Chebyshev-Cantelli PAC-Bayes-Bennett Inequality for the Weighted Majority Vote

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Abstract

We present a new second-order oracle bound for the expected risk of a weighted majority vote. The bound is based on a novel parametric form of the Chebyshev-Cantelli inequality (a.k.a. one-sided Chebyshev’s), which is amenable to efficient minimization. The new form resolves the optimization challenge faced by prior oracle bounds based on the Chebyshev-Cantelli inequality, the C-bounds [Germain et al., 2015], and, at the same time, it improves on the oracle bound based on second order Markov’s inequality introduced by Masegosa et al. [2020]. We also derive a new concentration of measure inequality, which we name PAC-Bayes-Bennett, since it combines PAC-Bayesian bounding with Bennett’s inequality. We use it for empirical estimation of the oracle bound. The PAC-Bayes-Bennett inequality improves on the PAC-Bayes-Bernstein inequality of Seldin et al. [2012]. We provide an empirical evaluation demonstrating that the new bounds can improve on the work of Masegosa et al. [2020]. Both the parametric form of the Chebyshev-Cantelli inequality and the PAC-Bayes-Bennett inequality may be of independent interest for the study of concentration of measure in other domains.

1 Introduction

Weighted majority vote is a central technique for combining predictions of multiple classifiers. It is an integral part of random forests [Breiman 1996, 2001], boosting [Freund and Schapire 1996], gradient boosting [Friedman 1999, 2001], and it is also used to combine predictions of heterogeneous classifiers. It is part of the winning strategies in many machine learning competitions. The power of the majority vote is in the cancellation of errors effect: when the errors of individual classifiers are independent or anticorrelated and the error probability of individual classifiers is smaller than 0.5, then the errors average out and the majority vote tends to outperform the individual classifiers.

Generalization bounds for weighted majority vote and theoretically-grounded approaches to weight-tuning are decades-old research topics. Berend and Kontorovich [2016] derived an optimal solution under the assumption of known error rates and independence of errors of individual classifiers, but neither of the two assumptions is typically satisfied in practice.

In absence of the independence assumption, the most basic result is the first order oracle bound, which is based on Markov’s inequality and bounds the expected loss of $\rho$-weighted majority vote by twice the $\rho$-weighted average of expected losses of the individual classifiers. This finding is so old and basic that Langford and Shawe-Taylor [2002] call it “the folk theorem”. The $\rho$-weighted average
of the expected losses is then bounded using PAC-Bayesian bounds, turning the oracle bound into an empirical bound [McAllester, 1998, Seeger, 2002, Langford and Shawe-Taylor, 2002]. While the translation from oracle to empirical bound is quite tight [Germain et al., 2009, Thiemann et al., 2017], the first order oracle bound ignores the correlation of errors, which is the main power of the majority vote. As a result, its minimization overconcentrates the weights on the best-performing classifiers, effectively reducing the majority vote to a very few or even just a single best classifier, which leads to a significant deterioration of the test error on held-out data [Lorenzen et al., 2019, Masegosa et al., 2020].

In order to take correlation of errors into account, [Lacasse et al., 2007] derived second order oracle bounds, the C-bounds, which are based on the Chebyshev-Cantelli inequality. The ideas were further developed by [Laviolette et al., 2011, Germain et al., 2015, and Laviolette et al., 2017]. However, they were only able to optimize the bounds in the highly restrictive setting of binary classification with self-complemented sets of classifiers and aligned priors and posteriors [Germain et al., 2015]. Several follow-up works resorted to minimization of heuristic surrogates rather than the bound itself [Bauvin et al., 2020, Viallard et al., 2021]. Furthermore, second order oracle quantities in the denominator of the oracle bounds lead to looseness in their translation to empirical bounds [Lorenzen et al., 2019].

Masegosa et al. [2020] proposed an alternative second-order oracle bound, the tandem bound, based on second order Markov’s inequality. While the second order Markov’s inequality is weaker than the Chebyshev-Cantelli inequality, the resulting bound has no oracle quantities in the denominator, which allows tight translation to an empirical bound. Additionally, Masegosa et al. proposed an efficient procedure for minimization of their empirical bound. They have shown that minimization of the empirical bound does not lead to deterioration of the test error.

Our work can be seen as a bridge between the tandem bound and the C-bounds, and as an improvement of both. The key novelty is a new parametric form of Chebyshev-Cantelli inequality, which preserves the tightness of Chebyshev-Cantelli, but avoids oracle quantities in the denominator. This allows both efficient translation to empirical bounds and efficient minimization. We derive two new second order oracle bounds based on the new inequality, one using the tandem loss and the other using the tandem loss with an offset. For empirical estimation of the latter we derive a PAC-Bayes-Bennett inequality. The overall contributions can be summarized as follows:

1. We propose a new parametric form of the Chebyshev-Cantelli inequality, which has no variance in the denominator and preserves tightness of the original bound. The new form allows efficient minimization and empirical estimation.

2. We propose two new second order oracle bounds for the weighted majority vote based on the new form of the Chebyshev-Cantelli inequality. The bounds have two advantages: (1) they are amenable to tight translation to empirical bounds; and (2) the resulting empirical bounds are amenable to efficient minimization.

3. We derive a new concentration of measure inequality, which we name the PAC-Bayes-Bennett inequality. It improves on the PAC-Bayes-Bernstein inequality of Seldin et al. [2012]. We use the inequality for bounding the tandem loss with an offset.

2 Problem setup

The problem setup and notations are borrowed from Masegosa et al. [2020].

Multiclass classification. We let \( S = \{(X_1, Y_1), \ldots, (X_n, Y_n)\} \) be an independent identically distributed sample from \( X \times Y \), drawn according to an unknown distribution \( D \), where \( Y \) is finite and \( X \) is arbitrary. A hypothesis is a function \( h : X \rightarrow Y \), and \( \mathcal{H} \) denotes a space of hypotheses. We evaluate the quality of \( h \) using the zero-one loss \( \ell(h(X), Y) = \mathbb{1}(h(X) \neq Y) \), where \( \mathbb{1}(\cdot) \) is the indicator function. The expected loss of \( h \) is denoted by \( L(h) = \mathbb{E}_{(X,Y) \sim D}[\ell(h(X), Y)] \) and the empirical loss of \( h \) on a sample \( S \) of size \( n \) is denoted by \( \hat{L}(h, S) = \frac{1}{n} \sum_{i=1}^{n} \ell(h(X_i), Y_i) \).

Randomized classifiers. A randomized classifier (a.k.a. Gibbs classifier) associated with a distribution \( \rho \) on \( \mathcal{H} \), for each input \( X \) randomly draws a hypothesis \( h \in \mathcal{H} \) according to \( \rho \) and predicts \( h(X) \). The expected loss of a randomized classifier is given by \( \mathbb{E}_{h \sim \rho}[L(h)] \) and the empirical loss by
Theorem 4 together with Lemma 2 leads to the following result, known as the \textit{C-bound}.

$$\mathbb{E}_{h \sim \rho} [\hat{L}(h, S)].$$ To simplify the notation we use $\mathbb{E}_D[\cdot]$ as a shorthand for $\mathbb{E}_{(X,Y) \sim D}[\cdot]$ and $\mathbb{E}_\rho[\cdot]$ as a shorthand for $\mathbb{E}_{h \sim \rho}[\cdot]$.

\textbf{Ensemble classifiers and majority vote.} Ensemble classifiers predict by taking a weighted aggregation of predictions by hypotheses from $\mathcal{H}$. The $\rho$-weighted majority vote $MV_\rho(X) = \arg \max_{y \in Y} \mathbb{E}_\rho[1(h(X) = y)]$, where ties can be resolved arbitrarily.

3 A review of prior first and second order oracle bounds

If majority voting makes an error, we know that at least a $\rho$-weighted half of the classifiers have made an error and, therefore, $\ell(MV_\rho(X), Y) \leq \mathbb{I}(\mathbb{E}_\rho[1(h(X) \neq Y)] \geq 0.5)$. This observation leads to the well-known first order oracle bound for the loss of weighted majority vote.

\textbf{Theorem 1 (First Order Oracle Bound).}

$$L(MV_\rho) \leq 2\mathbb{E}_\rho[L(h)].$$

\textbf{Proof.} We have $L(MV_\rho) = \mathbb{E}_D[\ell(MV_\rho(X), Y)] \leq \mathbb{P}(\mathbb{E}_\rho[1(h(X) \neq Y)] \geq 0.5)$. By applying Markov’s inequality to random variable $Z = \mathbb{E}_\rho[1(h(X) \neq Y)]$ we have:

$$L(MV_\rho) \leq \mathbb{P}(\mathbb{E}_\rho[1(h(X) \neq Y)] \geq 0.5) \leq 2\mathbb{E}_D[\mathbb{E}_\rho[1(h(X) \neq Y)] \geq 0.5] = 2\mathbb{E}_\rho[L(h)].$$

PAC-Bayesian analysis can be used to bound $\mathbb{E}_\rho[L(h)]$ in terms of $\mathbb{E}_\rho[\hat{L}(h, S)]$, thus turning the oracle bound into an empirical one. The disadvantage of the first order approach is that $\mathbb{E}_\rho[L(h)]$ ignores correlations of predictions, which is the main power of the majority vote.

\cite{massego2020} have used second order Markov’s inequality, by which for a non-negative random variable $Z$ and $\varepsilon > 0$

$$\mathbb{P}(Z \geq \varepsilon) = \mathbb{P}(Z^2 \geq \varepsilon^2) \leq \frac{\mathbb{E}[Z^2]}{\varepsilon^2}.$$

For pairs of hypotheses $h$ and $h'$ they have defined the \textit{tandem loss} $\ell(h(X), h'(X), Y) = 1(h(X) \neq Y \land h'(X) \neq Y) = 1(h(X) \neq Y)1(h'(X) \neq Y)$, also termed \textit{joint error} by \cite{lacasse2007}, which counts an error only if both $h$ and $h'$ err on a sample $(X, Y)$. The corresponding \textit{expected tandem loss} is defined by

$$L(h, h') = \mathbb{E}_D[1(h(X) \neq Y)1(h'(X) \neq Y)].$$

\cite{lacasse2007} and \cite{massego2020} have shown that expectation of the second moment of the weighted loss equals expectation of the tandem loss. Using $\rho^2$ as a shorthand for the product distribution $\rho \times \rho$ over $\mathcal{H} \times \mathcal{H}$ and $\mathbb{E}_{\rho^2}[L(h, h')]$ as a shorthand for $\mathbb{E}_{h \sim \rho, h' \sim \rho}[L(h, h')]$, the result is the following.

\textbf{Lemma 2 (Masegosa et al. 2020).} In multiclass classification

$$\mathbb{E}_D[\mathbb{E}_{\rho^2}[1(h(X) \neq Y)]^2] = \mathbb{E}_{\rho^2}[L(h, h')].$$

By combining second order Markov’s inequality with Lemma \cite{massego2020} \cite{massego2020} have shown the following result.

\textbf{Theorem 3 (Masegosa et al. 2020).} In multiclass classification

$$L(MV_\rho) \leq 4\mathbb{E}_{\rho^2}[L(h, h')].$$

\cite{lacasse2007} have used the Chebyshev-Cantelli inequality to derive a different form of a second order oracle bound. We use $\mathbb{V}[Z]$ to denote the variance of a random variable $Z$ in the statement of Chebyshev-Cantelli inequality.

