Foundational AI: a mathematician’s take

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CogX
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Prelude: towards Artificial General Intelligence (AGI)

Artificial entity capable of interacting and coexisting with its environment, especially humans:
- Complies to oral / written / visual instructions
- Initiates new decisions depending on environment
- Must be able to explain its actions (based on a rationale)
- Compliance to an overarching set of rules (morals, law, time/institution/task-dependent, etc.) likely to evolve
- Acknowledges its environment through "senses" (captors, ...) and ability to preserve it (especially living creatures such as humans!)

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Credits: blu.digital
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Can’t be hard-programmed! Must be able to **learn** from previous sample tasks / data / situations / . . . and **adapt** its behaviour.
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Must involve multi-disciplinary research efforts!

Some of the many fields involved in AGI

Statistics
Machine learning
Optimisation
Probability Theory
Robotics
Neurosciences
Psychology
Sociology
Among the many tasks needed to solve AGI, mostly interested in the learning + decision-making module.
It’s all connected

Theoreticians

Designers of algorithms

Practitioners of machine learning

The sensible world
The big picture

Solving AGI requires outstanding coordinated multi-disciplinary research efforts.

Where do we mathematicians and computer scientists fit in?
Contribute to understanding and designing AGI systems: machine learning, probability theory, optimisation, deep learning, computational statistics, reinforcement learning, ...

What about me?
Personal research obsession: rethinking generalisation!
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Learning is to be able to generalise
Learning is to be able to generalise

[Credits: Wikipedia]

From examples, what can a system learn about the underlying phenomenon?

Memorising the already seen data is usually bad $\rightarrow$ overfitting.

Generalisation is the ability to 'perform' well on unseen data.

A few of those slides are inspired by our ICML 2019 tutorial, "A Primer on PAC-Bayesian Learning", Guedj and Shawe-Taylor

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The simplest setting

Learning algorithm $A : \mathcal{Z}^m \rightarrow \mathcal{H}$

- $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$
- $\mathcal{H}$ = hypothesis class

Training set (aka sample): $S_m = ((X_1, Y_1), \ldots, (X_m, Y_m))$
a finite sequence of input-output examples.

- Data-generating distribution $\mathbb{P}$ over $\mathcal{Z}$.
- Learner doesn’t know $\mathbb{P}$, only sees the training set.
- The training set examples are i.i.d. from $\mathbb{P}$: $S_m \sim \mathbb{P}^m$
Generalisation

Loss function $\ell(h(X), Y)$ to measure the discrepancy between a predicted output $h(X)$ and the true output $Y$.

Empirical risk: $R_{\text{in}}(h) = \frac{1}{m} \sum_{i=1}^{m} \ell(h(X_i), Y_i)$ (in-sample)

Theoretical risk: $R_{\text{out}}(h) = \mathbb{E}[\ell(h(X), Y)]$ (out-of-sample)

Upper bounds: with high probability $\Delta(h) \leq \epsilon(m, \delta)$

Flavours:
- distribution-free
- algorithm-free
- distribution-dependent
- algorithm-dependent
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Theoretical risk:  
$$R_{\text{out}}(h) = \mathbb{E} [\ell(h(X), Y)]$$  
(out-of-sample)

If predictor $h$ does well on the in-sample $(X, Y)$ pairs...  
...will it still do well on out-of-sample pairs?

Generalisation gap:  
$$\Delta(h) = R_{\text{out}}(h) - R_{\text{in}}(h)$$

Upper bounds:  
with high probability  
$$\Delta(h) \leq \epsilon(m, \delta)$$

$\Rightarrow$  
$$R_{\text{out}}(h) \leq R_{\text{in}}(h) + \epsilon(m, \delta)$$

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The PAC framework

PAC stands for Probably Approximately Correct.

Roughly translated: with high probability, the error of an hypothesis \( h \) is at most something we can control and even compute. For any \( \delta > 0 \),

\[
\mathbb{P}\left[ R_{\text{out}}(h) \leq R_{\text{in}}(h) + \epsilon(m, \delta) \right] \geq 1 - \delta.
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Think of \( \epsilon(m, \delta) \) as Complexity \( \times \frac{\log \frac{1}{\delta}}{\sqrt{m}} \).
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Rich literature on PAC generalisation bounds, for many machine learning algorithms in a variety of settings.

See Guedj (2019) for a recent survey on PAC-Bayes
Generalisation bounds are a safety check: they give a theoretical guarantee on the performance of a learning algorithm on any unseen data.

Generalisation bounds:

- provide a computable control on the error on any unseen data with prespecified confidence
- explain why specific learning algorithms actually work
- and even lead to designing new algorithm which scale to more complex settings
Is deep learning breaking statistical learning theory?
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Neural networks architectures trained on massive datasets achieve **zero training error** which does not bode well for their performance: this strongly suggests **overfitting**...
Is deep learning breaking statistical learning theory?

