On generalisation and learning: towards principled frugal AI

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In a nutshell

Research at the crossroads of statistics, probability, machine learning, optimisation. ”Mathematical foundations of machine learning” says it all!

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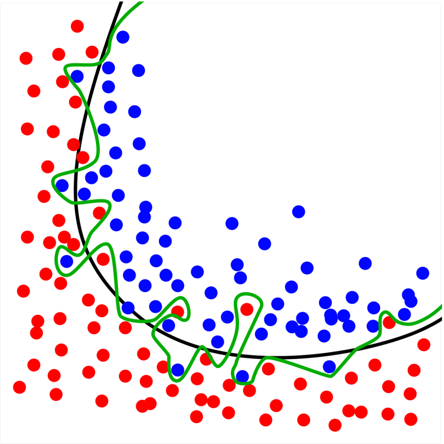
$\longrightarrow$ Project SHARP (PEPR IA) 2023-2027

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 $\longrightarrow$ overfitting

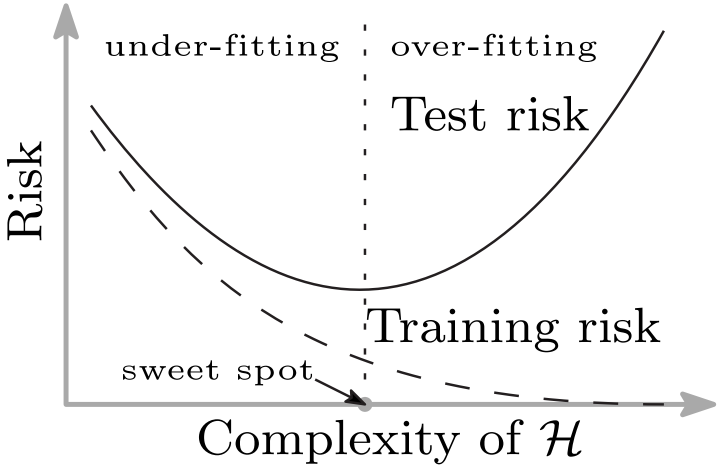
Generalisation is the ability to 'perform' well on unseen data.

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...

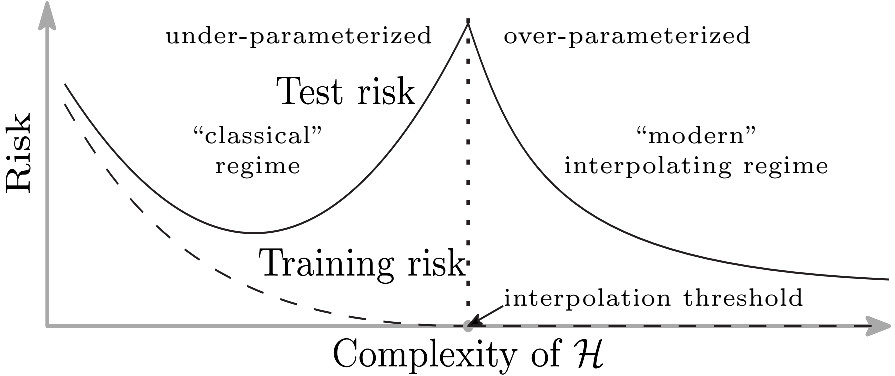
... yet they also achieve remarkably low errors on test sets!

A famous plot...



(Belkin et al., 2019)

... which might just be half of the picture



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Semantic representation to accelerate learning?

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).

(Noroozi and Favaro, 2016)

Semantic content of data is key! $\longrightarrow$ MURI project (2018-2023)

A tale of two learners

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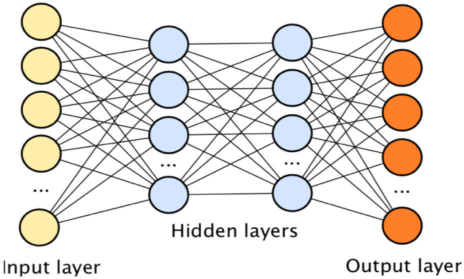
First contender: a deep neural network



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 and significant environmental footprint.