\textbf{Theorem 4 (Chebyshev-Cantelli inequality).} For $\varepsilon > 0$

$$\mathbb{P}(Z - \mathbb{E}[Z] \geq \varepsilon) \leq \frac{\mathbb{V}[Z]}{\varepsilon^2 + \mathbb{V}[Z]}.$$

Theorem \cite{massego2020} together with Lemma \cite{massego2020} leads to the following result, known as the \textit{C-bound}.
We present three main contributions: (1) a new form of the Chebyshev-Cantelli inequality, which can be seen as a refinement of second order Markov’s inequality or as an intermediate step in the proof of Theorem 6. However, the presence of $E_{\rho}[L(h, h')]$ and $E_{\rho}[L(h)]$ in the denominator make empirical estimation and optimization of the bound in Theorem 5 impractical, and Theorem 3 was the only practically applicable second order bound so far.

4 Main Contributions

We present three main contributions: (1) a new form of the Chebyshev-Cantelli inequality, which is convenient for optimization; (2) an application of the inequality to the analysis of weighted majority vote; and (3) a PAC-Bayes-Bennett inequality, which is used to bound the risk with an offset in the bound for weighted majority vote. We start with the new form of Chebyshev-Cantelli inequality, which can be seen as a refinement of second order Markov’s inequality or as an intermediate step in the proof of the Chebyshev-Cantelli inequality.

Theorem 5. [Lacasse et al., 2007; Masegosa et al., 2020] If $\mathbb{E}_\rho[L(h)] \leq \frac{1}{2}$, then

$$L(MV_\rho) \leq \frac{\mathbb{E}_{\rho'}[L(h, h')] - \mathbb{E}_{\rho}[L(h)]^2}{\frac{1}{4} + \mathbb{E}_{\rho'}[L(h, h')] - \mathbb{E}_{\rho}[L(h)]}.$$ 

Masegosa et al. have shown that the Chebyshev-Cantelli inequality is always at least as tight as second order Markov’s inequality (below we provide an alternative and more intuitive proof of this fact) and, therefore, the oracle bound in Theorem 5 is always at least as tight as the oracle bound in Theorem 3. However, the presence of $E_{\rho'}[L(h, h')]$ and $E_{\rho}[L(h)]$ in the denominator make empirical estimation and optimization of the bound in Theorem 5 impractical, and Theorem 3 was the only practically applicable second order bound so far.

Theorem 6. For any $\varepsilon > 0$ and all $\mu < \varepsilon$

$$P(Z \geq \varepsilon) \leq \mathbb{E} \left[ \frac{(Z - \mu)^2}{(\varepsilon - \mu)^2} \right].$$

Proof.

$$P(Z \geq \varepsilon) = P(Z - \mu \geq \varepsilon - \mu) \leq P((Z - \mu)^2 \geq (\varepsilon - \mu)^2) \leq \mathbb{E} \left[ \frac{(Z - \mu)^2}{(\varepsilon - \mu)^2} \right].$$

The inequality can also be written as

$$P(Z \geq \varepsilon) \leq \frac{\mathbb{E} \left[ (Z - \mu)^2 \right]}{(\varepsilon - \mu)^2} = \frac{\mathbb{E} \left[ Z^2 \right] - 2\mu \mathbb{E} \left[ Z \right] + \mu^2}{(\varepsilon - \mu)^2}. \quad (1)$$

The bound is minimized by $\mu^* = \mathbb{E} \left[ Z \right] - \frac{\mathbb{E} \left[ Z^2 \right]}{\mathbb{E} \left[ Z \right]}$, which can be verified by taking a derivative of the bound with respect to $\mu$. Note that $\mu^*$ can take negative values. Substitution of $\mu^*$ into the bound and simple algebraic manipulations recover the Chebyshev-Cantelli inequality, whereas $\mu = 0$ recovers second order Markov’s inequality. The main advantage of Theorem 6 over the Chebyshev-Cantelli inequality is ease of estimation and optimization due to absence of the variance term in the denominator.

Equation (1) leads to two new second order oracle bounds for the weighted majority vote, given in Theorems 7 and 8.

Theorem 7. In multiclass classification, for all $\rho$ and all $\mu < 0.5$

$$L(MV_\rho) \leq \frac{\mathbb{E}_{\rho'}[L(h, h')] - 2\mu \mathbb{E}_{\rho}[L(h)] + \mu^2}{(0.5 - \mu)^2}.$$ 

Proof. As in the previous section, we take $Z = \mathbb{E}_{\rho'}[\mathbb{1}(h(X) \neq Y)]$, so that $L(MV_\rho) \leq P(Z \geq 0.5)$. The result follows by (1) and the calculations of $E \left[ Z^2 \right]$ and $E \left[ Z \right]$ from the previous section. Note that the result is a deterministic statement. \hfill \square

For $\mu = 0$, Theorem 7 recovers Theorem 3, but if $\mu^* = \mathbb{E}_{\rho}[L(h)] - \frac{\mathbb{E}_{\rho'}[L(h, h')] - \mathbb{E}[L(h)]^2}{0.5 - \mathbb{E}[L(h)]} \neq 0$, then substitution of $\mu^*$ into the theorem yields a tighter oracle bound. At the same time, substitution of $\mu^*$ recovers Theorem 5, but the great advantage of Theorem 7 is that the bound allows easy empirical estimation and optimization with respect to $\rho$, due to absence of $\mathbb{E}_{\rho'}[L(h, h')]$ and $\mathbb{E}_{\rho}[L(h)]$ in the theorem.
denominator. Thus, Theorem [7] has the oracle tightness of Theorem [5] and the ease of estimation and optimization of Theorem [3]. The oracle quantities $E_{\rho,\gamma}[L(h, h')]$ and $E_{\rho}[L(h)]$ can be bounded using PAC-Bayes-kl or PAC-Bayes-\lambda inequalities, as discussed in the next section.

In order to present the second oracle bound we introduce a new quantity. For a pair of hypotheses $h$ and $h'$ and a constant $\mu$, we define tandem loss with $\mu$-offset, for brevity $\mu$-tandem loss, as

$$\ell_\mu(h(X), h'(X), Y) = (1(h(X) \neq Y) - \mu)(1(h'(X) \neq Y) - \mu).$$

(2)

Note that it can take negative values. We denote its expectation by

$$L_\mu(h, h') = E_D[\ell_\mu(h(X), h'(X), Y)] = E_D[(1(h(X) \neq Y) - \mu)(1(h'(X) \neq Y) - \mu)].$$

With $Z = E_{\rho}[1(h(X) \neq Y)]$ as before, we have

$$E[(Z - \mu)^2] = E_D[(E_{\rho}[(1(h(X) \neq Y) - \mu)])^2] = E_{\rho^2}[E_D[(1(h(X) \neq Y) - \mu)(1(h'(X) \neq Y) - \mu)]] = E_{\rho^2}[L_\mu(h, h')].$$

Now we present our second oracle bound.

**Theorem 8.** In multiclass classification, for all $\rho$ and all $\mu < 0.5$

$$L(MV_\rho) \leq \frac{E_{\rho^2}[L_\mu(h, h')]}{(0.5 - \mu)^2}.$$

**Proof.** The result follows by Theorem [6] and the calculation above. Note that the inequality is a deterministic statement. $\square$

In order to discuss the advantage of Theorem [8] we define the variance of the $\mu$-tandem loss

$$\mathcal{V}_\mu(h, h') = E_D[(1(h(X) \neq Y) - \mu)(1(h'(X) \neq Y) - \mu) - L_\mu(h, h')]^2].$$

If the variance of the $\mu$-tandem loss is small, we can use Bernstein-type inequalities to obtain tighter estimates compared to kl-type inequalities.

We bound the $\mu$-tandem loss using our next contribution, the PAC-Bayes-Bennett inequality, which improves on the PAC-Bayes-Bernstein inequality derived by Seldin et al. [2012] and may be of independent interest. The inequality holds for any loss function with bounded length of the range, we use $\ell$ and matching tilde-marked quantities to distinguish it from the zero-one loss $\ell$. We let $\hat{L}(h) = E_D[\ell(h(X), Y)]$ and $\hat{V}(h) = E_D[(\ell(h(X), Y) - \hat{L}(h))^2]$ be the expected tilde-loss of $h$ and its variance and let $\hat{L}(h, S) = \frac{1}{n} \sum_{i=1}^{n} \ell(h(X_i), Y_i)$ be the empirical tilde-loss of $h$ on a sample $S$.

**Theorem 9 (PAC-Bayes-Bennett inequality).** Let $\hat{\ell}(\cdot, \cdot)$ be an arbitrary loss function taking values in an interval of length $b$, and assume that $\hat{V}(h)$ is finite for all $h$. Let $\phi(x) = e^x - x - 1$. Then for any distribution $\pi$ on $\mathcal{H}$ that is independent of $S$ and any $\gamma > 0$ and $d \in (0, 1)$, with probability at least $1 - d$ over a random draw of $S$, for all distributions $\rho$ on $\mathcal{H}$ simultaneously:

$$E_{\rho}[\hat{L}(h)] \leq E_{\rho}[\hat{L}(h, S)] + \frac{\phi(\gamma b)}{\gamma b^2} E_{\rho}[\hat{V}(h)] + \frac{KL(\rho||\pi) + \ln \frac{1}{d}}{\gamma n}.$$  

The proof is based on a change of measure argument combined with Bennett’s inequality, the details are provided in Appendix [A]. Note that the result holds for a fixed (but arbitrary) $\gamma > 0$. In case of optimization with respect to $\gamma$ a union bound has to be applied. For a fixed $\rho$ the bound is convex in $\gamma$ and for a fixed $\gamma$ it is convex in $\rho$, although it is not necessarily jointly convex in $\rho$ and $\gamma$. See Appendix [D] for optimization details. The PAC-Bayes-Bennett inequality is identical to the PAC-Bayes-Bernstein inequality of Seldin et al. [2012] Theorem 7, except that in the latter the coefficient in front of $E_{\mu}[\hat{V}[h]]$ is $(e - 2)^2$ instead of $\frac{\phi(\gamma b)}{\gamma b}$.

The result improves on the result of Seldin et al. in two ways. First, in the result of Seldin et al. $\gamma$ is restricted to the $(0, 1/b]$ interval, whereas in our result $\gamma$ is unrestricted from above. And second, we can rewrite the coefficient in front of the variance as $\frac{\phi(\gamma b)}{\gamma b^2} = \frac{\phi(\gamma b)}{\gamma b} \gamma$, where $\frac{\phi(\gamma b)}{\gamma b}$ is a monotonically increasing function of $\gamma$, which in the interval $\gamma \in (0, 1/b]$ satisfies $\lim_{\gamma \to 0} \frac{\phi(\gamma b)}{\gamma b} = \frac{1}{2}$ and for $\gamma = 1/b$ it gives $\frac{\phi(\gamma b)}{\gamma b} = (e - 2)$. Thus, PAC-Bayes-Bennett is always at least as tight as PAC-Bayes-Bernstein and, at the same time, for $\gamma < 1/b$ it improves the constant coefficient in front of the variance from $(e - 2) \approx 0.72$ down to 0.5 for $\gamma \to 0$. For $\gamma > 1/b$ PAC-Bayes-Bennett also improves on PAC-Bayes-Bernstein, because PAC-Bayes-Bernstein uses the suboptimal value $\gamma = 1/b$ dictated by its restricted range of $\gamma$. 

5
5 From oracle to empirical bounds

We obtain empirical bounds on the oracle quantities \( \mathbb{E}_\rho[L(h, h')] \) and \( \mathbb{E}_\rho[L(h)] \) in Theorem 7 and \( \mathbb{E}_\rho[L(h, h')] \) in Theorem 8 by using PAC-Bayesian inequalities. The empirical counterpart of the expected tandem loss is the empirical tandem loss

\[
\hat{L}(h, h', S) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{I}(h(X_i) \neq Y_i) \mathbb{I}(h'(X_i) \neq Y_i).
\]

For bounding \( \mathbb{E}_\rho[L(h, h')] \) and \( \mathbb{E}_\rho[L(h)] \) we use either PAC-Bayes-kl or PAC-Bayes-\( \lambda \) inequalities, both cited below. We use KL(\( \rho \| \pi \)) to denote the Kullback-Leibler divergence between distributions \( \rho \) and \( \pi \) on \( \mathcal{H} \) and kl(\( \rho \| q \)) to denote the Kullback-Leibler divergence between two Bernoulli distributions with biases \( \rho \) and \( q \).

