A PAC-Bayesian Margin Bound for Linear Classifiers: Why SVMs work

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Abstract

We present a bound on the generalisation error of linear classifiers in terms of a refined margin quantity on the training set. The result is obtained in a PAC–Bayesian framework and is based on geometrical arguments in the space of linear classifiers. The new bound constitutes an exponential improvement of the so far tightest margin bound by Shawe-Taylor et al. [8] and scales logarithmically in the inverse margin. Even in the case of less training examples than input dimensions sufficiently large margins lead to non-trivial bound values and — for maximum margins — to a vanishing complexity term. Furthermore, the classical margin is too coarse a measure for the *essential quantity* that controls the generalisation error: the *volume ratio* between the whole hypothesis space and the subset of consistent hypotheses. The practical relevance of the result lies in the fact that the well-known support vector machine is optimal w.r.t. the new bound only if the feature vectors are all of the same length. As a consequence we recommend to use SVMs on normalised feature vectors only — a recommendation that is well supported by our numerical experiments on two benchmark data sets.

1 Introduction

Linear classifiers are exceedingly popular in the machine learning community due to their straight-forward applicability and high flexibility which has recently been boosted by the so-called kernel methods [13]. A natural and popular framework for the theoretical analysis of classifiers is the PAC (*probably approximately correct*) framework [11] which is closely related to Vapnik's work on the generalisation error [12]. For binary classifiers it turned out that the *growth function* is an appropriate measure of "complexity" and can tightly be upper bounded by the VC (Vapnik-Chervonenkis) dimension [14]. Later, *structural risk minimisation* [12] was suggested for directly minimising the VC dimension based on a training set and an *a priori* structuring of the hypothesis space.

In practice, e.g. in the case of linear classifiers, often a thresholded *real-valued* func-

tion is used for classification. In 1993, Kearns [4] demonstrated that considerably tighter bounds can be obtained by considering a scale-sensitive complexity measure known as the *fat shattering dimension*. Further results [1] provided bounds on the Growth function similar to those proved by Vapnik and others [14, 6]. The popularity of the theory was boosted by the invention of the *support vector machine* (SVM) [13] which aims at directly minimising the complexity as suggested by theory.

Until recently, however, the success of the SVM remained somewhat obscure because in PAC/VC theory the structuring of the hypothesis space must be *independent* of the training data — in contrast to the data-dependence of the canonical hyperplane. As a consequence Shawe-Taylor et.al. [8] developed the *luckiness framework*, where luckiness refers to a complexity measure that is a function of both hypothesis *and* training sample.

Recently, David McAllester presented some PAC-Bayesian theorems [5] that bound the generalisation error of Bayesian classifiers *independently* of the correctness of the prior and regardless of the underlying data distribution — thus fulfilling the basic desiderata of PAC theory. In [3] McAllester's bounds on the Gibbs classifier were extended to the Bayes (optimal) classifier. The PAC-Bayesian framework provides *a posteriori* bounds and is thus closely related in spirit to the luckiness framework[1].

In this paper we give a tight margin bound for linear classifiers in the PAC-Bayesian framework. The main idea is to identify the generalisation error of the classifier h of interest with that of the Bayes (optimal) classifier of a (point-symmetric) subset Q that is *summarised* by h. We show that for a uniform prior the *normalised margin* of h is *directly* related to the volume of a large subset Q summarised by h. In particular, the result suggests that a learning algorithm for linear classifiers should aim at maximising the normalised margin instead of the classical margin. In Section 2 and 3 we review the basic PAC-Bayesian theorem and show how it can be applied to single classifiers. In Section 4 we give our main result and outline its proof. In Section 5 we discuss the consequences of the new result for the application of SVMs and demonstrate experimentally that in fact a normalisation of the feature vectors leads to considerably superior generalisation performance.

We denote n–tuples by italic bold letters (e.g. $\boldsymbol{x} = (x_1, \ldots, x_n)$), vectors by roman bold letters (e.g. $\mathbf{x}$), random variables by sans serif font (e.g. X) and vector spaces by calligraphic capitalised letters (e.g. $\mathcal{X}$). The symbols $\mathsf{P}, \mathsf{E}, \mathsf{I}$ and ℓ_2^n denote a probability measure, the expectation of a random variable, the indicator function and the normed space (2–norm) of sequences of length n, respectively.

