An Introduction to PAC-Bayesian Analysis

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Learning is to be able to generalise

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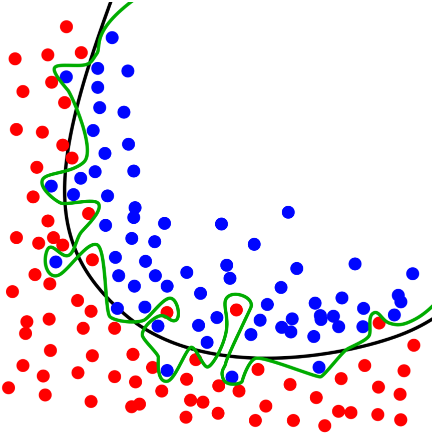

[Figure from Wikipedia]

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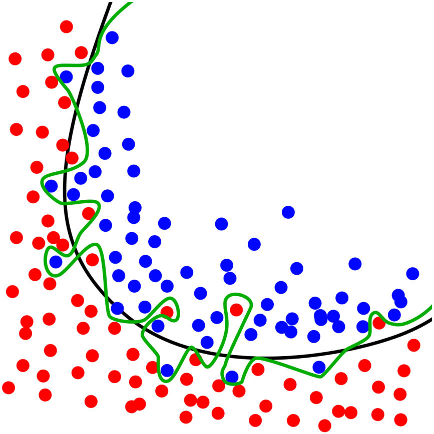

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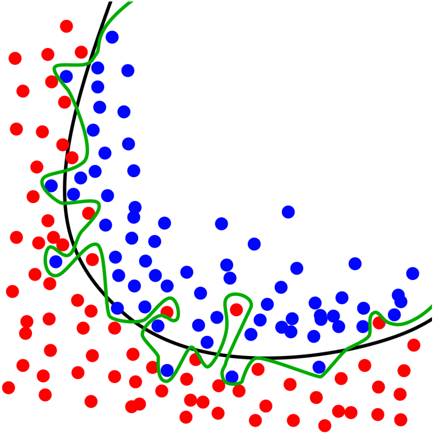

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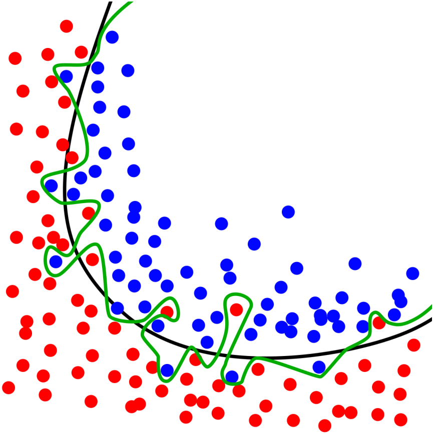

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Generalisation is the ability to 'perform' well on unseen data.

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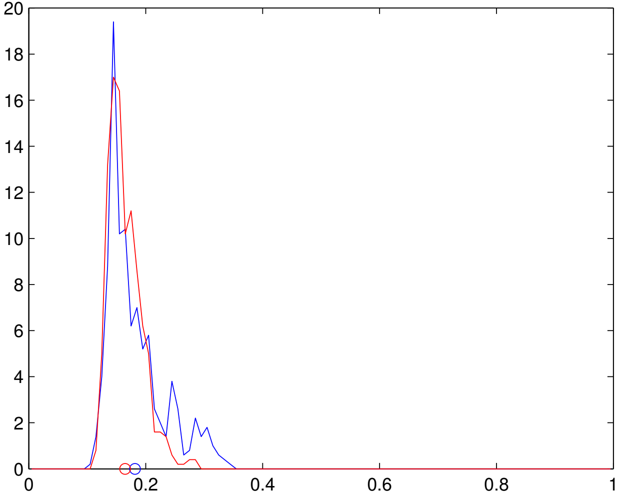
- Hence high confidence: $\mathbb{P}^m[\text{approximately correct}] \geqslant 1 - \delta$

Error distribution picture



means

95th percentiles

Mathematical formalization

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

- $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$
  $\mathcal{X}$ = set of inputs
  $\mathcal{Y}$ = set of outputs (e.g. labels)

- $\mathcal{H}$ = hypothesis class
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▷ these can be relaxed (mostly beyond the scope of this tutorial)

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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
- $\ell(h(X), Y) = -\log(h(X))$: log loss (density estimation)

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Flavours:

