A (condensed) primer on PAC-Bayesian Learning followed by A walkthrough of advanced PAC-Baves results

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Foundational AI Seminar Series June 16, 2020





The Institute

- Principal research fellow (~ associate professor) at UCL CS and AI,
- Tenured research scientist at Inria (Lille Nord Europe),
- Scientific director of the Inria London joint lab with UCL CS and AI,
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Most recent research: coupling machine learning and sleep deprivation.



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- Cover all of our ICML 2019 tutorial! See https://bguedj.github.io/icml2019/index.html
- Cover our NIPS 2017 workshop "(Almost) 50 Shades of Bayesian Learning: PAC-Bayesian trends and insights" See https://bguedj.github.io/nips2017/

# Take-home message

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MSc interns, PhD students, postdocs, visiting researchers

# Part I

#### A Primer on PAC-Bayesian Learning ICML 2019 tutorial



#### John

https://bguedj.github.io/icml2019/index.html Survey in the Journal of the French Mathematical Society: *Guedj (2019)* 





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

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For a fixed algorithm, function class and sample size, generating random samples  $\longrightarrow$  distribution of test errors

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- Hence high confidence:  $\mathbb{P}^m$ [approximately correct]  $\ge 1 \delta$

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

•  $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$  $\mathcal{X}$  = set of inputs  $\mathcal{Y}$  = set of outputs (e.g. labels) •  $\mathcal{H}$  = hypothesis class = set of predictors (e.g. classifiers) functions  $\mathcal{X} \rightarrow \mathcal{Y}$ 

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

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Actually these two goals interact with each other!

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

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$$R_{\mathrm{out}}(h) = \mathbb{E}[\ell(h(X), Y)]$$

Examples:

- $\ell(h(X), Y) = \mathbf{1}[h(X) \neq Y]$  : 0-1 loss (classification)
- $\ell(h(X), Y) = (Y h(X))^2$  : square loss (regression)
- $\ell(h(X), Y) = (1 Yh(X))_+$  : hinge loss
- $\ell(h(X), 1) = -\log(h(X))$  : log loss (density estimation)

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#### Flavours:

- distribution-free
- algorithm-free

- distribution-dependent
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- explain why specific learning algorithms actually work
- and even lead to designing new algorithm which scale to more complex settings

■ Single hypothesis *h* (building block):

with probability  $\ge 1 - \delta$ ,  $R_{\text{out}}(h) \le R_{\text{in}}(h) + \sqrt{\frac{1}{2m} \log(\frac{1}{\delta})}$ .

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 $\longrightarrow$  Extension: PAC-Bayes allows to consider  $\emph{distributions}$  over hypotheses.

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The risk measures  $R_{in}(h)$  and  $R_{out}(h)$  are extended by averaging:  $R_{in}(Q) \equiv \int_{\mathcal{H}} R_{in}(h) \, dQ(h) \qquad R_{out}(Q) \equiv \int_{\mathcal{H}} R_{out}(h) \, dQ(h)$ 

 $\operatorname{KL}(\boldsymbol{Q} \| \boldsymbol{P}) = \underset{h \sim \boldsymbol{Q}}{\mathbf{E}} \ln \frac{\boldsymbol{Q}(h)}{\boldsymbol{P}(h)}$  is the Kullback-Leibler divergence.

#### PAC-Bayes aka Generalised Bayes

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Prior	Bayesian inference Unique Statistical modelling (likelihood)	Posterior
Any distribution not depending on data	PAC-Bayes Model-free	Any distribution
	Inspired by the Bayesian update principle - Only depends on loss	(possibly) depending on data

"Prior": exploration mechanism of  ${\mathcal H}$  "Posterior" is the twisted prior after confronting with data

#### PAC-Bayes bounds vs. Bayesian learning
Prior

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- · Bayes: prior choice impacts inference

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#### Data distribution

- PAC-Bayes: bounds hold for any distribution
- · Bayes: randomness lies in the noise model generating the output

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

#### **McAllester Bound**

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

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

# A flexible framework

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Since 1997, PAC-Bayes has been successfully used in many machine learning settings (this list is by no means exhaustive).

