Chromatic PAC-Bayes Bounds for Non-IID Data

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Abstract

PAC-Bayes bounds are among the tightest generalization bounds for classifiers learned from IID data, especially for margin classifiers. However, there are many practical cases where the training data show some dependencies and where the usual IID assumption does not hold. Stating generalization bounds for such frameworks is therefore of the utmost interest, both from theoretical and practical standpoints. Here, we propose the first PAC-Bayes generalization bounds for classifiers trained on data exhibiting interdependencies. The approach undertaken to establish our results is based on the decomposition of a so-called dependency graph that encodes the dependencies within the data, in sets of independent data, through the tool of graph fractional covers. Our bounds are very general, since being able to find an upper bound on the (fractional) chromatic number of the dependency graph is sufficient to get new PAC-Bayes bounds for specific settings. We show how our results can be used to derive bounds for bipartite ranking and windowed prediction on sequential data.

1 Introduction

Recently, there has been much progress in the field of generalization bounds for classifiers. PAC-Bayes bounds, introduced in (McAllester, 1999), and refined in, e.g., (Seeger, 2002; Langford, 2005), are among the most appealing advances. Their possible tightness (Ambroladze et al., 2007) make them a possible route to do model selection. They can also be seen as theoretical tools to motivate new learning procedures.

Nevertheless, PAC-Bayes bounds have so far applied to classifiers trained from *independently and identically distributed* (IID) data. Yet, being able to learn from non-IID data while having strong theoretical guarantees is an actual problem in a number of real world applications such as, e.g., k-partite ranking or classification from sequential data. Here, we propose the first PAC-Bayes bounds for classifiers trained on non-IID data; they are a generalization of the IID PAC-Bayes bound and they are general enough to provide a principled way to establish generalization bounds for a number of non-IID settings. To establish these bounds, we make use of simple tools of probability theory, convexity properties of some functions, and we exploit the notion of graph *fractional covers*. This tool from graph theory has already been used for deriving concentration inequalities for non independent data (Janson, 2004) (see additional references therein) and for providing generalization bounds based on the *fractional Rademacher complexity* (Usunier et al., 2006).

The paper is organized as follows. Section 2 recalls the standard IID PAC-Bayes bound, introduces the notion of fractional covers and states the new *chromatic* PAC-*Bayes bounds*, which rely on the fractional chromatic number of the *dependency graph* of the data at hand. Section 3 is devoted to the proof of our main theorem. Section 4 provides specific versions of our bounds for the case of IID data (which gives back the standard IID bounds), for the case of bipartite ranking and for windowed prediction on sequential data.

2 Chromatic PAC-Bayes Bounds

2.1 IID PAC-Bayes Bound

We introduce notation that will hold from here on. We consider the problem of binary classification over

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the *input space* $\mathcal{X}$, and $\mathcal{Z}$ denotes the product space $\mathcal{X} \times \mathcal{Y}$, with $\mathcal{Y} = \{-1, +1\}$. $\mathcal{H} \subseteq \mathcal{Y}^{\mathcal{X}}$ is a family of classifiers from $\mathcal{X}$. D is a probability distribution defined on $\mathcal{Z}$ and $\mathbf{D}_m$ the distribution of an m-sample; for instance, $\mathbf{D}_m = \otimes_{i=1}^m D = D^m$ is the distribution of an IID sample $\mathbf{Z} = \{Z_i\}_{i=1}^m$ of size m ($Z_i \sim D$, $i = 1 \dots m$). P and Q are distributions over $\mathcal{H}$.

The IID PAC-Bayes bound, can be stated as follows (McAllester, 1999; Seeger, 2002).

Theorem 1 (IID PAC-Bayes Bound)**.** *$\forall m$, $\forall D$, $\forall \mathcal{H}$, $\forall \delta \in (0, 1]$, $\forall P$, with probability at least $1 - \delta$ over the random draw of $\mathbf{Z} \sim \mathbf{D}_m = D^m$, the following holds:*

$$\forall Q, kl(\hat{e}_Q || e_Q) \leq \frac{1}{m}\left[KL(Q||P) + \ln \frac{m+1}{\delta}\right]. \quad (1)$$

This theorem provides a generalization error bound for the *Gibbs classifier* g_Q: given a distribution Q, this stochastic classifier predicts a class for $\mathbf{x} \in \mathcal{X}$ by first drawing a hypothesis h according to Q and then outputting $h(\mathbf{x})$. Here, $\hat{e}_Q$ is the empirical error of g_Q on an IID sample $\mathbf{Z}$ of size m and e_Q is its true error:

$$\begin{aligned} \hat{e}_Q &= \mathbb{E}_{h\sim Q} \frac{1}{m} \sum_{i=1}^m r(h, Z_i) = \mathbb{E}_{h\sim Q} \hat{R}(h, \mathbf{Z}) \\ e_Q &= \mathbb{E}_{\mathbf{Z}\sim\mathbf{D}_m} \hat{e}_Q = \mathbb{E}_{\substack{Z\sim D \\ h\sim Q}} r(h, Z) = \mathbb{E}_{h\sim Q} R(h), \end{aligned} \quad (2)$$

where, for $Z = (X, Y)$, $r(h, Z) = \mathbb{I}_{h(X)\neq Y}$ and where the fact that $\mathbf{Z}$ is an (independently) identically distributed sample was used. $\mathrm{kl}(q||p)$ is the Kullback-Leibler divergence between the Bernoulli distributions with probabilities of success q and p, and $\mathrm{KL}(Q||P)$ is the Kullback-Leibler divergence between Q and P:

$$\mathrm{kl}(q||p) = q \ln \frac{q}{p} + (1-q) \ln \frac{1-q}{1-p}$$
$$\mathrm{KL}(Q||P) = \mathbb{E}_{h\sim Q} \ln \frac{Q(h)}{P(h)}.$$

Throughout, we assume that the posteriors are absolutely continuous with respect to the priors.

We note that even if the present bound applies to the risk e_Q of the stochastic classifier g_Q, a straightforward argument gives that, if b_Q is the (deterministic) Bayes classifier such that $b_Q(x) = \mathrm{sign}(\mathbb{E}_{h\sim Q} h(x))$, then $R(b_Q) \leq 2e_Q$ (Langford & Shawe-taylor, 2002).

The problem we focus on is that of generalizing Theorem 1 to the situation where there may exist probabilistic dependencies between the elements Z_i of $\mathbf{Z} = \{Z_i\}_{i=1}^m$ while the marginal distributions of the Z_i's are identical. In other words, we provide PAC-Bayes bounds for classifiers trained on *identically but not independently distributed data*. These results rely on properties of a dependency graph that is built according to the dependencies within $\mathbf{Z}$. Before stating our new bounds, we thus introduce the concepts of graph theory that will play a role in their statements.

2.2 Dependency Graph, Fractional Covers

Definition 1 (Dependency Graph)**.** Let $\mathbf{Z} = \{Z_i\}_{i=1}^m$ be a set of random variables taking values in some space $\mathcal{Z}$. The *dependency graph* $\Gamma(\mathbf{Z})$ of $\mathbf{Z}$ is such that: the set of vertices of $\Gamma(\mathbf{Z})$ is $\{1, \dots, m\}$ and there is an edge between i and j *if and only if* Z_i and Z_j are not independent (in the probabilistic sense).