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

Before PAC-Bayes

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

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

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

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

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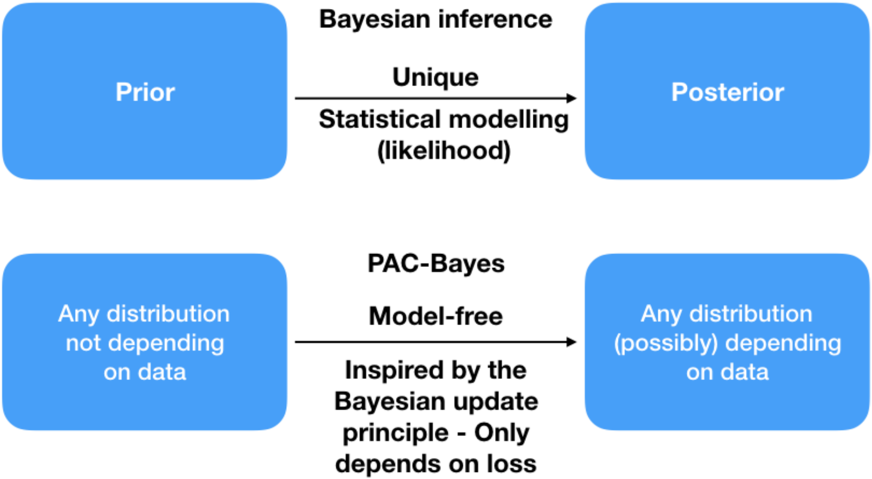

"Prior": exploration mechanism of $\mathcal{H}$

"Posterior" is the twisted prior after confronting with data

PAC-Bayes bounds vs. Bayesian learning

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

A General PAC-Bayesian Theorem

Δ-function: "distance" between $R_{\mathrm{in}}(Q)$ and $R_{\mathrm{out}}(Q)$

Convex function $\Delta : [0,1] \times [0,1] \to \mathbb{R}$.

General theorem (*Bégin et al. [7, 8], Germain [21]*)

For any distribution D on $\mathcal{X} \times \mathcal{Y}$, for any set $\mathcal{H}$ of voters, for any distribution P on $\mathcal{H}$, for any $\delta \in (0,1]$, and for any Δ-function, we have, with probability at least $1-\delta$ over the choice of $S \sim D^m$,

$$\forall\, Q \text{ on } \mathcal{H}: \quad \Delta\Big(R_{\mathrm{in}}(Q), R_{\mathrm{out}}(Q)\Big) \leqslant \frac{1}{m}\left[\mathrm{KL}(Q\|P) + \ln \frac{\mathcal{I}_\Delta(m)}{\delta}\right],$$

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where

$$\mathcal{I}_\Delta(m) = \sup_{r\in[0,1]} \left[\sum_{k=0}^{m} \underbrace{\binom{m}{k} r^k (1-r)^{m-k}}_{\mathbf{Bin}\left(k;m,r\right)} e^{m\Delta\left(\frac{k}{m}, r\right)} \right].$$

Proof of the general theorem

General theorem

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Proof ideas.

Change of Measure Inequality

For any P and Q on $\mathcal{H}$, and for any measurable function $\phi : \mathcal{H} \to \mathbb{R}$, we have

$$\begin{aligned}
-\ln\left(\mathop{\mathbf{E}}_{h\sim P} e^{\phi(h)}\right) &= -\ln \mathop{\mathbf{E}}_{h\sim Q}\left(\frac{P(h)}{Q(h)} e^{\phi(h)}\right) \\
&\leqslant \mathop{\mathbf{E}}_{h\sim Q} \ln\left(\frac{Q(h)}{P(h)}\right) - \mathop{\mathbf{E}}_{h\sim Q} \phi(h) \\
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Markov's inequality

for a random variable X satisfying $X \geqslant 0$

$$\Pr\left(X \geqslant a\right) \le \frac{\mathbf{E}\,X}{a} \quad\Longleftrightarrow\quad \Pr\left(X \leqslant \frac{\mathbf{E}\,X}{\delta}\right) \ge 1-\delta\,.$$

Proof of the general theorem

Probability of observing k misclassifications among m examples

Given a voter h, consider a **binomial variable** of m trials with **success** $R_{\mathrm{out}}(h)$:

$$\Pr_{S\sim D^m}\left(R_{\mathrm{in}}(h)=\tfrac{k}{m}\right) \quad = \quad \binom{m}{k}\Big(R_{\mathrm{out}}(h)\Big)^k\Big(1-R_{\mathrm{out}}(h)\Big)^{m-k} \;=\; \mathbf{Bin}\Big(k;m,R_{\mathrm{out}}(h)\Big)$$

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Proof.

$$m \cdot \Delta\Big(\mathop{\mathbf{E}}_{h\sim Q} R_{\text{in}}(h),\ \mathop{\mathbf{E}}_{h\sim Q} R_{\text{out}}(h)\Big)$$

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Jensen's Inequality $\qquad \leqslant \qquad \mathop{\mathbf{E}}_{h\sim Q} m\cdot\Delta\Big(R_{\mathrm{in}}(h), R_{\mathrm{out}}(h)\Big)$

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- So this result is no longer valid in the non iid case, even if General Theorem is.