2 A PAC Margin Bound

We consider learning in the PAC framework. Let $\mathcal{X}$ be the input space, and let $\mathcal{Y} = \{-1, +1\}$. Let a labelled training sample $\boldsymbol{z} = (\boldsymbol{x}, \boldsymbol{y}) \in (\mathcal{X} \times \mathcal{Y})^m = \mathcal{Z}^m$ be drawn iid according to some unknown probability measure $\mathsf{P}_\mathsf{Z} = \mathsf{P}_{\mathsf{Y}|\mathsf{X}}\mathsf{P}_\mathsf{X}$. Furthermore for a given hypothesis space $\mathcal{H} \subseteq \mathcal{Y}^\mathcal{X}$ we assume the existence of a "true" hypothesis $h^* \in \mathcal{H}$ that labelled the data

$$\mathsf{P}_{\mathsf{Y}|\mathsf{X}=x}(y) = \mathsf{I}_{y=h^*(x)} \,. \tag{1}$$

We consider linear hypotheses

$$\mathcal{H} = \{h_\mathbf{w} : x \mapsto \operatorname{sign}(\langle \mathbf{w}, \phi(x) \rangle_\mathcal{K}) \mid \mathbf{w} \in \mathcal{W}\}\,, \quad \mathcal{W} = \{\mathbf{w} \in \mathcal{K} \mid \|\mathbf{w}\|_\mathcal{K} = 1\}\,, \tag{2}$$

[1] In fact, even Shawe-Taylor et.al. concede that "... a Bayesian might say that luckiness is just a complicated way of encoding a prior. The sole justification for our particular way of encoding is that it allows us to get the PAC like results we sought..." [9, p. 4].

where the mapping $\phi : \mathcal{X} \to \mathcal{K} \subseteq \ell_2^n$ maps[2] the input data to some feature space $\mathcal{K}$ and $\|\mathbf{w}\|_{\mathcal{K}} = 1$ leads to a one-to-one correspondence of hypotheses $h_{\mathbf{w}}$ to their parameters $\mathbf{w}$. From the existence of h^* we know that there exists a version space $V(\boldsymbol{z}) \subseteq \mathcal{W}$,

$$V(\boldsymbol{z}) = \{\mathbf{w} \in \mathcal{W} \mid \forall (x,y) \in \boldsymbol{z} : h_{\mathbf{w}}(x) = y\} .$$

Our analysis aims at bounding the true risk $R[\mathbf{w}]$ of consistent hypotheses $h_{\mathbf{w}}$,

$$R[\mathbf{w}] = \mathbf{P}_{\mathsf{XY}}(h_{\mathbf{w}}(\mathsf{X}) \neq \mathsf{Y}) .$$

Since all classifiers $\mathbf{w} \in V(\boldsymbol{z})$ are indistinguishable in terms of number of errors committed on the given training set $\boldsymbol{z}$ let us introduce the concept of the *margin* $\gamma_{\boldsymbol{z}}(\mathbf{w})$ of a classifier $\mathbf{w}$, i.e.

$$\gamma_{\boldsymbol{z}}(\mathbf{w}) = \min_{(x_i,y_i)\in\boldsymbol{z}} \frac{y_i \langle \mathbf{w}, \mathbf{x}_i \rangle_{\mathcal{K}}}{\|\mathbf{w}\|_{\mathcal{K}}} . \tag{3}$$

The following theorem due to Shawe-Taylor et al. [8] bounds the generalisation errors $R[\mathbf{w}]$ of all classifier $\mathbf{w} \in V(\boldsymbol{z})$ in terms of the margin $\gamma_{\boldsymbol{z}}(\mathbf{w})$.

