On the Properties of Variational Approximations of Gibbs Posteriors

Pierre Alquier, James Ridgway & Nicolas Chopin
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Pierre Alquier (CREST-ENSAE),
James Ridgway (CREST-ENSAE and Université Paris Dauphine)
and Nicolas Chopin (CREST-ENSAE and HEC Paris)

The PAC-Bayesian approach is a powerful set of techniques to derive non-asymptotic risk bounds for random estimators. The corresponding optimal distribution of estimators, usually called the Gibbs posterior, is unfortunately intractable. One may sample from it using Markov chain Monte Carlo, but this is often too slow for big datasets. We consider instead variational approximations of the Gibbs posterior, which are fast to compute. We undertake a general study of the properties of such approximations. Our main finding is that such a variational approximation has often the same rate of convergence as the original PAC-Bayesian procedure it approximates. We specialise our results to several learning tasks (classification, ranking, matrix completion), discuss how to implement a variational approximation in each case, and illustrate the good properties of said approximation on real datasets.

1. Introduction

A Gibbs posterior, also known as a PAC-Bayesian or pseudo-posterior, is a probability distribution for random estimators of the form:

\[ \hat{\theta}_\lambda(d\theta) = \frac{\exp[-\lambda r_n(\theta)]}{\int \exp[-\lambda r_n]d\pi} \pi(d\theta). \]

More precise definitions will follow, but for now, \( \theta \) may be interpreted as a parameter (in a finite or infinite-dimensional space), \( r_n(\theta) \) as an empirical measure of risk (e.g. prediction error), and \( \pi(d\theta) \) a prior distribution.

We will follow in this paper the PAC (Probably Approximatively Correct)-Bayesian approach, which originates from machine learning [Shawe-Taylor and Williamson, 1997; McAllester, 1998; Catoni, 2004]; see Catoni [2007] for an exhaustive study, and Jiang and Tanner [2008], Yang [2004], Zhang [2006], Dalalyan and Tsybakov [2008] for related perspectives (such as the aggregation of estimators in the last 3 papers). There, \( \hat{\rho}_\lambda \) appears
as the probability distribution that minimises the upper bound of an oracle inequality on the risk of random estimators. The PAC-Bayesian approach offers sharp theoretical guarantees on the properties of such estimators, without assuming a particular model for the data generating process.

The Gibbs posterior has also appeared in other places, and under different motivations: in Econometrics, as a way to avoid direct maximisation in moment estimation [Chernozhukov and Hong, 2003]; and in Bayesian decision theory, as as way to define a Bayesian posterior distribution when no likelihood has been specified [Bissiri et al., 2013]. Another well-known connection, although less directly useful (for Statistics), is with thermodynamics, where $r_n$ is interpreted as an energy function, and $\lambda$ as the inverse of a temperature.

Whatever the perspective, estimators derived from Gibbs posteriors usually show excellent performance in diverse tasks, such as classification, regression, ranking, and so on, yet their actual implementation is still far from routine. The usual recommendation [Dalalyan and Tsybakov, 2012; Alquier and Biau, 2013; Guedj and Alquier, 2013] is to sample from a Gibbs posterior using MCMC [Markov chain Monte Carlo, see e.g. Green et al., 2015]: but constructing an efficient MCMC sampler is often difficult, and even efficient implementations are often too slow for practical uses when the dataset is very large.

In this paper, we consider instead VB (Variational Bayes) approximations, which have been initially developed to provide fast approximations of ‘true’ posterior distributions (i.e. Bayesian posterior distributions for a given model); see Jordan et al. [1999], MacKay [2002] and Chap. 10 in Bishop [2006].

Our main results are as follows: when PAC-Bayes bounds are available - mainly, when a strong concentration inequality holds - replacing the Gibbs posterior by a variational approximation does not affect the rate of convergence to the best possible prediction, on the condition that the Kullback-Leibler divergence between the posterior and the approximation is itself controlled in an appropriate way.

We also provide empirical bounds, which may be computed from the data so as to ascertain the actual performance of estimators obtained by variational approximation. All the results gives strong incentives, we believe, to recommend Variational Bayes as the default approach to approximate Gibbs posteriors.

The rest of the paper is organised as follows. In Section 2 we introduce the notations and assumptions. In Section 3 we introduce variational approximations and the corresponding algorithms. The main results are provided in general form in Section 4: in Subsection 4.1 we give results under the assumption that a Hoeffding type inequality holds (slow rates) and in Subsection 4.2 we give results under the assumption that a Bernstein type inequality holds (fast rates). Note that for the sake of shortness, we will refer to these settings as “Hoeffding assumption” and “Bernstein assumption” even if this terminology is non standard. We then apply these results in various settings: classification (Section 5), convex classification (Section 6), ranking (Section 7), and matrix completion (Section 8). In each case, we show how to specialise the general results of Section 4 to the considered application, so as to obtain the properties of the VB approx-
imation, and we also discuss its numerical implementation. All the proofs are collected in the Appendix.

2. PAC-Bayesian framework

We observe a sample \((X_1,Y_1),\ldots,(X_n,Y_n)\), taking values in \(\mathcal{X} \times \mathcal{Y}\), where the pairs \((X_i,Y_i)\) have the same distribution \(P\). We will assume explicitly that the \((X_i,Y_i)\)'s are independent in several of our specialised results, but we do not make this assumption at this stage, as some of our general results, and more generally the PAC-Bayesian theory, may be extended to dependent observations; see e.g. Alquier and Li [2012]. The label set \(\mathcal{Y}\) is always a subset of \(\mathbb{R}\). A set of predictors is chosen by the statistician: \(\{f_\theta : \mathcal{X} \to \mathbb{R}, \theta \in \Theta\}\). For example, in linear regression, we may have: \(f_\theta(x) = \langle \theta, x \rangle\), the inner product of \(\mathcal{X} = \mathbb{R}^d\), while in classification, one may have \(f_\theta(x) = I_{h(\theta,x) > 0}\) \(\{0,1\}\).

We assume we have at our disposal a risk function \(R(\theta)\); typically \(R(\theta)\) is a measure of the prevision error. We set \(R = R(\theta)\), where \(\theta = \arg \min_\Theta R\); i.e. \(f_\theta\) is an optimal predictor. We also assume that the risk function \(R(\theta)\) has an empirical counterpart \(r_n(\theta)\), and set \(r_n = r_n(\theta)\). Often, \(R\) and \(r_n\) are based on a loss function \(\ell : \mathbb{R} \to \mathbb{R}\); i.e. \(R(\theta) = \mathbb{E}[\ell(Y,f_\theta(X))]\) and \(r_n(\theta) = \frac{1}{n} \sum_{i=1}^n \ell(Y_i,f_\theta(X_i))\). (In this paper, the symbol \(\mathbb{E}\) will always denote the expectation with respect to the (unknown) law \(P\) of the \((X_i,Y_i)\)'s.) There are situations however (e.g. ranking), where \(R\) and \(r_n\) have a different form.

We define a prior probability measure \(\pi(\cdot)\) on the set \(\Theta\) (equipped with the standard \(\sigma\)-algebra for the considered context), and we let \(\mathcal{M}_+^1(\Theta)\) denote the set of all probability measures on \(\Theta\).

**Definition 2.1** We define, for any \(\lambda > 0\), the pseudo-posterior \(\hat{\pi}_\lambda\) by

\[
\hat{\pi}_\lambda(d\theta) = \frac{\exp[-\lambda r_n(\theta)]}{\int \exp[-\lambda r_n]d\pi} \pi(d\theta).
\]

The pseudo-posterior \(\hat{\pi}_\lambda\) (also known as the Gibbs posterior, Catoni [2004, 2007], or the exponentially weighted aggregate, Dalalyan and Tsybakov [2008]) plays a central role in the PAC-Bayesian approach. It is obtained as the distribution that minimises the upper bound of a certain oracle inequality applied to random estimators. Practical estimators (predictors) may be derived from the pseudo-posterior, by e.g. taking the expectation, or sampling from it. Of course, when \(\exp[-\lambda r_n(\theta)]\) may be interpreted as the likelihood of a certain model, \(\hat{\pi}_\lambda\) becomes a Bayesian posterior distribution, but we will not restrict our attention to this particular case.

