An Introduction to PAC-Bayesian Analysis

Benjamin Guedj John Shawe-Taylor

Supervised Learning
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Learning is to be able to generalise

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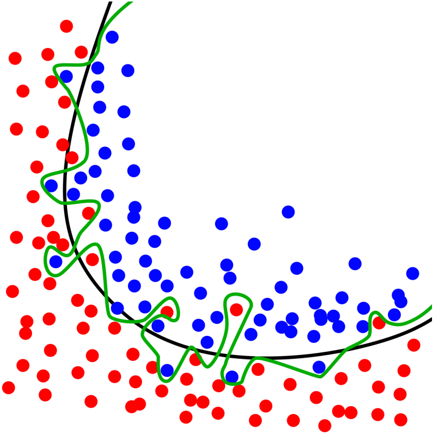

[Figure from Wikipedia]

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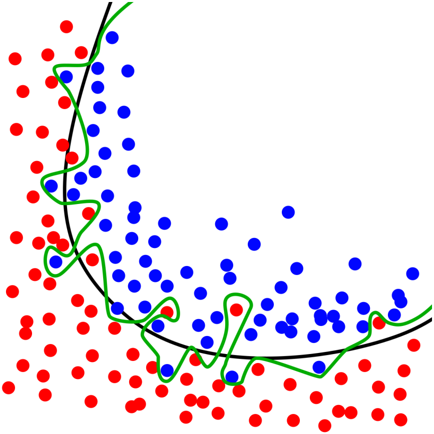

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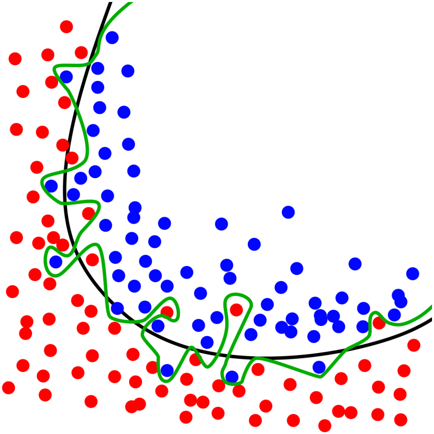

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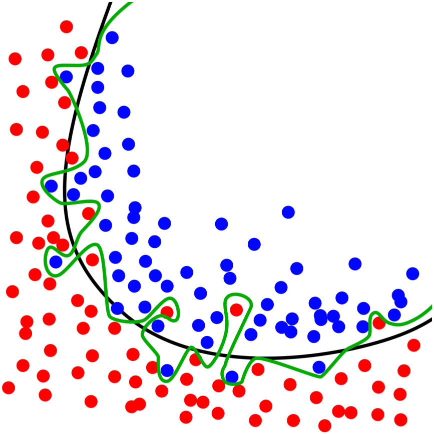

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Generalisation is the ability to 'perform' well on unseen data.

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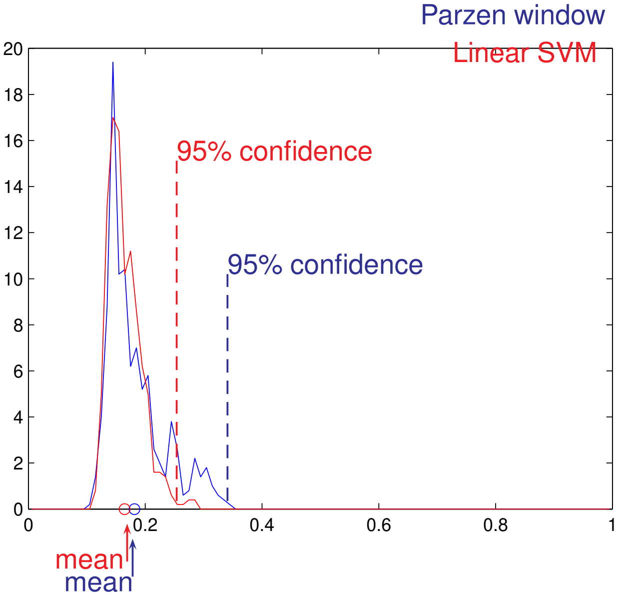
- Hence high confidence: $\mathbb{P}^m[\text{approximately correct}] \geqslant 1 - \delta$

Error distribution picture



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- $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$

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- $\mathcal{H}$ = 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) TODO