Theorem 10 (PAC-Bayes-kl Inequality, Seeger [2002], Maurer [2004]). For any probability distribution \( \pi \) on \( \mathcal{H} \) that is independent of \( S \) and any \( \delta \in (0, 1) \), with probability at least \( 1 - \delta \) over a random draw of a sample \( S \) for all distributions \( \rho \) on \( \mathcal{H} \) simultaneously:

\[
\text{kl} \left( \mathbb{E}_\rho[\hat{L}(h, S)] \bigg| \mathbb{E}_\rho[L(h)] \right) \leq \frac{\text{KL}(\rho \| \pi) + \ln(2\sqrt{n}/\delta)}{n}. \tag{3}
\]

Theorem 11 (PAC-Bayes-\( \lambda \) Inequality, Thiemann et al. [2017], Masegosa et al. [2020]). For any probability distribution \( \pi \) on \( \mathcal{H} \) that is independent of \( S \) and any \( \delta \in (0, 1) \), with probability at least \( 1 - \delta \) over a random draw of a sample \( S \), for all distributions \( \rho \) on \( \mathcal{H} \) and all \( \lambda \in (0, 2) \) and \( \gamma > 0 \) simultaneously:

\[
\begin{align*}
\mathbb{E}_\rho[L(h)] & \leq \frac{\mathbb{E}_\rho[\hat{L}(h, S)]}{1 - \frac{\gamma}{2}} + \frac{\text{KL}(\rho \| \pi) + \ln(2\sqrt{n}/\delta)}{\lambda(1 - \frac{\gamma}{2}) n}, \tag{4} \\
\mathbb{E}_\rho[L(h)] & \geq \left( 1 - \frac{\gamma}{2} \right) \mathbb{E}_\rho[\hat{L}(h, S)] - \frac{\text{KL}(\rho \| \pi) + \ln(2\sqrt{n}/\delta)}{\gamma n}. \tag{5}
\end{align*}
\]

(The upper bound (4) is due to Thiemann et al. [2017] and the lower bound (5) is due to Masegosa et al. [2020], and the two bounds hold simultaneously.) The PAC-Bayes-\( \lambda \) inequality is an optimization-friendly relaxation of the PAC-Bayes-kl inequality. Therefore, for optimization of \( \rho \) we use the PAC-Bayes-\( \lambda \) inequality, the upper bound for \( \mathbb{E}_\rho[L(h, h')] \) and the lower or upper bound for \( \mathbb{E}_\rho[L(h)] \), depending on the positiveness of \( \mu \), but once we have converged to a solution we use PAC-Bayes-kl to compute the final bound. The kl form provides both an upper and a lower bound through the upper and lower inverse of the kl[1]. Taking the oracle bound from Theorem 7 and bounding the oracle quantities using Theorem 11 we obtain the following result.

Theorem 12. For any distribution \( \pi \) on \( \mathcal{H} \) that is independent of \( S \), and any \( \delta \in (0, 1) \), with probability at least \( 1 - \delta \) over a random draw of \( S \), for all distributions \( \rho \) on \( \mathcal{H} \), and all \( \mu, \lambda, \) and \( \gamma > 0 \) in the ranges specified below simultaneously, we have:

- For \( \mu \in [0, 0.5), \lambda \in (0, 2), \) and \( \gamma > 0 \):

\[
L(MV_\rho) \leq \frac{1}{(0.5 - \mu)^2} \left[ \frac{\mathbb{E}_\rho[\hat{L}(h, h', S)]}{1 - \frac{\gamma}{2}} + \frac{2\text{KL}(\rho \| \pi) + \ln(4\sqrt{n}/\delta)}{\lambda(1 - \frac{\gamma}{2}) n} - 2\mu \left( \frac{1}{2} \mathbb{E}_\rho[\hat{L}(h, S)] - \frac{\text{KL}(\rho \| \pi) + \ln(4\sqrt{n}/\delta)}{\gamma n} \right) + \mu^2 \right].
\]

Reeb et al. [2018] and Letarte et al. [2019] provide alternative ways of direct minimization of the upper bound on \( \mathbb{E}_\rho[L(h)] \) given by the upper inverse of kl in the PAC-Bayes-kl bound. We use the PAC-Bayes-\( \lambda \) relaxation due to its simplicity, and because it provides an easy way of simultaneous optimization of an upper bound on \( \mathbb{E}_\rho[L(h, h')] \) and a lower or upper bound on \( \mathbb{E}_\rho[L(h)] \) (depending on \( \mu \)).
For $\mu < 0$, $\lambda \in (0, 2)$, and $\gamma \in (0, 2)$:

$$L(MV_\rho) \leq \frac{1}{(0.5 - \mu)^2} \left[ \frac{\mathbb{E}_{\rho'}[\hat{L}(h, h', S)]}{1 - \frac{\lambda}{2}} + \frac{2KL(\rho\|\pi) + \ln(4\sqrt{n}/\delta)}{\lambda \left(1 - \frac{\lambda}{2}\right)n} - 2\mu \left(\frac{\mathbb{E}_{\rho}[\hat{L}(h, S)]}{1 - \frac{\lambda}{2}} + \frac{KL(\rho\|\pi) + \ln(4\sqrt{n}/\delta)}{\gamma \left(1 - \frac{\gamma}{2}\right)n}\right) + \mu^2 \right].$$

**Proof.** The result follows by substitution of the upper bound (4) on $\mathbb{E}_{\rho'}[\hat{L}(h, h', S)]$ and the lower bound (5) on $\mathbb{E}_{\rho}[\hat{L}(h)]$ in the case of positive $\mu$, or the upper bound (4) on $\mathbb{E}_{\rho}[\hat{L}(h)]$ in the case of negative $\mu$, into Theorem 7. We note that $KL(\rho^2\|\pi^2) = 2KL(\rho\|\pi)$ [Germain et al. 2015], which gives the factor 2 in front of the first KL term. The factor 4 in the logarithms comes from a union bound over the bounds on $\mathbb{E}_{\rho'}[\hat{L}(h, h')]$ and $\mathbb{E}_{\rho}[\hat{L}(h)]$. □

We note that both the loss and the tandem loss are Bernoulli random variables, and for Bernoulli random variables the PAC-Bayes-kl inequality is tighter than the PAC-Bayes-Bennett [Tolstikhin and Seldin 2013]. However, the empirical counterpart of the expected $\mu$-tandem loss is the empirical $\mu$-tandem loss

$$\hat{L}_\mu(h, h', S) = \frac{1}{n} \sum_{i=1}^{n} (\mathbb{I}(h(X_i) \neq Y_i) - \mu)(\mathbb{I}(h'(X_i) \neq Y_i) - \mu),$$

and the $\mu$-tandem losses are not Bernoulli. Therefore, we use the PAC-Bayes-Bennett inequality, which provides an advantage if the variance of the $\mu$-tandem losses happens to be small. The expected and empirical variance of the $\mu$-tandem losses of a pair of hypotheses $h$ and $h'$ are, respectively, defined by

$$\forall_\mu(h, h') = \mathbb{E}_{\rho}[((\mathbb{I}(h(X) \neq Y) - \mu)(\mathbb{I}(h'(X) \neq Y) - \mu) - L_\mu(h, h')]^2],$$

$$\hat{\forall}_\mu(h, h', S) = \frac{1}{n-1} \sum_{i=1}^{n} ((\mathbb{I}(h(X_i) \neq Y_i) - \mu)(\mathbb{I}(h'(X_i) \neq Y_i) - \mu) - \hat{L}_\mu(h, h', S))^2.$$

The empirical variance $\hat{\forall}_\mu(h, h', S)$ is an unbiased estimate of $\forall_\mu(h, h')$.

Since the PAC-Bayes-Bennett inequality is stated in terms of the oracle variance $\mathbb{E}_\rho[\hat{V}(h)]$, we use the result by Tolstikhin and Seldin [2013] Equation (15) to bound it in terms of the empirical variance. For a general loss function $\ell(\cdot, \cdot)$ (not necessarily within $[0, 1]$), we define the empirical variance of the loss of $h$ by $\hat{V}(h, S) = \frac{1}{n-1} \sum_{i=1}^{n} (\ell(h(X_i), Y_i) - \hat{L}_\mu(h, h'))^2$. We recall that $\hat{L}, \hat{V}$, and $\hat{\ell}$ were defined above Theorem 9. We note that the result of Tolstikhin and Seldin assumes that the losses are bounded in the $[0, 1]$ interval. Rescaling to a general range introduces the squared range factor $c^2$ in front of the last term in the inequality below, since scaling a random variable by $c$ scales the variance by $c^2$.

**Theorem 13** (Tolstikhin and Seldin 2013). Let $\ell(\cdot, \cdot)$ be an arbitrary bounded loss function and let $c$ be the length of the loss range. Then for any distribution $\pi$ on $\mathcal{H}$ that is independent of $S$, any $\lambda \in \left(0, \frac{2(n-1)}{n}\right)$, and any $\delta \in (0, 1)$, with probability at least $1 - \delta$ over a random draw of the sample $S$, for all distributions $\rho$ on $\mathcal{H}$ simultaneously:

$$\mathbb{E}_\rho[\hat{V}(h)] \leq \frac{\mathbb{E}_\rho[\hat{V}(h, S)]}{1 - \frac{\lambda}{2(n-1)}} + c^2 \left(\frac{KL(\rho\|\pi) + \ln \frac{1}{\delta}}{n\lambda \left(1 - \frac{2\lambda}{2(n-1)}\right)}\right).$$

We note that, similar to the PAC-Bayes-Bennett inequality, but in contrast to the PAC-Bayes-$\lambda$ inequality, the inequality above holds for a fixed value of $\lambda$ and in case of optimization over $\lambda$ a union bound has to be applied.

The last thing that is left is to bound the length of the range of $\mu$-tandem losses defined in equation (2).
Lemma 14. For \( \mu < 0.5 \) we have that the length of the range of \( \ell_{\mu}(\cdot, \cdot) \) is \( K_\mu = \max\{1 - \mu, 1 - 2\mu\} \).

A proof is provided in Appendix B. Taking together the results of Theorems 8 and 13 and Lemma 14, we obtain the following result.

Theorem 15. For any parameter grid \( \{\gamma_1, \ldots, \gamma_k\} \) and \( \{\lambda_1, \ldots, \lambda_k\} \), where \( \gamma_i > 0 \) for all \( i \) and \( \lambda_i \in (0, \frac{2/(n-1)}{n}) \) for all \( i \), any distribution \( \pi \) on \( \mathcal{H} \) that is independent of \( S \), and any \( \delta \in (0, 1) \), with probability at least \( 1 - \delta \) over a random draw of \( S \), for all values of \( \mu \leq 0.5 \), all distributions \( \rho \) on \( \mathcal{H} \), and all values of \( \gamma \) and \( \lambda \) in the parameter grid simultaneously:

\[
L(M) \leq \frac{1}{(0.5 - \mu)^2} \left( \mathbb{E}_{\rho^2}[\hat{\ell}_{\mu}(h, h', S)] + \frac{2 \text{KL}(\rho||\pi) + \ln \frac{2k_\mu}{\delta}}{\gamma n} \right)
\]

\[
+ \frac{\phi(\gamma K_\mu)}{\gamma K_\mu} \left( \frac{\mathbb{E}_{\rho^2}[\hat{V}_{\mu}(h, h', S)]}{1 - \frac{\lambda n}{2(n-1)}} + \frac{K_\mu^2 \left( 2 \text{KL}(\rho||\pi) + \ln \frac{2k_\mu}{\delta} \right)}{n\lambda \left( 1 - \frac{\lambda n}{2(n-1)} \right)} \right).
\]

Proof. The result follows by reverse substitution of the result of Lemma 14 into Theorem 13, then into Theorem 9, and finally into Theorem 8. Since \( \text{KL}(\rho^2||\pi^2) = 2 \text{KL}(\rho||\pi) \), we have factor 2 in front of the KL terms. The factor \( 2k_\mu \) comes from a union bound over the parameter grid and the bounds in Theorems 9 and 13. \( \Box \)

6 Experiments

We start with a simulated comparison of the oracle bounds and then present an empirical evaluation on real data. The python source code for replicating the experiments is available at Github.