The following ‘theoretical’ counterpart of \(\hat{\pi}_\lambda\) will prove useful to state results.

**Definition 2.2** We define, for any \(\lambda > 0\), \(\pi_\lambda\) as

\[
\pi_\lambda(d\theta) = \frac{\exp[-\lambda R(\theta)]}{\int \exp[-\lambda R]d\pi} \pi(d\theta).
\]
We will derive PAC-Bayesian bounds on predictions obtained by variational approximations of \( \hat{\rho}_\lambda \) under two types of assumptions: a Hoeffding-type assumption, from which we may deduce slow rates of convergence (Subsection 4.1), and a Bernstein-type assumption, from which we may obtain fast rates of convergence (Subsection 4.2).

**Definition 2.3** We say that a Hoeffding assumption is satisfied for prior \( \pi \) when there is a function \( f \) and an interval \( I \subset \mathbb{R}^*_+ \) such that, for any \( \lambda \in I \), for any \( \theta \in \Theta \),

\[
\frac{\pi \left( \mathbb{E} \exp \left\{ \lambda |R(\theta) - R_n(\theta)| \right\} \right)}{\pi \left( \mathbb{E} \exp \left\{ \lambda |r_n(\theta) - R(\theta)| \right\} \right)} \leq \exp \left( f(\lambda, n) \right). \tag{1}
\]

Inequality (1) can be interpreted as an integrated version (with respect to \( \pi \)) of Hoeffding’s inequality, for which \( f(\lambda, n) \propto \lambda^2/n \). In many cases the loss will be bounded uniformly over \( \theta \); then Hoeffding’s inequality will directly imply (1). The expectation with respect to \( \pi \) in (1) allows us to treat some cases where the loss is not upper bounded by specifying a prior with sufficiently light tails.

**Definition 2.4** We say that a Bernstein assumption is satisfied for prior \( \pi \) when there is a function \( g \) and an interval \( I \subset \mathbb{R}^*_+ \) such that, for any \( \lambda \in I \), for any \( \theta \in \Theta \),

\[
\frac{\pi \left( \mathbb{E} \exp \left\{ \lambda |R(\theta) - R| - \lambda |r_n(\theta) - R_n| \right\} \right)}{\pi \left( \mathbb{E} \exp \left\{ \lambda |r_n(\theta) - R_n| - \lambda |R(\theta) - R| \right\} \right)} \leq \pi \left( \exp \left( g(\lambda, n)|R(\theta) - R| \right) \right). \tag{2}
\]

This assumption is satisfied for example by sums of i.i.d. sub-exponential random variables, see Subsection 2.4 p. 27 in Boucheron et al. 2013, when a margin assumption on the function \( R(\cdot) \) is satisfied [Tsybakov 2004]. This is discussed in Section 4.2. Again, extensions beyond the i.i.d. case are possible, see e.g. Wintenberger 2010 for a survey and new results. In all these examples, the important feature of the function \( g \) that we will use to derive rates of convergence is the fact that there is a constant \( c > 0 \) such that when \( \lambda = cn \), \( g(\lambda, n) = g(cn, n) \propto n \).

As mentioned previously, we will often consider \( r_n(\theta) = \frac{1}{n} \sum_{i=1}^n \ell(Y_i, f_\theta(X_i)) \), however, the previous assumptions can also be satisfied when \( r_n(\theta) \) is a U-statistic, using Hoeffding’s decomposition of U-statistics combined with the corresponding inequality for sums of independent variables [Hoeffding 1948]. This idea comes from Clémençon et al. 2008 and we will use it in our ranking application.

**Remark 2.1** We could consider more generally inequalities of the form

\[
\frac{\pi \left( \mathbb{E} \exp \left\{ \lambda |R(\theta) - R| - \lambda |r_n(\theta) - R_n| \right\} \right)}{\pi \left( \mathbb{E} \exp \left\{ \lambda |r_n(\theta) - R_n| - \lambda |R(\theta) - R| \right\} \right)} \leq \pi \left( \exp \left( g(\lambda, n)|R(\theta) - R|^\kappa \right) \right)
\]

that allow to use the more general form of the margin assumption of Mammen and Tsybakov 1999, Tsybakov 2004. PAC-Bayesian bounds in this context are provided by Catoni 2007. However, the techniques involved would require many pages to be described so we decided to focus on the cases \( \kappa = 0 \) and \( \kappa = 1 \) to keep the exposition simple.
3. Numerical approximations of the pseudo-posterior

3.1. Monte Carlo

As already explained in the introduction, the usual approach to approximate \( \hat{\rho}_\lambda \) is MCMC (Markov chain Monte Carlo) sampling. [Ridgway et al. 2014] proposed tempering SMC (Sequential Monte Carlo, e.g. Del Moral et al. [2006]) as an alternative to MCMC to sample from Gibbs posteriors: one samples sequentially from \( \hat{\rho}_{\lambda_i} \), with \( 0 = \lambda_0 < \cdots < \lambda_T = \lambda \) where \( \lambda \) is the desired temperature. One advantage of this approach is that it makes it possible to contemplate different values of \( \lambda \), and choose one by e.g. cross-validation. Another advantage is that such an algorithm requires little tuning; see Appendix B for more details on the implementation of tempering SMC. We will use tempering SMC as our gold standard in our numerical studies.

SMC and related Monte Carlo algorithms tend to be too slow for practical use in situations where the sample size is large, the dimension of \( \Theta \) is large, or \( f_\theta \) is expensive to compute. This motivates the use of fast, deterministic approximations, such as Variational Bayes, which we describe in the next section.

3.2. Variational Bayes

Various versions of VB (Variational Bayes) have appeared in the literature, but the main idea is as follows. We define a family \( \mathcal{F} \subset \mathcal{M}^+_1(\Theta) \) of probability distributions that are considered as tractable. Then, we define the VB-approximation of \( \hat{\rho}_\lambda: \tilde{\rho}_\lambda \).

**Definition 3.1** Let

\[
\tilde{\rho}_\lambda = \arg \min_{\rho \in \mathcal{F}} \mathcal{K}(\rho, \hat{\rho}_\lambda),
\]

where \( \mathcal{K}(\rho, \hat{\rho}_\lambda) \) denotes the KL (Kullback-Leibler) divergence of \( \hat{\rho}_\lambda \) relative to \( \rho: \mathcal{K}(m, \mu) = \int \log\left[ \frac{dm}{d\mu} \right] dm \) if \( m \ll \mu \) (i.e. \( \mu \) dominates \( m \)), \( \mathcal{K}(m, \mu) = +\infty \) otherwise.

The difficulty is to find a family \( \mathcal{F} \) (a) which is large enough, so that \( \tilde{\rho}_\lambda \) may be close to \( \hat{\rho}_\lambda \), and (b) such that computing \( \tilde{\rho}_\lambda \) is feasible. We now review two types of families popular in the VB literature.

- Mean field VB: for a certain decomposition \( \Theta = \Theta_1 \times \cdots \times \Theta_d \), \( \mathcal{F} \) is the set of product probability measures

\[
\mathcal{F}^{\text{MF}} = \left\{ \rho \in \mathcal{M}^+_1(\Theta) : \rho(d\theta) = \prod_{i=1}^d \rho_i(d\theta_i), \forall i \in \{1, \ldots, d\}, \rho_i \in \mathcal{M}^+_1(\Theta_i) \right\}.
\] (3)

The infimum of the KL divergence \( \mathcal{K}(\rho, \tilde{\rho}_\lambda) \), relative to \( \rho = \prod_i \rho_i \) satisfies the following fixed point condition [Parisi 1988, Bishop 2006, Chap. 10]:

\[
\forall j \in \{1, \cdots, d\} \quad \rho_j(d\theta_j) \propto \exp \left( \int \{-\lambda r_n(\theta) + \log \pi(\theta)\} \prod_{i \neq j} \rho_i(d\theta_i) \right) \pi(d\theta_j).
\] (4)
This leads to a natural algorithm where we update successively every \( \rho_j \) until stabilization.

