Summer School, Canberra, February 2002

Application — Kernel Classifiers

Consider learning algorithms for kernel classifiers, that is,

 $\mathfrak{H}_{\boldsymbol{\phi}} := \left\{ \boldsymbol{x} \mapsto \left\langle \boldsymbol{\phi} \left(\boldsymbol{x} \right), \boldsymbol{w} \right\rangle \; | \; \boldsymbol{w} \in \mathfrak{K} \right\} \;, \qquad \boldsymbol{\phi} : \mathfrak{X} \to \mathfrak{K} \subseteq \ell_2^n \,.$

Assume that the learning algorithms $\ensuremath{\mathcal{A}}$ have the property that

$$\mathcal{A}: \boldsymbol{z} = (\boldsymbol{x}, \boldsymbol{y}) \mapsto \langle \boldsymbol{\phi}(\boldsymbol{x}), \mathbf{w}_{\boldsymbol{z}} \rangle \text{ where } \mathbf{w}_{\boldsymbol{z}} = \sum_{x_i \in \boldsymbol{x}} \hat{\alpha}_i \boldsymbol{\phi}(x_i) \text{ and } \|\mathbf{w}_{\boldsymbol{z}}\| = 1.$$

Examples are SVMs, BPMs and the perceptron algorithm.

Let the (normalised) margin $\Gamma(z)$ be defined by

$$\Gamma(\boldsymbol{z}) := \min_{(x_i, y_i) \in \boldsymbol{z}} \frac{y_i \langle \boldsymbol{\phi}(x_i), \mathbf{w}_{\boldsymbol{z}} \rangle}{\|\boldsymbol{\phi}(x_i)\| \cdot \|\mathbf{w}_{\boldsymbol{z}}\|}$$





Application — Kernel Classifiers (cont.)



Margin Luckiness: Let $\varepsilon_i(\mathbf{x})$ be the smallest $\epsilon > 0$ such that $\{\phi(x_1), \ldots, \phi(x_m)\}$ can be covered by at most i balls of radius less than or equal to ϵ . For the loss $l(\hat{y}, y) = \mathbb{I}_{y\hat{y} \leq 0}$, the luckiness function



$$L_{\text{margin}}\left(\mathcal{A}, \boldsymbol{z}\right) = -\min\left\{i \in \mathbb{N} \mid i \geq \left(\frac{\varepsilon_{i}\left(\boldsymbol{x}\right)\sum_{j=1}^{m} |\hat{\alpha}_{j}|}{\Gamma\left(\boldsymbol{z}\right)}\right)^{2}\right\}$$

is ω -small at scale 1/2m where

$$\omega\left(\boldsymbol{L},\delta,1/2m\right) = \left(\frac{2em}{-L}\right)^{-2L}$$

The bound comprises 3 main terms: *margin* $\Gamma(\boldsymbol{z})$, *sparsity surrogate* $\sum_{j=1}^{m} |\hat{\alpha}_j|$ and a factor depending on the *distribution of the data* $\varepsilon_i(\boldsymbol{x})$.



The sequence $(\varepsilon_i(\boldsymbol{x}))_i$ measures how clumpy the data is.

A small number of small clumps means $\varepsilon_i(\boldsymbol{x})$ is small for small *i*.

Compare with the idea of "kernel alignment".





Makovoz theorem shows that for all $z \in \mathbb{Z}^m$ there exists a weight vector $\tilde{\mathbf{w}} = \sum_{i=1}^m \tilde{\alpha}_i \boldsymbol{\phi}(x_i)$ such that

$$\left\|\tilde{\mathbf{w}} - \mathbf{w}_{\boldsymbol{z}}\right\|^2 \le \Gamma^2\left(\boldsymbol{z}\right)$$

and $\| \tilde{\boldsymbol{\alpha}} \|_0 \leq -L_{ ext{margin}} \left(\boldsymbol{\mathcal{A}}, \boldsymbol{z} \right) =: -L_0.$



It follows that
$$\langle \mathbf{w}_{\boldsymbol{z}}, \tilde{\mathbf{w}} / \| \tilde{\mathbf{w}} \| \rangle \geq \sqrt{1 - \Gamma^2(\boldsymbol{z})}$$
; that is, $\tilde{\mathbf{w}}$ still correctly classifies \boldsymbol{z} .

For every of the no more than $\left(\frac{2em}{-L_0}\right)^{-L_0}$ many subsamples $\tilde{z} \subseteq z$, \tilde{w} lives in a space of dimension no more than $-L_0$. By an application of the growth function bound, each \tilde{w} can achieve no more than $\left(\frac{2em}{-L_0}\right)^{-L_0}$ many dichotomies on z.

Discussion Discussion



Algorithmic luckiness framework differs from classical statistical learning theory aproaches in that it does not use the crude step of viewing algorithms just in terms of their hypothesis space.

Generalization of standard VC results. Get agnostic and realizable bounds.

Example of maximum margin algorithm illustrates that the framework has the power to develop new insights into what makes algorithms perform well.

Main point is that it provides new theoretical tools for understanding algorithms "smarter" that Empirical Risk Minimization.

Hope is that by analysing algorithms in this (or related) ways, will be able to better discern the features about particular learning problems that make them easy or difficult.

References and Slides



Jack Kiefer, "Conditional Confidence Statements and Confidence Estimators," *Jouranl of the American Statistical Association*, **72**(360), pp. 789–827, (1977).

ames Berger, "The Frequentist Viewpoint and Conditioning", pp 5–44 in *Proceedings of the Berkeley Conference in Honour of Jerzy Veyman and Jack Kiefer*, Volume 1, Wadsworth, (1985).

George Casella, "Conditionally Acceptable Frequentist Solutions," pp. 73–117 in *Statistical Decision Theory and Related Topics IV*, Springer, New York (1988).

ohn Shawe-Taylor, Peter L. Bartlett, Robert C. Williamson and Martin Anthony, "Structural Risk Minimization over Data-Dependent Hierarchies," *IEEE Transactions on Information Theory*, **44**(5), 926–1940, (1998). http://axiom.anu.edu.au/~williams/papers/P85.ps

Ralf Herbrich, Learning Kernel Classifiers, MIT Press, (2002).

Ralf Herbrich and Robert C. Williamson, "Algorithmic Luckiness" ubmitted to *Journal of Machine Learning Research* (December 2001) http://axiom.anu.edu.au/~williams/papers/P159.ps.gz

Ralf Herbrich and Robert C. Williamson, "Learning and Generalization: Theoretical Bounds" to appear in Michael Arbib (Ed.) *Handbook of Brain Theory and Neural Networks*, 2nd Edition, MIT Press, (2002). http://axiom.anu.edu.au/~williams/papers/P158.ps.gz

Slides at http://axiom.anu.edu.au/~williams/papers/P156.pdf