Theorem 1 (PAC margin bound). *For all probability measures $\mathbf{P}_{\mathsf{Z}}$ such that $\mathbf{P}_{\mathsf{X}}(\|\phi(\mathsf{X})\|_{\mathcal{K}} \leq \varsigma) = 1$, for any $\delta > 0$ with probability at least $1-\delta$ over the random draw of the training set $\boldsymbol{z}$, if we succeed in correctly classifying m samples $\boldsymbol{z}$ with a linear classifier $\mathbf{w}$ achieving a positive margin $\gamma_{\boldsymbol{z}}(\mathbf{w}) > \sqrt{32\varsigma^2/m}$ then the generalisation $R[\mathbf{w}]$ of $\mathbf{w}$ is bounded from above by*

$$\frac{2}{m}\left(\kappa(\mathbf{w}) \log_2\left(\frac{8em}{\kappa(\mathbf{w})}\right) \log_2(32m) + \ln\left(\frac{m^2}{\delta}\right)\right), \quad \kappa(\mathbf{w}) = \left\lceil \left(\frac{8\varsigma}{\gamma_{\boldsymbol{z}}(\mathbf{w})}\right)^2 \right\rceil . \tag{4}$$

As the bound on $R[\mathbf{w}]$ depends linearly on $\gamma_{\boldsymbol{z}}^{-2}(\mathbf{w})$ we see that Theorem 1 provides a theoretical foundation of all algorithms that aim at maximising $\gamma_{\boldsymbol{z}}(\mathbf{w})$, e.g. SVMs and Boosting [13, 7].

3 PAC-Bayesian Analysis

We first present a result [5] that bounds the risk of the generalised Gibbs classification strategy $Gibbs_{W(\boldsymbol{z})}$ by the measure $\mathbf{P}_{\mathbf{W}}(W(\boldsymbol{z}))$ on a consistent subset $W(\boldsymbol{z}) \subseteq V(\boldsymbol{z})$. This average risk is then related via the Bayes-Gibbs lemma to the risk of the Bayes classification strategy $Bayes_{W(\boldsymbol{z})}$ on $W(\boldsymbol{z})$. For a single consistent hypothesis $\mathbf{w} \in \mathcal{W}$ it is then necessary to identify a consistent subset $Q(\mathbf{w})$ such that the Bayes strategy $Bayes_{Q(\mathbf{w})}$ on $Q(\mathbf{w})$ always agrees with $\mathbf{w}$. Let us define the Gibbs classification strategy $Gibbs_{W(\boldsymbol{z})}$ w.r.t. the subset $W(\boldsymbol{z}) \subseteq V(\boldsymbol{z})$ by

$$Gibbs_{W(\boldsymbol{z})}(x) = h_{\mathbf{w}}(x) , \qquad \mathbf{w} \sim \mathbf{P}_{\mathbf{W}|\mathbf{W}\in W(\boldsymbol{z})} . \tag{5}$$

Then the following theorem [5] holds for the risk of $Gibbs_{W(\boldsymbol{z})}$.

Theorem 2 (PAC-Bayesian bound for subsets of classifiers). *For any measure $\mathbf{P}_{\mathbf{W}}$ and any measure $\mathbf{P}_{\mathsf{Z}}$, for any $\delta > 0$ with probability at least $1-\delta$ over the random draw of the training set $\boldsymbol{z}$ for all subsets $W(\boldsymbol{z}) \subseteq V(\boldsymbol{z})$ such that $\mathbf{P}_{\mathbf{W}}(W(\boldsymbol{z})) > 0$ the generalisation error of the associated Gibbs classification strategy $Gibbs_{W(\boldsymbol{z})}$ is bounded from above by*

$$R\left[Gibbs_{W(\boldsymbol{z})}\right] \leq \frac{1}{m}\left(\ln\left(\frac{1}{\mathbf{P}_{\mathbf{W}}(W(\boldsymbol{z}))}\right) + 2\ln(m) + \ln\left(\frac{1}{\delta}\right) + 1\right) . \tag{6}$$

[2] For notational simplicity we sometimes abbreviate $\phi(x)$ by $\mathbf{x}$ which should not be confused with the sample $\boldsymbol{x}$ of training objects.