A tale of two learners

Second contender: young children
(here, aged 1 and 3)

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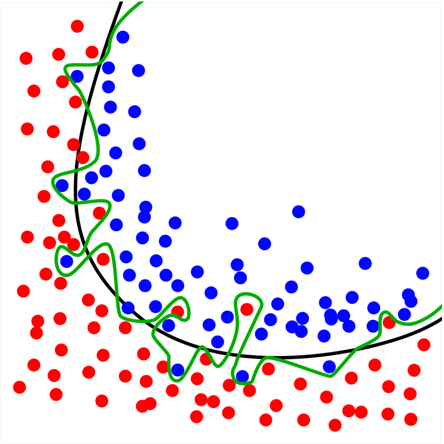
Identify horses with 100% accuracy. Also very good at transferring to *e.g.* zebras

Training samples: a handful of children books, bedtime stories and (poorly executed) drawings.

Also expensive training.

Learning is to be able to generalise...



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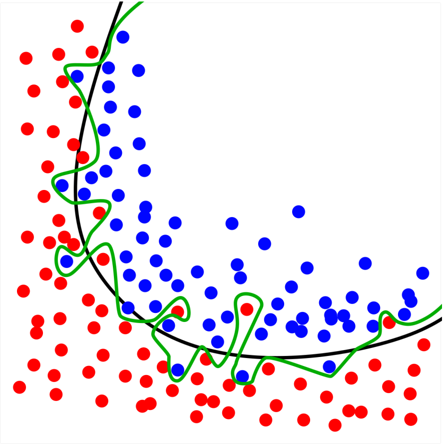

... but not from scratch! Tackling each learning task as a fresh draw unlikely to be efficient – must not be blind to context.

Need to incorporate structure / semantic information / implicit representations of the ”sensible” world.

Should lead to better algorithms design (more ”intelligent”, frugal / resources-efficient, etc.)

Part I

A Primer on PAC-Bayesian Learning
(embarrassingly short version of our ICML 2019 tutorial
with John Shawe-Taylor)

https://bguedj.github.io/icml2019/index.html

The simplest setting

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

- $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$
- $\mathcal{H}$ = 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 $\mathbb{P}$: $S_m \sim \mathbb{P}^m$

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- PAC: probably approximately correct (Valiant, 1984)

  Use a 'confidence parameter' δ: $\mathbb{P}^m[\text{large error}] \leqslant \delta$

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  δ is the probability of being misled by the training set
- Hence high confidence: $\mathbb{P}^m[\text{approximately correct}] \geqslant 1 - \delta$

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- what happens beyond the training set
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Actually these two goals interact with each other!

Generalisation

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

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

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

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 $\Delta(h) \leqslant \epsilon(m, \delta)$

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

Flavours:

- distribution-free
- algorithm-free
- distribution-dependent
- algorithm-dependent

The PAC (Probably Approximately Correct) framework

In a nutshell: with high probability, the generalisation error of an hypothesis h is at most something we can control and even compute. For any $\delta > 0$,

$$\mathbb{P}\left[R_{\mathrm{out}}(h) \leqslant R_{\mathrm{in}}(h) + \epsilon(m, \delta)\right] \geqslant 1 - \delta.$$

Think of $\epsilon(m, \delta)$ as $\mathrm{Complexity} \times \frac{\log \frac{1}{\delta}}{\sqrt{m}}$.

This is about high confidence statements on the tail of the distribution of test errors (compare to a statistical test at level $1 - \delta$).

PAC-Bayes is about PAC generalisation bounds for ***distributions over hypotheses***.

”Why should I care about generalisation?”

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 some specific learning algorithms actually work
- and even lead to designing new algorithms which scale to more complex settings

Take-home message

PAC-Bayes is a generic framework to efficiently rethink generalisation for numerous statistical learning algorithms. It leverages the flexibility of Bayesian inference and allows to derive new learning algorithms.