- **Parametric family:**
  \[
  \mathcal{F}^p = \{ \rho \in \mathcal{M}_1^+(\Theta) : \rho(d\theta) = f(\theta;m)d\theta, m \in M \};
  \]
  and \( M \) is finite-dimensional; say \( \mathcal{F}^p \) is the family of Gaussian distributions (of dimension \( d \)). In this case, several methods may be used to compute the infimum. As above, one may used fixed-point iteration, provided an equation similar to \( (4) \) is available. Alternatively, one may directly maximize \( \int \log[\exp[-\lambda r_n(\theta)]\frac{\pi(\theta)}{\rho(\theta)}]\rho(d\theta) \) with respect to parameter \( m \), using numerical optimization routines. This approach was used for instance in [Hoffman et al. 2013] with combination of some stochastic gradient descent to perform inference on a latent Dirichlet allocation model. See also e.g. [Khan 2014, Khan et al. 2013] for efficient algorithms for Gaussian variational approximation.

In what follows (Subsections 4.1 and 4.2) we provide tight bounds for the prevision risk of \( \tilde{\rho}_\lambda \). This leads to the identification of a condition on \( \mathcal{F} \) such that the risk of \( \tilde{\rho}_\lambda \) is not worse than the risk of \( \hat{\rho}_\lambda \). We will make this condition explicit in various examples, using either mean field VB or parametric approximations.

**Remark 3.1** An useful identity, obtained by direct calculations, is: for any \( \rho \ll \pi \),

\[
\log \int \exp[-\lambda r_n(\theta)]\pi(d\theta) = -\lambda \int r_n(\theta)\rho(d\theta) - K(\rho, \pi) + K(\rho, \hat{\rho}_\lambda). \tag{5}
\]

Since the left hand side does not depend on \( \rho \), one sees that \( \hat{\rho}_\lambda \), which minimises \( K(\rho, \hat{\rho}_\lambda) \) over \( \mathcal{F} \), is also the minimiser of:

\[
\hat{\rho}_\lambda = \arg\min_{\rho \in \mathcal{F}} \left\{ \int r_n(\theta)\rho(d\theta) + \frac{1}{\lambda} K(\rho, \pi) \right\}
\]

This equation will appear frequently in the sequel in the form of an empirical upper bound.

### 4. General results

This section gives our general results, under either a Hoeffding Assumption (Definition 2.3) or a Bernstein Assumption (Definition 2.4), on risks bounds for the variational approximation, and how it relates to risks bounds for Gibbs posteriors. These results will be specialised to several learning problems in the following sections.

#### 4.1. Bounds under the Hoeffding assumption

**4.1.1. Empirical bounds**

**Theorem 4.1** Under the Hoeffding assumption (Definition 2.3), for any \( \varepsilon > 0 \), with probability at least \( 1 - \varepsilon \) we have simultaneously for any \( \rho \in \mathcal{M}_1^+(\Theta) \),

\[
\int R d\rho \leq \int r_n d\rho + \frac{f(\lambda, n) + K(\rho, \pi) + \log(\frac{1}{\varepsilon})}{\lambda}.
\]
This result is a simple variant of a result in Catoni [2007] but for the sake of completeness, its proof is given in Appendix A. It gives us an upper bound on the risk of both the pseudo-posterior (take $\rho = \hat{\rho}_\lambda$) and its variational approximation (take $\rho = \tilde{\rho}_\lambda$). These bounds may be be computed from the data, and therefore provide a simple way to evaluate the performance of the corresponding procedure, in the spirit of the first PAC-Bayesian inequalities [Shawe-Taylor and Williamson, 1997, McAllester, 1998, 1999]. However, this bound do not provide the rate of convergence of these estimators. For this reason, we also provide oracle-type inequalities.

4.1.2. Oracle-type inequalities

Another way to use PAC-Bayesian bounds is to compare $\int Rd\hat{\rho}_\lambda$ to the best possible risk, thus linking this approach to oracle inequalities. This is the point of view developed in [Catoni 2004, 2007, Dalalyan and Tsybakov 2008].

Theorem 4.2 Assume that the Hoeffding assumption is satisfied (Definition 2.3). For any $\varepsilon > 0$, with probability at least $1 - \varepsilon$ we have simultaneously

$$\int Rd\hat{\rho}_\lambda \leq B_\lambda(\mathcal{M}_+^1(\Theta)) := \inf_{\rho \in \mathcal{M}_+^1(\Theta)} \left\{ \int Rd\rho + 2 \frac{f(\lambda, n) + K(\rho, \pi) + \log \left( \frac{2}{\lambda} \right)}{\lambda} \right\}$$

and

$$\int Rd\tilde{\rho}_\lambda \leq B_\lambda(\mathcal{F}) := \inf_{\rho \in \mathcal{F}} \left\{ \int Rd\rho + 2 \frac{f(\lambda, n) + K(\rho, \pi) + \log \left( \frac{2}{\lambda} \right)}{\lambda} \right\}.$$ 

Moreover,

$$B_\lambda(\mathcal{F}) = B_\lambda(\mathcal{M}_+^1(\Theta)) + \frac{2}{\lambda} \inf_{\rho \in \mathcal{F}} K(\rho, \pi)$$

where we remind that $\pi$ is defined in Definition 2.2.

In this way, we are able to compare $\int Rd\hat{\rho}_\lambda$ to the best possible aggregation procedure in $\mathcal{M}_+^1(\Theta)$ and $\int Rd\tilde{\rho}_\lambda$ to the best aggregation procedure in $\mathcal{F}$. More importantly, we are able to obtain explicit expressions for the right-hand side of these inequalities in various models, and thus to obtain rates of convergence. This will be done in the remaining sections. This leads to the second interest of this result: if there is a $\lambda = \lambda(n)$ that leads to $B_\lambda(\mathcal{M}_+^1(\Theta)) \leq \overline{R} + s_n$ with $s_n \to 0$ for the pseudo-posterior $\hat{\rho}_\lambda$, then we only have to prove that there is a $\rho \in \mathcal{F}$ such that $K(\rho, \pi) / \lambda \leq cs_n$ for some constant $c > 0$ to ensure that the VB approximation $\tilde{\rho}_\lambda$ also reaches the rate $s_n$.

We will see in the following sections several examples where the approximation does not deteriorate the rate of convergence. But first let us show the equivalent oracle inequality under the Bernstein assumption.
4.2. Bounds under the Bernstein assumption

In this context the empirical bound on the risk would depend on the minimal achievable risk \( \bar{r}_n \), and cannot be computed explicitly. We give the oracle inequality for both the Gibbs posterior and its VB approximation in the following theorem.