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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

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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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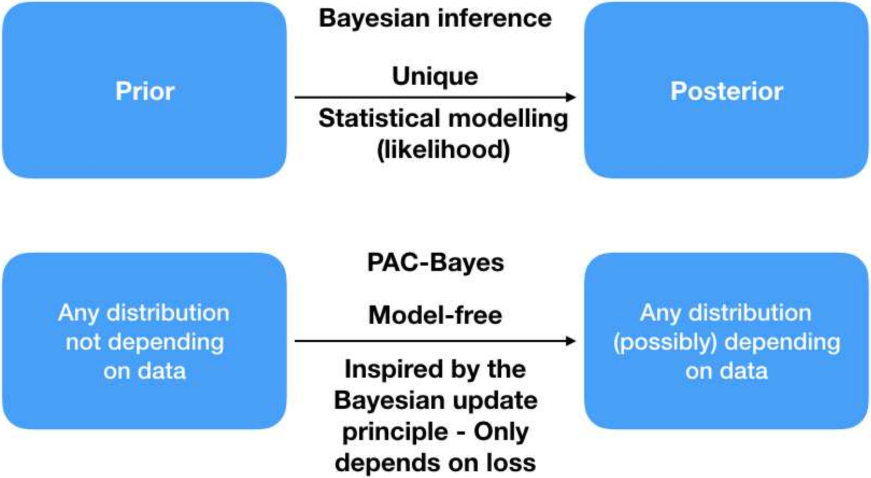

"Prior": exploration mechanism of $\mathcal{H}$

"Posterior" is the twisted prior after confronting with data

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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

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

Proof of the general theorem

General theorem

$$\Pr_{S\sim D^m}\left(\forall\, Q \text{ on } \mathcal{H}: \ \Delta\Big(R_{\rm in}(Q), R_{\rm out}(Q)\Big) \ \le\ \frac{1}{m}\left[\mathrm{KL}(Q\|P) + \ln\frac{\mathcal{I}_\Delta(m)}{\delta}\right]\right) \ \geqslant\ 1-\delta\,.$$

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** $R_{\mathrm{out}}(h)$:

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

$$\Pr_{S\sim D^m}\left(\forall\, Q \text{ on } \mathcal{H}:\ \Delta\Big(R_{\mathrm{in}}(Q), R_{\mathrm{out}}(Q)\Big) \leq \frac{1}{m}\left[\mathrm{KL}(Q\|P) + \ln\frac{\mathcal{J}_\Delta(m)}{\delta}\right]\right) \geqslant 1{-}\delta\,.$$

Proof.

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

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Proof.

$$
\begin{array}{lrl}
 & & m\cdot\Delta\Big(\mathop{\mathbf{E}}\limits_{h\sim Q} R_{\rm in}(h),\, \mathop{\mathbf{E}}\limits_{h\sim Q} R_{\rm out}(h)\Big) \\
\textbf{Jensen's Inequality} & \leqslant & \mathop{\mathbf{E}}\limits_{h\sim Q} m\cdot\Delta\Big(R_{\rm in}(h), R_{\rm out}(h)\Big) \\
\textbf{Change of measure} & \leqslant & \mathrm{KL}(Q\|P) + \ln \mathop{\mathbf{E}}\limits_{h\sim P} e^{m\Delta\left(R_{\rm in}(h), R_{\rm out}(h)\right)} \\
\textbf{Markov's Inequality} & \leq_{1-\delta} & \mathrm{KL}(Q\|P) + \ln \frac{1}{\delta} \mathop{\mathbf{E}}\limits_{S'\sim D^m} \mathop{\mathbf{E}}\limits_{h\sim P} e^{m\cdot\Delta(R_{\rm in}(h), R_{\rm out}(h))}
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Binomial law $= \mathrm{KL}(Q\|P) + \ln\frac{1}{\delta} \mathop{\mathbf{E}}_{h\sim P} \sum_{k=0}^{m} \mathbf{Bin}\Big(k; m, R_{\rm out}(h)\Big)\, e^{m\cdot\Delta(\frac{k}{m}, R_{\rm out}(h))}$

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Supremum over risk $\leqslant$ $$\mathrm{KL}(Q\|P) + \ln\frac{1}{\delta}\sup_{r\in[0,1]}\left[\sum_{k=0}^{m}\mathbf{Bin}\Big(k; m, r\Big)\, e^{m\Delta(\frac{k}{m}, r)}\right]$$