Comparison of the oracle bounds

Figure 1 depicts a comparison of the second order oracle bound based on the Chebyshev-Cantelli inequality (Theorems 5 and 8, which, as oracle bounds, are equivalent) and the second order oracle bound based on the second order Markov’s inequality (Theorem 3). We plot the ratio of the right hand side of the bound in Theorem 7 for the optimal value \( \mu^* = \mathbb{E}_\rho[L(h)] - \mathbb{E}_\rho[L(h', h)] - \mathbb{E}_\rho[L(h)]^2 \) over \( 0.5 - \mathbb{E}_\rho[L(h)] \) to the value of the right hand side of the bound in Theorem 3. A simple calculation shows that if \( \mathbb{E}_\rho[L(h, h')] = 0.5\mathbb{E}_\rho[L(h)] \), then \( \mu^* = 0 \), which recovers the bound in Theorem 3. The line \( \mathbb{E}_\rho[L(h, h')] = 0.5\mathbb{E}_\rho[L(h)] \) is shown in black in Figure 1. We also note that \( \mathbb{E}_\rho[L(h)]^2 \leq \mathbb{E}_\rho[L(h, h')] \leq \mathbb{E}_\rho[L(h)] \), which defines the feasible region in Figure 1. Whenever \( \mathbb{E}_\rho[L(h, h')] \neq 0.5\mathbb{E}_\rho[L(h)] \) the Chebyshev-Cantelli inequality provides an improvement over second order Markov’s inequality. The region above the black line, where \( \mathbb{E}_\rho[L(h, h')] > 0.5\mathbb{E}_\rho[L(h)] \), is the region of high correlation of errors and in this case majority vote yields little improvement over individual classifiers. In this region the first order oracle bound is tighter than the second order oracle bounds (see Appendix C). The region below the black line, where \( \mathbb{E}_\rho[L(h, h')] < 0.5\mathbb{E}_\rho[L(h)] \), is the region of low correlation of errors. In this region the second order oracle bounds are tighter than the first order oracle bound. Note that the potential for improvement below the black line is much higher than above it.

Empirical evaluation on real datasets

We studied the empirical performance of the bounds using standard random forest [Breiman 2001] and a combination of heterogeneous classifiers on a subset of data sets from UCI and LibSVM.

\[https://github.com/StephanLorenzen/MajorityVoteBounds\]
We derived an optimization-friendly form of the Chebyshev-Cantelli inequality and applied it to derive two new forms of second order oracle bounds for the weighted majority vote. The new oracle bounds bridge between the C-bounds [Germain et al., 2015] and the tandem bound [Masegosa et al., 2020].
and take the best of both: the tightness of the Chebyshev-Cantelli inequality and the optimization and estimation convenience of the tandem bound. We also derived the PAC-Bayes-Bennett inequality, improving on the PAC-Bayes-Bernstein inequality of Seldin et al. [2012].

Our paper opens several directions for future research. One of them is a better treatment of parameter search in parametric bounds that would give tighter bounds than a union bound over a grid. It would also be interesting to find other applications for the new form of Chebyshev-Cantelli inequality and the PAC-Bayes-Bennett inequality.

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A Proof of the PAC-Bayes-Bennett inequality (Theorem\(^9\)) and a comparison with the PAC-Bayes-Bernstein inequality

In this section we provide a proof of Theorem\(^9\) and a numerical comparison with the PAC-Bayes-Bernstein inequality. The proof is based on the standard change of measure argument. We use the following version by Tolstikhin and Seldin (2013).

**Lemma 16** (PAC-Bayes Lemma). For any function \( f_n : \mathcal{H} \times (X \times Y)^n \to \mathbb{R} \) and for any distribution \( \pi \) on \( \mathcal{H} \), such that \( \pi \) is independent of \( S \), with probability at least \( 1 - \delta \) over a random draw of \( S \), for all distributions \( \rho \) on \( \mathcal{H} \) simultaneously:

\[
\mathbb{E}_\rho[f_n(h, S)] \leq \text{KL}(\rho \| \pi) + \ln \frac{1}{\delta} + \ln \mathbb{E}_\pi[\mathbb{E}_{S'}[e^{f_n(h, S')}]].
\]

The second ingredient is Bennett’s lemma, which is a bound on the moment generating function used in the proof of Bennett’s inequality. Since we are unaware of a reference, we provide a proof below, which is essentially an intermediate step in the proof of Bennett’s inequality [Boucheron et al. 2013, Theorem 2.9].

**Lemma 17** (Bennett’s Lemma). Let \( b > 0 \) and let \( Z_1, \ldots, Z_n \) be i.i.d. zero-mean random variables with finite variance, such that \( Z_i \leq b \) for all \( i \). Let \( M_n = \sum_{i=1}^n Z_i \) and \( V_n = \sum_{i=1}^n \mathbb{E} [Z_i^2] \). Let \( \phi(u) = e^u - u - 1 \). Then for any \( \lambda > 0 \):

\[
\mathbb{E} \left[ e^{\lambda M_n - \frac{\phi(b \lambda)}{b^2} V_n} \right] \leq 1.
\]

**Proof.** Since \( u^{-2}\phi(u) \) is a non-decreasing function of \( u \in \mathbb{R} \) (where at zero we continuously extend the function), for all \( i \in [n] \) and \( \lambda > 0 \) we have

\[
e^{\lambda Z_i} - \lambda Z_i - 1 \leq Z_i^2 \frac{\phi(b \lambda)}{b^2},
\]

which implies

\[
\mathbb{E} \left[ e^{\lambda Z_i} \right] \leq 1 + \lambda \mathbb{E} [Z_i] + \frac{\phi(b \lambda)}{b^2} \mathbb{E} [Z_i^2] \leq e^{\frac{\phi(b \lambda)}{b^2} \mathbb{E} [Z_i^2]},
\]

where the second inequality uses the assumption that \( \mathbb{E} [Z_i] = 0 \) and the fact that \( 1 + x \leq e^x \) for all \( x \in \mathbb{R} \). By the above inequality and independence of the random variables,

\[
\mathbb{E} \left[ e^{\lambda M_n - \frac{\phi(b \lambda)}{b^2} V_n} \right] = \mathbb{E} \left[ \prod_{i=1}^n e^{\lambda Z_i - \frac{\phi(b \lambda)}{b^2} \mathbb{E} [Z_i^2]} \right] = \prod_{i=1}^n \mathbb{E} \left[ e^{\lambda Z_i - \frac{\phi(b \lambda)}{b^2} \mathbb{E} [Z_i^2]} \right] \leq 1.
\]

Now we are ready to prove the theorem.

**Proof of Theorem\(^9\)** We take \( f_n(h, S) = \gamma n \left( \tilde{L}(h) - \hat{L}(h, S) \right) - \frac{\phi(\gamma b)}{b^2} \gamma n \tilde{V}(h) \). Then by Lemma 17 we have \( \mathbb{E}_S[e^{f_n(h, S)}] \leq 1 \). By plugging this into Lemma 16, normalizing by \( \gamma n \), and changing sides, we obtain the result.

Numerical comparison of the PAC-Bayes-Bennett and PAC-Bayes-Bernstein bound

Figure 3 provides a numerical comparison of the PAC-Bayes-Bennett and PAC-Bayes-Bernstein inequalities (Theorem\(^9\) and Theorem 7 by Tolstikhin and Seldin (2013)).

B Proof of Lemma\(^{14}\)

**Proof.** Recall that

\[
\ell_\mu(h(X), h'(X), Y) = (1(h(X) \neq Y) - \mu)(1(h'(X) \neq Y) - \mu) \in \{(1 - \mu)^2, -\mu(1 - \mu), \mu^2\}.
\]
As most of the other PAC-Bayesian works, we take $\pi$ to be a union distribution over the hypotheses. We set $\text{KL}(\rho || \pi) = 5$ and $\delta = 0.05$. The value of $n$ is provided in the captions of the subfigures.

For $\mu < 0.5$, we have $-\mu(1-\mu) < (1-\mu)^2$ and $\mu^2 < (1-\mu)^2$. Therefore, $\ell_\mu(h(X), h'(X), Y) \leq (1-\mu)^2$.

Furthermore, for $\mu < 0$ we have $\mu^2 < -\mu(1-\mu)$, and for $\mu > 0$ we have $-\mu(1-\mu) \leq \mu^2$. Therefore, for $\mu < 0.5$ we have $\ell_\mu(h(X), h'(X), Y) \geq \min\{-\mu(1-\mu), \mu^2\}$.

By combining the upper and the lower bound, we obtain

$$K_\mu = (1-\mu)^2 - \min\{-\mu(1-\mu), \mu^2\} = \max\{(1-\mu)^2 - (-\mu(1-\mu)), (1-\mu)^2 - \mu^2\} = \max\{1-\mu, 1-2\mu\}.$$

\[\square\]

C Comparison of the first and second order oracle bounds

In this section we show that if $\mathbb{E}_\rho[L(h)] < 0.5$ and $\mathbb{E}_{\rho^2}[L(h, h')] > 0.5\mathbb{E}_\rho[L(h)]$, then the first order oracle bound is tighter than the second order oracle bounds, and if $\mathbb{E}_\rho[L(h)] < 0.5$ and $\mathbb{E}_{\rho^2}[L(h, h')] < 0.5\mathbb{E}_\rho[L(h)]$, then it is the other way around.

For comparison of the first order oracle bound $L(MV_\rho) \leq 2\mathbb{E}_\rho[L(h)]$ vs. the second order oracle tandem bound $L(MV_{\rho^2}) \leq 4\mathbb{E}_{\rho^2}[L(h, h')]$ the statement above is evident.

For the second order oracle bounds based on the Chebyshev-Cantelli inequality we have

$$\frac{\mathbb{E}_{\rho^2}[L(h, h')] - \mathbb{E}_\rho[L(h)]^2}{0.25 + \mathbb{E}_{\rho^2}[L(h, h')] - \mathbb{E}_\rho[L(h)]^2} \quad \text{vs.} \quad 2\mathbb{E}_\rho[L(h)],$$

$$\mathbb{E}_{\rho^2}[L(h, h')] - \mathbb{E}_\rho[L(h)]^2 \quad \text{vs.} \quad 0.5\mathbb{E}_\rho[L(h)] + 2\mathbb{E}_\rho[L(h)]\mathbb{E}_{\rho^2}[L(h, h')] - 2\mathbb{E}_\rho[L(h)]^2,$$

$$\mathbb{E}_{\rho^2}[L(h, h')] - (1-2\mathbb{E}_\rho[L(h)]) \quad \text{vs.} \quad 0.5\mathbb{E}_\rho[L(h)](1-2\mathbb{E}_\rho[L(h)]),$$

$$\mathbb{E}_{\rho^2}[L(h, h')] \quad \text{vs.} \quad 0.5\mathbb{E}_\rho[L(h)],$$

where under the assumption that $\mathbb{E}_\rho[L(h)] < 0.5$ we can cancel $(1 - 2\mathbb{E}_\rho[L(h)])$, since it is positive, and the result is again evident.