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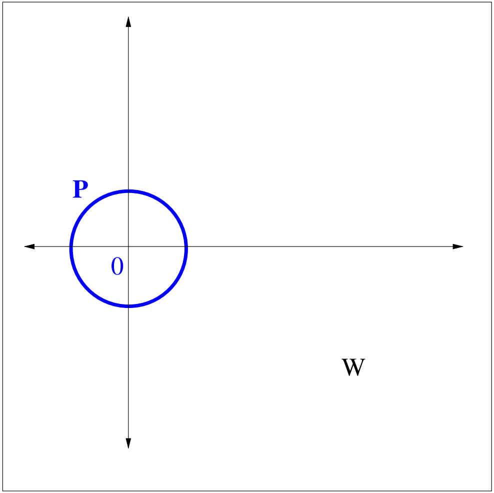
- The specification of the centre for the posterior $Q(\mathbf{w}, \mu)$ will be by a unit vector $\mathbf{m}w$ and a scale factor μ.

PAC-Bayes Bound for SVM (1/2)



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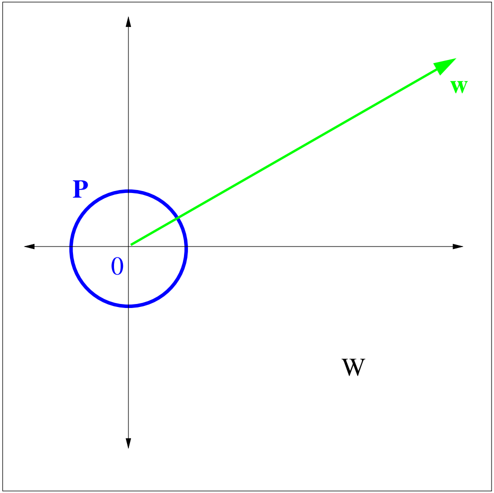

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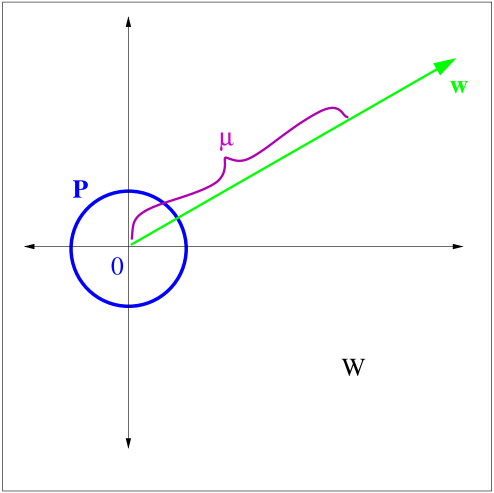

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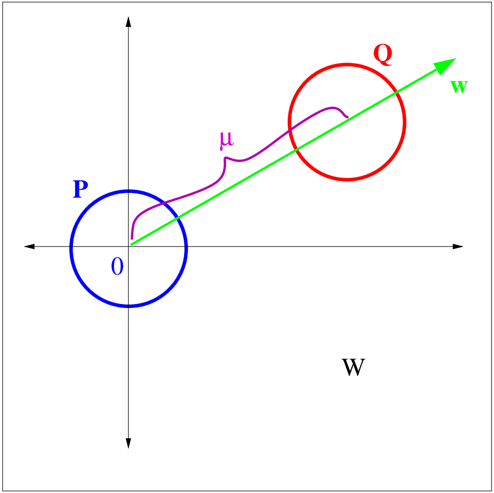

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$$\mathrm{KL}\big(\hat{Q}_S(\mathbf{w},\mu)\,\big\|\,\boxed{Q_{\mathcal{D}}(\mathbf{w},\mu)}\big) \leqslant \frac{\mathrm{KL}(P\|Q(\mathbf{w},\mu)) + \ln\frac{m+1}{\delta}}{m}$$

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- Hence its error bounded by $2Q_{\mathcal{D}}(\mathbf{m}w, \mu)$, since as observed above if $\mathbf{x}$ misclassified at least half of $c \sim Q$ err.