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General theorem

$$\Pr_{S\sim D^m}\left(\forall\, Q \text{ on } \mathcal{H}:\ \Delta\Big(R_{\mathrm{in}}(Q), R_{\mathrm{out}}(Q)\Big) \le \frac{1}{m}\left[\mathrm{KL}(Q\|P) + \ln\frac{\mathcal{I}_\Delta(m)}{\delta}\right]\right) \geqslant 1-\delta\,.$$

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[...] with probability at least $1-\delta$ *over the choice of* $S \sim D^m$*, for all* Q *on* $\mathcal{H}$ *:*

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

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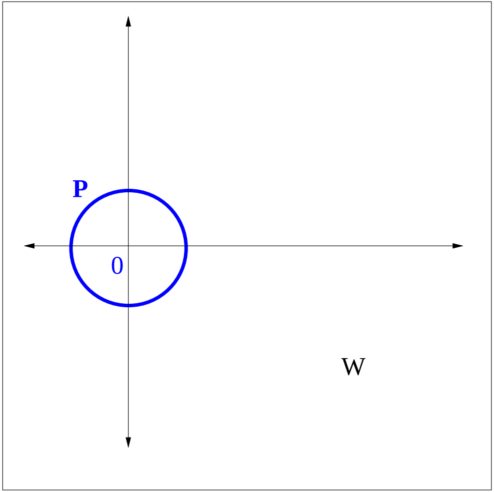
- The specification of the centre for the posterior $Q(\mathbf{w}, \mu)$ will be by a unit vector $\mathbf{m}w$ and a scale factor μ.

PAC-Bayes Bound for SVM (1/2)



- **Prior** *P* is Gaussian $\mathcal{N}(0, 1)$
-
-
-

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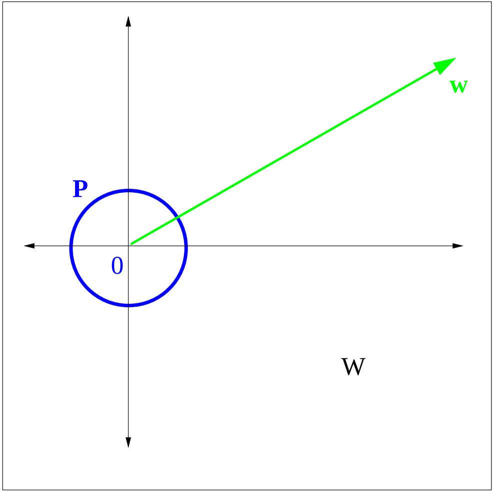

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-
-

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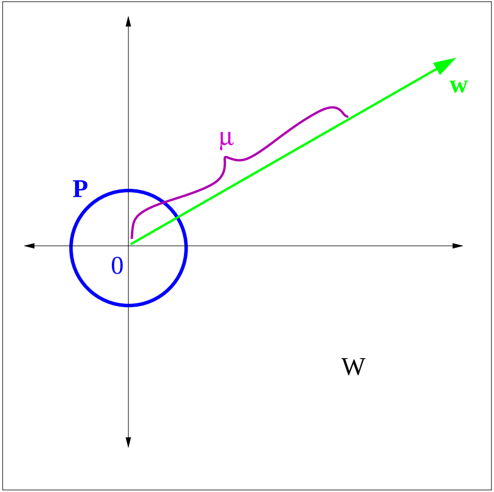

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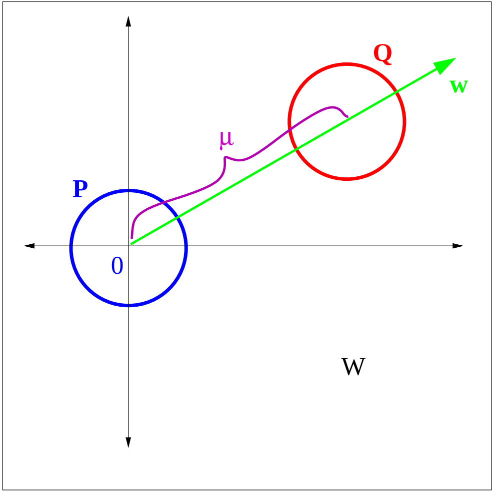

