Rethinking Generalisation: Beyond KL with Geometry and Comparators

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Mathematical foundations of intelligence

Research at the crossroads of statistics, probability theory, machine learning, optimisation. *Mathematical foundations of artificial intelligence* is a pretty good tagline.

Keywords: statistical learning theory, PAC-Bayes, generalisation bounds, concentration inequalities, computational statistics, theoretical analysis of deep learning and in particular generative models, information theory

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Generalisation theory is all about understanding how to design learning algorithm that learn well beyond training data.

In this talk I will present recent advances that move beyond classical generalisation bounds, replacing KL divergences with Wasserstein distances, and using comparators to make bounds tighter.

Outline

Generalisation in machine learning

Wasserstein-based deviation bounds

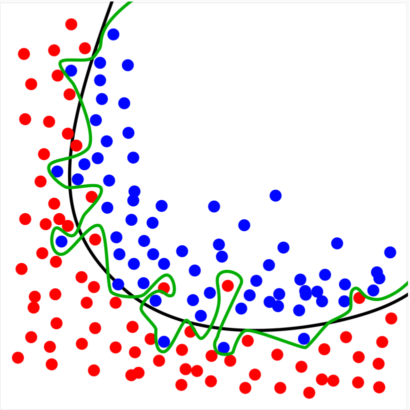
Interlude: generalisation-driven deep learning

Comparators in generalisation bounds

Information theory and PAC-Bayes united

Generalisation in machine learning

Learning is to be able to generalise



[Source: Wikipedia]

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

Memorising the already seen data is usually bad (overfitting)

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

The deep learning era puts generalisation on the spot

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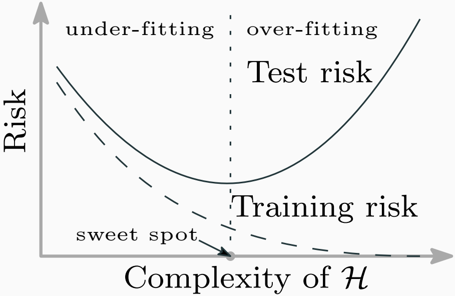

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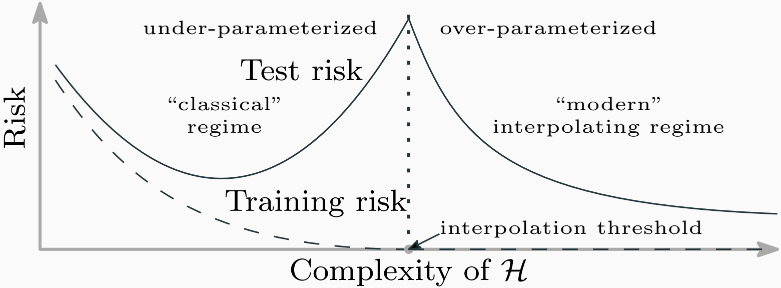

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Why generalisation matters in machine learning

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Let $(X_i, Y_i)_{i=1}^n \in (\mathcal{X} \times \mathcal{Y})^n$ be an iid sample drawn from some distribution $\mathcal{D}^{\otimes n}$, and let $\ell \colon \mathcal{Y} \times \mathcal{Y} \to [0, \infty)$ be a loss function. For any hypothesis $h \colon \mathcal{X} \to \mathcal{Y}$,

$$\widehat{L}(h) = \frac{1}{n} \sum_{i=1}^{n} \ell(h(X_i), Y_i), \quad L(h) = \mathbb{E}\ell(h(X), Y).$$

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- How can we certify that a hypothesis with good performance on training data has similarly good performance on new, unseen data?
- When does a low training loss imply a low population loss?

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This motivates *generalisation bounds*: $\Gamma(h) \leq \mathrm{Bound}$, with several flavours

- hypothesis-dependent vs. hypothesis-free
- (data generating) distribution-dependent vs. distribution-free
- in expectation
- with (arbitrarily) high probability

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Think of $\mathcal{B}(n, \delta)$ as $\mathrm{Complexity} \times \frac{\log 1/\delta}{\sqrt{n}}$. PAC bounds are high confidence statements on the tail of the distribution of population losses (think of a statistical test at level $1 - \delta$).

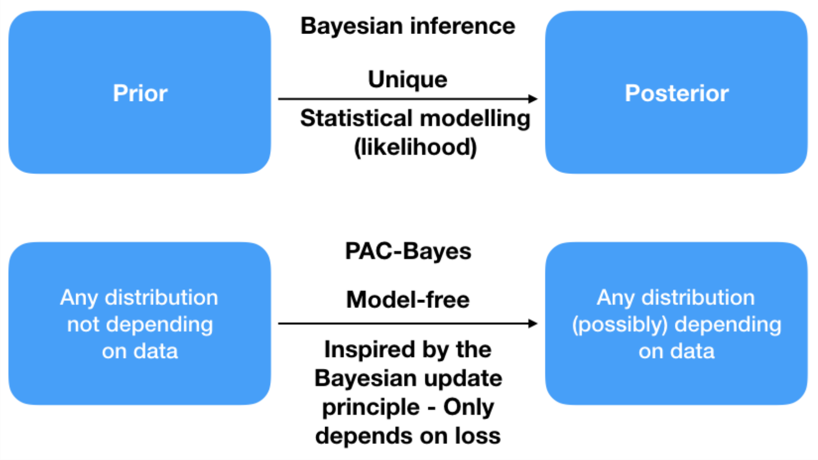
PAC-Bayes

PAC-Bayes is about PAC generalisation bounds for *distributions over hypotheses*. Let Q_n denote a posterior distribution that produces hypotheses,

