Introduction to the Theory of Machine Learning To Trust Models or Not To Trust Models

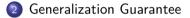
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IIIT Surat

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Outline





Occam's Razor

4 No Free Lunch



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 $x \in \mathcal{X}$ is a datapoint eg. a photo

 $y \in \mathcal{Y}$ is the label eg. Cat or Dog

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*The regression, we need to worry about the rain though.

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Does low Empirical Error imply low Test Error?

What we can see: $err_{S}(h)$

Error on training set

We can calculate it

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Expected error on new data We can't calculate it directly

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Expected error on new data We can't calculate it directly This is what we really care about!

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To Trust a Model or Not To Trust a Model?

If we have a PAC algorithm A, we can **trust*** a model *h* generated by it

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ERM to PAC

When can we say $\operatorname{err}_{\mathcal{D}}(h) < \epsilon$ with probability $1 - \delta$?

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^athat samples are drawn i.i.d. from a fixed, unknown ${\cal D}$



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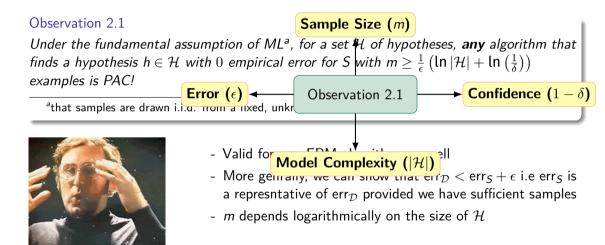
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- More genrally, we can show that $err_D < err_S + \epsilon$ i.e err_S is a representative of err_D provided we have sufficient samples
- m depends logarithmically on the size of ${\cal H}$



Observation 3.1 (Simplified Sample Complexity Bound)

 $h \in \mathcal{H}$ with $\operatorname{err}_{S}(h) = 0 \rightarrow \operatorname{err}_{\mathcal{D}}(h) < \epsilon$, provided S had $m \geq \frac{\ln |\mathcal{H}|}{\epsilon}$ samples.

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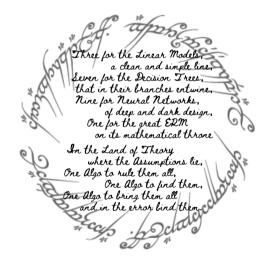
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- Simpler models (smaller $|\mathcal{H}|)$ are easier to work with and they provide better generalization



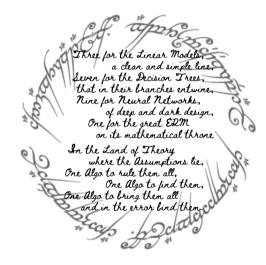


ERM: the master algorithm for ML?



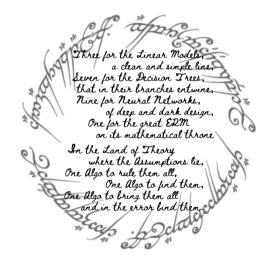
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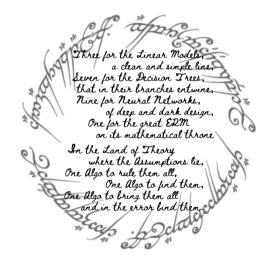


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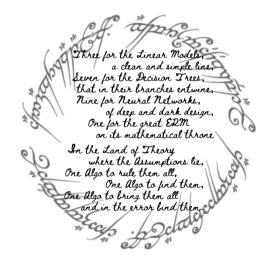
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Except it is not...

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Every algorithm makes a bet on the nature of the problem

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No Free Lunch Theorem (Informal)

For any learning algorithm A, there exists a distribution D on which it performs poorly. Averaged over all D, the performance of any two algorithms is **exactly the same**.

Complete Inductive Bias (Hardcoded System)

Zero Inductive Bias (Generic Learner)

Expert Systems

Complete Inductive Bias (Hardcoded System)

Zero Inductive Bias (Generic Learner)

Noam Chomsky: The ability to learn grammars is hard-wired into the brain. It is not possible to "learn" linguistic ability — rather, we are born with it.



Expert Systems

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Geoff Hinton: There exists some "universal" learning algorithm that can learn anything: language, vision, speech, etc. The brain is based on it, and we're working on uncovering it.

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Zero Inductive Bias (Generic Learner) More Data Required —>



Expert Systems

Linear Models, Simple Trees

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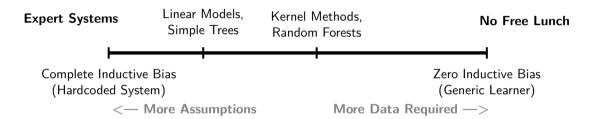
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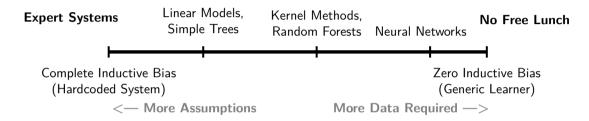




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Understand the problem well enough to **choose** an algorithm whose inductive bias matches the underlying structure of the data.

Questions?

The Linear Models, born of light, The branching Trees of wood and might, The Neural Networks, deep as night, Each claims its rule, and thinks it right.

But no single Algo to rule them all, Where one triumphs, one must fall. No master key for every door, No champion on every shore. Quest is not to find the One. Hone your bias, 'til the work is done.

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References

An excellent introductory course on Theory of ML: TTIC 31250 by Avrim Blum

THE textbook of ML: Understanding Machine Learning: From Theory to Algorithms by Shai Shalev-Shwartz and Shai Ben-David