**Theorem 4.3** Assume that the Bernstein assumption is satisfied (Definition 2.4). Assume that \( \lambda > 0 \) satisfies \( \lambda - g(\lambda, n) > 0 \). Then for any \( \varepsilon > 0 \), with probability at least \( 1 - \varepsilon \) we have simultaneously:

\[
\int R \hat{\rho}_\lambda - R \leq \mathcal{B}_\lambda(\mathcal{M}_+^1(\Theta)),
\]

\[
\int R \hat{\rho}_\lambda - R \leq \mathcal{B}_\lambda(\mathcal{F}),
\]

where, for either \( A = \mathcal{M}_+^1(\Theta) \) or \( A = \mathcal{F} \),

\[
\mathcal{B}_\lambda(A) = \frac{1}{\lambda - g(\lambda, n)} \inf_{\rho \in A} \left\{ [\lambda + g(\lambda, n)] \int (R - \bar{R}) d\rho + 2\mathcal{K}(\rho, \pi) + 2 \log \left( \frac{2}{\varepsilon} \right) \right\}.
\]

In addition,

\[
\mathcal{B}_\lambda(\mathcal{F}) = \mathcal{B}_\lambda(\mathcal{M}_+^1(\Theta)) + \frac{2}{\lambda - g(\lambda, n)} \inf_{\rho \in \mathcal{F}} \mathcal{K} \left( \rho, \pi_{\lambda + g(\lambda, n)} \right).
\]

The main difference with Theorem 4.2 is that the function \( R(\cdot) \) is replaced by \( R(\cdot) - \bar{R} \). This is well known way to obtain better rates of convergence.

5. Application to classification

5.1. Preliminaries

In all this section, we assume that \( Y = \{0, 1\} \) and we consider linear classification: \( \Theta = \mathcal{X} = \mathbb{R}^d \), \( f_\theta(x) = 1_{(\theta, x) \geq 0} \). We put \( r_n(\theta) = \frac{1}{n} \sum_{i=1}^n 1_{f_\theta(X_i) \neq Y_i} \), \( R(\theta) = \mathbb{P}(Y \neq f_\theta(X)) \) and assume that the \( [(X_i, Y_i)]_{i=1}^n \) are i.i.d. In this setting, it is well-known that the Hoeffding assumption always holds. We state as a reminder the following lemma.

**Lemma 5.1** Hoeffding assumption \[1\] is satisfied with \( f(\lambda, n) = \lambda^2/(2n) \).

The proof is given in Appendix A for the sake of completeness.

It is also possible to prove that Bernstein assumption \[2\] holds in the case where the so-called margin assumption of Mammen and Tsybakov is satisfied. This condition we use was introduced by Tsybakov [2004] in a classification setting, based on a related definition in Mammen and Tsybakov [1999].
Lemma 5.2 Assume that Mammen and Tsybakov’s margin assumption is satisfied: i.e., there is a constant $C$ such that

$$\mathbb{E}[(1_{f_\pi(X) \neq Y} - 1_{f_\pi(X) \neq Y})^2] \leq C[R(\theta) - \bar{R}].$$

Then Bernstein assumption (2) is satisfied with $g(\lambda, n) = \frac{C_0^2}{n^{\frac{1}{2}}}$.

Remark 5.1 We refer the reader to Tsybakov [2004] for a proof that $\mathbb{P}(0 < |(\theta, X)| \leq t) \leq C't$ for some constant $C' > 0$ implies the margin assumption. In words, when $X$ is not likely to be in the region $(\theta, X) \simeq 0$, where points are hard to classify, then the problem becomes easier and the classification rate can be improved.

We propose in this context a Gaussian prior: $\pi = N_d(0, \varphi^2 I_d)$, and we consider a VB approach based on Gaussian families. The corresponding optimization problem is not convex, but remains feasible as we explain below.

5.2. Three sets of Variational Gaussian approximations

Consider the three following Gaussian families

$$\mathcal{F}_1 = \left\{ \Phi_{m, \sigma^2} : m \in \mathbb{R}^d, \sigma^2 \in \mathbb{R}_+^d \right\},$$

$$\mathcal{F}_2 = \left\{ \Phi_{m, \sigma^2} : m \in \mathbb{R}^d, \sigma^2 \in \mathbb{R}_+^d \right\} \text{ (mean field approximation),}$$

$$\mathcal{F}_3 = \left\{ \Phi_{m, \Sigma} : m \in \mathbb{R}^d, \Sigma \in \mathcal{S}_{++}^d \right\} \text{ (full covariance approximation),}$$

where $\Phi_{m, \sigma^2}$ is Gaussian distribution $N_d(m, \sigma^2 I_d)$, $\Phi_{m, \sigma^2}$ is $N_d(m, \text{diag}(\sigma^2))$, and $\Phi_{m, \Sigma}$ is $N_d(m, \Sigma)$. Obviously, $\mathcal{F}_1 \subset \mathcal{F}_2 \subset \mathcal{F}_3 \subset \mathcal{M}_{++}^1(\Theta)$, and

$$B_\lambda(\mathcal{M}_{++}^1(\Theta)) \leq B_\lambda(\mathcal{F}_3) \leq B_\lambda(\mathcal{F}_2) \leq B_\lambda(\mathcal{F}_1). \quad (6)$$

Note that, for the sake of simplicity, we will use the following classical notations in the rest of the paper: $\varphi(\cdot)$ is the density of $\mathcal{N}(0, 1)$ w.r.t. the Lebesgue measure, and $\Phi(\cdot)$ the corresponding c.d.f. The rest of Section 5 is organized as follows. In Subsection 5.3 we calculate explicitly $B_\lambda(\mathcal{F}_2)$ and $B_\lambda(\mathcal{F}_1)$. Thanks to (6) this also gives an upper bound on $B_\lambda(\mathcal{F}_3)$ and proves the validity of the three types of Gaussian approximations. Then, we give details on algorithms to compute the variational approximation based on $\mathcal{F}_2$ and $\mathcal{F}_3$, and provide a numerical illustration on real data.

5.3. Theoretical analysis

We start with the empirical bound for $\mathcal{F}_2$ (and $\mathcal{F}_1$ as a consequence), which is a direct corollary of Theorem 4.1.
Corollary 5.3 For any $\varepsilon > 0$, with probability at least $1 - \varepsilon$ we have, for any $m \in \mathbb{R}^d$, $\sigma^2 \in (\mathbb{R}_+)^d$,

$$\int Rd\Phi_{m,\sigma^2} \leq \int r_n d\Phi_{m,\sigma^2} + \frac{\sigma^2}{2n} + \frac{\sum_{i=1}^{d} \left[ \frac{1}{\sigma_i} \log \left( \frac{\sigma_i^2}{\sigma_j^2} \right) \right] + \frac{\sigma_i^2}{\sigma_j^2} + \frac{\|m\|^2}{\sigma_j^2} - \frac{d}{2} + \log \left( \frac{1}{\varepsilon} \right).$$

We now want to apply Theorem 4.2 in this context. In order to do so, we introduce an additional assumption.

Definition 5.1 We say that Assumption A1 is satisfied when there is a constant $c > 0$ such that, for any $(\theta, \theta') \in \Theta^2$ with $\|\theta\| = \|\theta'\| = 1$, $\mathbb{P}(X(\theta, \theta') < 0) \leq c\|\theta - \theta'\|$.

Note that this is not a stringent assumption. For example, it is satisfied as soon as $X/\|X\|$ has a bounded density on the unit sphere.

Corollary 5.4 Assume that the VB approximation is done on either $F_1$, $F_2$ or $F_3$. Take $\lambda = \sqrt{nd}$ and $\vartheta = \frac{1}{\sqrt{d}}$. Under Assumption A1, for any $\varepsilon > 0$, with probability at least $1 - \varepsilon$ we have simultaneously

$$\int Rd\hat{\rho}_\lambda \leq \bar{R} + \sqrt{d} \log (4ne^2) + \frac{c}{\sqrt{n}} + \sqrt{\frac{d}{4n^3} + \frac{2\log \left( \frac{2}{\varepsilon} \right)}{\sqrt{nd}}}. $$

See the appendix for a proof. Note also that the values $\lambda = \sqrt{nd}$ and $\vartheta = \frac{1}{\sqrt{d}}$ allow to derive this almost optimal rate of convergence, but are not necessarily the best choices in practice.

