A (condensed) primer on PAC-Bayesian Learning
followed by
News from the PAC-Bayes frontline

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UCL Statistical Science Seminar
January 21, 2021

Greetings!

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PhD in mathematics and statistics, 2013 Sorbonne Univ. (France)

Since 2018, principal research fellow at CS and the AI Centre

Interests: statistical learning theory, PAC-Bayes, computational statistics, generalisation bounds for deep learning, and many others.

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Becoming quite an expert in coupling statistical learning and sleep deprivation.

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I won't...

- 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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PhD students, postdocs, tenured researchers, visiting positions
Through the Centre for AI at UCL,
and through the newly founded Inria London Programme

Part I

A Primer on PAC-Bayesian Learning
(short version of our ICML 2019 tutorial)

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

Learning is to be able to generalise

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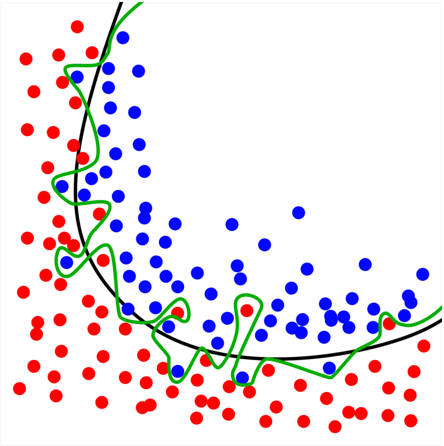

[Figure from Wikipedia]

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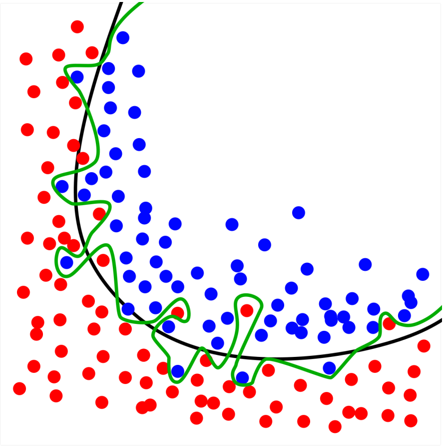

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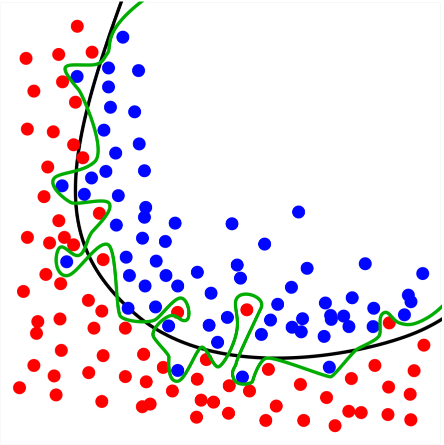

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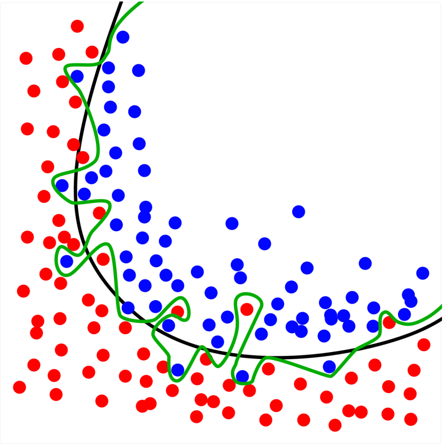

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Generalisation is the ability to 'perform' well on unseen data.

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

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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
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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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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
- algorithm-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

Before PAC-Bayes

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- Single hypothesis h (building block):

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

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The risk measures $R_{\rm in}(h)$ and $R_{\rm out}(h)$ are extended by averaging:

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

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

PAC-Bayes aka Generalised Bayes

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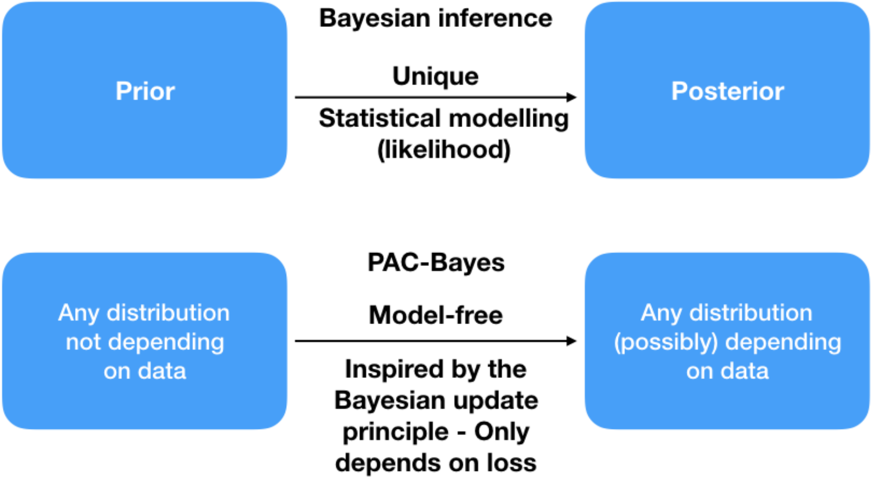

"Prior": exploration mechanism of $\mathcal{H}$

"Posterior" is the twisted prior after confronting with data

PAC-Bayes bounds vs. Bayesian learning

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  - Bayes: statistical modelling choices impact inference

A classical PAC-Bayesian bound

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Pre-history: PAC analysis of Bayesian estimators

Shawe-Taylor and Williamson (1997); Shawe-Taylor et al. (1998)

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

McAllester Bound

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

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

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, 2020); 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)*

…

PAC-Bayes-inspired learning algorithms

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

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

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

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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 $\int (\exp \circ \phi) \mathrm{d}P < \infty$,

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

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

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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

- ☑ 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 2020.
- ☑ Haddouche, Guedj, Rivasplata and Shawe-Taylor (2020). PAC-Bayes unleashed: generalisation bounds with unbounded losses, preprint.
- ■ Mhammedi, Guedj and Williamson (2020). PAC-Bayesian Bound for the Conditional Value at Risk, NeurIPS 2020 (spotlight).









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

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

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

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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

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- the moment $\mathcal{M}_q$ (which depends on the distribution of the data)
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For $p = q = 2$, w.p. $\geqslant 1 - \delta$, $R_{\mathrm{out}}(Q) \leqslant R_{\mathrm{in}}(Q) + \sqrt{\frac{\mathcal{V}}{m\delta} \int \left(\frac{\mathrm{d}Q}{\mathrm{d}P}\right)^2 \mathrm{d}P}$.

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Classification setting:

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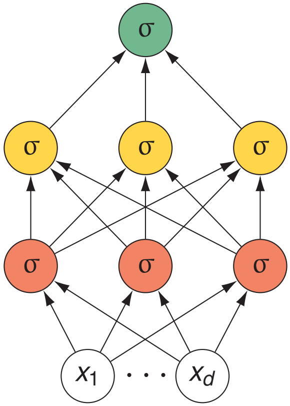

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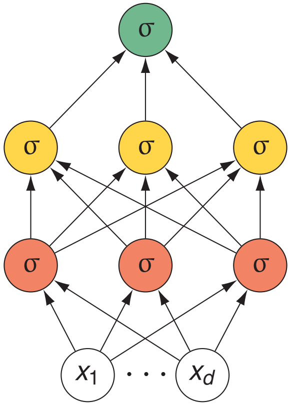


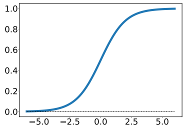
Prediction

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

PAC-Bayesian bounds for Stochastic NN

Langford and Caruana (2001)

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



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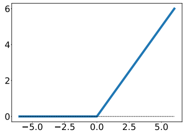

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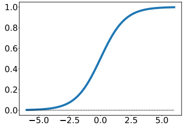

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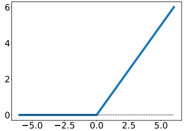

Idea: Bound the expected loss of the network under a Gaussian perturbation of the weights

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

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

Binary Activated Neural Networks

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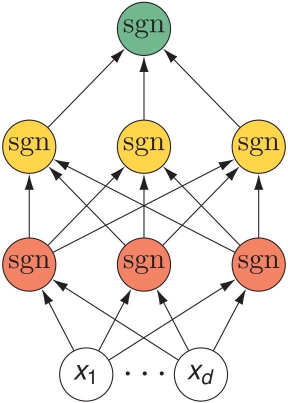


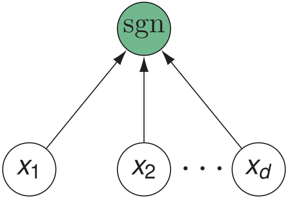
Prediction

$$f_\theta(\mathbf{x}) = \text{sgn}\Big(\mathbf{w}_L \text{sgn}\big(\mathbf{W}_{L-1} \text{sgn}\big(\ldots \text{sgn}\big(\mathbf{W}_1 \mathbf{x}\big)\big)\big)\Big),$$