$$\widehat{\mathcal{L}}(Q_n) = \mathbb{E}_{h\sim Q_n}\widehat{L}(h) = \frac{1}{n}\sum_{i=1}^{n}\mathbb{E}_{h\sim Q_n}\ell(h(X_i), Y_i),$$

$$\mathcal{L}(Q_n) = \mathbb{E}_{h\sim Q_n}L(h) = \mathbb{E}_{h\sim Q_n}\mathbb{E}\ell(h(X), Y).$$

We compare Q_n to a prior Q_0, typically through the KL divergence $\mathrm{KL}(Q_n||Q_0) = \mathbb{E}_{h\sim Q_n}\log\frac{Q_n(h)}{Q_0(h)}$.



Prior

Bayesian inference

Unique

Statistical modelling (likelihood)

Posterior

Any distribution not depending on data

PAC-Bayes

Model-free

Inspired by the Bayesian update principle - Only depends on loss

Any distribution (possibly) depending on data

What makes PAC-Bayes a post-Bayes approach?

- 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 PAC-Bayesian bound

Shawe-Taylor and Williamson, A PAC analysis of a Bayes estimator, COLT, 1997

McAllester, Some PAC-Bayesian theorems, COLT, 1998

McAllester, PAC-Bayesian model averaging, COLT, 1999

Prototypical bound

For any prior Q_0, any $\delta \in (0, 1]$, we have

$$\mathbb{P}\left(\forall\, Q_n : \; \mathcal{L}(Q_n) \leq \; \widehat{\mathcal{L}}(Q_n) + \sqrt{\frac{\mathrm{KL}(Q_n \| Q_0) + \log(2\sqrt{n}/\delta)}{2n}}\right) \geq 1 - \delta.$$

What is this useful for?

From

$$\mathbb{P}\left[\mathcal{L}(h) \leq \widehat{\mathcal{L}}(h) + \mathcal{B}(n, \delta, Q_n)\right] \geq 1 - \delta,$$

- We can compute the numerical value of the bound $\mathcal{B}(n, \delta, Q_n)$,
- We can train new algorithms and derive new hypotheses, with

$$Q^\star \in \operatorname*{arg\,inf}_{Q_n \ll Q_0} \left\{ \widehat{\mathcal{L}}(Q_n) + \mathcal{B}(n, \delta, Q_n) \right\}$$

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

Variational definition of the KL-divergence

- Csiszár., I-divergence geometry of probability distributions and minimization problems, Annals of Probability, 1975

- Donsker and Varadhan, Asymptotic evaluation of certain Markov process expectations for large time, Communications on Pure and Applied Mathematics, 1975

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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

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

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

Proof: let $Q \ll P$.

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Let $\lambda > 0$ and take $\phi = -\lambda \widehat{\mathcal{L}}$,

$$Q_\lambda \propto \exp \left(-\lambda \widehat{\mathcal{L}} \right) P = \operatorname*{arg\,inf}_{Q \ll P} \left\{ \widehat{\mathcal{L}}(Q) + \frac{\mathrm{KL}(Q \| P)}{\lambda} \right\}.$$

"Why should I care about generalisation?"

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Generalisation bounds are both a safety check (theoretical and possibly numerical guarantee on the performance of hypotheses on unseen data) and an original training objective.

Formalisms for generalisation

- Concentration inequalities
- Rademacher complexities
- VC-dimension
- Information-theoretic
- PAC-Bayes bounds

When classical PAC-Bayes bounds fall short

- **Geometry mismatch.** The usual KL divergence ignores the geometry of the data space.
  - KL blows up when $\rho \not\ll \pi$,
  - offers no notion of distance or curvature.

📕 Bégin, Germain, Laviolette & Roy, *PAC-Bayesian bounds based on the Rényi divergence*, AISTATS, 2016.

📕 Alquier & Guedj, *Simpler PAC-Bayesian bounds for hostile data*, Machine Learning, 2018.

- **Not all generalisation gaps are equal.** Standard PAC-Bayes bounds control a single scalar gap, but cannot adapt to the structure of the prediction problem.