Definition 2 (Fractional Covers, (Schreinerman & Ullman, 1997))**.** Let $\Gamma = (V, E)$ be an undirected graph, with $V = \{1, \dots, m\}$.

- $C \subseteq V$ is *independent* if the vertices in C are independent (no two vertices in C are connected).
- $\mathbf{C} = \{C_j\}_{j=1}^n$, with $C_j \subseteq V$, is a *proper cover* of V if each C_j is independent and $\bigcup_{j=1}^n C_j = V$. The size of $\mathbf{C}$ is n.
- $\mathbf{C} = \{(C_j, \omega_j)\}_{j=1}^n$, with $C_j \subseteq V$ and $\omega_j \in [0, 1]$, is a *proper exact fractional cover* of V if each C_j is independent and $\forall i \in V$, $\sum_{i=1}^n \omega_j \mathbb{I}_{i\in C_j} = 1$; $\omega(\mathbf{C}) = \sum_{j=1}^n w_i$ is the *chromatic weight* of $\mathbf{C}$.
- $\chi(\Gamma)$ ($\chi^*(\Gamma)$) is the minimum size (weight) over all proper exact (fractional) covers of Γ: it is the *(fractional) chromatic number* of Γ.

The problem of computing the (fractional) chromatic number of a graph is NP-hard (Schreinerman & Ullman, 1997). However, for some particular graphs as those that come from the settings we study in Section 4, this number can be evaluated precisely. The following property holds (Schreinerman & Ullman, 1997):

Property 1. *Let $\Gamma = (V, E)$ be a graph. Let $c(\Gamma)$ be the* clique number *of Γ, i.e. the order of the largest clique in Γ. Let $\Delta(\Gamma)$ be the maximum degree of a vertex in Γ. We have the following inequalities:*

$$1 \leq c(\Gamma) \leq \chi^*(\Gamma) \leq \chi(\Gamma) \leq \Delta(\Gamma) + 1.$$

In addition, $1 = c(\Gamma) = \chi^*(\Gamma) = \chi(\Gamma) = \Delta(\Gamma) + 1$ if and only if Γ is totally disconnected.

Remark 1. A cover can be thought of a fractional cover with every w_i equal to 1. Hence, all the results we state for fractional covers apply to the case of covers.

Remark 2. If $\mathbf{Z} = \{Z_i\}_{i=1}^m$ is a set of random variables over $\mathcal{Z}$ then a (fractional) proper cover of $\Gamma(\mathbf{Z})$, splits $\mathbf{Z}$ into subsets of independent random variables. This is a crucial feature to establish our results. In addition, we can see $\chi^*(\Gamma(\mathbf{Z}))$ and $\chi(\Gamma(\mathbf{Z}))$ as measures of the amount of dependencies within $\mathbf{Z}$.

The following lemma, also taken from (Janson, 2004), Lemma 3.1, will be very useful in the following.

Lemma 1. *If* $\mathbf{C} = \{(C_j, \omega_j)\}_{j=1}^n$ *is an exact fractional cover of* $\Gamma = (V, E)$*, with* $V = \{1, \ldots, m\}$*, then*

$$\forall \mathbf{t} \in \mathbb{R}^m, \ \sum_{i=1}^m t_i = \sum_{j=1}^n \omega_j \sum_{k \in C_j} t_k.$$

In particular $m = \sum_{j=1}^n |C_j|$.

2.3 Chromatic PAC-Bayes Bounds

We now provide new PAC-Bayes bounds for classifiers trained on samples $\mathbf{Z}$ drawn from distributions $\mathbf{D}_m$ where dependencies exist. We assume these dependencies are fully determined by $\mathbf{D}_m$ and we define the dependency graph $\Gamma(\mathbf{D}_m)$ of $\mathbf{D}_m$ to be $\Gamma(\mathbf{D}_m) = \Gamma(\mathbf{Z})$. As said before, the marginal distributions of $\mathbf{D}_m$ along each coordinate are equal to some distribution D.

We consider some additional notation. $\textsc{Pefc}(\mathbf{D}_m)$ is the set of proper exact fractional covers of $\Gamma(\mathbf{D}_m)$. Given a cover $\mathbf{C} = \{(C_j, \omega_j)\}_{j=1}^n \in \textsc{Pefc}(\mathbf{D}_m)$, $\mathbf{Z}^{(j)} = \{Z_k\}_{k \in C_j}$ and $\mathbf{D}_m^{(j)}$ is the distribution of $\mathbf{Z}^{(j)}$, it is therefore equal to $D^{|C_j|}$; $\boldsymbol{\alpha} \in \mathbb{R}^n$ is the vector of coefficients $\alpha_j = \omega_j / \omega(\mathbf{C})$ and $\boldsymbol{\pi} \in \mathbb{R}^n$ is the vector of coefficients $\pi_j = \omega_j |C_j| / m$. $\mathbf{P}_n$ and $\mathbf{Q}_n$ are distributions over $\mathcal{H}^n$, P_n^j and Q_n^j are the marginal distributions of $\mathbf{P}_n$ and $\mathbf{Q}_n$ with respect to the jth coordinate, respectively; $\mathbf{h} = (h_1, \ldots, h_n)$ is an element of $\mathcal{H}^n$.

We can now state our main results.

Theorem 2 (Chromatic PAC-Bayes Bound (I))**.** *$\forall m$, $\forall \mathbf{D}_m$, $\forall \mathcal{H}, \forall \delta \in (0, 1]$, $\forall \mathbf{C} = \{(C_j, \omega_j)\}_{j=1}^n \in \textsc{Pefc}(\mathbf{D}_m)$, $\forall \mathbf{P}_n$, with probability at least $1-\delta$ over the random draw of $\mathbf{Z} \sim \mathbf{D}_m$, the following holds: $\forall \mathbf{Q}_n$,*

$$kl(\bar{e}_{\mathbf{Q}_n} || e_{\mathbf{Q}_n}) \leq \frac{\omega}{m} \left[\sum_{j=1}^n \alpha_j KL(Q_n^j || P_n^j) + \ln \frac{m + \omega}{\delta \omega} \right], \quad (3)$$

where ω stands for $\omega(\mathbf{C})$ and $e_{\mathbf{Q}_n} = \mathbb{E}_{\mathbf{Z} \sim \mathbf{D}_m} \bar{e}_{\mathbf{Q}_n}$, with

$$\begin{aligned} \bar{e}_{\mathbf{Q}_n} &= \mathbb{E}_{\mathbf{h} \sim \mathbf{Q}_n} \frac{1}{m} \sum_{j=1}^n \omega_j \sum_{k \in C_j} r(h_j, Z_k) \\ &= \frac{1}{m} \sum_{j=1}^n \omega_j |C_j| \mathbb{E}_{h \sim Q_n^j} \frac{1}{|C_j|} \sum_{k \in C_j} r(h, Z_k) \\ &= \sum_{j=1}^n \pi_j \mathbb{E}_{h \sim Q_n^j} \hat{R}(h, \mathbf{Z}^{(j)}). \end{aligned}$$

The proof of this theorem is deferred to Section 3. The following proposition characterizes $\mathbb{E}_{\mathbf{Z} \sim \mathbf{D}_m} \bar{e}_{\mathbf{Q}_n}$.