Statistical learning theory Shawe-Taylor and Williamson (1997); McAllester (1998, 1999, 2003a,b); Seeger (2002, 2003); Maurer (2004); Catoni (2004, 2007); Audibert and Bousquet (2007); Thiemann et al. (2017); Guedj (2019); Mhammedi et al. (2019); Guedj and Pujol (2019); Haddouche et al. (2020)

- SVMs & linear classifiers Langford and Shawe-Taylor (2002); McAllester (2003a); Germain et al. (2009a)
- Supervised learning algorithms reinterpreted as bound minimizers Ambroladze et al. (2007); Shawe-Taylor and Hardoon (2009); Germain et al. (2009b)
- High-dimensional regression Alquier and Lounici (2011); Alquier and Biau (2013); Guedj and Alquier (2013); Li et al. (2013); Guedj and Robbiano (2018)

Classification Langford and Shawe-Taylor (2002); Catoni (2004, 2007); Lacasse et al. (2007); Parrado-Hernández et al. (2012)

# A flexible framework

Transductive learning, domain adaptation Derbeko et al. (2004); Bégin et al. (2014); Germain et al. (2016); Nozawa et al. (2020)

- Non-iid or heavy-tailed data Lever et al. (2010); Seldin et al. (2011, 2012); Alquier and Guedj (2018); Holland (2019)
- Density estimation Seldin and Tishby (2010); Higgs and Shawe-Taylor (2010) Reinforcement learning Fard and Pineau (2010); Fard et al. (2011); Seldin et al. (2011, 2012); Ghavamzadeh et al. (2015)
- Sequential learning Gerchinovitz (2011); Li et al. (2018)
- Algorithmic stability, differential privacy London et al. (2014); London (2017); Dziugaite and Roy (2018a,b); Rivasplata et al. (2018)
- Deep neural networks Dziugaite and Roy (2017); Neyshabur et al. (2017); Zhou et al. (2019); Letarte et al. (2019); Biggs and Guedj (2020)

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Error on unseen data  $\leq$  Error on sample + complexity term  $R_{\text{out}}(Q) \leq R_{\text{in}}(Q) + F(Q, \cdot)$ 

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$$h \sim Q^*$$
  
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(optimisation problem which can be solved or approximated by [stochastic] gradient descent-flavoured methods, Monte Carlo Markov Chain, (generalized) variational inference...)

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

Variational definition of  ${\rm KL}$ -divergence (Csiszár, 1975; Donsker and Varadhan, 1975; Catoni, 2004).

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Let (A, A) be a measurable space.

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

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

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

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

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

$$\begin{split} \log \int (\exp \circ \varphi) \mathrm{d} \boldsymbol{P} &= \sup_{\boldsymbol{Q} \ll \boldsymbol{P}} \left\{ \int \varphi \mathrm{d} \boldsymbol{Q} - \mathrm{KL}(\boldsymbol{Q}, \boldsymbol{P}) \right\}, \quad \frac{\mathrm{d} \boldsymbol{G}}{\mathrm{d} \boldsymbol{P}} &= \frac{\exp \circ \varphi}{\int (\exp \circ \varphi) \mathrm{d} \boldsymbol{P}}. \end{split}$$
Proof: let  $\boldsymbol{Q} \ll \boldsymbol{P}.$ 

$$-\operatorname{KL}(Q, G) = -\int \log \left( \frac{\mathrm{d}Q}{\mathrm{d}P} \frac{\mathrm{d}P}{\mathrm{d}G} \right) \mathrm{d}Q$$

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

$$Q_{\lambda} \propto \exp\left(-\lambda R_{\mathrm{in}}
ight) P = \operatorname*{arg\,inf}_{\mathcal{Q} \ll \mathcal{P}} \left\{ R_{\mathrm{in}}(\mathcal{Q}) + \dfrac{\mathrm{KL}(\mathcal{Q}, \mathcal{P})}{\lambda} 
ight\}.$$

What we've seen so far

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What is coming next

A small sample of what PAC-Bayes can offer!