Now consider the Bayes classifier $Bayes_{W(z)}$,

$$Bayes_{W(z)}(x) = \text{sign}\left(\mathbf{E}_{\mathbf{W}|\mathbf{W}\in W(z)}\left[h_{\mathbf{W}}(x)\right]\right) ,$$

where the expectation $\mathbf{E}_{\mathbf{W}|\mathbf{W}\in W(z)}$ is taken over a cut-off posterior given by combining the PAC-likelihood (1) and the prior $\mathbf{P}_{\mathbf{W}}$.

Lemma 1 (Bayes-Gibbs Lemma). *For any two measures* $\mathbf{P}_{\mathbf{W}}$ *and* $\mathbf{P}_{\mathsf{XY}}$ *and any set* $W \subseteq \mathcal{W}$

$$\mathbf{P}_{\mathsf{XY}}\left(Bayes_W(\mathsf{X}) \neq \mathsf{Y}\right) \leq 2 \cdot \mathbf{P}_{\mathsf{XY}}\left(Gibbs_W(\mathsf{X}) \neq \mathsf{Y}\right) . \tag{7}$$

Proof. (Sketch) Consider only the simple PAC setting we need. At all those points $x \in \mathcal{X}$ at which $Bayes_W$ is wrong by definition at least half of the classifiers $\mathbf{w} \in W$ under consideration make a mistake as well. □

The combination of Lemma 1 with Theorem 2 yields a bound on the risk of $Bayes_{W(z)}$. For a single hypothesis $\mathbf{w} \in \mathcal{W}$ let us find a (Bayes-admissible) subset $Q(\mathbf{w})$ of version space $V(z)$ such that $Bayes_{Q(\mathbf{w})}$ on $Q(\mathbf{w})$ agrees with $\mathbf{w}$ on every point in $\mathcal{X}$.

Definition 1 (Bayes-admissibility). Given the hypothesis space in (2) and a prior measure $\mathbf{P}_{\mathbf{W}}$ over $\mathcal{W}$ we call a subset $Q(\mathbf{w}) \subseteq \mathcal{W}$ *Bayes admissible w.r.t.* $\mathbf{w}$ *and* $\mathbf{P}_{\mathbf{W}}$ if and only if

$$\forall x \in \mathcal{X}: \qquad h_{\mathbf{w}}(x) = Bayes_{Q(\mathbf{w})}(x) .$$

Although difficult to achieve in general the following geometrically plausible lemma establishes Bayes-admissibility for the case of interest.

Lemma 2 (Bayes-admissibility for linear classifiers). *For uniform measure* $\mathbf{P}_{\mathbf{W}}$ *over* $\mathcal{W}$ *each ball* $Q(\mathbf{w}) = \{\mathbf{v} \in \mathcal{W} \mid \|\mathbf{w} - \mathbf{v}\|_{\mathcal{K}} \leq r\}$ *is Bayes admissible w.r.t. its centre* $\mathbf{w}$.

Please note that by considering a ball $Q(\mathbf{w})$ rather than just $\mathbf{w}$ we make use of the fact that $\mathbf{w}$ *summarises* all its neighbouring classifiers $\mathbf{v} \in Q(\mathbf{w})$. Now using a uniform prior $\mathbf{P}_{\mathbf{W}}$ the *normalised* margin

$$\Gamma_z(\mathbf{w}) = \min_{(x_i,y_i)\in z} \frac{y_i \langle \mathbf{w}, \mathbf{x}_i \rangle_{\mathcal{K}}}{\|\mathbf{w}\|_{\mathcal{K}} \|\mathbf{x}_i\|_{\mathcal{K}}} , \tag{8}$$

quantifies the relative volume of classifiers summarised by $\mathbf{w}$ and thus allows us to bound its risk. Note that in contrast to the classical margin γ_z (see 3) this *normalised* margin is a dimensionless quantity and constitutes a measure for the relative size of the version space invariant under rescaling of both weight vectors $\mathbf{w}$ and feature vectors $\mathbf{x}_i$.

4 A PAC-Bayesian Margin Bound

Combining the ideas outlined in the previous section allows us to derive a generalisation error bound for linear classifiers $\mathbf{w} \in V(z)$ in terms of their *normalised* margin $\Gamma_z(\mathbf{w})$.