Proposition 1. *$\forall m$, $\forall \mathbf{D}_m$, $\forall \mathcal{H}$, $\forall \mathbf{C} = \{(C_j, \omega_j)\}_{j=1}^n \in \textsc{Pefc}(\mathbf{D}_m)$, $\forall \mathbf{Q}_n$: $e_{\mathbf{Q}_n} = \mathbb{E}_{\mathbf{Z} \sim \mathbf{D}_m} \bar{e}_{\mathbf{Q}_n}$ is the error of the Gibbs classifier based on the mixture of distributions $Q^{\boldsymbol{\pi}} = \sum_{j=1}^n \pi_j Q_n^j$ over $\mathcal{H}$.*

Proof. From Definition 2, $\pi_j \geq 0$ and, according to Lemma 1, $\sum_{j=1}^n \pi_j = \frac{1}{m} \sum_{j=1}^n \omega_j |C_j| = 1$. Then,

$$\begin{aligned} \mathbb{E}_{\mathbf{Z} \sim \mathbf{D}_m} \bar{e}_{\mathbf{Q}_n} &= \sum_j \pi_j \mathbb{E}_{h \sim Q_j} \mathbb{E}_{\mathbf{Z} \sim \mathbf{D}_m} \hat{R}(h, \mathbf{Z}^{(j)}) \\ &= \sum_j \pi_j \mathbb{E}_{h \sim Q_j} \mathbb{E}_{\mathbf{Z}^{(j)} \sim \mathbf{D}_m^{(j)}} \hat{R}(h, \mathbf{Z}^{(j)}) \\ &= \sum_j \pi_j \mathbb{E}_{h \sim Q_n^j} R(h) \\ &= \mathbb{E}_{h \sim \pi_1 Q_n^1 + \ldots + \pi_j Q_n^j} R(h) = \mathbb{E}_{h \sim Q^{\boldsymbol{\pi}}} R(h). \end{aligned}$$

This closes the proof. □

Remark 3. The prior $\mathbf{P}_n$ and the posterior $\mathbf{Q}_n$ entering into play in Proposition 1 and Theorem 2 through their marginals only advocates for the following learning scheme. Given a cover and a (possibly factorized) prior $\mathbf{P}_n$, look for a factorized posterior $\mathbf{Q}_n = \otimes_{j=1}^n Q_j$ such that each Q_j independently minimizes the usual IID PAC-Bayes bound given in Theorem 1 on each $\mathbf{Z}^{(j)}$. Then make predictions according to the Gibbs classifier defined with respect to $Q^{\boldsymbol{\pi}} = \sum_j \pi_j Q_j$.

The following theorem gives a result that can be readily used without choosing a specific cover.

Theorem 3 (Chromatic PAC-Bayes Bound (II))**.** *$\forall m$, $\forall \mathbf{D}_m$, $\forall \mathcal{H}$, $\forall \delta \in (0, 1]$, $\forall P$, with probability at least $1-\delta$ over the random draw of $\mathbf{Z} \sim \mathbf{D}_m$, the following holds*

$$\forall Q, kl(\hat{e}_Q || e_Q) \leq \frac{\chi^*}{m} \left[KL(Q||P) + \ln \frac{m + \chi^*}{\delta \chi^*} \right], \quad (4)$$

where χ^* is the fractional chromatic number of $\Gamma(\mathbf{D}_m)$, and where $\hat{e}_Q$ and e_Q are defined as in (2).

Proof. This theorem is just a particular case of Theorem 2. Assume that $\mathbf{C} = \{(C_j, \omega_j)\}_{j=1}^n \in \textsc{Pefc}(\mathbf{D}_m)$ such that $\omega(C) = \chi^*(\Gamma(\mathbf{D}_m))$, $\mathbf{P}_n = \otimes_{j=1}^n P = P^n$ and $\mathbf{Q}_n = \otimes_{j=1}^n Q = Q^n$, for some P and Q.

For the right-hand side of (4), it directly comes that

$$\sum_j \alpha_j \mathrm{KL}(Q_n^j || P_n^j) = \sum_j \alpha_j \mathrm{KL}(Q||P) = \mathrm{KL}(Q||P).$$

It then suffices to show that $\bar{e}_{\mathbf{Q}_n} = \hat{e}_Q$:

$$\begin{aligned} \bar{e}_{\mathbf{Q}_n} &= \sum_j \pi_j \mathbb{E}_{h \sim Q_n^j} \hat{R}(h, \mathbf{Z}^{(j)}) = \sum_j \pi_j \mathbb{E}_{h \sim Q} \hat{R}(h, \mathbf{Z}^{(j)}) \\ &= \frac{1}{m} \sum_j \omega_j |C_j| \mathbb{E}_{h \sim Q} \frac{1}{|C_j|} \sum_k r(h, Z_k) \\ &= \mathbb{E}_{h \sim Q} \frac{1}{m} \sum_j \omega_j \sum_k r(h, Z_k) \\ &= \mathbb{E}_{h \sim Q} \frac{1}{m} \sum_i r(h, Z_i) = \mathbb{E}_{h \sim Q} \hat{R}(h, \mathbf{Z}) = \hat{e}_Q. \end{aligned}$$

□

Remark 4. This theorem says that even in the case of non IID data, a PAC-Bayes bound very similar to the IID PAC-Bayes bound (1) can be stated, with a worsening (since $\chi^* \geq 1$) proportional to χ^*, i.e proportional to the amount of dependencies in the data. In addition, the new PAC-Bayes bounds is valid with any priors and posteriors, without the need for these distributions nor their marginals to depend on the chosen cover (as is the case with the more general Theorem 2).

Remark 5. We note that among all elements of $\text{PEFC}(\mathbf{D}_m)$, χ^* is the best constant achievable in terms of the tightness of the bound. Indeed, the function $f_{m,\delta}(\omega) = \omega \ln \frac{m+\omega}{\delta\omega}$ is nondecreasing for all $m \in \mathbb{N}$ and $\delta \in (0,1]$, as indicated by the sign of $f'_{m,\delta} = \frac{df_{m,\delta}}{d\omega}$:

$$\begin{aligned} f'_{m,\delta}(\omega) &= -\ln \frac{\delta\omega}{m+\omega} + \frac{\omega}{m+\omega} - 1 \\ &\geq -\ln \frac{\omega}{m+\omega} + \frac{\omega}{m+\omega} - 1 \\ &\geq -\frac{\omega}{m+\omega} + 1 + \frac{\omega}{m+\omega} - 1 = 0 \end{aligned}$$

where we have used $\ln x \leq x - 1$. As χ^* is the smallest chromatic weight, it gives the tightest bound.

3 Proof of Theorem 2

A proof in three steps, following the lines of the proofs given in (Seeger, 2002) and (Langford, 2005) for the IID PAC-Bayes bound, can be provided for Theorem 2.

