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# 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<sup>1</sup>.

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.  $\mathbf{x} = (x_1, \dots, x_n)$ ), vectors by roman bold letters (e.g.  $\mathbf{x}$ ), random variables by sans serif font (e.g.  $\mathbf{X}$ ) and vector spaces by calligraphic capitalised letters (e.g.  $\mathcal{X}$ ). The symbols  $\mathbf{P}, \mathbf{E}, \mathbf{I}$  and  $\ell_2^n$  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  $\mathbf{z} = (\mathbf{x}, \mathbf{y}) \in (\mathcal{X} \times \mathcal{Y})^m = \mathcal{Z}^m$  be drawn iid according to some unknown probability measure  $\mathbf{P}_Z = \mathbf{P}_{Y|X}\mathbf{P}_X$ . 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

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

We consider linear hypotheses

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

<sup>1</sup>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  $\phi : \mathcal{X} \rightarrow \mathcal{K} \subseteq \ell_2^n$  maps<sup>2</sup> 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  $V(\mathbf{z}) \subseteq \mathcal{W}$ ,

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

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

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

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

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

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

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

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

As the bound on  $R[\mathbf{w}]$  depends linearly on  $\gamma_{\mathbf{z}}^{-2}(\mathbf{w})$  we see that Theorem 1 provides a theoretical foundation of all algorithms that aim at maximising  $\gamma_{\mathbf{z}}(\mathbf{w})$ , 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  $Gibbs_{W(\mathbf{z})}$  by the measure  $\mathbf{P}_{\mathbf{W}}(W(\mathbf{z}))$  on a consistent subset  $W(\mathbf{z}) \subseteq V(\mathbf{z})$ . This average risk is then related via the Bayes-Gibbs lemma to the risk of the Bayes classification strategy  $Bayes_{W(\mathbf{z})}$  on  $W(\mathbf{z})$ . 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  $Gibbs_{W(\mathbf{z})}$  w.r.t. the subset  $W(\mathbf{z}) \subseteq V(\mathbf{z})$  by

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

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

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

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

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

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

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

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  $\mathbf{P}_{XY}$  and any set  $W \subseteq \mathcal{W}$*

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

*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.  $\square$

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

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

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

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

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  $\gamma_z$  (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  $\Gamma_z(\mathbf{w})$ .

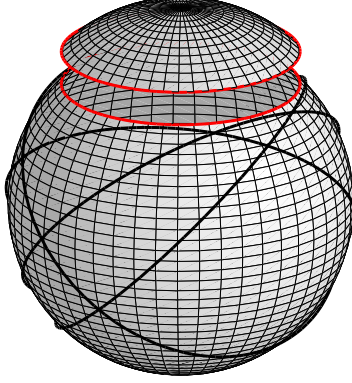


Figure 1: Illustration of the volume ratio for the classifier at the north pole. Four training points shown as grand circles make up version space — the polyhedron on top of the sphere. The radius of the “cap” of the sphere is proportional to the margin  $\Gamma_z$ , which *only* for constant  $\|\mathbf{x}_i\|_{\mathcal{K}}$  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  $\mathbf{P}_z$ , for any  $\delta > 0$  with probability at least  $1 - \delta$  over the random draw of the training set  $z$ , if we succeed in correctly classifying  $m$  samples  $z$  with a linear classifier  $\mathbf{w}$  achieving a positive margin  $\Gamma_z(\mathbf{w}) > 0$  then the generalisation error  $R[\mathbf{w}]$  of  $\mathbf{w}$  is bounded from above by*

$$\frac{2}{m} \left( d \ln \left( \frac{1}{1 - \sqrt{1 - \Gamma_z^2(\mathbf{w})}} \right) + 2 \ln(m) + \ln \left( \frac{1}{\delta} \right) + 2 \right). \quad (9)$$

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  $\mathbf{P}_w$  is uniform on the unit sphere as suggested by symmetry. Given the training set  $z$  and a classifier  $\mathbf{w}$  all classifiers  $\mathbf{v} \in Q(\mathbf{w})$

$$Q(\mathbf{w}) = \left\{ \mathbf{v} \in \mathcal{W} \mid \langle \mathbf{w}, \mathbf{v} \rangle_{\mathcal{K}} > \sqrt{1 - \Gamma_z^2(\mathbf{w})} \right\} \quad (10)$$

are within  $V(z)$  (For a proof see [2]). Such a set  $Q(\mathbf{w})$  is Bayes-admissible by Lemma 2 and hence we can use  $\mathbf{P}_w(Q(\mathbf{w}))$  to bound the generalisation error of  $\mathbf{w}$ . Since  $\mathbf{P}_w$  is uniform, the value  $-\ln(\mathbf{P}_w(Q(\mathbf{w})))$  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

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

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

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

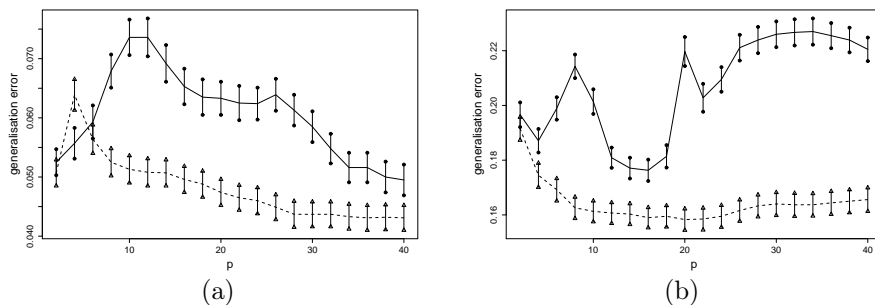


Figure 2: Generalisation errors of classifiers learned by an SVM with (dashed line) and without (solid line) normalisation of the feature vectors  $\mathbf{x}_i$ . The error bars indicate one standard deviation over 100 random splits of the data sets. The two plots are obtained on the **(a) thyroid**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

An appealing feature of equation (9) is that for  $\Gamma_{\mathbf{z}}(\mathbf{w}) = 1$  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  $\Gamma_{\mathbf{z}}(\mathbf{w}) > 0.91$  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  $V(\mathbf{z})$  (through a given training set  $\mathbf{z}$ ) find the classifier  $\mathbf{w}$  that maximises  $\Gamma_{\mathbf{z}}(\mathbf{w})$ . 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  $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$  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

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

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  $\Gamma_z$  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

**Acknowledgements** We would like to thank David McAllester, John Shawe-Taylor, Bob Williamson, Olivier Chapelle, John Langford, Alex Smola and Bernhard Schölkopf for interesting discussions and useful suggestions on earlier drafts.

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