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- $\tilde{F}(t) = 1 - \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{t} e^{-x^2/2}\mathrm{d}x$

PAC-Bayes Bound for SVM (2/2)

Linear classifiers performance may be bounded by

$$\mathrm{KL}(\hat{Q}_S(\mathbf{w},\mu)\|Q_{\mathcal{D}}(\mathbf{w},\mu)) \leqslant \frac{\boxed{\mathrm{KL}(P\|Q(\mathbf{w},\mu))} + \ln\frac{m+1}{\delta}}{m}$$

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- δ is the confidence
- The bound holds with probability $1-\delta$ over the random i.i.d. selection of the training data.

Form of the SVM bound

- Note that bound holds for all posterior distributions so that we can choose μ to optimise the bound

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- Note that bound holds for all posterior distributions so that we can choose μ to optimise the bound
- If we define the inverse of the KL by

$$\mathrm{KL}^{-1}(q, A) = \max\{p : \mathrm{KL}(q\|p) \leqslant A\}$$

then have with probability at least $1 - \delta$

$$Pr\left(\langle \mathbf{w}, \phi(\mathbf{x})\rangle \neq y\right) \leqslant 2 \min_{\mu} \mathrm{KL}^{-1}\left(\mathbb{E}_m[\tilde{F}(\mu\gamma(\mathbf{x}, y))], \frac{\mu^2/2 + \ln \frac{m+1}{\delta}}{m}\right)$$

Gives SVM Optimisation

- Primal form:

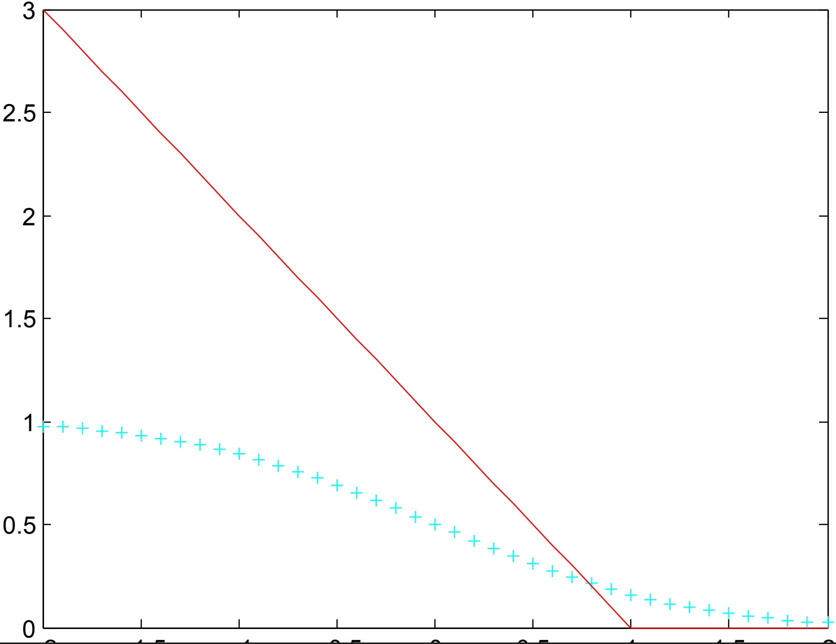
$$\begin{array}{lll} & \min_{\mathbf{w},\xi_i} \left[\frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^m \xi_i\right] & \\ \text{s.t.} & y_i \mathbf{w}^T \phi(\mathbf{x}_i) \geqslant 1 - \xi_i & i = 1, \ldots, m \\ & \xi_i \geqslant 0 & i = 1, \ldots, m \end{array}$$

- Dual form:

$$\begin{array}{ll} & \max_{\alpha} \left[\sum_{i=1}^m \alpha_i - \frac{1}{2}\sum_{i,j=1}^m \alpha_i \alpha_j y_i y_j \kappa(\mathbf{x}_i, \mathbf{x}_j)\right] \\ \text{s.t.} & 0 \leqslant \alpha_i \leqslant C \quad i = 1, \ldots, m \end{array}$$

where $\kappa(\mathbf{x}_i, \mathbf{x}_j) = \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle$ and $\langle \mathbf{w}, \phi(\mathbf{x}) \rangle = \sum_{i=1}^m \alpha_i y_i \kappa(\mathbf{x}_i, \mathbf{x})$.