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PAC-Bayes Bound for SVM (2/2)

Linear classifiers performance may be bounded by

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

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- SVM is deterministic classifier that exactly corresponds to $\mathrm{sgn}\left(\mathbb{E}_{c\sim Q(\mathbf{m}w,\mu)}[c(\mathbf{x})]\right)$ as centre of the Gaussian gives the same classification as halfspace with more weight.
- 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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- $\hat{Q}_S(\mathbf{w}, \mu)$ stochastic measure of the training error

PAC-Bayes Bound for SVM (2/2)

Linear classifiers performance may be bounded by

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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:

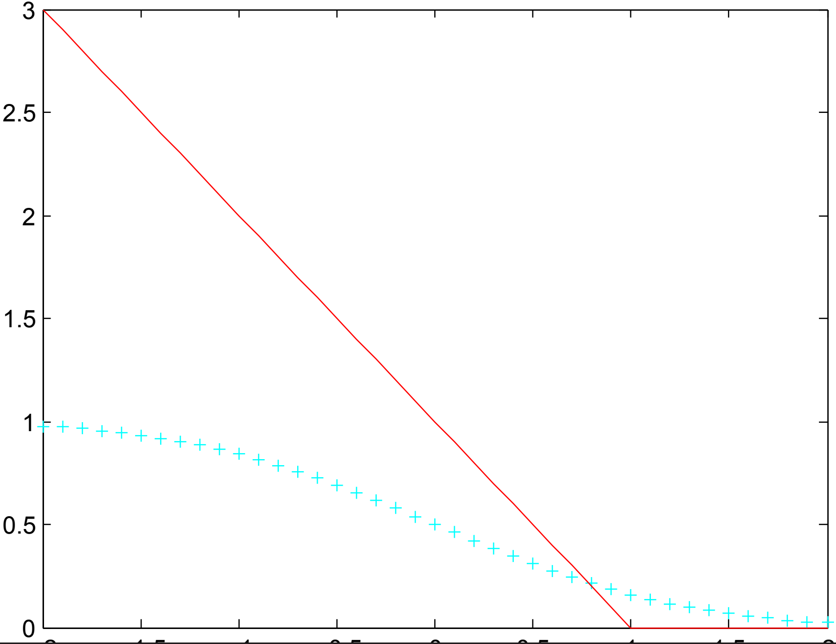
$$\begin{aligned}
&\min_{\mathbf{w},\xi_i} \left[\tfrac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{m}\xi_i\right] && \\
\text{s.t.}\quad & y_i\mathbf{w}^T\phi(\mathbf{x}_i) \geqslant 1-\xi_i && i=1,\ldots,m \\
& \xi_i \geqslant 0 && i=1,\ldots,m
\end{aligned}$$

- Dual form:

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

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



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  - defining the prior in terms of the *data generating distribution (aka localised PAC-Bayes)*.

Learning the prior (1/3)

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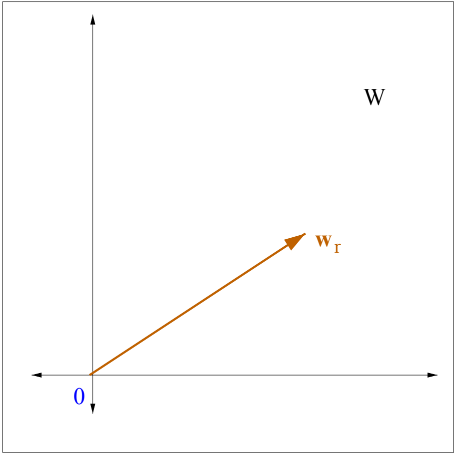
- Compute stochastic error with **remaining data**

New prior for the SVM (3/3)



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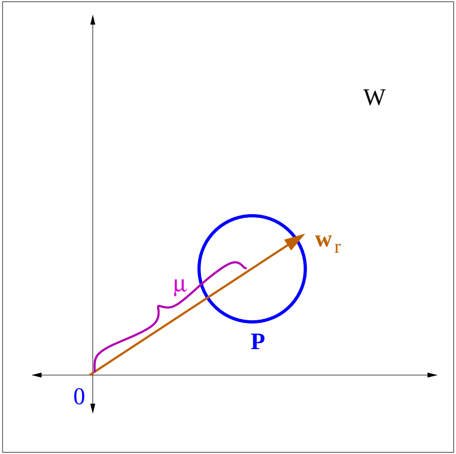