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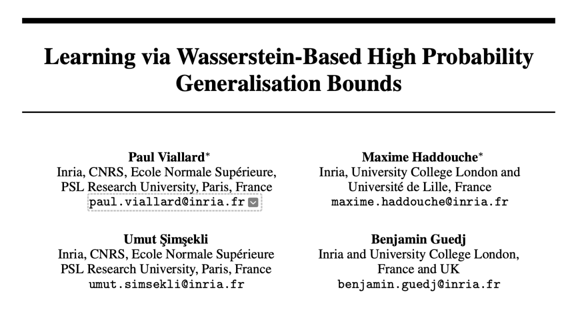
Two contributions

(1) geometric reformulation via Wasserstein distances,
(2) rethinking the notion of generalisation through comparators.

Wasserstein-based deviation bounds



Learning via Wasserstein-Based High Probability Generalisation Bounds

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Viallard, Haddouche, Simsekli and Guedj, *Learning via Wasserstein-based high probability generalisation bounds*, NeurIPS 2023.

Why Wasserstein instead of KL?

- Classical PAC-Bayes bounds use $\mathrm{KL}(\rho\|\pi)$, which can:
  - ignore geometry of $\mathcal{H}$ or $\mathcal{Z}$;
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  - be vacuous with heavy-tailed losses.
- The Wasserstein distance

$$W(\rho, \pi) = \inf_{\gamma \in \Gamma(\rho, \pi)} \mathbb{E}_{(h, h') \sim \gamma} \left[d(h, h') \right]$$

  encodes geometry and does not require absolute continuity.
- We provide high-probability PAC-Bayes bounds with W_1, valid under weak moment assumptions and even non-i.i.d. data.

Setup: priors and multiple priors

- Hypothesis space $\mathcal{H}$ with metric d; data $S = (z_1, \ldots, z_m) \sim \mu^m$.
- Prior $\pi \in \mathcal{M}(\mathcal{H})$, posterior $\rho \in \mathcal{M}(\mathcal{H})$.
- Split S into K disjoint subsets $S_1, \ldots, S_K$.
- Each prior $\pi_{i,S}$ is built from data disjoint from S_i (independence for the bound).

$\rightarrow$ Data-dependent priors remain valid via sample splitting.

Theorem 2: High-probability Wasserstein PAC-Bayes bound

Assume ℓ is L-Lipschitz in h and non-negative. For any $\delta \in (0,1]$, with probability at least $1-\delta$ over $S \sim \mu^m$, the following holds for the distributions $\pi_{i,S} := \pi_i(S,\cdot)$ and for any $\rho \in \mathcal{M}(\mathcal{H})$:

$$\boxed{\mathbb{E}_{h\sim\rho}\left[R_\mu(h) - \widehat{R}_S(h)\right] \;\leq\; \sum_{i=1}^{K} \frac{2|S_i|L}{m}\, W\!\left(\rho, \pi_{i,S}\right) \;+\; \sum_{i=1}^{K} \sqrt{\frac{2\,|S_i|\,\ln\!\left(K/\delta\right)}{m^2}}\;.}$$

Proof sketch

1. Prove a Wasserstein deviation inequality using the Kantorovich–Rubinstein dual for W_1.
2. Prove Catoni-type high-probability control.
3. Uniformise over all ρ via $W(\rho, \pi_{i,S})$ terms.
4. Use sample splitting to construct independent $\pi_{i,S}$ and take a union bound over $i = 1, \dots, K$.

$\rightarrow$ Geometry-aware, linear in W, high-probability bound.

From bound to learning objective

Minimising the RHS of Theorem 2 gives:

$$\rho^\star \in \arg \min_{\rho \in \mathcal{M}(\mathcal{H})} \left[\mathbb{E}_{h \sim \rho} \widehat{R}_S(h) + \sum_{i=1}^{K} \frac{2|S_i| L}{m} W\big(\rho, \pi_{i,S}\big) \right].$$

For deterministic predictors ($\rho = \delta_{h_w}$):

$$h_w^\star \in \arg \min_{w} \ \widehat{R}_S(h_w) + \varepsilon \sum_{i=1}^{K} \frac{|S_i|}{m} d\big(h_w, h_{w_i}\big).$$

$\rightarrow$ Wasserstein acts as a geometry-aware regulariser.

Interpreting the parameter ε

- In the deterministic case, $W(\rho, \pi_{i,S}) = d(h_w, h_{w_i})$.
- The theoretical weight $2L$ becomes a tunable ε:

$$h_w^\star = \arg\min_w \ \widehat{R}_S(h_w) + \varepsilon \sum_{i=1}^{K} \frac{|S_i|}{m} \, d(h_w, h_{w_i}).$$

- ε controls the trade-off between:
    - empirical risk minimisation (fit), and
    - geometric regularisation (proximity to priors).
- Analogous to the inverse temperature $1/\lambda$ in Gibbs posteriors.