Lemma 2. *$\forall m$, $\forall \mathbf{D}_m$, $\forall \delta \in (0,1]$, $\forall \mathbf{C} = \{(C_j, \omega_j)\}_{j=1}^n$, $\forall \mathbf{P}_n$, with probability at least $1-\delta$ over the random draw of $\mathbf{Z} \sim \mathbf{D}_m$, the following holds*

$$\mathbb{E}_{\mathbf{h}\sim\mathbf{P}_n} \sum_{j=1}^n \alpha_j e^{|C_j| kl(\hat{R}(h_j, \mathbf{Z}^{(j)})||R(h_j))} \leq \frac{m+\omega}{\delta\omega}, \quad (5)$$

where ω stands for $\omega(\mathbf{C})$.

Proof. We first observe the following:

$$\begin{aligned} &\mathbb{E}_{\mathbf{Z}\sim\mathbf{D}_m} \sum_j \alpha_j e^{|C_j| \text{kl}(\hat{R}(h_j, \mathbf{Z}^{(j)})||R(h_j))} \\ &= \sum_j \alpha_j \mathbb{E}_{\mathbf{Z}^{(j)}\sim\mathbf{D}_m^{(j)}} e^{|C_j| \text{kl}(\hat{R}(h, \mathbf{Z}^{(j)})||R(h))} \\ &\leq \sum_j \alpha_j (|C_j| + 1) \qquad \text{(Lemma 5, Appendix)} \\ &= \frac{1}{\omega} \sum_j \omega_j (|C_j| + 1) = \frac{m+\omega}{\omega}, \end{aligned}$$

where using Lemma 5 is made possible by the fact that $\mathbf{Z}^{(j)}$ are IID. Therefore,

$$\mathbb{E}_{\mathbf{Z}\sim\mathbf{D}_m} \mathbb{E}_{\mathbf{h}\sim\mathbf{P}_n} \sum_{j=1}^n \alpha_j e^{|C_j| \text{kl}(\hat{R}(h_j, \mathbf{Z}^{(j)})||R(h_j))} \leq \frac{m+\omega}{\omega}.$$

Applying Markov's inequality (Theorem 7, Appendix) to $\mathbb{E}_{\mathbf{h}\sim\mathbf{P}_n} \sum_j \alpha_j e^{|C_j| \text{kl}(\hat{R}(h_j, \mathbf{Z}^{(j)})||R(h_j))}$ gives the desired result. □

Lemma 3. *$\forall m$, $\forall \mathbf{D}_m$, $\forall \mathbf{C} = \{(C_j, \omega_j)\}_{j=1}^n$, $\forall \mathbf{P}_n$, $\forall \mathbf{Q}_n$, with probability at least $1-\delta$ over the random draw of $\mathbf{Z} \sim \mathbf{D}_m$, the following holds*

$$\begin{aligned} &\frac{m}{\omega} \sum_{j=1}^n \pi_j \mathbb{E}_{h\sim Q_n^j} kl(\hat{R}(h, \mathbf{Z}^{(j)})||R(h)) \quad (6) \\ &\qquad \leq \sum_{j=1}^n \alpha_j KL(Q_n^j||P_n^j) + \ln \frac{m+\omega}{\delta\omega}. \end{aligned}$$

Proof. It suffices to use Jensen's inequality with ln and the fact that $\mathbb{E}_{X\sim P} f(X) = \mathbb{E}_{X\sim Q} \frac{P(X)}{Q(X)} f(X)$, for all f, P, Q. Therefore, $\forall \mathbf{Q}_n$:

$$\begin{aligned} &\ln \mathbb{E}_{\mathbf{h}\sim\mathbf{P}_n} \sum_j \alpha_j e^{|C_j| \text{kl}\left(\hat{R}(h_j, \mathbf{Z}^{(j)})||R(h_j)\right)} \\ &= \ln \sum_j \alpha_j \mathbb{E}_{h\sim P_n^j} e^{|C_j| \text{kl}\left(\hat{R}(h, \mathbf{Z}^{(j)})||R(h)\right)} \\ &= \ln \sum_j \alpha_j \mathbb{E}_{h\sim Q_n^j} \frac{P_n^j(h)}{Q_n^j(h)} e^{|C_j| \text{kl}\left(\hat{R}(h, \mathbf{Z}^{(j)})||R(h)\right)} \\ &\geq \sum_j \alpha_j \mathbb{E}_{h\sim Q_n^j} \ln \left[\frac{P_n^j(h)}{Q_n^j(h)} e^{|C_j| \text{kl}\left(\hat{R}(h, \mathbf{Z}^{(j)})||R(h)\right)} \right] \\ &= -\sum_j \alpha_j \text{KL}(Q_n^j||P_n^j) \\ &\qquad + \sum_j \alpha_j |C_j| \mathbb{E}_{h\sim Q_n^j} \text{kl}\left(\hat{R}(h, \mathbf{Z}^{(j)})||R(h)\right) \\ &= -\sum_j \alpha_j \text{KL}(Q_n^j||P_n^j) \\ &\qquad + \frac{m}{\omega} \sum_j \pi_j \mathbb{E}_{h\sim Q_n^j} \text{kl}\left(\hat{R}(h, \mathbf{Z}^{(j)})||R(h)\right). \end{aligned}$$

Lemma 2 then gives the result. □

Lemma 4. *$\forall m$, $\forall \mathbf{D}_m$, $\forall \mathbf{C} = \{(C_j, \omega_j)\}_{j=1}^n$, $\forall \mathbf{Q}_n$,, the following holds*

$$\frac{m}{\omega} \sum_{j=1}^n \pi_j \mathbb{E}_{h\sim Q_n^j} kl(\hat{R}(h, \mathbf{Z}^{(j)})||R(h)) \geq kl(\bar{e}_Q||e_Q).$$

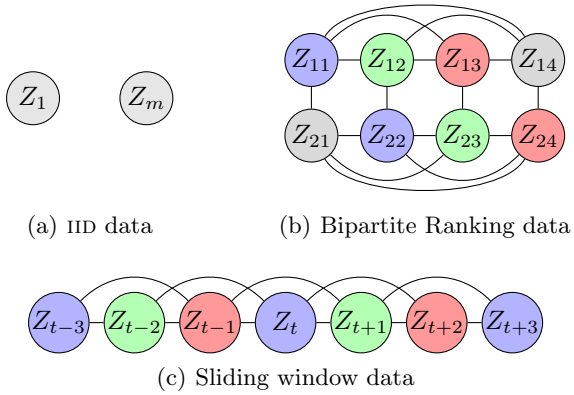
Proof. This simply comes from the application of Theorem 6 given in Appendix. This lemma, in combination with Lemma 3, closes the proof of Theorem 2. □

4 Examples

We give instances of Theorem 3 for various settings.