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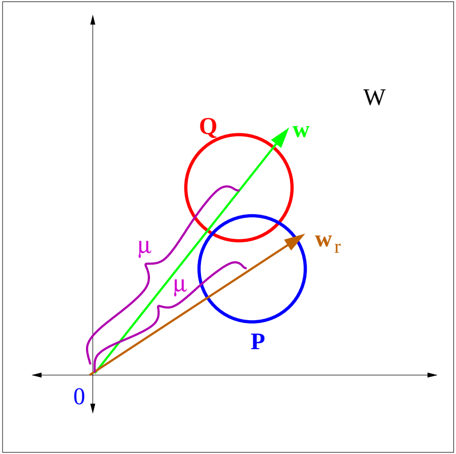

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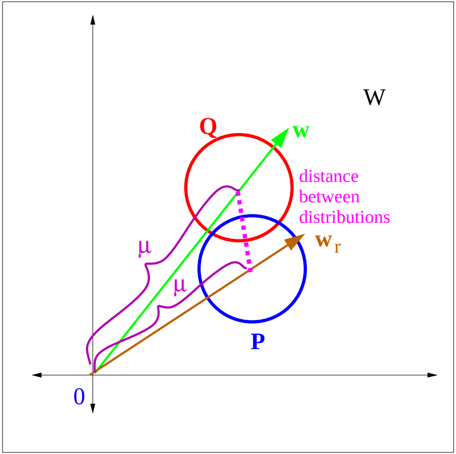

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- Prior in the **direction** $\mathbf{w}_r$
- **Posterior** like PAC-Bayes Bound
- **New bound** depends on $\mathrm{KL}(P \| Q)$

New Bound for the SVM (2/3)

SVM performance may be **tightly** bounded by

$$\mathrm{KL}(\hat{Q}_S(\mathbf{w},\mu) \| \boxed{Q_{\mathcal{D}}(\mathbf{w},\mu)}) \leqslant \frac{0.5\|\mu\mathbf{w} - \eta\mathbf{w}_r\|^2 + \ln\frac{(m-r+1)J}{\delta}}{m-r}$$

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- $Q_{\mathcal{D}}(\mathbf{w},\mu)$ true performance of the classifier

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- Penalty term only dependent on the remaining data $m-r$

Prior-SVM

- New bound proportional to $\|\mu\mathbf{w} - \eta\mathbf{w}_r\|^2$

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- The p-SVM is only solved with the **remaining points**

Bound for p-SVM

1. Determine the **prior** with a subset of the training examples to obtain $\mathbf{w}_r$

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4. **Linear search** to obtain the optimal value of μ. This introduces an insignificant extra penalty term

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- Prior is elongated along the line of $\mathbf{w}_r$ but spherical with variance 1 in other directions

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- Resulting bound depends on a benign parameter τ determining the variance in the direction $\mathbf{w}_r$

$$\mathrm{KL}(\hat{Q}_{S\setminus R}(\mathbf{w},\mu)\|Q_{\mathcal{D}}(\mathbf{w},\mu)) \leqslant$$
$$\frac{0.5(\ln(\tau^2)+\tau^{-2}-1+P^{\|}_{\mathbf{w}_r}(\mu\mathbf{w}-\mathbf{w}_r)^2/\tau^2+P^{\perp}_{\mathbf{w}_r}(\mu\mathbf{w})^2)+\ln(\frac{m-r+1}{\delta})}{m-r}$$

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  - 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

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- 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.
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- Consider P and Q are Gibbs-Boltzmann distributions

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- These distributions are hard to work with since we cannot apply the bound to a single weight vector, but the bounds can be very tight:

$$KL_+(\hat{Q}_S(\gamma) \| Q_{\mathcal{D}}(\gamma)) \leqslant \frac{1}{m}\left(\frac{\gamma}{\sqrt{m}}\sqrt{\ln\frac{8\sqrt{m}}{\delta}} + \frac{\gamma^2}{4m} + \ln\frac{4\sqrt{m}}{\delta}\right)$$

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- G. Lever, F. Laviolette, J. Shawe-Taylor. Distribution-Dependent PAC-Bayes Priors. Proceedings of the 21st International Conference on Algorithmic Learning Theory (ALT 2010), 119-133.