One Layer (linear predictor)

Germain et al. (2009a)

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



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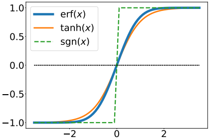
PAC-Bayes analysis:

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



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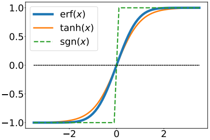
PAC-Bayes analysis:

- Space of all linear classifiers $\mathcal{F}_d \stackrel{\text{def}}{=} \{f_{\mathbf{v}} | \mathbf{v} \in \mathbb{R}^d\}$
- Gaussian posterior $Q_{\mathbf{w}} \stackrel{\text{def}}{=} \mathcal{N}(\mathbf{w}, I_d)$ over $\mathcal{F}_d$



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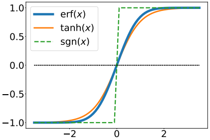

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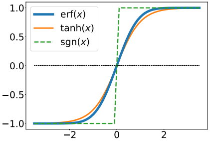

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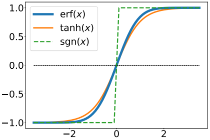

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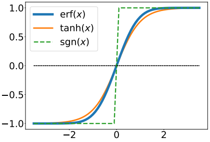
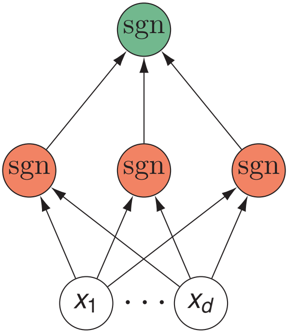


Bound minimisation — under the linear loss $\ell(y, y') := \frac{1}{2}(1 - yy')$

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

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

$$f_\theta(\mathbf{x}) = \mathrm{sgn}\big(\mathbf{w}_2 \cdot \mathrm{sgn}(\mathbf{W}_1 \mathbf{x})\big) \,.$$

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

$$f_\theta(\mathbf{x}) = \mathrm{sgn}\big(\mathbf{w}_2 \cdot \mathrm{sgn}(\mathbf{W}_1 \mathbf{x})\big) .$$

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

Two Layers (shallow network)

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

$$f_\theta(\mathbf{x}) = \mathrm{sgn}\big(\mathbf{w}_2 \cdot \mathrm{sgn}(\mathbf{W}_1\mathbf{x})\big)\,.$$

$$\begin{aligned}
F_\theta(\mathbf{x}) &= \mathop{\mathbf{E}}_{\tilde\theta\sim Q_\theta} f_{\tilde\theta}(\mathbf{x}) \\
&= \int_{\mathbb{R}^{d_1\times d_0}} Q_1(\mathbf{V}_1) \int_{\mathbb{R}^{d_1}} Q_2(\mathbf{v}_2)\mathrm{sgn}(\mathbf{v}_2\cdot\mathrm{sgn}(\mathbf{V}_1\mathbf{x}))\,d\mathbf{v}_2\,d\mathbf{V}_1 \\
&= \int_{\mathbb{R}^{d_1\times d_0}} Q_1(\mathbf{V}_1)\,\mathrm{erf}\left(\frac{\mathbf{w}_2\cdot\mathrm{sgn}(\mathbf{V}_1\mathbf{x})}{\sqrt{2}\|\mathrm{sgn}(\mathbf{V}_1\mathbf{x})\|}\right) d\mathbf{V}_1 \\
&= \sum_{\mathbf{s}\in\{-1,1\}^{d_1}} \mathrm{erf}\left(\frac{\mathbf{w}_2\cdot\mathbf{s}}{\sqrt{2d_1}}\right) \int_{\mathbb{R}^{d_1\times d_0}} \mathbb{1}[\mathbf{s} = \mathrm{sgn}(\mathbf{V}_1\mathbf{x})]\,Q_1(\mathbf{V}_1)\,d\mathbf{V}_1 \\
&= \sum_{\mathbf{s}\in\{-1,1\}^{d_1}} \underbrace{\mathrm{erf}\left(\frac{\mathbf{w}_2\cdot\mathbf{s}}{\sqrt{2d_1}}\right)}_{F_{\mathbf{w}_2}(\mathbf{s})} \underbrace{\prod_{i=1}^{d_1}\left[\frac{1}{2} + \frac{s_i}{2}\,\mathrm{erf}\left(\frac{\mathbf{w}_1^i\cdot\mathbf{x}}{\sqrt{2}\,\|\mathbf{x}\|}\right)\right]}_{\Pr(\mathbf{s}|\mathbf{x},\mathbf{W}_1)}\,.
\end{aligned}$$

Stochastic Approximation

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

Monte Carlo sampling

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

Stochastic Approximation

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

Monte Carlo sampling

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

Prediction.