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◇ New monograph Hellström, Durisi, Guedj and Raginsky (2023), ”Generalization Bounds: Perspectives from Information Theory and PAC-Bayes” `https://arxiv.org/abs/2309.04381`

◇ New ICML 2023 workshop ”PAC-Bayes meets interactive learning” `https://bguedj.github.io/icml2023-workshop/`

◇ ICML 2019 tutorial ”A Primer on PAC-Bayesian Learning” `https://bguedj.github.io/icml2019/`

◇ Survey in the Journal of the French Mathematical Society: Guedj (2019) `https://arxiv.org/abs/1901.05353`

◇ NeurIPS 2017 workshop ”(Almost) 50 Shades of Bayesian Learning: PAC-Bayesian trends and insights”

`https://bguedj.github.io/nips2017/`

Before PAC-Bayes

- Single hypothesis *h* (building block):

  with probability $\geqslant 1-\delta$, $\quad R_{\text{out}}(h) \leqslant R_{\text{in}}(h) + \sqrt{\frac{1}{2m}\log\left(\frac{1}{\delta}\right)}.$

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  w.p. $\geqslant 1-\delta, \quad \forall h \in \mathcal{H}, \quad R_{\text{out}}(h) \leqslant R_{\text{in}}(h) + \sqrt{\frac{1}{2m}\log\left(\frac{|\mathcal{H}|}{\delta}\right)}$

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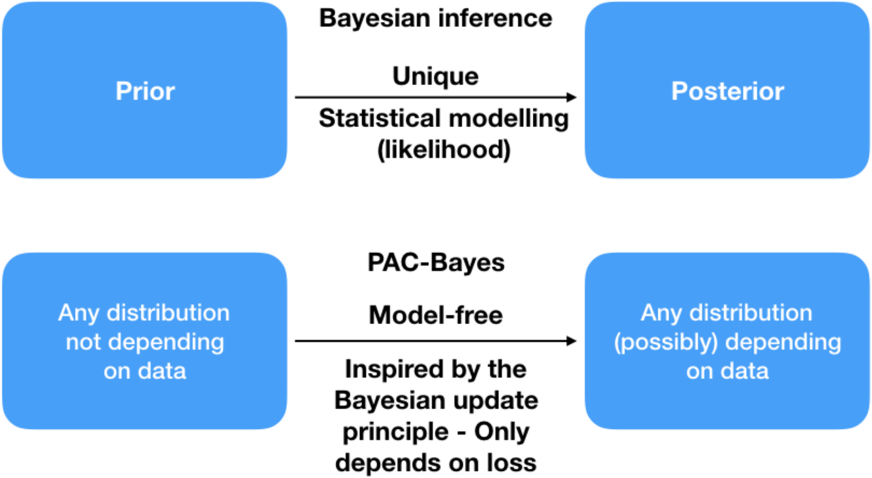
$\longrightarrow$ Extension: PAC-Bayes allows to consider *distributions* over hypotheses.

PAC-Bayes



"Prior": exploration mechanism of $\mathcal{H}$

"Posterior" is the twisted prior after confronting with data

PAC-Bayes bounds vs. Bayesian inference

Prior P, posterior $Q \ll P$. Define the risk of a distribution:

$$R_{\text{in}}(Q) \equiv \int_{\mathcal{H}} R_{\text{in}}(h)\, dQ(h) \qquad R_{\text{out}}(Q) \equiv \int_{\mathcal{H}} R_{\text{out}}(h)\, dQ(h)$$

Kullback-Leibler divergence $\mathrm{KL}(Q\|P) = \mathop{\mathbf{E}}_{h\sim Q} \ln \frac{Q(h)}{P(h)}$.

- **Prior**
  - PAC-Bayes: bounds hold for any distribution
  - Bayes: prior choice impacts inference
- **Posterior**
  - PAC-Bayes: bounds hold for any distribution
  - Bayes: posterior uniquely defined by prior and statistical model
- **Data distribution**
  - PAC-Bayes: bounds hold for any distribution
  - Bayes: statistical modelling choices impact inference

A classical PAC-Bayesian bound

Pre-history: PAC analysis of Bayesian estimators
(Shawe-Taylor and Williamson, 1997)

Birth: PAC-Bayesian bound
(McAllester, 1998, 1999)

Prototypical bound

For any prior P, any $\delta \in (0, 1]$, we have

$$\mathbb{P}^m\left(\forall\, Q \text{ on } \mathcal{H}:\ R_{\text{out}}(Q) \leqslant R_{\text{in}}(Q) + \sqrt{\frac{\mathrm{KL}(Q\|P) + \ln \frac{2\sqrt{m}}{\delta}}{2m}}\right) \geqslant 1 - \delta\,,$$