Neural networks architectures trained on massive datasets achieve zero training error which does not bode well for their performance: this strongly suggests overfitting...

... yet they also achieve remarkably low errors on test sets!
A famous plot...

Belkin et al. (2019)
... which might just be half of the picture

Belkin et al. (2019)
The jigsaw problem

... a.k.a. representations matter.

Fig. 1: What image representations do we learn by solving puzzles? Left: The image from which the tiles (marked with green lines) are extracted. Middle: A puzzle obtained by shuffling the tiles. Some tiles might be directly identifiable as object parts, but their identification is much more reliable once the correct ordering is found and the global figure emerges (Right).

Credits: Noroozi and Favaro (2016)
A tale of two learners – 1

Deep neural network typically identifies a specific item (say, a horse) in an image with accuracy > 99%. Training samples: millions of annotated images of horses – GPU-expensive training.
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D. (2.5 yo)
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Training samples: a handful of children books, bedtime stories and (poorly executed) drawings.
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Training samples: a handful of children books, bedtime stories and (poorly executed) drawings.

Also expensive training.
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Potential game-changer for algorithms design (more "intelligent", resources-efficient, etc.) and practitioners.
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Potential game-changer for algorithms design (more "intelligent", resources-efficient, etc.) and practitioners.

Very exciting research avenue for theoreticians for the next decade(s)!
Going further


Connect with the UCL Centre for Artificial Intelligence (home to our UKRI Centre for Doctoral Training in Foundational Artificial Intelligence)
https://www.ucl.ac.uk/ai-centre/
Thanks!

Feel free to reach out!

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@bguedj


Case study:
Generalisation bounds for deep neural networks

Context
Context

- **PAC-Bayes** has been successfully used to analyse and understand generalisation abilities of machine learning algorithms.
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Context

- **PAC-Bayes** has been successfully used to analyse and understand generalisation abilities of machine learning algorithms.

- Most PAC-Bayes generalisation bounds are **computable** tight upper bounds on the population error, *i.e.* an estimate of the error on any unseen future data.

- PAC-Bayes bounds hold for **any distribution on hypotheses**. As such, they are a principled way to **invent new learning algorithms**.
This spotlight


This spotlight


We focused on DNN with a **binary activation function**: surprisingly **effective** while preserving low **computing and memory footprints**.
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  **Breakthrough**: training by minimising the bound (SGD + tricks)
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- Who cares? Generalisation bounds are a theoretician’s concern!
  Breakthrough: Our bound is computable and serves as a safety check to practitioners
**Binary Activated Neural Networks**

- $x \in \mathbb{R}^{d_0}$, $y \in \{-1, 1\}$

**Architecture:**

- $L$ fully connected layers
- $d_k$ denotes the number of neurons of the $k^{th}$ layer
- $\text{sgn}(a) = 1$ if $a > 0$ and $\text{sgn}(a) = -1$ otherwise

**Parameters:**

- $W_k \in \mathbb{R}^{d_k \times d_{k-1}}$ denotes the weight matrices.
- $\theta = \text{vec}(\{W_k\}_{k=1}^L) \in \mathbb{R}^D$

**Prediction**

$$f_\theta(x) = \text{sgn}(w_L \text{sgn}(w_{L-1} \text{sgn}(\ldots \text{sgn}(w_1 x))))$$
Generalisation bound

For an arbitrary number of layers and neurons, with probability at least \(1 - \delta\), for any \(\theta \in \mathbb{R}^D\),

\[
R_{\text{out}}(F_\theta) \leq \inf_{C > 0} \left\{ \frac{1}{1 - \exp(-CR_{\text{in}}(F_\theta))} - \frac{1}{2} ||\theta - \theta_0||^2 + \log \frac{2}{\sqrt{m} \delta} \right\},
\]

where

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R_{\text{in}}(F_\theta) = \mathbb{E}_{\theta' \sim \mathcal{Q}} R_{\text{in}}(f_{\theta'}) = \frac{1}{m} \sum_{i=1}^{m} \left[ \frac{1}{2} - \frac{1}{2} y_i F_{\theta}(x_i) \right].
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where

$$R_{\text{in}}(F_\theta) = \mathbb{E}_{\theta' \sim Q_\theta} R_{\text{in}}(f_{\theta'}) = \frac{1}{m} \sum_{i=1}^{m} \left[ \frac{1}{2} - \frac{1}{2}y_i F_\theta(x_i) \right].$$
(A selection of) numerical results

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<th>Model name</th>
<th>Cost function</th>
<th>Train split</th>
<th>Valid split</th>
<th>Model selection</th>
<th>Prior</th>
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<td>MLP–tanh</td>
<td>linear loss, L2 regularized</td>
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<td>– pretrain</td>
<td>linear loss (20 epochs)</td>
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<td>– final</td>
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