Theorem 4: Online Wasserstein PAC-Bayes bound (statement)

Assume the loss $\ell : \mathcal{H} \times \mathcal{Z} \to \mathbb{R}_+$ is L-Lipschitz in h, and that priors $\pi_i(S, \cdot)$ satisfy bounded conditional second moments:

$$\forall i, S : \quad \mathbb{E}_{h \sim \pi_i(S,\cdot)}\Big[\mathbb{E}_{i-1}\big[\ell(h, z_i)^2\big]\Big] \leq 1.$$

Then for any $\delta \in (0, 1]$, with probability at least $1 - \delta$ over $S \sim \mu^m$, for data-dependent priors $\pi_{i,S} = \pi_i(S, \cdot)$ and any posterior sequence $(\rho_i)_{i=1}^m$,

$$\boxed{\frac{1}{m}\sum_{i=1}^{m} \mathbb{E}_{h \sim \rho_i}\Big[\mathbb{E}[\ell(h, z_i) \mid \mathcal{F}_{i-1}] - \ell(h, z_i)\Big] \leq \frac{2L}{m}\sum_{i=1}^{m} W(\rho_i, \pi_{i,S}) + \sqrt{\frac{2\ln(1/\delta)}{m}}\ .}$$

Theorem 4: interpretation and learning rule

- This is the first online PAC-Bayes bound using Wasserstein regularisation.
- Controls the expected regret of the online learner:

$$\text{Regret} = \frac{1}{m}\sum_{i=1}^{m}\Big(\mathbb{E}_{h\sim\rho_i}[\ell(h,z_i)] - \mathbb{E}_{h\sim\pi_{i,S}}[\ell(h,z_i)]\Big).$$

- The additional term $\frac{2L}{m}\sum_i W(\rho_i,\pi_{i,S})$ penalises geometric deviation from the prior sequence.
- The corresponding online update rule:

$$\rho_i \in \arg\min_{\rho}\ \mathbb{E}_{h\sim\rho}[\ell(h,z_i)] + 2L\,W(\rho,\pi_{i,S}), \qquad i = 1,\dots,m.$$

- For deterministic learners:

$$h_i \in \arg\min_{h}\ \ell(h,z_i) + d(h,h_{i-1}), \quad d(h,h_{i-1}) \le 1.$$

$\rightarrow$ Geometry-aware online learning with transport regularisation.

Take-home message

- High-probability Wasserstein PAC-Bayes bounds for batch and online settings.
- Linear W_1-terms $\Rightarrow$ optimisable objectives and deterministic predictors.
- Especially robust under heavy tails and geometry-sensitive $\mathcal{H}$.

Interlude: generalisation-driven deep learning

Letarte, Germain, Guedj and Laviolette, Dichotomize and generalize: PAC-Bayesian binary activated deep neural networks, NeurIPS, 2019

Biggs and Guedj, Differentiable PAC-Bayes Objectives with Partially Aggregated Neural Networks, Entropy, 2021

Biggs and Guedj, On Margins and Derandomisation in PAC-Bayes, AISTATS, 2022

Cherief-Abdellatif, Shi, Doucet and Guedj, On PAC-Bayesian reconstruction guarantees for VAEs, AISTATS, 2022

Biggs and Guedj, Non-Vacuous Generalisation Bounds for Shallow Neural Networks, ICML, 2022

Common trait of these works: for specific architectures of deep neural networks, we obtain PAC-Bayes generalisation bounds which are

- used as a training objective – delivering networks which achieve the best generalisation performance
- evaluated numerically: all are non-vacuous

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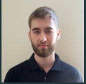
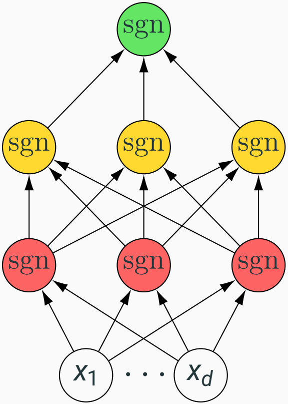
Binary Activated Networks (NeurIPS 2019)



$\mathbf{x} \in \mathbb{R}^{d_0}$, $y \in \{-1, 1\}$. Architecture:

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



Parameters:

- $\mathbf{W}_k \in \mathbb{R}^{d_k \times d_{k-1}}$ denotes the weight matrices.
- $\theta = \operatorname{vec}\left(\{\mathbf{W}_k\}_{k=1}^{L}\right) \in \mathbb{R}^D$

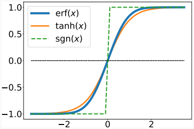
Prediction

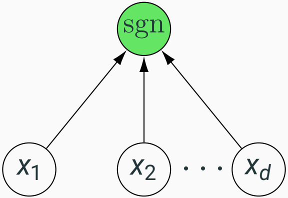
$$f_\theta(\mathbf{x}) = \operatorname{sgn}\left(\mathbf{w}_L \operatorname{sgn}\left(\mathbf{W}_{L-1} \operatorname{sgn}\left(\ldots \operatorname{sgn}\left(\mathbf{W}_1 \mathbf{x}\right)\right)\right)\right),$$

Building block: one layer (aka linear predictor)

Model $f_{\mathbf{w}}(\mathbf{x}) \overset{\text{def}}{=} \operatorname{sgn}(\mathbf{w} \cdot \mathbf{x})$, with $\mathbf{w} \in \mathbb{R}^d$.