Remark 5.2 Note that Assumption A1 is not necessary to obtain oracle inequalities on the risk integrated under $\hat{\rho}_\lambda$. We refer the reader to Chapter 1 in Catoni [2007] for such assumption-free bounds. However, it is clear that without this assumption the shape of $\hat{\rho}_\lambda$ and $\tilde{\rho}_\lambda$ might be very different. Thus, it seems reasonable to require that A1 is satisfied for the approximation of $\hat{\rho}_\lambda$ by $\tilde{\rho}_\lambda$ to make sense.

We finally provide an application of Theorem 4.3. Under the additional constraint that the margin assumption is satisfied, we obtain a better rate.

Corollary 5.5 Assume that the VB approximation is done on either $F_1$, $F_2$ or $F_3$. Under Assumption A1 (Definition 5.1 page 10), and under Mammen and Tsybakov margin assumption, with $\lambda = \frac{2n}{d + 2}$ and $\vartheta > 0$, for any $\varepsilon > 0$, with probability at least $1 - \varepsilon$,

$$\int Rd\hat{\rho}_\lambda \leq \bar{R} + \frac{(C + 2)(C + 1)}{2} \left\{ \frac{d \log \frac{d}{\varepsilon}}{n} + \frac{2d\vartheta}{n^2} + \frac{2}{\vartheta n} + \frac{2}{n} \log \frac{2}{\varepsilon} \right\} + \frac{\sqrt{d}2c(2C + 1)}{n}.$$ 

The prior variance optimizing the bound is $\vartheta = d/(d + 2d/n)$, this choice or any constant instead will lead to a rate in $d \log(n)/n$. Note that the rate $d/n$ is minimax-optimal in this context. This is, for example, a consequence of more general results in Lecue [2007] under a general form of the the margin assumption. See the Appendix for a proof.
5.4. Implementation and numerical results

For family $\mathcal{F}_2$ (mean field), the variational lower bound (5) equals

$$L_{\lambda,\theta}(\mathbf{m},\mathbf{\sigma}) = -\frac{\lambda}{n} \sum_{i=1}^{n} \Phi \left( -Y_i \frac{X_i \mathbf{m}}{\sqrt{X_i \text{diag}(\mathbf{\sigma}^2) X_i}} \right) - \frac{\mathbf{m}^T \mathbf{m}}{2\theta} + \frac{1}{2} \sum_{k=1}^{d} \left( \log \sigma_k^2 - \frac{\sigma_k^2}{\theta} \right),$$

while for family $\mathcal{F}_3$ (full covariance), it equals

$$L_{\lambda,\theta}(\mathbf{m},\mathbf{\Sigma}) = -\frac{\lambda}{n} \sum_{i=1}^{n} \Phi \left( -Y_i \frac{X_i \mathbf{m}}{\sqrt{X_i \Sigma X_i}} \right) - \frac{\mathbf{m}^T \mathbf{m}}{2\theta} + \frac{1}{2} \left( \log |\mathbf{\Sigma}| - \frac{1}{\theta} \text{tr} \mathbf{\Sigma} \right).$$

Both functions are non-convex, but the multimodality of the latter may be more severe due to the larger dimension of $\mathcal{F}_3$. To address this issue, we recommend to use the reparametrisation of Opper and Archambeau (2009), which makes the dimension of the latter optimisation problem $O(n)$; see Khan (2014) for a related approach. In both cases, we found that deterministic annealing to be a good approach to optimise such non-convex functions. We refer to Appendix B for more details on deterministic annealing and on our particular implementation.

We now compare the numerical performance of the mean field and full covariance VB approximations to the Gibbs posterior (as approximated by SMC, see Section 3.1) for the classification of standard datasets; see Table 1. We also include results for a kernel SVM (support vector machine); this comparison is not entirely fair, since SVM is a non-linear classifier, while all the other classifiers are linear. Still, except for the Glass dataset, the full covariance VB approximation performs as well or better than both SMC and SVM (while being much faster to compute, especially compared to SMC).

<table>
<thead>
<tr>
<th>Dataset</th>
<th>Covariates</th>
<th>Mean Field ($\mathcal{F}_2$)</th>
<th>Full cov. ($\mathcal{F}_3$)</th>
<th>SMC</th>
<th>SVM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pima</td>
<td>7</td>
<td>31.0</td>
<td>21.3</td>
<td>22.3</td>
<td>30.4</td>
</tr>
<tr>
<td>Credit</td>
<td>60</td>
<td>32.0</td>
<td>33.6</td>
<td>32.0</td>
<td>32.0</td>
</tr>
<tr>
<td>DNA</td>
<td>180</td>
<td>23.6</td>
<td>23.6</td>
<td>23.6</td>
<td>20.4</td>
</tr>
<tr>
<td>SPECTF</td>
<td>22</td>
<td>08.0</td>
<td>06.9</td>
<td>08.5</td>
<td>10.1</td>
</tr>
<tr>
<td>Glass</td>
<td>10</td>
<td>34.6</td>
<td>19.6</td>
<td>23.3</td>
<td>4.7</td>
</tr>
<tr>
<td>Indian</td>
<td>11</td>
<td>48.0</td>
<td>25.5</td>
<td>26.2</td>
<td>26.8</td>
</tr>
<tr>
<td>Breast</td>
<td>10</td>
<td>35.1</td>
<td>1.1</td>
<td>1.1</td>
<td>1.7</td>
</tr>
</tbody>
</table>

Table 1: Comparison of misclassification rates (%).

Misclassification rates for different datasets and for the proposed approximations of the Gibbs posterior. The last column is the misclassification rate given by a kernel-SVM with radial kernel. The hyper-parameters are chosen by cross-validation.
Interestingly, VB outperforms SMC in certain cases. This might be due to the fact that a VB approximation tends to be more concentrated around the mode than the Gibbs posterior it approximates. Mean field VB does not perform so well on certain datasets (e.g. Indian). This may due either to the approximation family being too small, or to the corresponding optimisation problem to be strongly multi-modal.

6. Application to classification under convexified loss

Compared to the previous section, the advantage of convex classification is that the corresponding variational approximation will amount to minimising a convex function. This means that (a) the minimisation problem will be easier to deal with; and (b) we will be able to compute a bound for the integrated risk after a given number of steps of the minimisation procedure.

The setting is the same as in the previous section, except that for convenience we now take $Y = \{-1, 1\}$, and the risk is based on the hinge loss,

$$r_n^H(\theta) = \frac{1}{n} \sum_{i=1}^{n} \max(0, 1 - Y_i < \theta, X_i >).$$

We will write $R^H$ for the theoretical counterpart and $\hat{R}^H$ for its minimum in $\theta$. We keep the superscript $H$ in order to allow comparison with the risk $R$ under the $0-1$ loss. We assume in this section that the $X_i$ are uniformly bounded by a constant, $|X_i| < c_x$. Note that we do not require an assumption of the form (A1) to obtain the results of this section, as we rely directly on the Lipschitz continuity of the hinge risk.

6.1. Theoretical Results

Contrarily to the previous section, the risk is not bounded in $\theta$, and we must specify a prior distribution for the Hoeffding assumption to hold.

**Lemma 6.1** Under a independent Gaussian prior $\pi$ such that each component is $N(0, \vartheta^2)$, and for $\lambda < \frac{2}{\sqrt{2}} \sqrt{\frac{\lambda}{\vartheta}}$ and with bounded design $|X_{ij}| < c_x$, Hoeffding assumption \(\text{[1]}\) is satisfied with $f(\lambda, n) = \lambda^2/(4n) - \frac{1}{2} \log \left(1 - \frac{\alpha^2 c_x^2}{4n \lambda^2}\right)$.

The main impact of such a bound is that the prior variance cannot be taken too big relative to $\lambda$.