Slack variable conversion



Model Selection with the new bound: setup

- Comparison of 10-fold Xvalidation, PAC-Bayes Bound and the Prior PAC-Bayes Bound

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  - For 10-F XV select the pair that minimize the validation error
  - For PAC-Bayes Bound and Prior PAC-Bayes Bound select the pair that minimize the bound

Results

		Classifier					
		SVM				ηPrior SVM	
Problem		2FCV	10FCV	PAC	PrPAC	PrPAC	τ-PrPAC
digits	Bound	–	–	0.175	0.107	0.050	**0.047**
	TE	**0.007**	**0.007**	**0.007**	0.014	0.010	0.009
waveform	Bound	–	–	0.203	0.185	0.178	**0.176**
	TE	0.090	0.086	**0.084**	0.088	0.087	0.086
pima	Bound	–	–	0.424	0.420	0.428	**0.416**
	TE	0.244	0.245	**0.229**	**0.229**	0.233	0.233
ringnorm	Bound	–	–	0.203	0.110	0.053	**0.050**
	TE	**0.016**	**0.016**	0.018	0.018	**0.016**	**0.016**
spam	Bound	–	–	0.254	0.198	0.186	**0.178**
	TE	0.066	**0.063**	0.067	0.077	0.070	0.072
Average	TE	0.0846	0.0834	**0.081**	0.0852	0.0832	0.0832

Take home messages

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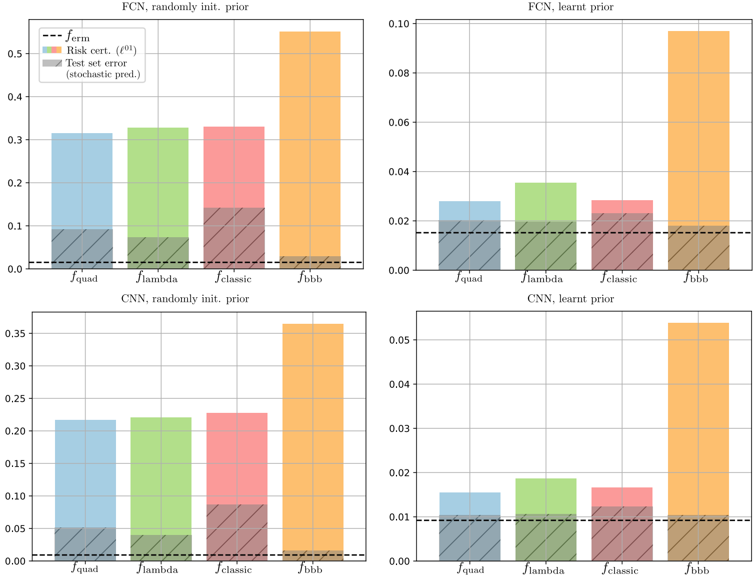
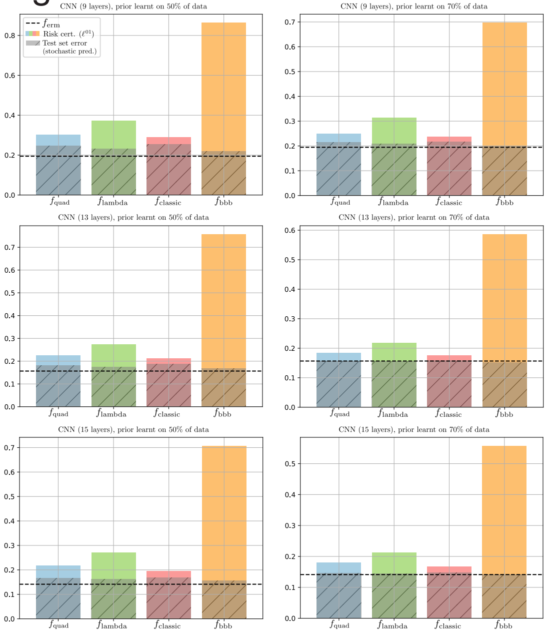
- Bounds are remarkably tight: for final column average factor between bound and TE is under 3.
- Model selection from the bounds is as good as 10FCV: in fact all but one of the PAC-Bayes model selections give better averages for TE.
- The better bounds do not appear to give better model selection - best model selection is from the simplest bound.

  - A. Ambroladze, E. Parrado-Hernández, and J. Shawe-Taylor. Tighter PAC-Bayes bounds. In *Advances in Neural Information Processing Systems* 18, (2006) Pages 9-16.
  - P. Germain, A. Lacasse, F. Laviolette and M. Marchand. PAC-Bayesian learning of linear classifiers, in *Proceedings of the 26nd International Conference on Machine Learning* (ICML'09, Montréal, Canada.). ACM Press (2009), 382, Pages 453-460.