- Linear classifiers $\mathcal{F}_d \overset{\text{def}}{=} \{f_{\mathbf{v}} | \mathbf{v} \in \mathbb{R}^d\}$
- Predictor
  $F_{\mathbf{w}}(\mathbf{x}) \overset{\text{def}}{=} \mathbf{E}_{\mathbf{v}\sim Q_{\mathbf{w}}} f_{\mathbf{v}}(\mathbf{x}) \;=\; \operatorname{erf}\left(\frac{\mathbf{w}\cdot\mathbf{x}}{\sqrt{d}\|\mathbf{x}\|}\right)$
- Sampling + closed form of the KL + a few other tricks + extension to an arbitrary number of layers





Generalisation bound

Let F_θ denote the network with parameter θ. With probability at least $1-\delta$, for any $\theta \in \mathbb{R}^D$

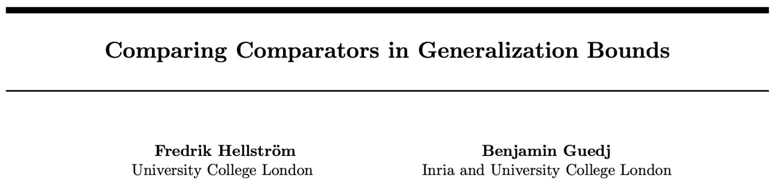
$$\mathcal{L}(F_\theta) \leq$$
$$\inf_{C>0} \left\{ \frac{1}{1-e^{-C}} \left(1 - \exp\left(-C\widehat{\mathcal{L}}(F_\theta) - \frac{\mathrm{KL}(\theta, \theta_0) + \log \frac{2\sqrt{m}}{\delta}}{m} \right) \right) \right\}.$$

Numerical experiments

Model name	Cost function	Train split	Valid split	Model selection	Prior
MLP–tanh	linear loss, L2 regularized	80%	20%	valid linear loss	-
PBGNet$_\ell$	linear loss, L2 regularized	80%	20%	valid linear loss	random init
PBGNet	**PAC-Bayes bound**	**100 %**	**-**	**PAC-Bayes bound**	**random init**
PBGNet$_{\text{pre}}$					
– pretrain	linear loss (20 epochs)	50%	-	-	random init
– final	PAC-Bayes bound	50%	-	PAC-Bayes bound	pretrain

Dataset	MLP–tanh		PBGNet$_\ell$		PBGNet			PBGNet$_{\text{pre}}$		
	$\mathcal{L}$	$\widehat{\mathcal{L}}$	$\widehat{\mathcal{L}}$	$\widehat{\mathcal{L}}$	$\mathcal{L}$	$\widehat{\mathcal{L}}$	Bound	$\mathcal{L}$	$\widehat{\mathcal{L}}$	Bound
ads	0.021	0.037	0.018	**0.032**	0.024	0.038	0.283	0.034	0.033	0.058
adult	0.128	0.149	0.136	**0.148**	0.158	0.154	0.227	0.153	0.151	0.165
mnist17	0.003	**0.004**	0.008	0.005	0.007	0.009	0.067	0.003	0.005	0.009
mnist49	0.002	**0.013**	0.003	0.018	0.034	0.039	0.153	0.018	0.021	0.030
mnist56	0.002	0.009	0.002	0.009	0.022	0.026	0.103	0.008	**0.008**	0.017
mnistLH	0.004	**0.017**	0.005	0.019	0.071	0.073	0.186	0.026	0.026	0.033

Comparators in generalisation bounds



Comparing Comparators in Generalization Bounds

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Benjamin Guedj
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Hellström and Guedj, Comparing comparators in generalization bounds, AISTATS, 2024

The typical approach

- Most generalisation bounds are about bounding the difference $\mathcal{L} - \widehat{\mathcal{L}}$
- Simple, and easy to interpret, but not always tight!
- Can we do better?

Generalising with Comparator Functions

We define the comparator function as $\Delta\colon [0,\infty)^2 \to [0,\infty)$ convex.

A comparator function computes a discrepancy between the training and population loss.