D Minimization of the bounds

In this section we provide technical details on minimization of the bounds in Theorems 12 and 15.

Figure 3: The ratio of PAC-Bayes Bennett to PAC-Bayes Bernstein bound as a function of $\mathbb{E}_\rho[\hat{L}(h, S)]$ and $\mathbb{E}_\rho[\bar{V}(h)]$. We set $\text{KL}(\rho || \pi) = 5$ and $\delta = 0.05$. The value of $n$ is provided in the captions of the subfigures.

(a) $n = 1000$

(b) $n = 10000$
in both cases. As discussed in Section 6 we build a set of data-dependent hypotheses by splitting the data set \( S = T_h \cup S_h \), such that \( T_h \cap S_h = \emptyset \), training \( h \) on \( T_h \) and calculating an unbiased loss estimate \( \hat{L}(h, S_h) \) on \( S_h \). For tandem losses we compute the unbiased estimates \( \hat{L}(h', S_h \cap S_{h'}) \) on the intersections of the corresponding sets \( S_h \) and \( S_{h'} \).

### D.1 Minimization of the bound in Theorem 12

The adjustment of the bound from Theorem 9 to this construction is for \( \mu \geq 0 \):

\[
L(MV, \rho) \leq \frac{1}{(5 - \mu)^2} \left[ \mathbb{E}_{\rho} \left[ \hat{L}(h, h', S_h \cap S_{h'}) \right] + \frac{2 \text{KL}(\rho || \pi) + \ln(4\sqrt{m} / \delta)}{\lambda (1 - \frac{3}{2}) m} \right.
- 2\mu \left( 1 - \frac{\gamma}{2} \right) \mathbb{E}_{\rho} [\hat{L}(h, S_h)] - \frac{\text{KL}(\rho || \pi) + \ln(4\sqrt{n} / \delta)}{\gamma n} + \mu^2 \left],
\]

and for \( \mu < 0 \):

\[
L(MV, \rho) \leq \frac{1}{(5 - \mu)^2} \left[ \mathbb{E}_{\rho} \left[ \hat{L}(h, h', S_h \cap S_{h'}) \right] + \frac{2 \text{KL}(\rho || \pi) + \ln(4\sqrt{m} / \delta)}{\lambda (1 - \frac{3}{2}) m} \right.
- 2\mu \left( 1 - \frac{\gamma}{2} \right) \mathbb{E}_{\rho} [\hat{L}(h, S_h)] - \frac{\text{KL}(\rho || \pi) + \ln(4\sqrt{n} / \delta)}{\gamma (1 - \frac{3}{2}) n} + \mu^2 \left],
\]

where \( m = \min_{h, h'} |S_h \cap S_{h'}| \) and \( n = \min_h |S_h| \). Below we provide the pseudocode and derive update rules for \( \mu \), \( \lambda \), \( \gamma \), and \( \rho \) for alternating minimization of this bound.

#### Algorithm 1: Minimization of the bound in Theorem 12

**Input:** \( m, n \), tandem losses \( \hat{L}(h, h', S_h \cap S_{h'}) \) for all \( h, h' \), and Gibbs losses \( \hat{L}(h, S_h) \) for all \( h 
**Initialize:** \( \rho = \pi \) and \( \mu = 0 
**while** The improvement of the bound is larger than \( 10^{-9} \) do

- Compute \( \lambda^*_\rho \), the optimal \( \lambda \) given \( \rho \)
- Compute \( \gamma^*_\rho \), the optimal \( \gamma \) given \( \rho \) and \( \mu \)
- Compute the bound using \( \rho \), \( \mu \), \( \lambda^*_\rho \) and \( \gamma^*_\rho \)
- Compute new \( \mu^*_\rho \), the optimal \( \mu \) given \( \rho \), \( \lambda^*_\rho \) and \( \gamma^*_\rho \)
- Update the new distribution \( \rho' \) with gradient descent given \( \mu, \lambda^*_\rho \) and \( \gamma^*_\rho \)
- Let \( \rho = \rho' \) and \( \mu = \mu^*_\rho \)
**end while**

**Optimal \( \lambda \) given \( \rho \)** Minimization of the bound with respect to \( \lambda \) is identical to minimization of the tandem bound by [Masegosa et al., 2020, Theorem 9]. [Masegosa et al.] derive the optimal value of \( \lambda \):

\[
\lambda^*_\rho = \frac{2}{\sqrt{\frac{2mE_{\rho}[\hat{L}(h, h', S_h \cap S_{h'})]}{2KL(\rho || \pi) + \ln(4\sqrt{m} / \delta)}} + 1} + 1
\]

**Optimal \( \gamma \) given \( \rho \) and \( \mu \)** Minimization of the bound with respect to \( \gamma \) in the case of \( \mu \geq 0 \) is analogous to minimization of the bound by [Masegosa et al., 2020, Theorem 10] with respect to \( \gamma \). [Masegosa et al.] derive the optimal value of \( \gamma \):

\[
\gamma^*_\rho = \frac{2 \text{KL}(\rho || \pi) + \ln(16n/\delta^2)}{nE_{\rho}[\hat{L}(h, S_h)]}.
\]

On the other hand, the optimal \( \gamma \) in the case of \( \mu < 0 \) is analogous to the optimal \( \lambda \) above:

\[
\gamma^*_\rho = \frac{2}{\sqrt{\frac{2mE_{\rho}[\hat{L}(h, S_h)]}{\text{KL}(\rho || \pi) + \ln(4\sqrt{n} / \delta)}} + 1} + 1.
\]
Optimal $\mu$ given $\rho$ Given $\rho$, we can compute the optimal $\lambda^*_\rho$ and $\gamma^*_\rho$ by the above formulas. Let

$$U_T(\rho) := \frac{\mathbb{E}_\rho[\hat{L}(h, h', S_h \cap S_{h'})]}{1 - \frac{\lambda^*_\rho}{2}} + \frac{2 \text{KL}(\rho(\pi) + \ln(4\sqrt{\delta/n}))}{\mu^*_\rho \left(1 - \frac{\lambda^*_\rho}{2}\right)n},$$

$$L_G(\rho) := \left\{ \begin{array}{ll}
\left(1 - \frac{\gamma^*_\rho}{2}\right) \mathbb{E}_\rho[\hat{L}(h, S_h)] - \frac{\text{KL}(\rho(\pi) + \ln(4\sqrt{\delta/n}))}{\gamma^*_\rho \left(1 - \frac{\gamma^*_\rho}{2}\right)n}, & \mu \geq 0 \\
\frac{\mathbb{E}_\rho[\hat{L}(h, S_h)]}{1 - \frac{\gamma^*_\rho}{2}} + \frac{\text{KL}(\rho(\pi) + \ln(4\sqrt{\delta/n}))}{\gamma^*_\rho \left(1 - \frac{\gamma^*_\rho}{2}\right)n}, & \mu < 0
\end{array} \right.\right.$$

Then the optimal $\mu$ is

$$\mu^*_\rho = \frac{1}{2} L_G(\rho) - U_T(\rho).$$

Gradient w.r.t. $\rho$ given $\lambda$, $\gamma$ and $\mu$ Minimization of the bound w.r.t. $\rho$ is equivalent to constrained optimization of $f(\rho) = a\mathbb{E}_\rho[\hat{L}(h, h', S_h \cap S_{h'})] - 2b\mathbb{E}_\rho[\hat{L}(h, S_h)] + 2c \text{KL}(\rho(\pi)), \text{ where for } \mu \geq 0,$

$$a = \frac{1}{1 - \lambda/2}, \quad b = \mu(1 - \gamma/2) \text{ and } c = \frac{1}{(\lambda(1 - \lambda/2)m) + \mu(\gamma n)}, \text{ and for } \mu < 0,$

$$a = \frac{1}{1 - \lambda/2}, \quad b = \mu(1 - \gamma/2) \text{ and } c = \frac{1}{(\lambda(1 - \lambda/2)m) - \mu(1 - \gamma/2)n}.$$ The constraint is that $\rho$ is a probability distribution. We optimize $\rho$ by projected gradient descent, where we iteratively take steps in the direction of the negative gradient of $f$ and project the result onto the probability simplex.

We use $\hat{L}$ to denote the vector of empirical losses and $L_{\text{tand}}$ to denote the matrix of tandem losses. Let $\nabla f$ denote the gradient of $f$ w.r.t. $\rho$ and $(\nabla f)_h$ the $h$-th coordinate of the gradient. We have:

$$(\nabla f)_h = 2 \left( a \sum_{h'} \rho(h') \hat{L}(h, h', S_h \cap S_{h'}) - b \hat{L}(h, S_h) + c \left(1 + \ln \frac{\rho(h)}{\pi(h)}\right)\right),$$

$$\nabla f = 2 \left(a L_{\text{tand}} \rho - b \hat{L} + c \left(1 + \ln \frac{\rho}{\pi}\right)\right).$$

Gradient descent optimization w.r.t. $\rho$ To optimize the weighting $\rho$, we applied iRProp+ for the gradient based optimization, a first order method with adaptive individual step sizes [Igel and Hüsken 2003, Florescu and Igel 2018], until the bound did not improve for 10 iterations.

D.2 Minimization of the bound in Theorem 15

We start with the details on construction of the grid of $\mu$, $\lambda$ and $\gamma$.

D.2.1 The $\mu$ grid for Theorem 15

We were unable to find a closed-form solution for minimization of the bound w.r.t. $\mu$ and applied a heuristic. Empirically we observed that the bound was quasiconvex in $\mu$ (we were unable to prove that it is always the case) and applied binary search for $\mu$ in the grid. Note that even if we take a grid of $\mu$, we don’t need a union bound since the bound holds with high probability for all $\mu$ simultaneously.

We then consider the relevant range of $\mu$. By Theorem 6, we have $\mu < 0.5$. At the same time, $\mu^* = \frac{0.3\mathbb{E}_\rho[\hat{L}(h) - \mathbb{E}_\rho[\hat{L}(h,h)]]}{\mathbb{E}_\rho[\hat{L}(h,h)]}$, and in Section 6 we have shown that the primary region of interest is where $\mathbb{E}_\rho[\hat{L}(h,h')] < 0.5 \mathbb{E}_\rho[\hat{L}(h)]$, which corresponds to $\mu^* > 0$. However, since $\mathbb{E}_\rho[\hat{L}(h,h')]$ and $\mathbb{E}_\rho[\hat{L}(h)]$ are unobserved and we use an upper bound for the first and a lower bound for the second instead, we take a broader range of $\mu$. By making a mild assumption that the upper bound for the tandem loss $\mathbb{E}_\rho[\hat{L}(h,h')]$ is at most 0.25 and the lower bound for the Gibbs loss $\mathbb{E}_\rho[\hat{L}(h)]$ is at most 0.5, we have $\mu \in [-0.5, 0.5]$. We take 400 uniformly spaced points in the selected range for the CCPBB bound.