4.1 IID case

In this case, the training sample $\mathbf{Z} = \{(X_i, Y_i)\}_{i=1}^m$ is distributed according to $\mathbf{D}_m = D^m$ and the fractional chromatic number of $\Gamma(\mathbf{D}_m)$ is $\chi^* = 1$. Plugging in this value of χ^* in the bound of Theorem 3 gives the IID



(a) IID data (b) Bipartite Ranking data

(c) Sliding window data

Figure 1: Dependency graphs for the different settings described in section 4. Nodes of the same color are part of the same cover element; henceforth, they are independent. (a) When the data are IID , the dependency graph is disconnected and the fractional number is $\chi^* = 1$; (b) a dependency graph obtained for bipartite ranking from a sample containing 4 positive instances and 2 negative instances: $\chi^* = 4$; (c) a dependency graph obtained with the technique of sliding windows for sequence data, for a window parameter $r = 1$ (see text for details): $\chi^* = 2r + 1$.

PAC-Bayes bound of Theorem 1. This emphasizes the fact that the standard PAC-Bayes bound is a special case of our more general results.

4.2 Bipartite Ranking

Let $\overline{D}$ be a distribution over $\overline{\mathcal{X}} \times \overline{\mathcal{Y}}$ and $\overline{D}_{+1}$ ($\overline{D}_{-1}$) be the class conditional distribution $\overline{D}_{X|Y=+1}$ ($\overline{D}_{X|Y=-1}$) with respect to $\overline{D}$. In the bipartite ranking problem (see, e.g. (Agarwal et al., 2005)), one tries to control the misranking risk, defined for $f \in \mathbb{R}^{\mathcal{X}}$ by

$$R^{\text{rank}}(f) = \mathbb{P}_{\substack{\overline{X}^+ \sim \overline{D}_{+1} \\ \overline{X}^- \sim \overline{D}_{-1}}} \left(f(\overline{X}^+) \leq f(\overline{X}^-)\right). \quad (7)$$

f can be interpreted as a scoring function. Given an IID sample $\mathbf{S} = \{(\overline{X}_i, \overline{Y}_i)\}_{i=1}^{\ell}$ distributed according to $\overline{\mathbf{D}}_\ell = \overline{D}^\ell$, a usual strategy to minimize (7) is to minimize (a possibly regularized form of)

$$\hat{R}^{\text{rank}}(f, \mathbf{S}) = \frac{1}{\ell^+ \ell^-} \sum_{\substack{i:\overline{Y}_i=+1 \\ j:\overline{Y}_j=-1}} r(f, (\overline{X}_i, \overline{X}_j)), \quad (8)$$

where $r(f, (\overline{X}_i, \overline{X}_j)) = \mathbb{I}_{f(\overline{X}_i) \leq f(\overline{X}_j)}$ and ℓ^+ (ℓ^-) is the number of positive (negative) data in $\mathbf{S}$. This empirical risk, closely related to the Area under the ROC curve, or AUC[1] (Agarwal et al., 2005; Cortes & Mohri, 2004), estimates the fraction of pairs $(\overline{X}_i, \overline{X}_j)$ that are ranked incorrectly (given that $\overline{Y}_i = +1$ and $\overline{Y}_j = -1$) and is an unbiased estimator of $R^{\text{rank}}(h)$. The entailed problem can be seen as that of learning a classifier from the training set $\mathbf{Z} = \{Z_{ij}\}_{ij} = \{(X_{ij} = (\overline{X}_i, \overline{X}_j), 1)\}_{ij}$. This reveals the non-IID nature of the data, as Z_{ij} depends on $\{Z_{pq} : p = i \text{ or } q = j\}$ (see Figure 1).

[1] It is actually 1-AUC.

Using Theorem 3, we have the following result:

Theorem 4. *$\forall \ell$, $\forall \overline{D}$ over $\overline{\mathcal{X}} \times \overline{\mathcal{Y}}$, $\forall \overline{\mathcal{H}} \subseteq \mathbb{R}^{\overline{\mathcal{X}}}$, $\forall \delta \in (0, 1]$, $\forall \overline{P}$ over $\overline{\mathcal{H}}$, with probability at least $1 - \delta$ over the random draw of $\mathbf{S} \sim \overline{D}^\ell$, the following holds*

$$\forall \overline{Q} \text{ over } \overline{\mathcal{H}}, kl(\hat{e}^{rank}_{\overline{Q}} || e^{rank}_{\overline{Q}}) \leq \frac{1}{\ell_{\min}} \left[KL(\overline{Q}||\overline{P}) + \ln \frac{\ell_{\min} + 1}{\delta} \right], \quad (9)$$

where $\ell_{\min} = \min(\ell^+, \ell^-)$, and $\hat{e}^{rank}_{\overline{Q}}$ and $e^{rank}_{\overline{Q}}$ are the Gibbs ranking error counterparts of (2) based on (7) and (8), respectively.

Proof. The proof works in three parts and borrows ideas from (Agarwal et al., 2005). The first two parts are necessary to deal with the fact that the dependency graph of $\mathbf{Z}$, as implied by $\mathbf{S}$, does not have a deterministic structure.

Conditioning on $\mathbf{Y} = \mathbf{y}$. Let $\mathbf{y} \in \{-1, +1\}^\ell$ be a fixed vector and $\ell^+_{\mathbf{y}}$ and $\ell^-_{\mathbf{y}}$ the number of positive and negative labels, respectively. We define the distribution $\overline{\mathbf{D}}_{\mathbf{y}}$ as $\overline{\mathbf{D}}_{\mathbf{y}} = \otimes_{i=1}^{\ell} \overline{D}_{y_i}$; this is a distribution on $\overline{\mathcal{X}}^\ell$. With a slight abuse of notation, $\overline{\mathbf{D}}_{\mathbf{y}}$ will also be used to denote the distribution over $(\overline{\mathcal{X}} \times \overline{\mathcal{Y}})^\ell$ of samples $\mathbf{S} = \{(\overline{X}_i, y_i)\}_{i=1}^{\ell}$ such that the sequence $\{\overline{X}_i\}_{i=1}^{\ell}$ is distributed according to $\overline{\mathbf{D}}_{\mathbf{y}}$. It is easy to check that $\forall f \in \overline{\mathcal{H}}$, $\mathbb{E}_{\mathbf{S} \sim \overline{\mathbf{D}}_{\mathbf{y}}} \hat{R}^{\text{rank}}(f, \mathbf{S}) = R^{\text{rank}}(f)$ (cf. (7)).

Given $\mathbf{S}$, defining the random variable Z_{ij} as $Z_{ij} = ((X_i, X_j), 1)$, $\mathbf{Z} = \{Z_{ij}\}_{i:y_i=1, j:y_j=-1}$ is a sample of identically distributed variables, each with distribution $D_{\pm 1} = \overline{D}_{+1} \otimes \overline{D}_{-1} \otimes \mathbf{1}$ over $\mathcal{X} \times \mathcal{Y}$, where $\mathcal{X} = \overline{\mathcal{X}} \times \overline{\mathcal{X}}$, $\mathcal{Y} = \{-1, +1\}$ and $\mathbf{1}$ is the distribution that produces 1 with probability 1.