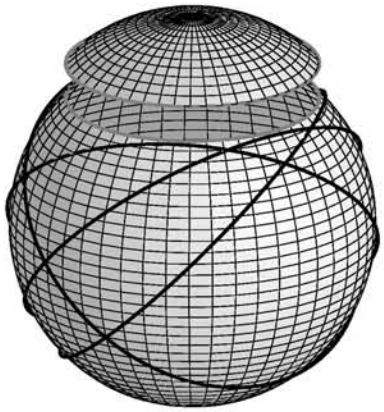

Figure 1: Illustration of the volume ratio for the classifier at the north pole. Four training points shown as grand circles make up version space — the polyhedron on top of the sphere. The radius of the "cap" of the sphere is proportional to the margin $\Gamma_{\boldsymbol{z}}$, which *only* for constant $\|\mathbf{x}_i\|_{\mathcal{K}}$ is maximised by the SVM.

Theorem 3 (PAC-Bayesian margin bound). *Suppose $\mathcal{K} \subseteq \ell_2^n$ is a given feature space of dimensionality n. For all probability measures P_Z, for any $\delta > 0$ with probability at least $1 - \delta$ over the random draw of the training set $\boldsymbol{z}$, if we succeed in correctly classifying m samples $\boldsymbol{z}$ with a linear classifier $\mathbf{w}$ achieving a positive margin $\Gamma_{\boldsymbol{z}}(\mathbf{w}) > 0$ then the generalisation error $R[\mathbf{w}]$ of $\mathbf{w}$ is bounded from above by*

$$\frac{2}{m}\left(d \ln\left(\frac{1}{1-\sqrt{1-\Gamma_{\boldsymbol{z}}^2(\mathbf{w})}}\right) + 2\ln(m) + \ln\left(\frac{1}{\delta}\right) + 2\right). \tag{9}$$

where $d = \min(m, n)$.

Proof. Geometrically the hypothesis space $\mathcal{W}$ is the unit sphere in $\mathbb{R}^n$ (see Figure 1). Let us assume that $\mathsf{P}_{\mathbf{W}}$ is uniform on the unit sphere as suggested by symmetry. Given the training set $\boldsymbol{z}$ and a classifier $\mathbf{w}$ all classifiers $\mathbf{v} \in Q(\mathbf{w})$

$$Q(\mathbf{w}) = \left\{\mathbf{v} \in \mathcal{W} \;\middle|\; \langle \mathbf{w}, \mathbf{v} \rangle_{\mathcal{K}} > \sqrt{1-\Gamma_{\boldsymbol{z}}^2(\mathbf{w})}\right\} \tag{10}$$

are within $V(\boldsymbol{z})$ (For a proof see [2]). Such a set $Q(\mathbf{w})$ is Bayes-admissible by Lemma 2 and hence we can use $\mathsf{P}_{\mathbf{W}}(Q(\mathbf{w}))$ to bound the generalisation error of $\mathbf{w}$. Since $\mathsf{P}_{\mathbf{W}}$ is uniform, the value $-\ln(\mathsf{P}_{\mathbf{W}}(Q(\mathbf{w})))$ is simply the logarithm of the *volume ratio* between the surface of the unit sphere and the surface of all $\mathbf{v}$ fulfilling equation (10). In [2] it is shown that this ratio is *exactly* given by

$$\ln\left(\frac{\int_0^{2\pi} \sin^{n-2}(\theta)\, d\theta}{\int_0^{\arccos\left(\sqrt{1-\Gamma_{\boldsymbol{z}}^2(\mathbf{w})}\right)} \sin^{n-2}(\theta)\, d\theta}\right).$$

It can be shown that this ratio is tightly bounded from above by

$$n \ln\left(\frac{1}{1-\sqrt{1-\Gamma_{\boldsymbol{z}}^2(\mathbf{w})}}\right) + \ln(2).$$