D.2.2 The $\lambda$ grid for Theorem 15

The parameter $\lambda$ comes from Theorem 15. The theorem is identical to the result by Tolstikhin and Seldin [2013, Equation (15)], except rescaling, but rescaling happens on top of the bound and has no
We use $V$ we have $\lambda$ $W$ where

Thus, the optimal value of $\gamma$ comes from Theorem 9. By taking the first two derivatives we can verify that for a fixed $\rho$ the PAC-Bayes-Bennett bound is convex in $\gamma$ and at the minimum point the optimal value of $\gamma$ satisfies

$$e^{(\gamma^* b - 1)} (\gamma^* b - 1) = \frac{1}{e} \left( b^2 \frac{KL(\rho||\pi) + \ln \frac{1}{\delta^2}}{nE_\rho[\tilde{V}(h)]} - 1 \right).$$

Thus, the optimal value of $\gamma$ is given by

$$\gamma^*_\rho = \frac{1}{b} \left( W_0 \left( \frac{1}{e} \left( b^2 \frac{KL(\rho||\pi) + \ln \frac{1}{\delta^2}}{nE_\rho[\tilde{V}(h)]} - 1 \right) \right) + 1 \right),$$

where $W_0$ is the principal branch of the Lambert W function, which is defined as the inverse of the function $f(x) = xe^x$.

In order to define a grid for $\gamma$ we first determine the relevant range for $\gamma^*_\rho$. We note that the variance $E_\rho[\tilde{V}(h)]$ is estimated using Theorem 13, which assumes that the length of the range of the loss $\tilde{\ell}(\cdot, \cdot)$ is $c$. The loss range provides a trivial upper bound on the variance $E_\rho[\tilde{V}(h)] \leq \frac{c^2}{\sqrt{T}}$. At the same time, we have $\lambda \left( 1 - \frac{\lambda n}{2(n-1)} \right) \leq \frac{n-1}{2n}$ (it is a downward-pointing parabola) and, therefore, the right hand side of the bound in Theorem 13 is at least the value of its second term, which is at least

$$\frac{2c^2 \ln \frac{1}{\delta}}{n-1},$$

since $KL(\rho||\pi) \geq 0$. Thus, we obtain that the estimate of $E_\rho[\tilde{V}(h)]$ is in the range $\left( \frac{2c^2 \ln \frac{1}{\delta}}{n-1}, \frac{c^2}{\sqrt{T}} \right]$.

We use $V_{\min} = \frac{2c^2 \ln \frac{1}{\delta}}{n-1}$ to denote the lower bound of this range.

Since $W_0(\cdot)$ is a monotonically increasing function, $KL(\rho||\pi) \geq 0$, and the estimate of $E_\rho[\tilde{V}(h)]$ is at most $\frac{c^2}{\sqrt{T}}$, we obtain that $\gamma^*_\rho$ satisfies

$$\gamma^*_\rho = \frac{1}{b} \left( W_0 \left( \frac{1}{e} \left( b^2 \frac{KL(\rho||\pi) + \ln \frac{1}{\delta^2}}{nE_\rho[\tilde{V}(h)]} - 1 \right) \right) + 1 \right) \geq \frac{1}{b} \left( W_0 \left( \frac{1}{e} \left( \frac{4b^2}{nc^2} \ln \frac{1}{\delta^2} - 1 \right) \right) + 1 \right) \overset{\text{def}}{=} \gamma_{\min}.$$  

For an upper bound we observe that since $E_\rho[\tilde{L}(h)] - E_\rho[\tilde{L}(h, S)]$ is trivially bounded by $b$, the bound in Theorem 13 is only interesting if it is smaller than $b$ and, in particular, $\frac{\phi(\gamma^*_\rho)}{\gamma^*_\rho^2} E_\rho[\tilde{V}(h)] \leq b$. This gives

$$b \geq \frac{\phi(\gamma^*_\rho)}{\gamma^*_\rho^2} E_\rho[\tilde{V}(h)] \geq \frac{\phi(\gamma^*_\rho)}{\gamma^*_\rho^2} V_{\min}.$$  

Thus, $\gamma$ should satisfy

$$\phi(\gamma b) \leq \frac{\gamma b^3}{V_{\min}}.$$
which gives that the maximal value of $\gamma$, denoted $\gamma_{\text{max}}$, is the positive root of

$$H(\gamma) = e^{\gamma b} - \gamma b \left( 1 + \frac{b^2}{V_{\text{min}}} \right) - 1 = 0.$$ 

Let $\alpha = (1 + b^2/V_{\text{min}})^{-1} \in (0, 1)$, and $x = -\gamma b - \alpha$. Then the above problem is equivalent to finding the root of $f(x) = xe^x - d$ for $d = -\alpha e^{-\alpha}$, which can again be solved by applying the Lambert $W$ function. Since for $\alpha \in (0, 1)$, we have $d \in (-1/e, 0)$, which indicates that there are two roots [Corless et al., 1996]. We denote the root greater than $-1$ as $W_0(d)$ and the root less than $-1$ as $W_{-1}(d)$. It is obvious that $W_0(d) = -1$. However, $W_0(d)$ is not the desired solution, since for $b > 0$, $x = -\alpha$ implies $\gamma = 0$, but we assume $\gamma > 0$. Hence, $W_{-1}(d)$ is the desired root, which gives the corresponding $\gamma = -\frac{1}{b}(W_{-1}(d) + \alpha) > 0$. Thus, we obtain

$$\gamma_{\text{max}} = -\frac{1}{b} W_{-1} \left( \frac{1}{1 + \frac{b^2}{V_{\text{min}}} \cdot e^{-\frac{1}{b} W_{-1}(d)}} \right).$$

We construct the grid by taking $\gamma_i = c_2^{-1} \gamma_{\text{min}}$ for $i \in \{1, \ldots, k_{\gamma}\}$, were $k_{\gamma} = \mid \ln(\gamma_{\text{max}}/\gamma_{\text{min}})/\ln c_2 \mid$. In the experiments we took $c_2 = 1.05$, and $\delta_1 = \delta_2 = \delta/2$.

### D.2.4 Minimization of the bound

The adjustment of the bound in Theorem 15 to our hypothesis space construction, as described above, is:

$$L(MV) \leq \frac{1}{(0.5 - \mu)^2} \left( \mathbb{E}_{\rho^2} \left[ \hat{L}_\mu(h, h', S_h \cap S_{h'}) \right] + \frac{2 \text{KL}(\rho\|\pi)}{\gamma n} + \phi(\gamma K_\mu) \left( \mathbb{E}_{\rho^2} \left[ \hat{V}_\mu(h, h', S_h \cap S_{h'}) \right] \cdot 1 - \frac{\lambda_{n-1}}{2} \right) + \frac{K_\mu^2}{n \lambda} \left( \frac{2 \text{KL}(\rho\|\pi) + \ln \frac{2k}{\delta}}{2(n-1)} - 1 \right) \right),$$

where $n = \min_{h,h'} |S_h \cap S_{h'}|$ and $k = k_{\gamma} k_{\lambda}$. We minimize the bound without considering $k_{\gamma}$ and $k_{\lambda}$ since we define the grid without taking them into consideration. However, we put back $k_{\gamma}$ and $k_{\lambda}$ when computing the generalization bound. Thus, when doing the optimization we take $k = 1$, but when we compute the bound we take the proper $k = k_{\gamma} k_{\lambda}$.

### Algorithm 2: Minimization of the bound in Theorem 15

**Input:** $n$, grid of $\mu$ and losses $I(h(X_i) \neq Y_i)$ for all $(X_i, Y_i) \in S_h$ for all $h$

for $\mu$ selected by the binary search in the grid do

**Initialize:** $\rho = \pi$

Compute $\hat{L}_\mu(h, h', S_h \cap S_{h'})$ and $\hat{V}_\mu(h, h', S_h \cap S_{h'})$ for all $h, h'$

while The improvement of the bound for a fixed $\mu$ is larger than $10^{-9}$ do

Compute $\lambda^*_{\mu,\rho}$, the optimal $\lambda$ given $\rho$ and $\mu$

Compute $\gamma^*_{\mu,\rho}$, the optimal $\gamma$ given $\rho$ and $\mu$

Apply gradient descent to the bound w.r.t. $\rho$ given $\mu$, $\lambda^*_{\mu,\rho}$ and $\gamma^*_{\mu,\rho}$

end while

Proceed to the next $\mu$ in the grid proposed by the binary search

end for

**Optimal $\lambda$ given $\mu$ and $\rho$**

Given $\mu$ and $\rho$, $\lambda$ can be computed in the same way as in the optimization of Theorem 15 since the optimization problem is the same, and get

$$\lambda_{\mu,\rho} = \frac{2(n-1)}{n} \left( \frac{2(n-1)\mathbb{E}_{\rho^2}[\hat{V}_\mu(h, h', S_h \cap S_{h'})]}{K_\mu^2(2 \text{KL}(\rho\|\pi) + \ln \frac{2k}{\delta})} + 1 \right)^{-1}.$$ 

In our implementation at every optimization step we took the closest $\lambda$ to the above value from the $\lambda$-grid.
We construct the ensemble from decision trees available in scikit-learn. For each data set, an ensemble of 100 trees is trained using bagging (as described in Section 6). For each tree, the Gini criterion is used for splitting and \( \sqrt{d} \) features are considered in each split.

**E Experiments**

**E.1 Data sets**

As mentioned, we considered data sets from the UCI and LibSVM repositories [Dua and Graff, 2019; Chang and Lin, 2011], as well as Fashion-MNIST (Fashion) from Zalando Research. We used data sets with size \( 3000 \leq N \leq 70000 \) and dimension \( d \leq 1000 \). These relatively large data sets were chosen in order to provide meaningful bounds in the standard bagging setting, where individual trees are trained on \( n = 0.8N \) randomly subsampled points with replacement and the size of the overlap of out-of-bag sets is roughly \( n/9 \). An overview of the data sets is given in Table 1.

For all experiments, we removed patterns with missing entries and made a stratified split of the data set. For data sets with a training and a test set (SVMGuide1, Splice, Adult, w1a, MNIST, Shuttle, Pendigits, Protein, SatImage, USPS) we combined the training and test sets and shuffled the entire set before splitting.

**E.2 Optimized weighted random forest**

Experimental Setting

This section describes in detail the settings and the results of the empirical evaluation using random forest (RF) majority vote classifiers.

We construct the ensemble from decision trees available in scikit-learn. For each data set, an ensemble of 100 trees is trained using bagging (as described in Section 6). For each tree, the Gini criterion is used for splitting and \( \sqrt{d} \) features are considered in each split.