Generic PAC-Bayes Bound with a comparator

Theorem
Assume the loss ℓ is bounded by 1. For any comparator Δ,

$$\mathbb{P}\left[\Delta(\widehat{\mathcal{L}}, \mathcal{L}) \leq \frac{\mathrm{KL}(Q_n \| Q_0) + \log \frac{\Upsilon_\Delta(n)}{\delta}}{n}\right] \geq 1 - \delta,$$

where

$$\Upsilon_\Delta(n) = \sup_{r \in [0,1]} \sum_{k=0}^{n} \binom{n}{k} r^k (1-r)^{n-k} e^{n\Delta(k/n, r)}.$$

Bégin et al., PAC-Bayesian bounds based on the Rényi divergence, AISTATS, 2016

Many known bounds arise as instances of the bound from Bégin et al. (2016). Examples:

- Difference: $\Delta(p,q) = p - q$, we obtain McAllester's bound

$$\mathbb{P}\left(\mathcal{L}(Q_n) \leq \widehat{\mathcal{L}}(Q_n) + \sqrt{\frac{\mathrm{KL}(Q_n \| Q_0) + \log(2\sqrt{n}/\delta)}{2n}}\right) \geq 1-\delta.$$

- Catoni's family, for any $\gamma \in \mathbb{R}$

$$\Delta_\gamma(p,q) = \gamma q - \log(1 - p + pe^\gamma),$$

  and we get the bound

$$\mathbb{P}\left(\Delta_\gamma(\widehat{\mathcal{L}}(Q_n), \mathcal{L}(Q_n)) \leq \frac{\mathrm{KL}(Q_n \| Q_0) + \log\frac{1}{\delta}}{n}\right) \geq 1 - \delta,$$

- Binary KL divergence

$$
\begin{aligned}
\Delta(p,q) = \mathsf{kl}(q,p) = \mathrm{KL}(\mathrm{Bern}(q) \,\|\, \mathrm{Bern}(p)) \\
= q \log \frac{q}{p} + (1-q) \log \frac{1-q}{1-p},
\end{aligned}
$$

and we get the Maurer-Langford-Seeger bound

$$
\mathbb{P}\left(\mathsf{kl}(\widehat{\mathcal{L}}(Q_n), \mathcal{L}(Q_n)) \leq \frac{\mathrm{KL}(Q_n \| Q_0) + \log \frac{2\sqrt{n}}{\delta}}{n} \right) \geq 1 - \delta.
$$

So which comparator gives the best bound?

When the loss is bounded, the kl is the optimal comparator (up to a log term), as established by Foong et al. (2021).

📕 Foong et al., How Tight Can PAC-Bayes be in the Small Data Regime?, NeurIPS, 2021

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In this work we relax the boundedness assumption.

Bounds in expectation

We let

$$\widehat{\mathcal{L}}(Q_n) = \mathbb{E}_{h\sim Q_n}\mathbb{E}\left[\frac{1}{n}\sum_{i=1}^{n}\ell(h(X_i), Y_i)\right],$$
$$\mathcal{L}(Q_n) = \mathbb{E}_{h\sim Q_n}\mathbb{E}\left[\ell(h(X), Y)\right].$$

Let X be a real-valued random variable. The **cumulant generating function (CGF)** of X is

$$\Psi_X(t) = \log \mathbb{E}\left[e^{tX}\right].$$

Theorem — Average Case Generalisation Bound

Let $\mathcal{P}$ be a set of distributions such that for all $r \in [0, \infty)$, there exists $P_r \in \mathcal{P}$ with mean r. Let $\mathcal{C}$ be the set of proper, convex, lower semicontinuous functions $\mathbb{R}^2 \to \mathbb{R}$, and let $\mathcal{F} \subset \mathcal{C}$ be the set of f satisfying:

$$\mathbb{E}\left[e^{f(\widehat{\mathcal{L}}(h), \mathcal{L}(h))}\right] \leq \mathbb{E}_{x \sim P_{\mathcal{L}(h)}}\left[e^{f(\bar{x}, \mathcal{L}(h))}\right].$$

Then for all $\Delta \in \mathcal{F}$ and all $Q_n \ll Q_0$:

$$\Delta(\widehat{\mathcal{L}}(Q_n), \mathcal{L}(Q_n)) \leq \frac{\mathrm{KL}(Q_n D^n \| Q_0 D^n) + \log \Upsilon_{\Delta}^{\mathcal{P}}(n)}{n},$$

where

$$\Upsilon_{\Delta}^{\mathcal{P}}(n) = \sup_{r \in [0, \infty)} \mathbb{E}_{x \sim P_r}\left[\exp\left(n \Delta(\bar{x}, r)\right)\right].$$

How do we make this relevant beyond bounded losses?

Recall that σ-sub-Gaussian random variables are characterized by having a CGF that is dominated by the CGF of some Gaussian distribution with variance σ^2, with similar notions for, *e.g.*, sub-gamma and sub-exponential random variables.

The convex conjugate of a function f is given by

$$f^*(y) = \sup_x \{\langle x, y\rangle - f(x)\}.$$

Definition of Sub-$\mathcal{P}$ Losses

Let $\mathcal{P}$ be a set of distributions such that, for all $r \in [0, \infty)$, there exists $P_r \in \mathcal{P}$ with first moment r.