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

Stochastic Approximation

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

Monte Carlo sampling

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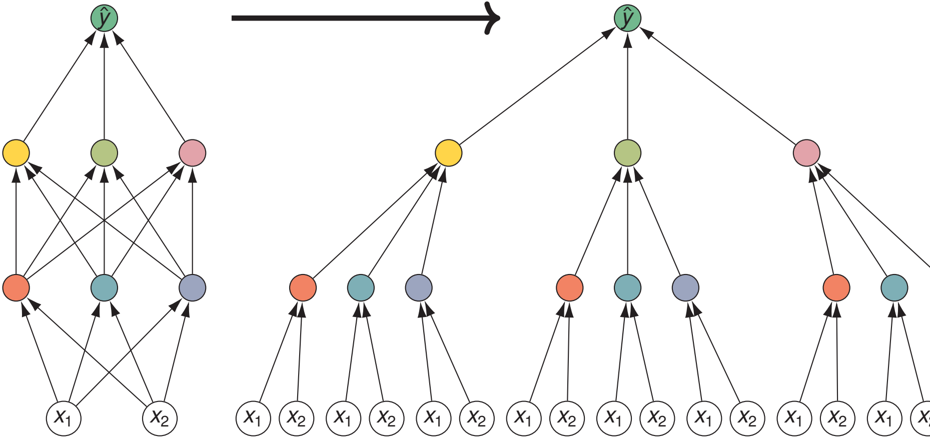
Prediction.

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

Derivatives.

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

More Layers (deep)



$$F_1^{(j)}(\mathbf{x}) = \operatorname{erf}\left(\frac{\mathbf{w}_1^j \cdot \mathbf{x}}{\sqrt{2}\|\mathbf{x}\|}\right), \qquad F_{k+1}^{(j)}(\mathbf{x}) = \sum_{\mathbf{s}\in\{-1,1\}^{d_k}} \operatorname{erf}\left(\frac{\mathbf{w}_{k+1}^j \cdot \mathbf{s}}{\sqrt{2d_k}}\right) \prod_{i=1}^{d_k} \left(\frac{1}{2} + \frac{1}{2} s_i \times F_k^{(i)}(\mathbf{x})\right)$$

Generalisation bound

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

$$R_{\mathrm{out}}(G_\theta) \leqslant$$

$$\inf_{C>0} \left\{ \frac{1}{1-e^{-C}} \left(1 - \exp\left(-C R_{\mathrm{in}}(G_\theta) - \frac{\mathrm{KL}(\theta, \theta_0) + \log \frac{2\sqrt{m}}{\delta}}{m} \right) \right) \right\}.$$

Numerical results

Model name	Cost function	Train split	Valid split	Model selection	Prior
MLP–tanh	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

Numerical results

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Dataset	MLP–tanh		PBGNet$_\ell$		PBGNet			PBGNet$_{\text{pre}}$		
	E_S	E_T	E_S	E_T	E_S	E_T	Bound	E_S	E_T	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

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, 2020)
- PAC-Bayes and robust learning (Guedj and Pujol, 2019)
- PAC-Bayesian online clustering (Li et al., 2018)
- PAC-Bayesian bipartite ranking (Guedj and Robbiano, 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)
- Contrastive unsupervised learning (Nozawa et al., 2020)
- Image denoising (Guedj and Rengot, 2020)
- Matrix factorisation (Alquier and Guedj, 2017; Chrétien and Guedj, 2020)
- Preventing model overfitting (Zhang et al., 2019)
- Decentralised learning with aggregation (Klein et al., 2019)
- Ensemble learning (nonlinear aggregation) in Python (Guedj and Srinivasa Desikan, 2018, 2020)
- Identifying subcommunities in social networks (Vendeville et al., 2020b,a)
- Prediction with multi-task Gaussian processes (Leroy et al., 2020)
- + a few others in the pipe, hopefully soon on arXiv!

This talk: `https://bguedj.github.io/talks/2021-01-21-seminar-ucl-stat`

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