**E.3 Optimized weighted random forest**

**Gradient w.r.t. \( \rho \) given \( \lambda, \gamma, \) and \( \mu \)**

Optimizing the bound w.r.t. \( \rho \) is equivalent to constrained optimization of \( f(\rho) = \mathbb{E}_{\rho, \pi} [\hat{L}_\mu(h, h', S')] + a \mathbb{E}_{\mu} [\hat{V}_\mu(h, h', S')] + 2b \mathbb{KL}(\rho \| \pi) \), where

\[
\begin{align*}
\phi(K_{\mu}\gamma) = & \frac{\phi(K_{\mu}\gamma)}{K_{\mu}^2} \frac{1}{1 - \frac{n\lambda}{2(n-1)}},
\end{align*}
\]

and the constraint is that \( \rho \) must be a probability distribution. We optimize \( \rho \) in the same way as presented in Appendix D.1. We use \( \hat{L}_\mu \) to denote the matrix of empirical \( \mu \)-tandem losses and \( \hat{V}_\mu \) to denote the matrix of empirical variance of the \( \mu \)-tandem losses. Then, the gradient w.r.t. \( \rho \) is given by:

\[
(\nabla f)_h = 2 \left( \sum_{h'} \rho(h') (\hat{L}_\mu(h, h', S') + a \hat{V}_\mu(h, h', S')) + b \left( 1 + \ln \frac{\rho(h)}{\pi(h)} \right) \right),
\]

\[
\nabla f = 2 \left( \hat{L}_\mu \rho + a \hat{V}_\mu \rho + b \left( 1 + \ln \frac{\rho}{\pi} \right) \right).
\]

We applied gradient descent in the same way as presented in Appendix D.1.
Table 1: Data set overview. \(c_{\text{min}}\) and \(c_{\text{max}}\) denote the minimum and maximum class frequency.

| Data set   | \(N\)  | \(d\) | \(c\) | \(c_{\text{min}}\) | \(c_{\text{max}}\) | Source          |
|------------|--------|-------|------|-----------------|-----------------|----------------|
| Adult      | 32561  | 123   | 2    | 0.2408          | 0.7592          | LIBSVM (a1a)   |
| Cod-RNA    | 59535  | 8     | 2    | 0.3333          | 0.6667          | LIBSVM         |
| Connect-4  | 67557  | 126   | 3    | 0.0955          | 0.6583          | LIBSVM         |
| Fashion    | 70000  | 784   | 10   | 0.1000          | 0.1000          | Zalando Research|
| Letter     | 20000  | 16    | 26   | 0.3333          | 0.6667          | UCI            |
| MNIST      | 70000  | 780   | 10   | 0.0992          | 0.1125          | LIBSVM         |
| Mushroom   | 8124   | 22    | 2    | 0.4820          | 0.5180          | LIBSVM         |
| Pendigits  | 10992  | 16    | 10   | 0.0960          | 0.1041          | LIBSVM         |
| Phishing   | 11055  | 68    | 2    | 0.4431          | 0.5569          | LIBSVM         |
| Protein    | 24387  | 357   | 3    | 0.2153          | 0.4638          | LIBSVM         |
| SVMGuide1  | 3089   | 4     | 2    | 0.3525          | 0.6475          | LIBSVM         |
| SatImage   | 6435   | 36    | 10   | 0.0973          | 0.2382          | LIBSVM         |
| Sensorless | 58509  | 48    | 11   | 0.0909          | 0.0909          | LIBSVM         |
| Shuttle    | 58000  | 9     | 7    | 0.0002          | 0.7860          | LIBSVM         |
| Splice     | 3175   | 60    | 2    | 0.4809          | 0.5191          | LIBSVM         |
| USPS       | 9298   | 256   | 10   | 0.0761          | 0.1670          | LIBSVM         |
| w1a        | 49749  | 300   | 2    | 0.0297          | 0.9703          | LIBSVM         |

Table 2: Numerical values of the test loss obtained by the RFs with optimized weighting. The smallest loss is highlighted in bold, while the smallest optimized loss is underlined.

| Data set   | \(L(\text{MV}_u)\) | \(L(\text{MV}_{\rho_u})\) | \(L(\text{MV}_{\text{TND}})\) | \(L(\text{MV}_{\text{CCTND}})\) | \(L(\text{MV}_{\text{CCPBB}})\) |
|------------|--------------------|--------------------------|-------------------------------|-------------------------------|-------------------------------|
| SVMGuide1  | 0.0284 (0.0037)    | 0.0372 (0.0066)          | 0.0287 (0.0035)               | 0.0286 (0.0036)               | 0.0287 (0.0039)               |
| Phishing   | 0.0292 (0.004)     | 0.0371 (0.0073)          | 0.0292 (0.0036)               | 0.0292 (0.0036)               | 0.0292 (0.004)                |
| Mushroom   | 0.0 (0.0)          | 0.0 (0.0)                | 0.0 (0.0)                     | 0.0 (0.0)                     | 0.0 (0.0)                     |
| Splice     | 0.0299 (0.009)     | 0.1087 (0.021)           | 0.0306 (0.0099)               | 0.0309 (0.0092)               | 0.0302 (0.01)                 |
| w1a        | 0.0108 (0.0007)    | 0.016 (0.0025)           | 0.0108 (0.0006)               | 0.0107 (0.0006)               | 0.0108 (0.0006)               |
| Cod-RNA    | 0.0402 (0.0013)    | 0.0712 (0.0064)          | 0.0395 (0.0014)               | 0.0395 (0.0014)               | 0.0395 (0.0015)               |
| Adult      | 0.1693 (0.0027)    | 0.1942 (0.0151)          | 0.1698 (0.0031)               | 0.1701 (0.003)                | 0.1698 (0.0031)               |
| Connect-4  | 0.1706 (0.0023)    | 0.2803 (0.0165)          | 0.1699 (0.002)                | 0.1705 (0.0024)               | 0.1695 (0.0019)               |
| Shuttle    | 0.0002 (0.0001)    | 0.0003 (0.0002)          | 0.0002 (0.0001)               | 0.0002 (0.0001)               | 0.0002 (0.0001)               |
| Pendigits  | 0.0096 (0.0023)    | 0.0452 (0.0012)          | 0.0092 (0.0022)               | 0.0093 (0.0021)               | 0.0092 (0.0025)               |
| Letter     | 0.0378 (0.0036)    | 0.1408 (0.0356)          | 0.0398 (0.0041)               | 0.0402 (0.0042)               | 0.0383 (0.0034)               |
| SatImage   | 0.0828 (0.0068)    | 0.1321 (0.0268)          | 0.0835 (0.0061)               | 0.0839 (0.0062)               | 0.0832 (0.006)                |
| Sensorless | 0.0014 (0.0004)    | 0.0138 (0.0019)          | 0.0012 (0.0003)               | 0.0012 (0.0003)               | 0.0012 (0.0003)               |
| USPS       | 0.0394 (0.0043)    | 0.1325 (0.0251)          | 0.0401 (0.0055)               | 0.0405 (0.0052)               | 0.0404 (0.005)                |
| MNIST      | 0.0316 (0.0017)    | 0.16 (0.0352)            | 0.0323 (0.0017)               | 0.0324 (0.0017)               | 0.0317 (0.0014)               |
| Fashion    | 0.1175 (0.0018)    | 0.2122 (0.0299)          | 0.1192 (0.0022)               | 0.1197 (0.0022)               | 0.1178 (0.0023)               |

We compare the RF using the default uniform weighting \(\rho_u\) and the optimized weighting obtained by FO [Thiemann et al., 2016], TND [Masegosa et al., 2020], CCTND (Theorem 12) and CCPBB (Theorem 15). Optimization is based on the out-of-bag sets (see Section 6). For each optimized RF, we also compute the optimized bound.

Numerical Results

This section lists the numerical results for the empirical evaluation using RF. Table 2 provides the numerical values of the test loss obtained by the RFs with uniform weighting and with weighting optimized by FO, TND, CCTND and CCPBB; a visual presentation is given in Figure 2a. As observed by Masegosa et al. [2020], optimization using FO leads to overfitting, while the second-order bounds does not significantly degrade the performance. Among the second-order bounds, optimizing using CCPBB produces the best classifier in most cases.

Table 3 provides the numerical values of the optimized bounds; a visual presentation is given in Figure 2b. Table 4 provides the recorded Gibbs loss and tandem loss using the optimized \(\rho\). The optimal \(\mu\) found is reported for CCTND and CCPBB as well.
Table 3: Numerical values of the bounds for the RFs with optimized weighting. The tightest bound is highlighted in bold, while the tightest second-order bound is underlined.

| Data set     | FO($\rho_L$) | TND($\rho_TND$) | CCTND($\rho_{CCTND}$) | CCPBB($\rho_{CCPBB}$) |
|--------------|--------------|-----------------|------------------------|------------------------|
| SVMGuide1    | 0.1079 (0.0079) | 0.1836 (0.0062) | 0.1853 (0.0059) | 0.2806 (0.0071) |
| Phishing     | 0.1189 (0.0035) | 0.1642 (0.0043) | 0.1674 (0.0042) | 0.2336 (0.005) |
| Mushroom     | 0.0068 (0.0001) | 0.0353 (0.0002) | 0.0388 (0.0002) | 0.1121 (0.0006) |
| Splice       | 0.3245 (0.0218) | 0.4077 (0.0062) | 0.4247 (0.0065) | 0.6562 (0.0056) |
| w1a          | 0.0424 (0.0015) | 0.0633 (0.0009) | 0.0642 (0.0009) | 0.0805 (0.0011) |
| Cod-RNA      | 0.1629 (0.0018) | 0.1663 (0.0014) | 0.1698 (0.0014) | 0.19 (0.0018) |
| Adult        | 0.4388 (0.0042) | 0.5701 (0.0051) | 0.5508 (0.0004) | 0.5976 (0.0042) |
| Connect-4    | 0.5978 (0.0067) | 0.6831 (0.0039) | 0.6758 (0.0036) | 0.7112 (0.0038) |
| Shuttle      | 0.0026 (0.0002) | 0.0078 (0.0002) | 0.0083 (0.0002) | 0.018 (0.0003) |
| Pendigits    | 0.142 (0.0035)  | 0.1445 (0.0026) | 0.1504 (0.0042) | 0.2155 (0.0003) |
| Letter       | 0.3858 (0.0067) | 0.4504 (0.0032) | 0.4513 (0.003)  | 0.5134 (0.0039) |
| SatImage     | 0.3762 (0.0075) | 0.4902 (0.0079) | 0.4851 (0.007)  | 0.6158 (0.0083) |
| Sensorless   | 0.0348 (0.0031) | 0.0257 (0.0006) | 0.0265 (0.0006) | 0.0376 (0.0007) |
| USPS         | 0.3394 (0.0065) | 0.4059 (0.0048) | 0.4097 (0.0044) | 0.5086 (0.0042) |
| MNIST        | 0.3795 (0.0031) | 0.3537 (0.0014) | 0.3598 (0.0014) | 0.3853 (0.0014) |
| Fashion      | 0.4806 (0.0003) | 0.5436 (0.0023) | 0.5408 (0.0021) | 0.5728 (0.0021) |

Table 4: Numerical values for Gibbs loss, tandem loss and optimized $\mu$ for the RFs with optimized weighting. We use $\mathbb{E}_\rho[L]$ and $\mathbb{E}_\mu[L]$ as short-hands for the Gibbs and the tandem loss respectively.

| Data set     | $\mathbb{E}_\rho[L]$ | $\mathbb{E}_\mu[L]$ | $\mathbb{E}_{\rho[T]}[L]$ | $\mathbb{E}_{\mu[T]}[L]$ | $\mathbb{E}_{\rho[CCT]}[L]$ | $\mathbb{E}_{\mu[CCT]}[L]$ | $\mathbb{E}_{\mu[L]}$ | $\mathbb{E}_{\rho[L]}$ | $\mu$ |
|--------------|-----------------------|-----------------------|---------------------------|---------------------------|---------------------------|---------------------------|-----------------------|-----------------------|-------|
| SVMGuide1    | 0.0325 0.0217 0.0406 0.0185 0.0403 0.0184 0.0527 0.0413 0.0194 0.0258 |              |                          |                          |                          |                          |                      |                      |       |
| Phishing     | 0.041 0.0255 0.0486 0.0197 0.0484 0.0196 0.0295 0.049 0.0202 0.0125 |              |                          |                          |                          |                          |                      |                      |       |
| Mushroom     | 0.0 0.0 0.0002 0.0 0.0 0.0 0.0317 0.0002 0.0 0.01 |
| Splice       | 0.1068 0.0903 0.1564 0.0424 0.1522 0.0415 0.057 0.16 0.044 0.0045 |
| w1a          | 0.0156 0.0123 0.0179 0.0091 0.0179 0.009 0.0111 0.018 0.0092 0.0065 |
| Cod-RNA      | 0.0712 0.0602 0.0802 0.0314 0.0803 0.0314 0.0178 0.0815 0.0318 0.0102 |
| Adult        | 0.1995 0.1474 0.2061 0.1184 0.2056 0.1182 0.1216 0.2068 0.1194 0.0918 |
| Connect-4    | 0.2824 0.2564 0.2953 0.1523 0.2943 0.1521 0.0959 0.2974 0.1535 0.0615 |
| Shuttle      | 0.0003 0.0001 0.0006 0.0002 0.0006 0.0002 0.0044 0.0006 0.0002 0.0 |
| Pendigits    | 0.0502 0.0346 0.061 0.0163 0.0609 0.0163 0.0099 0.0614 0.0166 0.0992 |
| Letter       | 0.1685 0.1249 0.1803 0.0851 0.1797 0.0849 0.0501 0.1816 0.0861 0.0228 |
| SatImage     | 0.1478 0.0968 0.1612 0.0746 0.1602 0.0741 0.1104 0.1617 0.0755 0.0535 |
| Sensorless   | 0.0325 0.0113 0.0192 0.0027 0.0192 0.0027 0.0008 0.0195 0.0027 0.01 |
| USPS         | 0.1363 0.0989 0.1517 0.0644 0.1509 0.0641 0.0153 0.1522 0.0603 0.0173 |
| MNIST        | 0.1763 0.1286 0.1837 0.075 0.1835 0.075 0.0281 0.185 0.0756 0.037 |
| Fashion      | 0.2256 0.1715 0.2325 0.1196 0.2322 0.1195 0.0577 0.2334 0.1203 0.0382 |

E.3 Ensemble of multiple heterogeneous classifiers

Experimental Setting

This section describes in detail the settings and the results of the experimental evaluation using an ensemble of multiple heterogeneous classifiers.