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  - Trick here is that the error measures only depend on the posterior Q, while the bound depends on KL between posterior and prior: an estimate of this KL is made without knowing the prior explicitly
- the Gibbs distributions are hard to sample from so not easy to work with this bound.

Other distribution defined priors

- An alternative distribution defined prior for an SVM is to place symmetrical Gaussian at the weight vector: $\mathbf{w}_p = \mathbb{E}_{(\mathbf{x},y)\sim D}(y\,\boldsymbol{\phi}(\mathbf{x}))$ to give distributions that are easier to work with, but results not impressive...

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- What if we were to take the expected weight vector returned from a random training set of size m: then the KL between posterior and prior is related to the concentration of weight vectors from different training sets

Other distribution defined priors

- An alternative distribution defined prior for an SVM is to place symmetrical Gaussian at the weight vector: $\mathbf{w}_p = \mathbb{E}_{(\mathbf{x},y)\sim D}(y\boldsymbol{\phi}(\mathbf{x}))$ to give distributions that are easier to work with, but results not impressive...
- What if we were to take the expected weight vector returned from a random training set of size m: then the KL between posterior and prior is related to the concentration of weight vectors from different training sets
- This is connected to stability...

Outline

- stability

Stability

Uniform hypothesis sensitivity β at sample size m:

$$\| \mathsf{A}(z_{1:m}) - \mathsf{A}(z'_{1:m}) \| \leqslant \beta \sum_{i=1}^{m} \mathbf{1}[z_i \neq z'_i]$$

$(z_1, \ldots, z_m)$

- $\mathsf{A}(z_{1:m}) \in \mathcal{H}$ normed space
- $w_m = \mathsf{A}(z_{1:m})$ ‘weight vector’

$(z'_1, \ldots, z'_m)$

- Lipschitz
- smoothness

Uniform loss sensitivity β at sample size m:

$$|\ell(\mathsf{A}(z_{1:m}), z) - \ell(\mathsf{A}(z'_{1:m}), z)| \leqslant \beta \sum_{i=1}^{m} \mathbf{1}[z_i \neq z'_i]$$

- worst-case
- data-insensitive
- distribution-insensitive
- Open: data-dependent?

Generalization from Stability

If A has sensitivity β at sample size m, then for any $\delta \in (0, 1)$,

w.p. $\geqslant 1 - \delta$, $\quad R_{\mathrm{out}}(h) \leqslant R_{\mathrm{in}}(h) + \epsilon(\beta, m, \delta)$

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- the intuition is that if individual examples do not affect the loss of an algorithm then it will be concentrated
- can be applied to kernel methods where β is related to the regularisation constant, but bounds are quite weak
- question: algorithm output is highly concentrated
  $\Longrightarrow$ stronger results?

Stability + PAC-Bayes I

If A has uniform hypothesis stability β at sample size n, then for any $\delta \in (0,1)$, w.p. $\geqslant 1 - 2\delta$,

$$\mathrm{KL}\big(R_{\mathrm{in}}(Q) \| R_{\mathrm{out}}(Q)\big) \leqslant \frac{\frac{n\beta^2}{2\sigma^2}\left(1 + \sqrt{\frac{1}{2}\log\left(\frac{1}{\delta}\right)}\,\right)^2 + \log\left(\frac{n+1}{\delta}\right)}{n}$$

Gaussian randomization

- $P = \mathcal{N}(\mathbb{E}[W_n], \sigma^2 I)$
- $Q = \mathcal{N}(W_n, \sigma^2 I)$
- $\mathrm{KL}(Q\|P) = \frac{1}{2\sigma^2}\|W_n - \mathbb{E}[W_n]\|^2$

Main proof components:

- w.p. $\geqslant 1 - \delta$, $\quad \mathrm{KL}\big(R_{\mathrm{in}}(Q) \| R_{\mathrm{out}}(Q)\big) \leqslant \frac{\mathrm{KL}(Q\|Q_0) + \log\left(\frac{n+1}{\delta}\right)}{n}$
- w.p. $\geqslant 1 - \delta$, $\quad \|W_n - \mathbb{E}[W_n]\| \leqslant \sqrt{n}\,\beta\left(1 + \sqrt{\frac{1}{2}\log\left(\frac{1}{\delta}\right)}\right)$

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]*
- ...

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