Letting $m = \ell^+_{\mathbf{y}} \ell^-_{\mathbf{y}}$ we denote by $\mathbf{D}_{\mathbf{y},m}$ the distribution of the training sample $\mathbf{Z}$, within which interdependencies exist (see Figure 1). Theorem 2 can thus be directly applied to classifiers trained on $\mathbf{Z}$, the structure of $\Gamma(\mathbf{D}_{\mathbf{y},m})$ and its corresponding fractional chromatic number $\chi^*_{\mathbf{y}}$ being completely determined by $\mathbf{y}$. Letting $\mathcal{H} \subseteq \mathcal{Y}^{\mathcal{X}}$, $\forall \delta \in (0, 1]$, $\forall P$ over $\mathcal{H}$, with probability at least $1 - \delta$ over the random draw of $\mathbf{Z} \sim \mathbf{D}_{\mathbf{y},m}$,

$$\forall Q \text{ over } \mathcal{H}, \text{kl}(\hat{e}_Q || e_Q) \leq \frac{\chi^*_{\mathbf{y}}}{m} \left[\text{KL}(Q||P) + \ln \frac{m + \chi^*_{\mathbf{y}}}{\delta \chi^*_{\mathbf{y}}} \right].$$

Given $f \in \overline{\mathcal{H}}$, it is obvious that for $h_f \in \mathcal{Y}^{\mathcal{X}}$ defined as $h_f((X, X')) = \text{sign}(f(X) - f(X'))$, with $\text{sign}(x) = +1$

if $x > 0$ and -1 otherwise, $\hat{R}(h_f, \mathbf{Z}) = \hat{R}^{\text{rank}}(f, \mathbf{S})$ and $\mathbb{E}_{\mathbf{Z}\sim\mathbf{D}_{\mathbf{y},m}} \hat{R}(h_f, \mathbf{Z}) = \mathbb{E}_{\mathbf{S}\sim\overline{\mathbf{D}}_{\mathbf{y}}} \hat{R}^{\text{rank}}(f, \mathbf{S}) = R^{\text{rank}}(f)$. Hence, $\forall \delta \in (0, 1]$, $\forall \overline{P}$ over $\overline{\mathcal{H}}$, with probability at least $1 - \delta$ over the random draw of $\mathbf{S} \sim \overline{\mathbf{D}}_{\mathbf{y}}$,

$$\forall \overline{Q}, \text{kl}(\hat{e}^{\text{rank}}_{\overline{Q}} || e^{\text{rank}}_{\overline{Q}}) \leq \frac{\chi^*_{\mathbf{y}}}{m} \left[\text{KL}(\overline{Q}||\overline{P}) + \ln \frac{m + \chi^*_{\mathbf{y}}}{\delta \chi^*_{\mathbf{y}}} \right]. \quad (10)$$

Integrating over Y. As proposed in (Agarwal et al., 2005), let us call $\Phi(\overline{P}, \mathbf{S}, \delta)$ the event (10); we just stated that $\forall \mathbf{y} \in \{-1, +1\}^{\ell}$, $\forall \overline{P}$, $\forall \delta \in (0, 1]$, $\mathbb{P}_{\mathbf{S}\sim\overline{\mathbf{D}}_{\mathbf{y}}}(\Phi(\overline{P}, \mathbf{S}, \delta)) \geq 1 - \delta$. Then, $\forall \overline{P}, \forall \delta \in (0, 1]$,

$$\begin{aligned}
\mathbb{P}_{\mathbf{S}\sim\overline{\mathbf{D}}_{\ell}}(\Phi(\overline{P}, \mathbf{S}, \delta)) &= \mathbb{E}_{\mathbf{Y}}[\mathbb{E}_{\mathbf{S}\sim\overline{\mathbf{D}}_{\mathbf{Y}}} \mathbb{I}_{\Phi(\overline{P}, \mathbf{S}, \delta)}] \\
&= \sum_{\mathbf{y}} \mathbb{E}_{\mathbf{S}\sim\overline{\mathbf{D}}_{\mathbf{y}}} \mathbb{I}_{\Phi(\overline{P}, \mathbf{S}, \delta)} \mathbb{P}(\mathbf{Y} = \mathbf{y}) \\
&= \sum_{\mathbf{y}} \mathbb{P}_{\mathbf{S}\sim\overline{\mathbf{D}}_{\mathbf{y}}}(\Phi(\overline{P}, \mathbf{S}, \delta)) \mathbb{P}(\mathbf{Y} = \mathbf{y}) \\
&\geq \sum_{\mathbf{y}} (1 - \delta) \mathbb{P}(\mathbf{Y} = \mathbf{y}) = 1 - \delta.
\end{aligned}$$

Hence, $\forall \delta \in (0, 1]$, $\forall \overline{P}$ over $\overline{\mathcal{H}}$, with probability at least $1 - \delta$ over the random draw of $\mathbf{S} \sim \overline{\mathbf{D}}_{\ell}$,

$$\forall \overline{Q}, \text{kl}(\hat{e}^{\text{rank}}_{\overline{Q}} || e^{\text{rank}}_{\overline{Q}}) \leq \frac{\chi^*_{\mathbf{S}}}{m_{\mathbf{S}}} \left[\text{KL}(\overline{Q}||\overline{P}) + \ln \frac{m_{\mathbf{S}} + \chi^*_{\mathbf{S}}}{\delta \chi^*_{\mathbf{S}}} \right]. \quad (11)$$

where $\chi^*_{\mathbf{S}}$ is the fractional chromatic number of the graph $\Gamma(\mathbf{Z})$, with $\mathbf{Z}$ defined from $\mathbf{S}$ as in the first part of the proof (taking into account the observed labels in $\mathbf{S}$); here $m_{\mathbf{S}} = \ell^+ \ell^-$, where ℓ^+ (ℓ^-) is the number of positive (negative) data in $\mathbf{S}$.

Computing the Fractional Chromatic Number. In order to finish the proof, it suffices to observe that, for $\mathbf{Z} = \{Z_{ij}\}_{ij}$, letting $\ell_{\max} = \max(\ell^+, \ell^-)$, the fractional chromatic number of $\Gamma(\mathbf{Z})$ is $\chi^* = \ell_{\max}$.

Indeed, the clique number of $\Gamma(\mathbf{Z})$ is $\ell_{\max}$ as for all $i = 1, \ldots, \ell^+$ ($j = 1, \ldots, \ell^-$), $\{Z_{ij} : j = 1, \ldots, \ell^-\}$ ($\{Z_{ij} : i = 1, \ldots, \ell^+\}$) defines a clique of order ℓ^- (ℓ^+) in $\Gamma(\mathbf{Z})$. Thus, from Property 1: $\chi \geq \chi^* \geq \ell_{\max}$.