The ensemble is defined by a set of standard classifiers available in scikit-learn:

- **Linear Discriminant Analysis**, with default parameters, which includes a singular value decomposition solver.
- Three versions of **k-Nearest Neighbors**: (i) $k=3$ and uniform weights (i.e., all points in each neighborhood are weighted equally); (ii) $k=5$ and uniform weights; and (iii) $k=5$ where points are weighted by the inverse of their distance. In all cases, it is employed the Euclidean distance.
- **Decision Tree**, with default parameters, which includes Gini criterion for splitting and no maximum depth.
- **Logistic Regression**, with default parameters, which includes L2 penalization.
Table 5: Numerical values of the test loss obtained by ensembles of multiple heterogeneous classifiers with optimized weighting. The smallest loss is highlighted in **bold**, while the smallest optimized loss is underlined.

| Data set     | \( L(MV_u) \) (0.005) | \( L(b_{best}) \) (0.0047) | \( L(MV_{ρTND}) \) (0.005) | \( L(MV_{ρCCTND}) \) (0.005) | \( L(MV_{ρCCPBB}) \) (0.005) |
|--------------|------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|
| SVMGuide1    | 0.0357 (0.005)         | 0.0404 (0.0047)             | 0.0352 (0.0051)             | 0.0348 (0.0053)             | **0.0343 (0.0059)**        |
| Phishing     | 0.0353 (0.0055)        | 0.0459 (0.0058)             | **0.0333 (0.0031)**         | 0.0337 (0.0028)             | 0.0335 (0.0032)            |
| Mushroom     | 0.0001 (0.0002)        | 0.0002 (0.0004)             | **0.0 (0.0)**                | 0.0001 (0.0002)             | 0.0001 (0.0002)            |
| Splice       | 0.1055 (0.0104)        | 0.0768 (0.0098)             | **0.0768 (0.0098)**         | 0.0768 (0.0098)             | **0.069 (0.0082)**        |
| CoR-RNA      | 0.0707 (0.0022)        | 0.064 (0.0022)              | 0.064 (0.0022)              | **0.0551 (0.0019)**         | 0.0581 (0.0023)            |
| Adult        | 0.1627 (0.0036)        | 0.1543 (0.0039)             | 0.1543 (0.0039)             | 0.1563 (0.0042)             | **0.1541 (0.0039)**       |
| Protein      | 0.3491 (0.0066)        | 0.3251 (0.0061)             | 0.3251 (0.0061)             | **0.3176 (0.0052)**         | 0.3251 (0.0061)            |
| Connect-4    | 0.2039 (0.0035)        | 0.2433 (0.0032)             | 0.2433 (0.0032)             | **0.1989 (0.0033)**         | 0.1992 (0.0032)            |
| Shuttle      | 0.0012 (0.0002)        | **0.0005 (0.0002)**         | **0.0005 (0.0002)**         | 0.0006 (0.0002)             | 0.0006 (0.0002)            |
| Pendigits    | 0.0111 (0.0016)        | 0.0092 (0.0017)             | 0.0092 (0.0017)             | 0.0086 (0.0016)             | 0.0087 (0.0016)            |
| Letter       | 0.069 (0.0041)         | 0.0673 (0.0052)             | 0.0673 (0.0052)             | 0.0538 (0.0043)             | **0.0526 (0.0041)**       |
| SaltImage    | 0.097 (0.0089)         | 0.1054 (0.0046)             | 0.1053 (0.0046)             | 0.0939 (0.0061)             | 0.0954 (0.0063)            |
| Sensorless   | 0.1816 (0.0121)        | **0.0213 (0.0018)**         | **0.0213 (0.0018)**         | **0.0213 (0.0018)**         | **0.0213 (0.0018)**       |
| USPS         | 0.0359 (0.0054)        | 0.0375 (0.0038)             | 0.0375 (0.0038)             | **0.0324 (0.0044)**         | 0.0326 (0.0042)            |
| MNIST        | 0.0356 (0.005)         | 0.0349 (0.0017)             | 0.0349 (0.0017)             | **0.0304 (0.0017)**         | **0.0304 (0.0017)**       |
| Fashion      | 0.1341 (0.0019)        | 0.154 (0.0028)              | 0.154 (0.0028)              | **0.1323 (0.003)**          | 0.1341 (0.0037)            |

- **Gaussian Naive Bayes**, with default parameters.

We included three versions of the kNN classifier to test if our bounds could deal with a heterogeneous set of classifiers where some of them are expected to provide highly correlated errors while others are expected to provide much less correlated errors.

Each of the seven classifiers of the ensemble was learned from a bootstrap sample of the training data set. We did it in the way to be able to compute and optimize our bounds with the out-of-bag-samples as described in Section 6.

**Numerical Results**

This section lists the numerical results for the empirical evaluation using ensembles of multiple heterogeneous classifiers.

Table 5 provides the numerical values of the test loss obtained by these ensembles with uniform weighting and with weighting optimized by FO, TND, CCTND and CCPBB; a visual presentation is given in Figure 2c. In this case, uniform voting is not a competitive weighting scheme. The second-order bounds perform much better than uniform weighting and than the weights computed according to the first-order bound. There is not any clear winner among the second-order bounds.

Table 6 provides the numerical values of the optimized bounds; a visual presentation is given in Figure 2d. Among the second-order bounds, the CCTND bound is often tighter in this setting.

Table 7 provides the recorded Gibbs loss and tandem loss using the optimized \( \rho \). The optimal \( \mu \) found is reported for CCTND and CCPBB as well.
Table 6: Numerical values of the bounds for ensembles of multiple heterogeneous classifiers with optimized weighting. The tightest bound is highlighted in **bold**, while the tightest second-order bound is underlined.

| Data set     | FO($\rho_\lambda$) | TND($\rho_{TND}$) | CCTND($\rho_{CCTND}$) | CCPBB($\rho_{CCPBB}$) |
|--------------|---------------------|--------------------|------------------------|------------------------|
| SVMGuide1    | 0.1133 (0.0053)     | 0.221 (0.0127)     | 0.2183 (0.0112)        | 0.3142 (0.0116)        |
| Phishing     | 0.1242 (0.0056)     | 0.1957 (0.0075)    | 0.1977 (0.0072)        | 0.2658 (0.0074)        |
| Mushroom     | 0.0078 (0.0008)     | 0.0412 (0.0019)    | 0.0441 (0.0019)        | 0.1162 (0.0026)        |
| Splice       | 0.2361 (0.0186)     | 0.4772 (0.0286)    | 0.4613 (0.0242)        | 0.6769 (0.0288)        |
| w1a          | 0.0392 (0.0015)     | 0.0694 (0.0021)    | 0.0703 (0.0021)        | 0.0879 (0.0022)        |
| Cod-RNA      | 0.1448 (0.0026)     | 0.2164 (0.0032)    | 0.2148 (0.0031)        | 0.2445 (0.0033)        |
| Adult        | 0.3343 (0.0071)     | 0.5648 (0.0077)    | 0.5366 (0.0066)        | 0.5857 (0.0064)        |
| Protein      | 0.6944 (0.0057)     | 1.0 (0.0)          | 0.9078 (0.0034)        | 1.0 (0.0)              |
| Connect-4    | 0.5157 (0.0047)     | 0.7272 (0.0099)    | 0.6733 (0.0068)        | 0.7107 (0.0064)        |
| Shuttle      | 0.0033 (0.0008)     | 0.0106 (0.0012)    | 0.0111 (0.0012)        | 0.0215 (0.0011)        |
| Pendigits    | 0.0335 (0.0033)     | 0.0838 (0.0062)    | 0.0856 (0.0061)        | 0.1412 (0.0067)        |
| Letter       | 0.1591 (0.0053)     | 0.2682 (0.0092)    | 0.2627 (0.0084)        | 0.3154 (0.0099)        |
| SatImage     | 0.2711 (0.0146)     | 0.4908 (0.0123)    | 0.4593 (0.011)         | 0.5857 (0.0122)        |
| Sensorless   | 0.0523 (0.0031)     | 0.1173 (0.0057)    | 0.2054 (0.0279)        | 0.1357 (0.0064)        |
| USPS         | 0.1069 (0.0053)     | 0.2183 (0.0074)    | 0.2142 (0.0066)        | 0.2932 (0.0084)        |
| MNIST        | 0.0811 (0.0022)     | 0.139 (0.0049)     | 0.1383 (0.0046)        | 0.1574 (0.0051)        |
| Fashion      | 0.3291 (0.0033)     | 0.4945 (0.0066)    | 0.4709 (0.0049)        | 0.5049 (0.0045)        |

Table 7: Numerical values for Gibbs loss, tandem loss and optimized $\mu$ for the heterogeneous classifiers with optimized weighting. We use $E_\mu[L]$ and $E_{\mu^2}[L]$ as short-hands for the Gibbs loss and the tandem loss respectively.

| Data set     | FO | TND | CCTND | CCPBB |
|--------------|----|-----|-------|-------|
| SVMGuide1    | 0.0365 | 0.031 | 0.0457 | 0.026 |
| Phishing     | 0.0447 | 0.0383 | 0.059 | 0.0262 |
| Mushroom     | 0.0001 | 0.0041 | 0.0003 | 0.0029 |
| Splice       | 0.0754 | 0.0754 | 0.1265 | 0.0552 |
| w1a          | 0.0147 | 0.0134 | 0.0204 | 0.0106 |
| Cod-RNA      | 0.0638 | 0.0572 | 0.0737 | 0.0425 |
| Adult        | 0.1502 | 0.1484 | 0.2049 | 0.1181 |
| Protein      | 0.3224 | 0.3153 | 0.4052 | 0.2645 |
| Connect-4    | 0.2438 | 0.236 | 0.2612 | 0.1634 |
| Shuttle      | 0.0005 | 0.0004 | 0.0019 | 0.0004 |
| Pendigits    | 0.008 | 0.0069 | 0.0156 | 0.0062 |
| Letter       | 0.0644 | 0.0587 | 0.0768 | 0.0454 |
| SatImage     | 0.1032 | 0.0928 | 0.1246 | 0.0766 |
| Sensorless   | 0.0208 | 0.0208 | 0.0345 | 0.0198 |
| MNIST        | 0.0345 | 0.0304 | 0.0428 | 0.026 |
| Fashion      | 0.1528 | 0.1488 | 0.1665 | 0.1081 |