PAC-Bayes-driven learning algorithms

With an arbitrarily high probability and for any posterior distribution Q,

$$\text{Error on unseen data} \leqslant \text{Error on sample} + \text{complexity term}$$

$$R_{\mathrm{out}}(Q) \leqslant R_{\mathrm{in}}(Q) + F(Q, \cdot)$$

This defines a principled strategy to obtain new learning algorithms:

$$h \sim Q^\star$$

$$Q^\star \in \underset{Q \ll P}{\arg\inf} \left\{ R_{\mathrm{in}}(Q) + F(Q, \cdot) \right\}$$

(optimisation problem which can be solved or approximated by [stochastic] gradient descent-flavoured methods, Monte Carlo Markov Chain, variational inference...)

SVMs, KL-regularized Adaboost, exponential weights are all minimisers of PAC-Bayes bounds.

Variational definition of KL-divergence (Csiszár, 1975; Donsker and Varadhan, 1975; Catoni, 2004).

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Let $(A, \mathcal{A})$ be a measurable space.

(i) For any probability P on $(A, \mathcal{A})$ and any measurable function $\phi : A \to \mathbb{R}$ such that $\int (\exp \circ \phi) \mathrm{d}P < \infty$,

$$\log \int (\exp \circ \phi) \mathrm{d}P = \sup_{Q \ll P} \left\{ \int \phi \mathrm{d}Q - \mathrm{KL}(Q, P) \right\}.$$

(ii) If ϕ is upper-bounded on the support of P, the supremum is reached for the Gibbs distribution G given by

$$\frac{\mathrm{d}G}{\mathrm{d}P}(a) = \frac{\exp \circ \phi(a)}{\int (\exp \circ \phi) \mathrm{d}P}, \quad a \in A.$$

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Proof: let $Q \ll P$.

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Let $\lambda > 0$ and take $\phi = -\lambda R_{\mathrm{in}}$,

$$Q_\lambda \propto \exp(-\lambda R_{\mathrm{in}}) \, P = \arg\inf_{Q \ll P} \left\{ R_{\mathrm{in}}(Q) + \frac{\mathrm{KL}(Q, P)}{\lambda} \right\}.$$

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What is coming next

- What we've been up to with PAC-Bayes recently!

Part II

News from the PAC-Bayes frontline

- Guedj and Robbiano (2018). PAC-Bayesian high dimensional bipartite ranking, Journal of Statistical Planning and Inference.
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Some of my partners in crime

On Margins and Derandomisation in PAC-Bayes

AISTATS 2022

We provide a unified framework for derandomising PAC-Bayes bounds with margins, leading to new bounds or greatly simplified proofs for

- L_2 and L_1 normed linear predictors,
- Linear predictors with a learned randomised feature space,
- One-hidden-layer neural networks with erf activations,
- Deep ReLU networks.

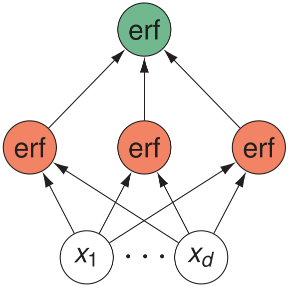
Key idea: PAC-Bayes bounds are (mostly) SOTA, but apply for non-deterministic randomised predictions. Large margin deterministic predictors give similar predictive performance to their randomised counterparts.

SHEL: An unusual neural architecture

Binary $\mathcal{Y} = \{\pm 1\}$ or multiclass classification $\mathcal{Y} = \{1, \ldots, c\}$. Predictors f are score-valued: $f(x) \in \mathbb{R}^c$ (multiclass) or $f(x) \in \mathbb{R}$ (binary). We define the binary margin $M_{\text{bin}}(f,(x,y)) = yf(x)$ and multiclass margin $M_{\text{multi}}(f,(x,y)) = f(x)[y] - \max_{k \neq y} f(x)[k]$.