# Part II

A (gentle) walkthrough of state-of-the-art PAC-Bayes

- Guedj and Robbiano (2018). PAC-Bayesian high dimensional bipartite ranking, Journal of Statistical Planning and Inference.
- Alquier and Guedj (2018). Simpler PAC-Bayesian bounds for hostile data, Machine Learning.
- Letarte, Germain, Guedj and Laviolette (2019). Dichotomize and generalize: PAC-Bayesian binary activated deep neural networks, NeurIPS 2019.
- Nozawa, Germain and Guedj (2020). PAC-Bayesian contrastive unsupervised representation learning, UAI.


# Bipartite ranking

Goal: design an order relationship on  $\mathbb{R}^d$  which is consistent with the order on  $\{\pm 1\}$ . Scoring function  $s: \mathbb{R}^d \to \mathbb{R}$ 

$$\forall (\mathbf{x}, \mathbf{x}') \in \mathbb{R}^d \times \mathbb{R}^d, \qquad \mathbf{x} \preceq_s \mathbf{x}' \Leftrightarrow s(\mathbf{x}) \leqslant s(\mathbf{x}').$$

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Idea: build s such that

$$\forall (\bm{x}, \bm{x}') \in \mathbb{R}^d \times \mathbb{R}^d, \quad \textit{s}(\bm{x}) \leqslant \textit{s}(\bm{x}') \Leftrightarrow \eta(\bm{x}) \leqslant \eta(\bm{x}').$$

### PAC-Bayes ranking

Ranking risk of a scoring function s and empirical counterpart

$$L(s) = \mathbb{P}\left[ (s(\mathbf{X}) - s(\mathbf{X}'))(Y - Y') < 0 \right].$$
  
$$L_m(s) = \frac{1}{m(m-1)} \sum_{i \neq j} \mathbf{1}_{\{(s(\mathbf{X}_i) - s(\mathbf{X}_j))(Y_i - Y_j) < 0\}}.$$

Dictionary of deterministic functions  $\mathbb{D} = \{ \phi_1, \dots, \phi_M \},\$ 

$$\mathbb{S}_{\Theta} = \left\{ \boldsymbol{s}_{\theta} \colon \boldsymbol{\mathbf{x}} \mapsto \sum_{j=1}^{d} \sum_{k=1}^{M} \theta_{jk} \phi_{k}(\boldsymbol{x}_{j}) = \langle \theta, \mathbb{D}(\boldsymbol{\mathbf{x}}) \rangle, \quad \theta \in \mathbb{R}^{dM} \right\}.$$

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Gibbs measure  $Q_{\lambda}(d\theta) \propto \exp[-\lambda L_n(s_{\theta})]P(d\theta), \lambda > 0$ . PAC-Bayes predictor

$$\widehat{\boldsymbol{s}} = \boldsymbol{s}_{\widehat{\boldsymbol{\theta}}} \colon \boldsymbol{x} \mapsto \sum_{j=1}^{d} \sum_{k=1}^{M} \widehat{\boldsymbol{\theta}}_{jk} \boldsymbol{\varphi}_{k}(\boldsymbol{x}_{j}) = \langle \widehat{\boldsymbol{\theta}}, \mathbb{D}(\boldsymbol{x}) \rangle, \quad \widehat{\boldsymbol{\theta}} \sim \boldsymbol{Q}_{\lambda}.$$

MCMC implementation (Metropolised Carlin and Chib)

#### Oracle generalisation bounds

For any distribution of (**X**, *Y*), any prior *P*, any  $\delta \in (0, 1)$ ,

$$\begin{split} \mathbb{P}\left[L(\widehat{s}) - L(\eta) \leqslant \inf_{Q \ll P} \left\{ \int L(s)Q(\mathrm{d}s) - L(\eta) \right. \\ \left. + \frac{1/2 + 2\log(2/\delta) + 2\mathrm{KL}(Q, P)}{\sqrt{m}} \right\} \right] \geqslant 1 - \delta. \end{split}$$

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Optimal sparse scoring functions

$$\mathbb{P}\left[L(\widehat{s}) - L(\eta) \leqslant \inf_{\substack{k=1,\dots,d \ \theta : \ |\theta|_0 = k}} \left\{L(s_{\theta}) - L(\eta) + \frac{3/2 + 2\log(2/\delta) + \log(\sqrt{m}) + k\log\frac{dM}{k}}{\sqrt{m}}\right\}\right] \ge 1 - \delta.$$

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Under a margin condition on  $\eta$ , we proved the first minimax optimal rates for high dimensional bipartite ranking.