For all $r \in [0, \infty)$, let $\mathcal{T}_r \subset \mathbb{R}$ and $\mathcal{T} = \{\mathcal{T}_r : r \in [0, \infty)\}$. We say that the loss is *sub*-$(\mathcal{P}, \mathcal{T})$ if, for all h and $t \in \mathcal{T}_{\mathcal{L}(h)}$, we have

$$\mathbb{E}\left[\exp(t\,\ell(h(X), Y))\right] \leq \mathbb{E}_{x \sim P_{\mathcal{L}(h)}}\left[\exp(tx)\right].$$

If $\mathcal{T}_r = \mathbb{R}$ for all $r \in [0, \infty)$, we say that the loss is *sub*-$\mathcal{P}$.

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A sub-$\mathcal{P}$ loss never has heavier tails than those of $\mathcal{P}$.

Theorem — Optimal Comparator and Bound

Assume that the loss is sub-$(\mathcal{P}, \mathcal{T})$. Let $\Psi_p(t) = \log \mathbb{E}_{x \sim P_p}[e^{tx}]$ be the CGF of the distribution P_p, and let the Cramér function be defined as

$$\Delta_{\mathcal{P}}^{\Psi}(q, p) = \Psi_p^*(q) = \sup_{t \in \mathcal{T}_p} \{tq - \Psi_p(t)\}.$$

Define the bound functional

$$\widehat{B}_n^{\Delta}(\alpha, \beta, \iota) = \sup_{\rho \in \mathcal{L}} \left\{ \rho : \Delta(\alpha, \rho) \leq \frac{\beta + \log \iota(n)}{n} \right\}.$$

Then, for any $\Delta \in \mathcal{F}$, we have

$$\begin{aligned} \widehat{\mathcal{L}}(Q_n) &\leq \widehat{B}_n^{\Delta_{\mathcal{P}}^{\Psi}} \left(\widehat{\mathcal{L}}(Q_n), \mathrm{KL}(Q_n D^n \| Q_0 D^n), 1 \right) \\ &\leq \widehat{B}_n^{\Delta} \left(\widehat{\mathcal{L}}(Q_n), \mathrm{KL}(Q_n D^n \| Q_0 D^n), \Upsilon_{\mathcal{P}}^{\Delta}(n) \right). \end{aligned}$$

In other words, the optimal average generalisation bound is obtained with the Cramér function as comparator.

For independent and identically distributed random variables, the Cramér function characterises the probability of rare events. Thus, the connection to generalisation bounds is somewhat natural.

📕 Cramér, On a new limit theorem of the theory of probability, Uspekhi Mathematicheskikh Nauk, 1944

📕 Boucheron et al., Concentration inequalities, A nonasymptotic theory of independence, Oxford University Press, 2013

The case of natural exponential families

- If $\mathcal{P}$ is a NEF, the Cramér function is a KL

$$\Delta_{\mathcal{P}}^{\Psi}(q,p) = \Psi_p^*(q) = \mathrm{KL}(P_q \,\|\, P_p).$$

- For the case of Gaussian distributions with known variance, the optimal comparator is given by

$$\mathrm{KL}\left(\mathcal{N}(q,\sigma^2) \,\|\, \mathcal{N}(p,\sigma^2)\right) = \frac{(q-p)^2}{2\sigma^2}.$$

Examples of Cramér Functions

- Bounded loss: binary KL $\mathrm{kl}(q, p)$,
- Sub-Gaussian: $\frac{(q-p)^2}{2\sigma^2}$,
- Sub-Poisson: $p - q + q \log(q/p)$,
- Sub-Gamma: $k(\frac{q}{p} - 1 - \log \frac{q}{p})$,
- Sub-Laplacian:

$$\begin{aligned}\Delta^{\Psi}_{\mathrm{Lap}}(q, p) = \frac{\sqrt{(q-p)^2 + b^2}}{b} - 1 \\ + \log\left(\frac{2\left(b\sqrt{(q-p)^2 + b^2} - b^2\right)}{(q-p)^2}\right).\end{aligned}$$

Theorem — Generic PAC-Bayesian Bound for Sub-$\mathcal{P}$ losses

Assume the loss is Sub-$\mathcal{P}$. Then for any $\Delta \in \mathcal{F}$, with probability at least $1 - \delta$, the following holds simultaneously for all posteriors $Q_n \ll Q_0$

$$\Delta\left(\widehat{\mathcal{L}}(Q_n), \mathcal{L}(Q_n)\right) \leq \frac{\mathrm{KL}(Q_n \| Q_0) + \log \frac{\Upsilon_{\Delta}^{\mathcal{P}}(n)}{\delta}}{n}.$$

Theorem — Near-Optimality of the Cramér Comparator i

Assume that the loss is sub-$(\mathcal{P}, \mathcal{T})$. Then, for any $\Delta \in \mathcal{F}$, the following holds:

$$B_n^{\Delta_{\mathcal{P}}^{\Psi}}(\widehat{\mathcal{L}}(Q_n), \mathrm{KL}(Q_n \| Q_0), 1) \leq B_n^{\Delta}\left(\widehat{\mathcal{L}}(Q_n), \mathrm{KL}(Q_n \| Q_0), \Upsilon_{\Delta}^{\mathcal{P}}(n)\right).$$