$R_{\text{out}}(f) = \Pr\{(x,y) : M(f,(x,y)) \leqslant 0\}$, $R_{\text{in},\gamma}(f) = m^{-1}|\{(x,y) \in S : M(f,(x,y)) \leqslant \gamma\}|$.

SHEL network: elementwise error function activations $F_{U,V}(x) = V\text{erf}(Ux)$.

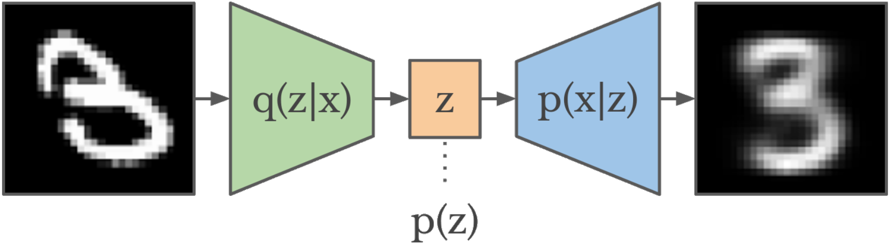


Theorem. For SHEL network with K hidden units,

$$R_{\text{out}}(F_{U,V}) \leqslant R_{\text{in},\gamma}(F_{U,V}) + \widetilde{\mathcal{O}}\left(\frac{\sqrt{K}}{\gamma\sqrt{m}}(\|V\|_{\max}\|U - U^0\|_F + \|V\|_F)\right).$$

On PAC-Bayesian reconstruction guarantees for VAEs

AISTATS 2022



x → encoder → Latent representation → decoder → $\widehat{x} = d(e(x))$

[Credits: Danijar Hafner]

An attempt at summarising my research

Quest for generalisation guarantees (about half *via* PAC-Bayes)

Directions:

- Generic bounds (relaxing assumptions such as iid or boundedness, new concentration inequalities, ...)
- Tight bounds for self-certifying specific algorithms (deep neural networks, NMF, ...)
- Towards new measures of performance (CVaR, ranking, contrastive losses, ...)
- Coupling theory and implemented algorithms: bound-driven algorithms
- Impact beyond learning theory (providing guidelines to machine learning users, sustainable / frugal machine learning)

Thanks!

What this talk could have been about...

- Tighter PAC-Bayes bounds (Mhammedi et al., 2019)
- PAC-Bayes for conditional value at risk (Mhammedi et al., 2020)
- PAC-Bayes-driven deep neural networks (Biggs and Guedj, 2021, 2022; Pérez-Ortiz et al., 2021a,b)
- PAC-Bayes and robust learning (Guedj and Pujol, 2021)
- PAC-Bayes for unbounded losses (Haddouche et al., 2021)
- PAC-Bayesian online clustering (Li et al., 2018)
- PAC-Bayesian bipartite ranking (Guedj and Robbiano, 2018)
- Online k-means clustering (Cohen-Addad et al., 2021)
- Sequential learning of principal curves (Li and Guedj, 2021)
- PAC-Bayes for heavy-tailed, dependent data (Alquier and Guedj, 2018)
- Stability and generalisation (Celisse and Guedj, 2016)
- Additive regression (Guedj and Alquier, 2013)
- Stochastic majority votes (Zantedeschi et al., 2021)

+ a few more in the pipe, soon on arXiv

- Contrastive unsupervised learning (Nozawa et al., 2020)
- Generalisation bounds for structured prediction (Cantelobre et al., 2020)
- MMD aggregated two sample tests (Schrab et al., 2023)
- Image denoising (Guedj and Rengot, 2020)
- Matrix factorisation (Alquier and Guedj, 2017; Chrétien and Guedj, 2020)
- Preventing model overfitting (Zhang et al., 2023)
- Decentralised learning with aggregation (Klein et al., 2020)
- Ensemble learning and nonlinear aggregation (Biau et al., 2016) in Python (Guedj and Srinivasa Desikan, 2018, 2020)
- Identifying subcommunities in social networks and application to forecasting elections (Vendeville et al., 2021, 2022)
- Upper and lower bounds for kernel PCA (Haddouche et al., 2020)
- Prediction with multi-task Gaussian processes (Leroy et al., 2022, 2023)

NOW HIRING

`https://bguedj.github.io`

`@bguedj`

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