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$$\mathcal{M}_q := \int \mathbb{E} \left( |R_{\mathrm{in}}(h) - R_{\mathrm{out}}(h)|^q \right) \mathrm{d}P(h).$$

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Csiszár *f*-divergence: let *f* be a convex function with f(1) = 0,

$$D_f(Q, P) = \int f\left(\frac{\mathrm{d}Q}{\mathrm{d}P}\right) \mathrm{d}P$$

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The KL is given by the special case  $\operatorname{KL}(Q \| P) = D_{x \log(x)}(Q, P)$ .

Power function:  $\phi_p$ :  $x \mapsto x^p$ .

Fix p > 1,  $q = \frac{p}{p-1}$  and  $\delta \in (0, 1)$ . With probability at least  $1 - \delta$  we have for any distribution Q

$$|R_{\text{out}}(Q) - R_{\text{in}}(Q)| \leq \left(\frac{\mathfrak{M}_{q}}{\delta}\right)^{\frac{1}{q}} \left(D_{\varphi_{p}-1}(Q, P) + 1\right)^{\frac{1}{p}}$$

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Again, strong incitement to define the posterior as the minimizer of the right-hand side!

For 
$$p = q = 2$$
, w.p.  $\geq 1 - \delta$ ,  $R_{\text{out}}(Q) \leq R_{\text{in}}(Q) + \sqrt{\frac{v}{m\delta}} \int \left(\frac{\mathrm{d}Q}{\mathrm{d}P}\right)^2 \mathrm{d}P$ .

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Proof Let Δ(

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$$\left| \int \mathcal{R}_{out} \mathrm{d}\mathcal{Q} - \int \mathcal{R}_{in} \mathrm{d}\mathcal{Q} \right|$$
Jensen
 $\leqslant \int \Delta \mathrm{d}\mathcal{Q}$ 

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- **x**  $\in \mathbb{R}^{d_0}$
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- L fully connected layers
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- $\label{eq:static} \ensuremath{{\rm \blacksquare}} \ensuremath{\,\sigma}: \ensuremath{\mathbb{R}} \to \ensuremath{\mathbb{R}} \ensuremath{\,\text{is the activation function}}$

Parameters:

■  $\mathbf{W}_k \in \mathbb{R}^{d_k \times d_{k-1}}$  denotes the weight matrices,  $D = \sum_{k=1}^{L} d_{k-1} d_k$ .

$$\bullet \theta = \operatorname{vec}\left(\{\mathbf{W}_k\}_{k=1}^L\right) \in \mathbb{R}^D$$



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Parameters:

### Prediction

$$f_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sigma \big( \boldsymbol{w}_L \sigma \big( \boldsymbol{W}_{L-1} \sigma \big( \dots \sigma \big( \boldsymbol{W}_1 \boldsymbol{x} \big) \big) \big) \big) \,.$$



# PAC-Bayesian bounds for Stochastic NN

### Langford and Caruana (2001)

- Shallow networks (L = 2)
- Sigmoid activation functions

### Dziugaite and Roy (2017)

- Deep networks (*L* > 2)
- ReLU activation functions





# PAC-Bayesian bounds for Stochastic NN



**Idea:** Bound the expected loss of the network under a Gaussian perturbation of the weights

 $\mathsf{Empirical \ loss:} \underset{\theta' \sim \mathcal{N}(\theta, \Sigma)}{\mathsf{E}} R_{\mathrm{in}}(f_{\theta'}) \longrightarrow \mathsf{estimated \ by \ sampling}$ 

Complexity term:  $\mathrm{KL}(\mathcal{N}(\theta, \Sigma) \| \mathcal{N}(\theta_0, \Sigma_0)) \longrightarrow \text{closed form}$ 

### Binary Activated Neural Networks $\mathbf{x} \in \mathbb{R}^{d_0}$

■  $y \in \{-1, 1\}$ 

Architecture:

- L fully connected layers
- *d<sub>k</sub>* denotes the number of neurons of the *k*<sup>th</sup> layer
- sgn(a) = 1 if a > 0 and sgn(a) = −1 otherwise

Parameters:

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### Prediction





Germain et al. (2009a)

$$\mathbf{x}_{\mathbf{w}}^{\mathsf{def}}(\mathbf{x}) \stackrel{\mathsf{def}}{=} \operatorname{sgn}(\mathbf{w} \cdot \mathbf{x}), \, \mathsf{with} \, \mathbf{w} \in \mathbb{R}^{d_0}.$$



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PAC-Bayes analysis:

**Space of all linear classifiers**  $\mathcal{F}_d \stackrel{\text{def}}{=} \{ f_{\mathbf{V}} | \mathbf{V} \in \mathbb{R}^d \}$ 



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# One Layer (linear predictor)

Germain et al. (2009a)

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- **Space of all linear classifiers**  $\mathcal{F}_d \stackrel{\text{\tiny def}}{=} \{ f_{\mathbf{V}} | \mathbf{V} \in \mathbb{R}^d \}$
- Gaussian posterior  $Q_{\mathbf{w}} \stackrel{\text{def}}{=} \mathcal{N}(\mathbf{w}, I_d)$  over  $\mathcal{F}_d$
- Gaussian prior  $P_{\mathbf{w}_0} \stackrel{\text{def}}{=} \mathcal{N}(\mathbf{w}_0, I_d)$  over  $\mathcal{F}_d$
- Predictor  $F_{\mathbf{w}}(\mathbf{x}) \stackrel{\text{def}}{=} \mathbf{E}_{\mathbf{v} \sim Q_{\mathbf{w}}} f_{\mathbf{v}}(\mathbf{x}) = \operatorname{erf}\left(\frac{\mathbf{w} \cdot \mathbf{x}}{\sqrt{d} \|\mathbf{x}\|}\right)$



Bound minimisation — under the linear loss  $\ell(y, y') \coloneqq \frac{1}{2}(1 - yy')$ 

$$CmR_{\rm in}(F_{\mathbf{w}}) + {\rm KL}(Q_{\mathbf{w}} || P_{\mathbf{w}_0}) = C \frac{1}{2} \sum_{i=1}^m \operatorname{erf}\left(-y_i \frac{\mathbf{w} \cdot \mathbf{x}_i}{\sqrt{d} || \mathbf{x}_i ||}\right) + \frac{1}{2} || \mathbf{w} - \mathbf{w}_0 ||^2.$$

# Two Layers (shallow network)



## Two Layers (shallow network) Posterior $Q_{\theta} = \mathcal{N}(\theta, I_D)$ , over the family of all networks $\mathcal{F}_D = \{f_{\tilde{\theta}} \mid \tilde{\theta} \in \mathbb{R}^D\}$ , where

 $f_{\Theta}(\mathbf{x}) = \operatorname{sgn}(\mathbf{w}_2 \cdot \operatorname{sgn}(\mathbf{W}_1 \mathbf{x})).$ 

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$$F_{\theta}(\mathbf{x}) = \mathop{\mathbf{E}}_{\tilde{\theta} \sim Q_{\theta}} f_{\tilde{\theta}(\mathbf{x})}$$

#### Two Layers (shallow network) Posterior $Q_{\theta} = \mathcal{N}(\theta, I_D)$ , over the family of all networks $\mathcal{F}_D = \{f_{\tilde{a}} \mid \tilde{\theta} \in \mathbb{R}^D\}$ , where