Deep Learning Results



Deep Learning Results



A flexible framework

A flexible framework

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

Statistical learning theory *Audibert and Bousquet [6], Catoni [9, 10], Guedj [25], Guedj and Pujol [27], Maurer [39], McAllester [41, 42, 44, 45], Mhammedi et al. [46], Seeger [51, 52], Shawe-Taylor and Williamson [56], Thiemann et al. [58]*

SVMs & linear classifiers *Germain et al. [19], Langford and Shawe-Taylor [32], McAllester [44]*

Supervised learning algorithms reinterpreted as bound minimizers *Ambroladze et al. [5], Germain et al. [22], Shawe-Taylor and Hardoon [57]*

High-dimensional regression *Alquier and Biau [1], Alquier and Lounici [2], Guedj and Robbiano [24], Guedj and Alquier [26], Li et al. [35]*

Classification *Catoni [9, 10], Lacasse et al. [30], Langford and Shawe-Taylor [32], Parrado-Hernández et al. [49]*

A flexible framework

Transductive learning, domain adaptation *Bégin et al. [7], Derbeko et al. [12], Germain et al. [20], Nozawa et al. [48]*

Non-iid or heavy-tailed data *Alquier and Guedj [3], Holland [29], Lever et al. [34], Seldin et al. [54, 55]*

Density estimation *Higgs and Shawe-Taylor [28], Seldin and Tishby [53]*

Reinforcement learning *Fard and Pineau [16], Fard et al. [17], Ghavamzadeh et al. [23], Seldin et al. [54, 55]*

Sequential learning *Gerchinovitz [18], Li et al. [36]*

Algorithmic stability, differential privacy *Dziugaite and Roy [13, 14], London [37], London et al. [38], Rivasplata et al. [50]*

Deep neural networks *Dziugaite and Roy [15], Letarte et al. [33], Neyshabur et al. [47], Zhou et al. [60]*

...

References I

[1] P. Alquier and G. Biau. Sparse single-index model. *Journal of Machine Learning Research*, 14:243–280, 2013.

[2] P. Alquier and K. Lounici. PAC-Bayesian theorems for sparse regression estimation with exponential weights. *Electronic Journal of Statistics*, 5:127–145, 2011.

[3] Pierre Alquier and Benjamin Guedj. Simpler PAC-Bayesian bounds for hostile data. *Machine Learning*, 107(5):887–902, 2018.

[4] Pierre Alquier, James Ridgway, and Nicolas Chopin. On the properties of variational approximations of Gibbs posteriors. *ArXiv e-prints*, 2015. URL `http://arxiv.org/abs/1506.04091`.

[5] A. Ambroladze, E. Parrado-Hernández, and J. Shawe-taylor. Tighter PAC-Bayes bounds. In *Advances in Neural Information Processing Systems, NIPS*, pages 9–16, 2007.

[6] Jean-Yves Audibert and Olivier Bousquet. Combining PAC-Bayesian and generic chaining bounds. *Journal of Machine Learning Research*, 2007.

[7] Luc Bégin, Pascal Germain, François Laviolette, and Jean-Francis Roy. PAC-Bayesian theory for transductive learning. In *AISTATS*, 2014.

[8] Luc Bégin, Pascal Germain, François Laviolette, and Jean-Francis Roy. PAC-Bayesian bounds based on the Rényi divergence. In *AISTATS*, 2016.

[9] O. Catoni. *Statistical Learning Theory and Stochastic Optimization*. École d'Été de Probabilités de Saint-Flour 2001. Springer, 2004.

[10] O. Catoni. *PAC-Bayesian Supervised Classification: The Thermodynamics of Statistical Learning*, volume 56 of *Lecture notes – Monograph Series*. Institute of Mathematical Statistics, 2007.

[11] Olivier Catoni. *PAC-Bayesian supervised classification: the thermodynamics of statistical learning*, volume 56. Inst. of Mathematical Statistic, 2007.

[12] Philip Derbeko, Ran El-Yaniv, and Ron Meir. Explicit learning curves for transduction and application to clustering and compression algorithms. *J. Artif. Intell. Res. (JAIR)*, 22, 2004.

[13] G. K. Dziugaite and D. M. Roy. Data-dependent PAC-Bayes priors via differential privacy. In *NeurIPS*, 2018.

[14] G. K. Dziugaite and D. M. Roy. Entropy-SGD optimizes the prior of a PAC-Bayes bound: Generalization properties of Entropy-SGD and data-dependent priors. In *International Conference on Machine Learning*, pages 1376–1385, 2018.