**Corollary 6.2** Assume that the VB approximation is done on either $\mathcal{F}_1$, $\mathcal{F}_2$ or $\mathcal{F}_3$. Take $\lambda = \frac{1}{c_x} \sqrt{\frac{d}{n}}$ and $\vartheta = \frac{1}{\sqrt{d}}$. For any $\varepsilon > 0$, with probability at least $1 - \varepsilon$ we have simultaneously

$$\int R^H d\hat{\pi}_\lambda \leq R^H + \frac{c_x}{2} \sqrt{\frac{d}{n}} \log n d + 2c_x \frac{d}{n} + \frac{1}{\sqrt{nd}} \left(\frac{c_x^2 + 1}{2c_x} + 2c_x \log \frac{2}{\varepsilon}\right)$$
The oracle inequality in the above corollary enjoys the same rate of convergence as the equivalent result in the preceding section. In the following we link the two results.

**Remark 6.1** As stated in the beginning of the section we can use the estimator specified under the hinge loss to bound the excess risk of the 0-1 loss. We write $R^*$ and $R_{H^*}$ the respective risk for their corresponding Bayes classifiers. From Zhang [2004] (section 3.3) we have the following inequality, linking the excess risk under the hinge loss and the 0–1 loss,

$$R(\theta) - R^* \leq R_{H}(\theta) - R_{H^*}$$

for every $\theta \in \mathbb{R}^p$. By integrating with respect to $\tilde{\rho}^H$ (the VB approximation on any $\mathcal{F}_1, \mathcal{F}_2, \mathcal{F}_3$ of the Gibbs posterior for the hinge risk) and making use of Corollary 6.2, we have with high probability,

$$\tilde{\rho}^H (R(\theta)) - R^* \leq \inf_{\theta \in \mathbb{R}^p} R_{H}(\theta) - R_{H^*} + O \left( \sqrt{\frac{d}{n} \log \left( \frac{n}{d} \right)} \right).$$

### 6.2. Numerical application

We have motivated the introduction of the hinge loss as a convex upper bound. In the sequel we show that the resulting VB approximation also leads to a convex optimization problem. This has the advantage of opening a range of possible optimization algorithms [Nesterov, 2004]. In addition we are able to bound the error of the approximated measure after a fixed number of iterations (see Theorem 6.3).

Under the model $\mathcal{F}_1$ each individual risk is given by:

$$\rho_{m,\sigma}(r_i(\theta)) = (1 - \Gamma_i m) \Phi \left( \frac{1 - \Gamma_i m}{\sigma \| \Gamma_i \|_2} \right) + \sigma \| \Gamma_i \| \varphi \left( \frac{1 - \Gamma_i m}{\sigma \| \Gamma_i \|_2} \right) := \Xi_i \left( \begin{pmatrix} m \\ \sigma \end{pmatrix} \right),$$

writing $\Gamma_i := Y_i X_i$.

Hence the lower bound to be maximized is given by

$$\mathcal{L}(m, \sigma) = -\lambda \left\{ \frac{1}{n} \sum_{i=1}^{n} (1 - \Gamma_i m) \Phi \left( \frac{1 - \Gamma_i m}{\sigma \| \Gamma_i \|_2} \right) + \sum_{i=1}^{n} \sigma \| \Gamma_i \| \varphi \left( \frac{1 - \Gamma_i m}{\sigma \| \Gamma_i \|_2} \right) \right\}$$

$$- \frac{\| m \|_2^2}{2 \rho} + \frac{d}{2} \left( \log \sigma^2 - \frac{\rho}{\sigma^2} \right).$$

It is easy to see that the function is convex in $(m, \sigma)$, first note that the map

$$\Psi \left( \begin{pmatrix} x \\ y \end{pmatrix} \right) \mapsto x \Phi \left( \frac{x}{y} \right) + y \varphi \left( \frac{x}{y} \right),$$

is convex and note that we can write $\Xi_i \left( \begin{pmatrix} m \\ \sigma \end{pmatrix} \right) = \Psi \left( A \left( \begin{pmatrix} x \\ y \end{pmatrix} \right) + b \right)$ hence by composition of convex function with linear mappings we have the result. Similar reasoning
could be held for the case $\mathcal{F}_2$ and $\mathcal{F}_3$, where in later the parametrization should be done in C such that $\Sigma = CC^t$. The bound is however not universally Lipschitz in $\sigma$, this impacts the optimization algorithms.

On the class of function $\mathcal{F}_0 = \left\{ \Phi_m \frac{1}{2}, m \in \mathbb{R}^d \right\}$, for which our Oracle inequalities still hold we could get faster numerical algorithms. The objective function has Lipschitz continuous derivatives and we would get a rate of $\frac{L}{(1+k)^2}$.

Other convex loss could be considered which could lead to convex optimization problems. For instance one could consider the exponential loss.

<table>
<thead>
<tr>
<th>Dataset</th>
<th>Covariates</th>
<th>Hinge loss</th>
<th>SMC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pima</td>
<td>7</td>
<td>21.8</td>
<td>22.3</td>
</tr>
<tr>
<td>Credit</td>
<td>60</td>
<td>27.2</td>
<td>32.0</td>
</tr>
<tr>
<td>DNA</td>
<td>180</td>
<td>4.2</td>
<td>23.6</td>
</tr>
<tr>
<td>SPECTF</td>
<td>22</td>
<td>19.2</td>
<td>08.5</td>
</tr>
<tr>
<td>Glass</td>
<td>10</td>
<td>26.12</td>
<td>23.3</td>
</tr>
<tr>
<td>Indian</td>
<td>11</td>
<td>26.2</td>
<td>25.5</td>
</tr>
<tr>
<td>Breast</td>
<td>10</td>
<td>0.5</td>
<td>1.1</td>
</tr>
</tbody>
</table>

Table 2: Comparison of misclassification rates (%). Misclassification rates for different datasets and for the proposed approximations of the Gibbs posterior. The hyperparameters are chosen by cross-validation. This is to be compared to Table 1.

**Theorem 6.3** Assume that the VB approximation is done on $\mathcal{F}_1, \mathcal{F}_2$ or $\mathcal{F}_3$. Denote by $\tilde{\rho}_k(d\theta)$ the VB approximated measure after the $k$th iteration of an optimal convex solver using the hinge loss. Take $\lambda = \sqrt{nd}$ and $\vartheta = \frac{1}{\sqrt{d}}$ then under the hypothesis of Corollary 6.2 with probability $1 - \epsilon$

$$\int R^H \tilde{\rho}_k \leq R^H + \frac{LM}{1+k} + \frac{c_x}{2} \sqrt{\frac{d}{n}} \log \frac{n}{d} + 2c_x \frac{d}{n} + \frac{1}{\sqrt{nd}} \left( \frac{c_x^2 + 1}{2c_x} + 2c_x \log \frac{2}{\epsilon} \right)$$

where $L$ is the Lipschitz coefficient on a ball of radius $M$ of the objective function maximized in VB.

From Theorem 6.3 we can compute the number of iterations to get a given level of error at a given probability.

We find that on average the misclassification error (Table 2) is lower than for the 0-1 loss where we have no guarantees that the maximum is attained.
7. Application to ranking

7.1. Preliminaries

In this section we take \( \mathcal{Y} = \{0, 1\} \) and consider again linear classifiers: \( \Theta = \mathcal{X} = \mathbb{R}^d \), \( f_\theta(x) = 1_{(\theta,x) \geq 0} \). We consider however a different criterion: in ranking, not only we want to classify well an object \( x \), but we want to make sure that given two different objects, the one that is more likely to correspond to a label 1 will be assigned a larger score through the function \( f_\theta \).

A usual way to measure this is to introduce the risk function

\[
R(\theta) = \mathbb{P}(Y_1 - Y_2)(f_\theta(X_1) - f_\theta(X_2)) < 0
\]

and the empirical risk

\[
r_n(\theta) = \frac{1}{n(n-1)} \sum_{1 \leq i \neq j \leq n} 1_{(Y_i - Y_j)(f_\theta(X_i) - f_\theta(X_j)) < 0}.
\]

Then, again, we recall classical results.