 $f_{\Theta}(\mathbf{x}) = \operatorname{sgn}(\mathbf{w}_2 \cdot \operatorname{sgn}(\mathbf{W}_1 \mathbf{x}))$ .  $F_{\theta}(\mathbf{x}) = \mathop{\mathbf{E}}_{\tilde{\theta} \sim O_{\theta}} t_{\tilde{\theta}(\mathbf{x})}$  $= \int_{\mathbf{r} d \cdot \mathbf{v} d \cdot} Q_1(\mathbf{V}_1) \int_{\mathbf{r} d \cdot} Q_2(\mathbf{v}_2) \operatorname{sgn}(\mathbf{v}_2 \cdot \operatorname{sgn}(\mathbf{V}_1 \mathbf{x})) d\mathbf{v}_2 d\mathbf{V}_1$  $= \left[ \sup_{\mathbf{v} \in \mathbf{V}, \mathbf{v} \in \mathbf{V}} Q_1(\mathbf{V}_1) \operatorname{erf} \left( \frac{\mathbf{w}_2 \cdot \operatorname{sgn}(\mathbf{V}_1 \mathbf{x})}{\sqrt{2} \|\operatorname{sgn}(\mathbf{V}_1 \mathbf{x})\|} \right) d\mathbf{V}_1 \right]$  $= \sum_{\mathbf{r}: d_1 \times d_2} \operatorname{erf}\left(\frac{\mathbf{w}_2 \cdot \mathbf{s}}{\sqrt{2d_1}}\right) \int_{\mathbf{r}: d_1 \times d_2} \operatorname{sgn}(\mathbf{V}_1 \mathbf{x}) [\mathbf{Q}_1(\mathbf{V}_1) \, d\mathbf{V}_1]$  $s \in \{-1, 1\}^{d_1}$  $= \sum_{\mathbf{s} \in \{-1,1\}^{d_1}} \underbrace{\operatorname{erf}\left(\frac{\mathbf{w}_2 \cdot \mathbf{s}}{\sqrt{2d_1}}\right)}_{\mathbf{x} = 1} \underbrace{\prod_{i=1}^{d_1} \left[\frac{1}{2} + \frac{s_i}{2} \operatorname{erf}\left(\frac{\mathbf{w}_1^i \cdot \mathbf{x}}{\sqrt{2} \|\mathbf{x}\|}\right)\right]}_{\mathbf{x} = 1}.$ 

 $Pr(\mathbf{s}|\mathbf{x},\mathbf{W}_1)$ 

## Stochastic Approximation

$$F_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sum_{\boldsymbol{s} \in \{-1,1\}^{d_1}} F_{\boldsymbol{w}_2}(\boldsymbol{s}) \operatorname{Pr}(\boldsymbol{s} | \boldsymbol{x}, \boldsymbol{W}_1)$$

Monte Carlo sampling

We generate *T* random binary vectors  $\{\mathbf{s}^t\}_{t=1}^T$  according to  $\Pr(\mathbf{s}|\mathbf{x}, \mathbf{W}_1)$ 

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$$F_{\theta}(\mathbf{x}) \approx \frac{1}{T} \sum_{t=1}^{T} F_{\mathbf{w}_2}(\mathbf{s}^t).$$

Derivatives.

$$\frac{\partial}{\partial \mathbf{w}_1^k} F_{\theta}(\mathbf{x}) \approx \frac{\mathbf{x}}{2^{\frac{3}{2}} \|\mathbf{x}\|} \operatorname{erf}'\left(\frac{\mathbf{w}_1^k \cdot \mathbf{x}}{\sqrt{2} \|\mathbf{x}\|}\right) \frac{1}{7} \sum_{t=1}^T \frac{s_k^t}{\Pr(s_k^t | \mathbf{x}, \mathbf{w}_1^k)} F_{\mathbf{w}_2}(\mathbf{s}^t) \,.$$

More Layers (deep)  $(x_1)$   $(x_2)$   $(x_1)$   $(x_2)$   $(x_1)$   $(x_2)$   $(x_1)$   $(x_2)$   $(x_1)$   $(x_2)$   $(x_1)$   $(x_2)$   $(x_1)$   $(x_2)$  $(x_1)(x_2)$ (**x**<sub>2</sub>)  $X_2$  $(x_1)$ *X*1  $F_{1}^{(j)}(\mathbf{x}) = \operatorname{erf}\left(\frac{\mathbf{w}_{1}^{j} \cdot \mathbf{x}}{\sqrt{2}\|\mathbf{x}\|}\right), \qquad F_{k+1}^{(j)}(\mathbf{x}) = \sum_{i=1}^{n} \operatorname{erf}\left(\frac{\mathbf{w}_{k+1}^{i} \cdot \mathbf{s}}{\sqrt{2d_{k}}}\right) \prod_{i=1}^{d_{k}} \left(\frac{1}{2} + \frac{1}{2}s_{i} \times F_{k}^{(i)}(\mathbf{x})\right)$  $s \in \{-1, 1\}^{d_k}$ 