A proper exact cover $\mathbf{C} = \{C_k\}_{k=1}^{\ell_{\max}}$ of $\Gamma(\mathbf{Z})$ can be constructed as follows[2]. Suppose that $\ell_{\max} = \ell^+$, then $C_k = \{Z_{i\sigma_k(i)} : i = 1, \ldots, \ell^-\}$, with

$$\sigma_k(i) = (i + k - 2 \mod \ell^+) + 1,$$

is an independent set: no two variables Z_{ij} and Z_{pq} in C_k are such that $i = p$ or $j = q$. In addition, it is straightforward to check that $\mathbf{C}$ is indeed a cover of $\Gamma(\mathbf{Z})$. This cover is of size $\ell^+ = \ell_{\max}$, which means that it achieves the minimal possible weight over proper exact (fractional) covers since $\chi^* \geq \ell_{\max}$. Hence, $\chi^* = \chi = \ell_{\max} (= c(\Gamma))$. Plugging in this value of χ^* in (11), and noting that $m_{\mathbf{S}} = \ell_{\max} \ell_{\min}$ with $\ell_{\min} = \min(\ell^+, \ell^-)$, closes the proof. □

[2]Note that the cover defined here considers elements C_k containing random variables themselves instead of their indices. This abuse of notation is made for sake of readability.

As proposed by (Langford, 2005), the PAC-Bayes bound of Theorem 4 can be specialized to the case where $\overline{\mathcal{H}} = \{\overline{f} : f(x) = w \cdot x, w \in \overline{\mathcal{X}}\}$. In this situation, for $f \in \overline{\mathcal{H}}$, $h_f((X, X')) = \text{sign}(f(X) - f(X')) = \text{sign}(w \cdot (X - X'))$ is simply a linear classifier (next result therefore carries over to kernel classifiers). Hence, assuming an isotropic Gaussian prior $P = \mathcal{N}(0, I)$ and a family of posteriors $Q_{w,\mu}$ parameterized by $w \in \overline{\mathcal{X}}$ and $\mu > 0$ such that $Q_{w,\mu}$ is $\mathcal{N}(\mu, 1)$ in the direction w and $\mathcal{N}(0, 1)$ in all perpendicular directions, we arrive at the following theorem (of which we omit the proof):

Theorem 5. *$\forall \ell, \forall \overline{D}$ over $\overline{\mathcal{X}} \times \overline{\mathcal{Y}}$, $\forall \delta \in (0, 1]$, the following holds with prob. at least $1 - \delta$ over the draw of $\mathbf{S} \sim \overline{D}^{\ell}$:*

$$\forall w, \mu > 0, kl(\hat{R}^{rank}_{Q_{w,\mu}} || R^{rank}_{Q_{w,\mu}}) \leq \frac{1}{\ell_{\min}} \left[\frac{\mu^2}{2} + \ln \frac{\ell_{\min} + 1}{\delta} \right].$$

The bounds given in Theorem 4 and Theorem 5 are very similar to what we would get if applying IID PAC-Bayes bound to one (independent) element C_j of a minimal cover (i.e. its weight equals the fractional chromatic number) $\mathbf{C} = \{C_j\}_{j=1}^n$ such as the one we used in the proof of Theorem 4. This would imply the empirical error $\hat{e}^{\text{rank}}_{\overline{Q}}$ to be computed on only one specific C_j and not all the C_j's simultaneously, as is the case for the new results. It turns out that, for proper exact fractional covers $\mathbf{C} = \{(C_j, \omega)\}_{j=1}^n$ with elements C_j having the same size, it is better, in terms of absolute moments of the empirical error, to assess it on the whole dataset, rather than on only one C_j. The following proposition formalizes this.

Proposition 2. *$\forall m$, $\forall \mathbf{D}_m$, $\forall \mathcal{H}$, $\forall \mathbf{C} = \{(C_j, \omega_j\}_{j=1}^n \in \text{PEFC}(\mathbf{D}_m)$, $\forall Q$, $\forall r \in \mathbb{N}, r \geq 1$, if $|C_1| = \ldots = |C_n|$ then*

$$\mathbb{E}_{\mathbf{Z}\sim\mathbf{D}_m} |\hat{e}_Q - e_Q|^r \leq \mathbb{E}_{\mathbf{Z}^{(j)}\sim\mathbf{D}_m^{(j)}} |\hat{e}^{(j)}_Q - e_Q|^r, \forall j \in \{1, \ldots n\},$$

where $\hat{e}^{(j)}_Q = \mathbb{E}_{h\sim Q} \hat{R}(h, \mathbf{Z}^{(j)})$.

Proof. Using the convexity of $|\cdot|^r$ for $r \geq 1$, the linearity of $\mathbb{E}$ and the notation of section 2, for $\mathbf{Z} \sim \mathbf{D}_m$:

$$\begin{aligned}
|\hat{e}_Q - e_Q|^r &= |\sum_j \pi_j \mathbb{E}_{h\sim Q}(\hat{R}(h, \mathbf{Z}^{(j)}) - R(h))|^r \\
&\leq \sum_j \pi_j |\mathbb{E}_{h\sim Q}(\hat{R}(h, \mathbf{Z}^{(j)}) - R(h))|^r \\
&= \sum_j \pi_j |\hat{e}^{(j)}_Q - e_Q|^r.
\end{aligned}$$

Taking the expectation of both sides with respect to $\mathbf{Z}$ and noting that the random variables $|\hat{e}_Q^{(j)} - e_Q|^r$, have the same distribution, gives the result. □

4.3 Sliding Windows for Sequence Data

There are many situations, such as in bioinformatics, where a classifier must be learned from a training sample $\mathbf{S} = \{(\overline{X}_t, \overline{Y}_t)\}_{t=1}^T \in (\overline{\mathcal{X}} \times \overline{\mathcal{Y}})^T$ where it is known that there is a sequential dependence between the X_t's. A typical approach to tackle the problem of learning from such data is the following: in order to predict $\overline{Y}_t$, information from a *window* $\{\overline{X}_{t+\tau}\}_{\tau=-r}^r$ of $2r+1$ data centered on $\overline{X}_t$ is considered, r being set according to some prior knowledge or after a cross-validation process. This problem can be cast in another classification problem using a training sample $\mathbf{Z} = \{Z_t\}_{t=1}^T$, with $Z_t = ((\overline{X}_{t-r}, \ldots, \overline{X}_t, \ldots, \overline{X}_{t+r}), \overline{Y}_t)$, with special care taken for $t \leq r+1$ and $t > T-r$. Considering that $\overline{\mathcal{Y}} = \{-1, +1\}$, the input space and output space to be considered are therefore $\mathcal{X} = \overline{\mathcal{X}}^{2r+1}$ and $\mathcal{Y} = \overline{\mathcal{Y}}$; the product space is $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$. As with the bipartite ranking problem, we end up with a learning problem from non-IID data, $\mathbf{Z}$ having a dependency graph $\Gamma(\mathbf{Z})$ as the one depicted on Figure 1.

It is easy to see that the clique number of $\Gamma(\mathbf{Z})$ is $2r+1$. Besides, one can construct a proper exact cover $\mathbf{C} = \{C_j\}_{j=1}^{2r+1}$ of minimal size/weight by taking $C_j = \{Z_{j+p(2r+1)} : p = 0, \ldots, \lfloor \frac{T-j}{2r+1} \rfloor\}$, for $j = 1, \ldots, 2r+1$ – we make the implicit and reasonable assumption that $T > 2r+1$. This cover is proper and has size $2r+1$. Invoking Property 1 gives that $\chi = \chi^* = 2r+1$.