**Lemma 7.1** The Hoeffding-type assumption is satisfied with \( f(\lambda, n) = \frac{\lambda^2}{n-1} \).

The variant of the margin assumption adapted to ranking was established by Robbiano [2013] and Ridgway et al. [2014].

**Lemma 7.2** Assume the following margin assumption:

\[
\mathbb{E}[(1_{[f_\theta(X_1) - f_\theta(X_2)](Y_1 - Y_2) < 0} - 1_{[f_\varphi(X_1) - f_\varphi(X_2)](Y_1 - Y_2) < 0}^2) \leq C[R(\theta) - \mathcal{R}].
\]

Then Bernstein assumption (2) is satisfied with \( g(\lambda, n) = \frac{C\lambda^2}{n-1-\lambda} \).

We still consider a Gaussian prior

\[
\pi(d\theta) = \prod_{i=1}^d \varphi(\theta_i; 0, \sigma_i^2)d\theta_i
\]

and the approximation families will be the same as in Section 5:

\( \mathcal{F}_1 = \{\Phi_{m,\sigma^2}, m \in \mathbb{R}^d, \sigma^2 \in \mathbb{R}^*_+\} \), \( \mathcal{F}_2 = \{\Phi_{m,\sigma^2}, m \in \mathbb{R}^d, \sigma^2 \in (\mathbb{R}^*_+)^2\} \) and \( \mathcal{F}_3 = \{\Phi_{m,\Sigma}, m \in \mathbb{R}^d, \Sigma \in \mathcal{S}^{d+}\} \).

7.2. Theoretical study

Here again, we start with the empirical bound.

**Corollary 7.3** For any \( \varepsilon > 0 \), with probability at least \( 1 - \varepsilon \) we have, for any \( m \in \mathbb{R}^d \), \( \sigma^2 \in (\mathbb{R}^*_+)^d \),

\[
\int R \Phi_{m,\sigma^2} \leq \int r_n d\Phi_{m,\sigma^2} + \frac{\lambda}{n-1} + \frac{\sum_{j=1}^d \left[ \frac{1}{2} \log \left( \frac{\sigma_j^2}{\varphi_j^2}\right) + \frac{\sigma_j^2}{\varphi_j^2}\right]}{\lambda} + \frac{\|m\|^2}{\sigma^2} - \frac{d}{2} + \log \left( \frac{1}{\varepsilon}\right).
\]
In order to derive a theoretical bound, we introduce the following variant of Assumption A1.

**Definition 7.1** We say that Assumption A2 is satisfied when there is a constant \( c > 0 \) such that, for any \((\theta, \theta') \in \Theta^2\) with \( \|\theta\| = \|\theta'\| = 1\), \( \mathbb{P}(\langle X_1 - X_2, \theta \rangle \langle X_1 - X_2, \theta' \rangle < 0) \leq c \|\theta - \theta'\| \).

Assumption A2 is satisfied as soon as \((X_1 - X_2)/\|X_1 - X_2\|\) has a bounded density on the unit sphere.

**Corollary 7.4** Use either \( F_1, F_2 \) or \( F_3 \). Take \( \vartheta = q/d(\sqrt{n}) \) and \( \# = 1 \). Under (A2), for any \( \varepsilon > 0 \), with probability at least \( 1 - \varepsilon \),

\[
\frac{\int R d\hat{\rho}_\lambda}{\int R d\hat{\rho}_\lambda} \leq \bar{R} + \sqrt{\frac{2d}{n-1}} \left( 1 + \frac{1}{2} \log (2d(n-1)) \right) + \frac{c\sqrt{2}}{\sqrt{n-1}} + \frac{2\sqrt{2}\log (\frac{2n}{d})}{(n-1)d}.
\]

Finally, under an additional margin assumption, we have:

**Corollary 7.5** Under Assumption A2 and the margin assumption of Lemma (7.2), for \( \lambda = \frac{d+2}{\vartheta^2} \) and \( \vartheta > 0 \), for any \( \varepsilon > 0 \), with probability at least \( 1 - \varepsilon \),

\[
\frac{\int R d\hat{\rho}_\lambda}{\int R d\hat{\rho}_\lambda} \leq \bar{R} + \frac{(C + 5)(C + 1)}{2} \left\{ \frac{d\log \frac{n}{\vartheta}}{n-1} + \frac{2d\vartheta}{n(n-1)} + \frac{2}{\vartheta} - \frac{d}{\vartheta n - 1} + \frac{2}{n - 1} \log \frac{2n}{d} \right\} + \frac{\sqrt{d\log(C + 1)}}{n}.
\]

The prior variance optimizing the bound is \( \vartheta = d/(d + 2 + 2d/n) \). The proof is similar to the ones of Corollaries 5.4, 5.5 and 7.4.

As in the case of classification, ranking under an AUC loss can be done by replacing the indicator function by the corresponding upper bound given by an hinge loss. In this case we can derive similar results as for the convexified classification in particular we can get a convex minimization problem and obtain result without requiring assumption (A2).

### 7.3. Algorithms and numerical results

As an illustration we focus here on family \( F_2 \) (mean field). In this case the VB objective to maximize is given by:

\[
\mathcal{L}(m, \sigma^2) = -\frac{\lambda}{n+n} \sum_{i:y_i=1,j:y_j=0} \Phi \left( -\frac{\Gamma_{ij} m}{\sqrt{\sum_{k=1}^{d} (\gamma_{ij}^k)^2 \sigma_k^2}} \right) - \frac{\|m\|_2^2}{2\vartheta} + \frac{1}{2} \sum_{k=1}^{d} \left[ \log \sigma_k^2 - \frac{\sigma_k^2}{\vartheta} \right],
\]

where \( \Gamma_{ij} = X_i - X_j \), and where \((\gamma_{ij}^k)_k\) are the elements of \( \Gamma \).

This function is expensive to compute, as it involves \( n_+ n_- \) terms, the computation of which is \( \mathcal{O}(p) \).
We propose to use a stochastic gradient descent in the spirit of [Hoffman et al., 2013]. The model we consider is not in an exponential family, meaning we cannot use the trick developed by these authors. We propose instead to use a standard descent.

The idea is to replace the gradient by an unbiased version based on a batch of size $B$ as described in Algorithm 4 in the Appendix. Robbins and Monro [1951] show that for a step-size $(\lambda_t)_t$ such that $\sum t \lambda_t^2 < \infty$ and $\sum t \lambda_t = \infty$ the algorithm converges to a local optimum.

In our case we propose to sample pairs of data with replacement and use the unbiased version of the derivative of the risk component. We use a simple gradient descent without any curvature information. One could also use recent research on stochastic quasi Newton-Raphson [Byrd et al., 2014].

For illustration, we consider a small dataset (Pima), and a larger one (Adult). The latter is already quite challenging with $n_+ n_- = 193,829,520$ pairs to compare. In both cases with different size of batches convergence is obtained with a few iterations only and leads to acceptable bounds.

In Figure 1 we show the empirical bound on the AUC risk as a function of the iteration of the algorithm, for several batch sizes. The bound is taken for 95% probability, the batch sizes are taken to be $B = 1, 10, 20, 50$ for the Pima dataset, and 50 for the Adult dataset. The figure shows an additional feature of VB approximation in the context of Gibbs posterior: namely the possibility of computing the empirical upper bound given by Corollary 7.3. That is we can check the quality of the bound at each iteration of the algorithm, or for different values of the hyperparameters.

8. Application to matrix completion

The matrix completion problem has received increasing attention recently, partly due to spectacular theoretical results [Candès and Tao, 2010], and to challenging applications like the Netflix challenge [Bennett and Lanning, 2007]. In the perspective of this paper, the specific interest of this application is twofold. First, this is a case where the family of approximations is not parametric, but rather of the form (3), i.e. the family of products of independent components. Then, there is no known theoretical result for the Gibbs estimator in the considered model, yet we can still directly bound the loss induced by the variational approximation.