## Generalisation bound

Let  $G_{\theta}$  denote the predictor with posterior mean as parameters. With probability at least  $1 - \delta$ , for any  $\theta \in \mathbb{R}^{D}$ 

$$R_{\text{out}}(G_{\theta}) \leq \inf_{C>0} \left\{ \frac{1}{1 - e^{-C}} \left( 1 - \exp\left( -CR_{\text{in}}(G_{\theta}) - \frac{\text{KL}(\theta, \theta_{0}) + \log\frac{2\sqrt{m}}{\delta}}{m} \right) \right) \right\}$$

# Numerical results

Model name	Cost function	Train split	Valid split	Model selection	Prior	
MLP–tanh PBGNetℓ <b>PBGNet</b>	linear loss, L2 regularized linear loss, L2 regularized <b>PAC-Bayes bound</b>	80% 80% <b>100 %</b>	20% 20% -	valid linear loss valid linear loss <b>PAC-Bayes bound</b>	- random init <b>random init</b>	
PBGNet <sub>pre</sub> – pretrain – final	linear loss (20 epochs) PAC-Bayes bound	50% 50%	-	- PAC-Bayes bound	random init pretrain	

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	MLP-tanh		Р	PBGNetℓ		PBGNet			PBGNetpre		
Dataset	E <sub>S</sub>	ET	ES	E <sub>T</sub>	E <sub>S</sub>	E <sub>T</sub>	Bound	Es	E <sub>T</sub>	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	

# Contrastive unsupervised representation learning (aka CURL)

SOTA technique to learn representations (as a set of features) from unlabelled data (e.g., word2vec, image classification). Contrastive loss differentiates inputs by similarity.

Arora et al. (2019): first theoretical results on CURL, using Rademacher complexity. In a nutshell, for any predictor *f* and  $\hat{f}$  an ERM, w.p.  $\ge 1 - \delta$ ,

$$\text{Loss}_{\text{sup}}(\widehat{f}) \leqslant C_1 \text{Loss}_{\text{uns}}(f) + C_2\left(\frac{\text{Rad}}{m} + \sqrt{\frac{\log(1/\delta)}{m}}\right)$$

We proposed a PAC-Bayes version which improves on their results by removing the iid assumption and by deriving a SOTA learning algorithm. For any prior *P*, any posterior *Q*, any  $\lambda > 0$ , w.p.  $\ge 1 - \delta$ 

$$\mathsf{Loss}_{\mathsf{sup}}(Q) \leqslant C \left( \begin{array}{c} \frac{1 - \exp\left(-\lambda \widehat{\mathsf{Loss}}_{\mathsf{uns}}(Q) - \frac{\mathrm{KL}(Q, P) + \log(1/\delta)}{m}\right)}{1 - \exp(-\lambda)} \right)$$

# Thanks!

#### What this talk could have been about...

- Tighter PAC-Bayes bounds (Mhammedi et al., 2019)
- PAC-Bayes and robust learning (Guedj and Pujol, 2019; Haddouche et al., 2020)
- PAC-Bayesian online clustering (Li et al., 2018)
- Online k-means clustering (Cohen-Addad et al., 2019)
- Sequential learning of principal curves (Guedj and Li, 2018)
- Stability and generalisation (Celisse and Guedj, 2016)
- Decentralised learning with aggregation (Klein et al., 2019)
- Image denoising (Guedj and Rengot, 2020)
- Matrix factorisation (Alquier and Guedj, 2017; Chrétien and Guedj, 2020)
- Preventing model overfitting (Zhang et al., 2019)
- / a few others... (very) soon on arXiv

#### = PAC-Bayes

"Wait, I can talk about other stuff too!"

#### This talk:

https://bguedj.github.io/talks/2020-06-16-seminar-faicdt

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