It is therefore easy to get a new PAC-Bayes theorem for the case of windowed prediction, by replacing χ^* by $2r+1$ and m by T in the bound (4) of Theorem 3. We do not state it explicitly for sake of conciseness.

5 Conclusion

In this work, we propose the first PAC-Bayes bounds applying for classifiers trained on non-IID data. The derivation of these results rely on the use of fractional covers of graphs, convexity and standard tools from probability theory. The results that we provide are very general and can easily be instantiated for specific learning settings such as bipartite ranking and windowed prediction for sequence data.

This work gives rise to many interesting questions. First, it seems that using a fractional cover to decompose the non-IID training data into sets of IID data and then tightening the bound through the use of the chromatic number is some form of variational relaxation as often encountered in the context of inference in graphical models, the graphical model under consideration in this work being one that encodes the dependencies in $\mathbf{D}_m$. It might be interesting to make this connection clearer to see if, for instance, tighter and still general bounds can be obtained with more appropriate variational relaxations than the one incurred by the use of fractional covers.

Besides, Theorem 2 advocates for the learning algorithm described in Remark 3. We would like to see how such a learning algorithm based on possibly multiple priors/multiple posteriors could perform empirically and how tight the proposed bound could be.

On another empirical side, we are planning to run intensive numerical simulations on bipartite ranking problems to see how accurate the bound of Theorem 5 can be: we expect the results to be of good quality, because of the resemblance of the bound of the theorem with the IID PAC-Bayes theorem for margin classifiers, which has proven to be rather accurate (Langford, 2005). Likewise, it would be interesting to see how the possibly more accurate PAC-Bayes bound for large margin classifiers proposed by (Langford & Shawe-taylor, 2002), which should translate to the case of bipartite ranking as well, performs empirically.

The question remains as to what kind of strategies to learn the prior(s) could be used to render the bound of Theorem 2 the tightest possible. This is one of the most stimulating question as performing such prior learning makes it possible to obtain very accurate generalization bound (Ambroladze et al., 2007).

Finally, assuming the data are identically distributed might be too strong an assumption. This brings up the question on whether it is possible to derive the same kind of results as those provided here in the case where the variables do not have the same marginals: we have recently obtained a positive answer on deriving such a bound (Ralaivola, 2009), by directly leveraging a concentration inequality given in (Janson, 2004). We are also currently investigating how PAC-Bayes bounds could be derived for a different setting that gives rise to non-IID data, namely mixing processes.

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Appendix

Lemma 5. *Let D be a distribution over $\mathcal{Z}$.*

$$\forall h \in \mathcal{H}, \mathbb{E}_{\mathbf{Z} \sim D^m} e^{mkl\left(\hat{R}(h,\mathbf{Z}) || R(h)\right)} \leq m+1.$$

Proof. Let $h \in \mathcal{H}$. For $\mathbf{z} \in \mathcal{Z}^m$, we let $q(\mathbf{z}) = \hat{R}(h, \mathbf{z})$; we also let $p = R(h)$. Note that since $\mathbf{Z}$ is i.i.d, $mq(\mathbf{Z})$ is binomial with parameters m and p (recall that $r(h, Z)$ takes the values 0 and 1 upon correct and erroneous classification of Z by h, respectively).

$$\begin{aligned}
&\mathbb{E}_{\mathbf{Z}\sim D^m} e^{m\mathrm{kl}(q(\mathbf{Z})||p)} \\
&\quad = \sum_{\mathbf{z}\in\mathcal{Z}^m} e^{m\mathrm{kl}(q(\mathbf{z})||p)} \mathbb{P}_{\mathbf{Z}\sim D^m}(\mathbf{Z} = \mathbf{z}) \\
&\quad = \sum_{0\le k\le m} e^{m\mathrm{kl}\left(\frac{k}{m}||p\right)} \mathbb{P}_{\mathbf{Z}\sim D^m}(mq(\mathbf{Z}) = k) \\
&\quad = \sum_{0\le k\le m} \binom{m}{k} e^{m\mathrm{kl}\left(\frac{k}{m}||p\right)} p^k (1-p)^{m-k} \\
&\quad = \sum_{0\le k\le m} \binom{m}{k} e^{m\left(\frac{k}{m}\ln\frac{k}{m} + (1-\frac{k}{m})\ln(1-\frac{k}{m})\right)} \\
&\quad = \sum_{0\le k\le m} \binom{m}{k} \left(\frac{k}{m}\right)^k \left(1-\frac{k}{m}\right)^{m-k}.
\end{aligned}$$

However, it is obvious that, from the definition of the binomial distribution,

$$\forall m \in \mathbb{N}, \forall k \in [0, m], \forall t \in [0, 1], \binom{m}{k} t^k (1-t)^{m-k} \le 1.$$

This is obviously the case for $t = \frac{k}{m}$, which gives

$$\sum_{0\le k\le m} \binom{m}{k} \left(\frac{k}{m}\right)^k \left(1-\frac{k}{m}\right)^{m-k} \le \sum_{0\le k\le m} 1 = m + 1.$$

□

Theorem 6 (Jensen's inequality)**.** *Let $f \in \mathbb{R}^{\mathcal{X}}$ be a convex function. For all probability distribution P on $\mathcal{X}$:*

$$f(\mathbb{E}_{X\sim P} X) \le \mathbb{E}_{X\sim P} f(X).$$

Proof. Directly comes by induction on the definition of a convex function. □

Theorem 7 (Markov's Inequality)**.** *Let X be a positive random variable on $\mathbb{R}$, such that $\mathbb{E}X < \infty$.*

$$\forall t \in \mathbb{R}, \mathbb{P}_X\left\{X \ge \frac{\mathbb{E}X}{t}\right\} \le \frac{1}{t}.$$

Consequently: $\forall M \ge \mathbb{E}X, \forall t \in \mathbb{R}, \mathbb{P}_X\left\{X \ge \frac{M}{t}\right\} \le \frac{1}{t}$.

Proof. In almost all textbooks on probability. □

Lemma 6. $\forall p, q, r, s \in [0, 1], \forall \alpha \in [0, 1]$,

$$\begin{aligned}
&kl(\alpha p + (1-\alpha)q||\alpha r + (1-\alpha)s) \\
&\qquad \le \alpha kl(p||r) + (1-\alpha) kl(q||s).
\end{aligned}$$

Proof. It suffices to see that $f \in \mathbb{R}^{[0,1]^2}$, $f(\mathbf{v} = [p\ q]) = \mathrm{kl}(q||p)$ is convex over $[0, 1]^2$: the Hessian H of f is

$$H = \begin{bmatrix} \frac{q}{p^2} + \frac{1-q}{(1-p)^2} & -\frac{1}{p} - \frac{1}{1-p} \\ -\frac{1}{p} - \frac{1}{1-p} & \frac{1}{q} + \frac{1}{1-q} \end{bmatrix},$$

and, for $p, q \in [0, 1]$, $\frac{q}{p^2} + \frac{1-q}{(1-p)^2} \ge 0$ and $\det H = \frac{(p-q)^2}{q(1-q)p^2(1-p)^2} \ge 0$: $H \succeq 0$ and f is indeed convex. □

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