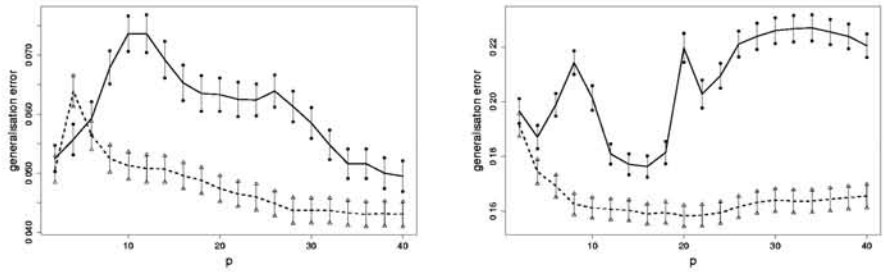

Figure 2: Generalisation errors of classifiers learned by an SVM with (dashed line) and without (solid line) normalisation of the feature vectors $\mathbf{x}_i$. The error bars indicate one standard deviation over 100 random splits of the data sets. The two plots are obtained on the **(a)** `thyroid` and **(b)** `sonar` data set.

With $\ln(2) < 1$ we obtain the desired result. Note that m points maximally span an m–dimensional space and thus we can marginalise over the remaining $n - m$ dimensions of feature space $\mathcal{K}$. This gives $d = \min(m, n)$. □

An appealing feature of equation (9) is that for $\Gamma_{\boldsymbol{z}}(\mathbf{w}) = 1$ the bound reduces to $\frac{2}{m}(2\ln(m) - \ln(\delta) + 2)$ with a rapid decay to zero as m increases. In case of margins $\Gamma_{\boldsymbol{z}}(\mathbf{w}) > 0.91$ the troublesome situation of $d = m$, which occurs e.g. for RBF kernels, is compensated for. Furthermore, upper bounding $1/(1 - \sqrt{1 - \Gamma})$ by $2/\Gamma$ we see that Theorem 3 is an exponential improvement of Theorem 1 in terms of the attained margins. It should be noted, however, that the new bound depends on the dimensionality of the input space via $d = \min(m, n)$.

5 Experimental Study

Theorem 3 suggest the following learning algorithm: given a version space $V(\boldsymbol{z})$ (through a given training set $\boldsymbol{z}$) find the classifier $\mathbf{w}$ that maximises $\Gamma_{\boldsymbol{z}}(\mathbf{w})$. This algorithm, however, is given by the SVM *only if* the training data in feature space $\mathcal{K}$ are normalised. We investigate the influence of such a normalisation on the generalisation error in the feature space $\mathcal{K}$ of all monomials up to the p–th degree (well-known from handwritten digit recognition, see [13]). Since the SVM learning algorithm as well as the resulting classifier only refer to inner products in $\mathcal{K}$, it suffices to use an easy-to-calculate kernel function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ such that for all $x, x' \in \mathcal{X}$, $k(x, x') = \langle \phi(x), \phi(x') \rangle_{\mathcal{K}}$, given in our case by the polynomial kernel

$$\forall p \in \mathbb{N}: \qquad k(x, x') = (\langle x, x' \rangle_{\mathcal{X}} + 1)^p \ .$$

Earlier experiment have shown [13] that without normalisation too large values of p may lead to "overfitting". We used the UCI [10] data sets `thyroid` ($d = 5$, $m = 140$, $m_{\text{test}} = 75$) and `sonar` ($d = 60$, $m = 124$, $m_{\text{test}} = 60$) and plotted the generalisation error of SVM solutions (estimated over 100 different splits of the data set) as a function of p (see Figure 2). As suggested by Theorem 3 in almost all cases the normalisation improved the performance of the support vector machine solution at a statistically significant level. As a consequence, we recommend:

When training an SVM, always normalise your data in feature space.

Intuitively, it is only the *spatial direction* of both weight vector and feature vectors that determines the classification. Hence the different lengths of feature vectors in the training set should not enter the SVM optimisation problem.

6 Conclusion

The PAC-Bayesian framework together with simple geometrical arguments yields the so far tightest margin bound for linear classifiers. The role of the normalised margin $\Gamma_{\boldsymbol{z}}$ in the new bound suggests that the SVM is theoretically justified only for input vectors of constant length. We hope that this result is recognised as a useful bridge between theory and practice in the spirit of Vapnik's famous statement:

> Nothing is more practical than a good theory

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