References II

[15] Gintare K. Dziugaite and Daniel M. Roy. Computing nonvacuous generalization bounds for deep (stochastic) neural networks with many more parameters than training data. In *Proceedings of Uncertainty in Artificial Intelligence (UAI)*, 2017.

[16] Mahdi Milani Fard and Joelle Pineau. PAC-Bayesian model selection for reinforcement learning. In *Advances in Neural Information Processing Systems (NIPS)*, 2010.

[17] Mahdi Milani Fard, Joelle Pineau, and Csaba Szepesvári. PAC-Bayesian Policy Evaluation for Reinforcement Learning. In *UAI, Proceedings of the Twenty-Seventh Conference on Uncertainty in Artificial Intelligence*, pages 195–202, 2011.

[18] S. Gerchinovitz. *Prédiction de suites individuelles et cadre statistique classique : étude de quelques liens autour de la régression parcimonieuse et des techniques d'agrégation*. PhD thesis, Université Paris-Sud, 2011.

[19] P. Germain, A. Lacasse, F. Laviolette, and M. Marchand. PAC-Bayesian learning of linear classifiers. In *Proceedings of the 26th Annual International Conference on Machine Learning, ICML*, 2009.

[20] P. Germain, A. Habrard, F. Laviolette, and E. Morvant. A new PAC-Bayesian perspective on domain adaptation. In *Proceedings of International Conference on Machine Learning*, volume 48, 2016.

[21] Pascal Germain. *Généralisations de la théorie PAC-bayésienne pour l'apprentissage inductif, l'apprentissage transductif et l'adaptation de domaine.* PhD thesis, Université Laval, 2015.

[22] Pascal Germain, Alexandre Lacasse, Mario Marchand, Sara Shanian, and François Laviolette. From PAC-Bayes bounds to KL regularization. In *Advances in Neural Information Processing Systems*, pages 603–610, 2009.

[23] M. Ghavamzadeh, S. Mannor, J. Pineau, and A. Tamar. Bayesian reinforcement learning: A survey. *Foundations and Trends in Machine Learning*, 8(5-6):359–483, 2015.

[24] B. Guedj and S. Robbiano. PAC-Bayesian high dimensional bipartite ranking. *Journal of Statistical Planning and Inference*, 196:70 – 86, 2018. ISSN 0378-3758.

[25] Benjamin Guedj. A primer on PAC-Bayesian learning. *arXiv:1901.05353*, 2019. To appear in the Proceedings of the French Mathematical Society.

[26] Benjamin Guedj and Pierre Alquier. PAC-Bayesian estimation and prediction in sparse additive models. *Electron. J. Statist.*, 7: 264–291, 2013.

[27] Benjamin Guedj and Louis Pujol. Still no free lunches: the price to pay for tighter PAC-Bayes bounds. *arXiv preprint arXiv:1910.04460*, 2019.

References III

[28] Matthew Higgs and John Shawe-Taylor. A PAC-Bayes bound for tailored density estimation. In *Proceedings of the International Conference on Algorithmic Learning Theory (ALT)*, 2010.

[29] Matthew J Holland. PAC-Bayes under potentially heavy tails. *arXiv:1905.07900*, 2019. To appear in NeurIPS.

[30] A. Lacasse, F. Laviolette, M. Marchand, P. Germain, and N. Usunier. PAC-Bayes bounds for the risk of the majority vote and the variance of the Gibbs classifier. In *Advances in Neural information processing systems*, pages 769–776, 2007.

[31] John Langford and Matthias Seeger. Bounds for averaging classifiers. Technical report, Carnegie Mellon, Departement of Computer Science, 2001.

[32] John Langford and John Shawe-Taylor. PAC-Bayes & margins. In *Advances in Neural Information Processing Systems (NIPS)*, 2002.

[33] Gaël Letarte, Pascal Germain, Benjamin Guedj, and François Laviolette. Dichotomize and Generalize: PAC-Bayesian Binary Activated Deep Neural Networks. *arXiv:1905.10259*, 2019. To appear at NeurIPS.

[34] G. Lever, F. Laviolette, and J. Shawe-Taylor. Distribution-dependent PAC-Bayes priors. In *International Conference on Algorithmic Learning Theory*, pages 119–133. Springer, 2010.

[35] C. Li, W. Jiang, and M. Tanner. General oracle inequalities for Gibbs posterior with application to ranking. In *Conference on Learning Theory*, pages 512–521, 2013.

[36] Le Li, Benjamin Guedj, and Sébastien Loustau. A quasi-Bayesian perspective to online clustering. *Electron. J. Statist.*, 12(2): 3071–3113, 2018.