Furthermore, letting $\bar{\Upsilon}(\mathcal{P}) := \Upsilon_{\Delta_{\mathcal{P}}^{\Psi}}^{\mathcal{P}}$, we have:

$$\mathcal{L}(Q_n) \leq B_n^{\Delta_{\mathcal{P}}^{\Psi}}\left(\widehat{\mathcal{L}}(Q_n), \mathrm{KL}(Q_n \| Q_0), \bar{\Upsilon}(\mathcal{P})\right).$$

Finally, for any fixed $t \in \mathcal{T}_p$, define $\Delta_{\mathcal{P}}^{t}(q, p) = tq - \Psi_p(t)$. Then:

$$\mathcal{L}(Q_n) \leq B_n^{\Delta_{\mathcal{P}}^{t}}\left(\widehat{\mathcal{L}}(Q_n), \mathrm{KL}(Q_n \| Q_0), 1\right).$$

Theorem — Near-Optimality of the Cramér Comparator ii

The first inequality shows that the Cramér comparator gives the smallest possible bound up to the normalisation factor.

The second inequality is a valid PAC-Bayesian generalisation bound using $\Delta_{\mathcal{P}}^{\Psi}$.

The third provides a parametric bound for fixed t, useful for optimisation.

Main takeaways

- Comparator choice is crucial in generalisation
- The optimal choice for unbounded losses: Cramér function derived from CGF
- For NEFs, this is equivalent to using the KL divergence

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- The optimal choice for unbounded losses: Cramér function derived from CGF
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In a nutshell

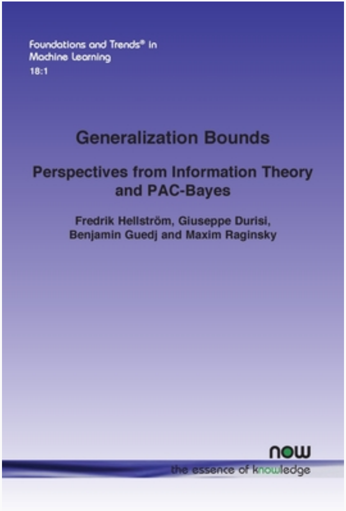
The tightest (up to log terms) generalisation bounds with controllable moment-generating functions are obtained with the Cramér function as the comparator function.

Open Questions

- Can we extend beyond CGF-controlled losses?
- Can we eliminate the log slack?
- Does this strategy apply to heavy-tailed losses?
- Can we derive conditional mutual information bounds?
- Empirical calibration of CGFs in practice

Information theory and PAC-Bayes united

Everything you've ever wanted to know about generalisation



Foundations and Trends® in Machine Learning
18:1

Generalization Bounds

Perspectives from Information Theory and PAC-Bayes

Fredrik Hellström, Giuseppe Durisi,
Benjamin Guedj and Maxim Raginsky

now
the essence of knowledge

Hellström, Durisi, Guedj, and Raginsky, Generalization Bounds: Perspectives from Information Theory and PAC-Bayes, Foundations and Trends in Machine Learning, 2025

What the book is about

- Offers a unified view of generalisation through two complementary theories:
    - PAC-Bayes bounds: relate predictors to priors and posteriors;
    - Information-theoretic bounds: relate data to algorithms.

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  1. control exponential moments of the loss;
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- Both rely on the same three-step reasoning:
    1. control exponential moments of the loss;
    2. perform a change of measure;
    3. derive a concentration inequality.
- The book presents this pattern in a modular way, with examples from algorithmic stability and deep learning.

→ One common foundation for modern generalisation theory.

Bridging two ways of reasoning

- PAC-Bayes view: compares the learner's average performance under a posterior and a prior.
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- PAC-Bayes view: compares the learner's average performance under a posterior and a prior.
- Information-theoretic view: quantifies how much the algorithm reveals about its training data.
- These perspectives are mathematically equivalent: a PAC-Bayes bound can be written as an information-theoretic bound with a matched reference distribution.
- PAC-Bayes is *constructive* — it suggests training objectives. Information theory is *diagnostic* — it measures complexity and stability.

→ Two complementary lenses on generalisation.

Practical lessons

- Concentration regimes link data behaviour, noise, and geometry:
    - Quadratic (sub-Gaussian): KL-based bounds for light-tailed data;
    - Bernoulli (bounded): finite-range losses such as 0–1 classification;
    - Catoni / robust (heavy-tailed): variance control via truncation;
    - Wasserstein (geometric): replaces KL by transport cost.

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- Each regime suggests a training principle: KL $\rightarrow$ exponential posteriors; Catoni $\rightarrow$ variance-controlled losses; Wasserstein $\rightarrow$ geometry-aware regularisation.
- Together, they form a continuum from information-theoretic to geometric learning.

$\rightarrow$ One toolbox, spanning theory and practice.

Thank you!