[37] B. London. A PAC-Bayesian analysis of randomized learning with application to stochastic gradient descent. In *Advances in Neural Information Processing Systems*, pages 2931–2940, 2017.

[38] B. London, B. Huang, B. Taskar, and L. Getoor. PAC-Bayesian collective stability. In *Artificial Intelligence and Statistics*, pages 585–594, 2014.

[39] A. Maurer. A note on the PAC-Bayesian Theorem. *arXiv preprint cs/0411099*, 2004.

[40] D. A. McAllester. PAC-Bayesian stochastic model selection. *Machine Learning*, 51(1):5–21, 2003.

[41] David McAllester. Some PAC-Bayesian theorems. In *Proceedings of the International Conference on Computational Learning Theory (COLT)*, 1998.

References IV

[42] David McAllester. Some PAC-Bayesian theorems. *Machine Learning*, 37, 1999.

[43] David McAllester. Some PAC-Bayesian theorems. *Machine Learning*, 37(3), 1999.

[44] David McAllester. PAC-Bayesian stochastic model selection. *Machine Learning*, 51(1), 2003.

[45] David McAllester. Simplified PAC-Bayesian margin bounds. In *COLT*, 2003.

[46] Zakaria Mhammedi, Peter D. Grunwald, and Benjamin Guedj. PAC-Bayes Un-Expected Bernstein Inequality. *arXiv preprint arXiv:1905.13367*, 2019. Accepted at NeurIPS 2019.

[47] B. Neyshabur, S. Bhojanapalli, D. A. McAllester, and N. Srebro. Exploring generalization in deep learning. In *Advances in Neural Information Processing Systems*, pages 5947–5956, 2017.

[48] Kento Nozawa, Pascal Germain, and Benjamin Guedj. PAC-Bayesian contrastive unsupervised representation learning. *arXiv preprint arXiv:1910.04464*, 2019.

[49] E. Parrado-Hernández, A. Ambroladze, J. Shawe-Taylor, and S. Sun. PAC-Bayes bounds with data dependent priors. *Journal of Machine Learning Research*, 13:3507–3531, 2012.

[50] O. Rivasplata, E. Parrado-Hernandez, J. Shawe-Taylor, S. Sun, and C. Szepesvari. PAC-Bayes bounds for stable algorithms with instance-dependent priors. In *Advances in Neural Information Processing Systems*, pages 9214–9224, 2018.

[51] M. Seeger. PAC-Bayesian generalization bounds for gaussian processes. *Journal of Machine Learning Research*, 3:233–269, 2002.

[52] M. Seeger. *Bayesian Gaussian Process Models: PAC-Bayesian Generalisation Error Bounds and Sparse Approximations*. PhD thesis, University of Edinburgh, 2003.

[53] Y. Seldin and N. Tishby. PAC-Bayesian analysis of co-clustering and beyond. *Journal of Machine Learning Research*, 11: 3595–3646, 2010.

[54] Y. Seldin, F. Laviolette, N. Cesa-Bianchi, J. Shawe-Taylor, and P. Auer. PAC-Bayesian inequalities for martingales. *IEEE Transactions on Information Theory*, 58(12):7086–7093, 2012.

[55] Yevgeny Seldin, Peter Auer, François Laviolette, John Shawe-Taylor, and Ronald Ortner. PAC-Bayesian analysis of contextual bandits. In *Advances in Neural Information Processing Systems (NIPS)*, 2011.

References V

[56] J. Shawe-Taylor and R. C. Williamson. A PAC analysis of a Bayes estimator. In *Proceedings of the 10th annual conference on Computational Learning Theory*, pages 2–9. ACM, 1997. doi: 10.1145/267460.267466.

[57] John Shawe-Taylor and David Hardoon. Pac-bayes analysis of maximum entropy classification. In *Proceedings on the International Conference on Artificial Intelligence and Statistics (AISTATS)*, 2009.

[58] Niklas Thiemann, Christian Igel, Olivier Wintenberger, and Yevgeny Seldin. A Strongly Quasiconvex PAC-Bayesian Bound. In *International Conference on Algorithmic Learning Theory, ALT*, pages 466–492, 2017.

[59] L. G. Valiant. A theory of the learnable. *Communications of the ACM*, 27(11):1134–1142, 1984.

[60] Wenda Zhou, Victor Veitch, Morgane Austern, Ryan P. Adams, and Peter Orbanz. Non-vacuous generalization bounds at the imagenet scale: a PAC-bayesian compression approach. In *ICLR*, 2019.