We observe i.i.d. pairs $((X_i, Y_i))_{i=1}^n$ where $X_i \in \{1, \ldots, m_1\} \times \{1, \ldots, m_2\}$, and we assume that there is a $m_1 \times m_2$-matrix $M$ such that $Y_i = M X_i + \varepsilon_i$ and the $\varepsilon_i$ are centred. Assuming that $X_i$ is uniform on $\{1, \ldots, m_1\} \times \{1, \ldots, m_2\}$, that $f_\theta(X_i) = \theta X_i$, and taking the quadratic risk, $R(\theta) = \mathbb{E} [(Y_i - \theta X_i)^2]$, we have that

$$R(\theta) - \bar{R} = \frac{1}{m_1 m_2} \|\theta - M\|_F^2$$

where $\|\cdot\|_F$ stands for the Frobenius norm.

A common way to parametrise the problem is

$$\Theta = \{\theta = UV^T, U \in \mathbb{R}^{m_1 \times K}, V \in \mathbb{R}^{m_2 \times K}\}.$$
Figure 1: Error bound at each iteration, stochastic descent, Pima and Adult datasets.

Stochastic VB with fixed temperature $\lambda = 100$ for Pima and $\lambda = 1000$ for adult. The left panel shows several curves that correspond to different batch sizes; these curves are hard to distinguish. The right panel is for a batch size of 50. The adult dataset has $n = 32556$ observation and $n_+n_- = 193829520$ possible pairs. The convergence is obtained in order of seconds. The bounds are the empirical bounds obtained in Corollary 7.3 for a probability of 95%.

where $K$ is large; e.g. $K = \min(m_1, m_2)$. Following Salakhutdinov and Mnih [2008], we define the following prior distribution: $U_{:,j} \sim \mathcal{N}(0, \gamma_j I)$, $V_{:,j} \sim \mathcal{N}(0, \gamma_j I)$ where the $\gamma_j$’s are i.i.d. from an inverse gamma distribution, $\gamma_j \sim \Gamma(a, b)$.

Note that VB algorithms were used in this context by Lim and Teh [2007] (with a slightly simpler prior however: the $\gamma_j$’s are fixed rather than random). Since then, this prior and variants were used in several papers [e.g. Lawrence and Urtasun, 2009; Zhou et al., 2010]. Until now, no theoretical results were proved up to our knowledge. Two papers prove minimax-optimal rates for slightly modified estimators (by truncation), for which efficient algorithms are unknown [Mai and Alquier, 2015; Suzuki, 2014]. However, using Theorems 4.2 and 4.3 we are able to prove the following: if there is a PAC-Bayesian bound leading to a rate for $\hat{\rho}_\lambda$ in this context, then the same rate holds for $\bar{\rho}_\lambda$. In other words: if someone proves the conjecture that the Gibbs estimator is minimax-optimal (up to log terms) in this context, then the VB approximation will enjoy automatically the same property.
We propose the following approximation:

\[
\mathcal{F} = \left\{ \rho(d(U, V)) = \prod_{i=1}^{m_1} u_i(dU_i, \cdot) \prod_{j=1}^{m_2} v_j(dV_j, \cdot) \right\}.
\]

**Theorem 8.1** Assume that \( M = UV^T \) with \( |U_{i,k}|, |V_{j,k}| \leq C \). Assume that \( \text{rank}(M) = r \) so that we can assume that \( U_{.,r+1} = \cdots = U_{.,K} = V_{.,r+1} = \cdots = V_{.,K} = 0 \) (note that the prior \( \pi \) does not depend on the knowledge of \( r \) though). Choose the prior distribution on the hyper-parameters \( \gamma_j \) as inverse gamma \( \text{Inv-}\Gamma(a, b) \) with \( b \leq 1/[2\beta(m_1 \vee m_2) \log(2K(m_1 \vee m_2))] \). Then there is a constant \( C(a, C) \) such that, for any \( \beta > 0 \),

\[
\inf_{\rho \in \mathcal{F}} \mathcal{K}(\rho, \pi_\beta) \leq \mathcal{C}(a, C) \left\{ r(m_1 + m_2) \log [\beta b(m_1 + m_2)K] + \frac{1}{\beta} \right\}.
\]

See the Appendix for a proof.

For instance, in Theorem 4.3, in classification and ranking we had \( \lambda, \lambda - g(\lambda, n) \) and \( \lambda + g(\lambda, n) \) of order \( O(n) \). In this case we would have:

\[
\frac{2}{\lambda - g(\lambda, n)} \inf_{\rho \in \mathcal{F}} \mathcal{K}(\rho, \pi_{\lambda + g(\lambda, n)}) = O \left( \frac{\mathcal{C}(a, C)r(m_1 + m_2) \log [nb(m_1 + m_2)K]}{n} \right),
\]

and note that in this context it is known that the minimax rate is at least \( r(m_1 + m_2)/n \) [Koltchinskii et al., 2011].

### 8.1. Algorithm

As already mentioned, the approximation family is not parametric in this case, but rather of type mean field. The corresponding VB algorithm amounts to iterating equation (4), which takes the following form in this particular case:

\[
\begin{align*}
\lambda_j(dU_{\cdot,j}) \propto & \exp \left\{ -\frac{\lambda}{n} \sum_i \mathbb{E}_{U_{\cdot,j}} \left[ (Y_{X_i} - (UV^T)X_i)^2 \right] - \sum_{k=1}^{K} \mathbb{E}_{\gamma_j} \left[ \frac{1}{2\gamma_k} U_{\cdot,jk}^2 \right] \right\} \\
v_j(dV_{\cdot,j}) \propto & \exp \left\{ -\frac{\lambda}{n} \sum_i \mathbb{E}_{V_{\cdot,j}} \left[ (Y_{X_i} - (UV^T)X_i)^2 \right] - \sum_{k=1}^{K} \mathbb{E}_{\gamma_j} \left[ \frac{1}{2\gamma_k} V_{\cdot,jk}^2 \right] \right\} \\
p(\gamma_k) \propto & \exp \left\{ -\frac{1}{2\gamma_k} \left( \sum_j \mathbb{E}_{U} U_{\cdot,jk}^2 + \sum_i \mathbb{E}_{V} V_{\cdot,ik}^2 \right) + (\alpha + 1) \log \frac{1}{\gamma_k} - \frac{\beta}{\gamma_k} \right\}
\end{align*}
\]

where the expectations are taken with respect to the thus defined variational approximations. One recognises Gaussian distributions for the first two, and an inverse Gamma distribution for the third. We refer to [Lim and Teh, 2007] for more details on this algorithm and for a numerical illustration.
9. Discussion

We showed in several important scenarios that approximating a Gibbs posterior through VB (Variational Bayes) techniques does not deteriorate the rate of convergence of the corresponding procedure. We also described practical algorithms for fast computation of these VB approximations, and provided empirical bounds that may be computed from the data to evaluate the performance of the so-obtained VB-approximated procedure. We believe these results provide a strong incentive to recommend VB as the default approach to approximate Gibbs posteriors, in lieu of Monte Carlo methods.

We hope to extend our results to other applications beyond those discussed in this paper, such as regression. One technical difficulty with regression is that the risk function is not bounded, which makes our approach a bit less direct to apply. In many papers on PAC-Bayesian bounds for regression, the noise can be unbounded (usually, it is assumed to be sub-exponential), but one assumes that the predictors are bounded, see e.g. Alquier and Biau [2013]. However, using the robust loss function of Audibert and Catoni, it is possible to relax this assumption [Audibert and Catoni 2011, Catoni 2012]. This requires a more technical analysis, which we leave for further work.

References


A. Proofs

A.1. Preliminary remarks

We start by a general remark. Let \( h : \Theta \to \mathbb{R}_+ \) with \( \int \exp[-h(\theta)] \pi(d\theta) < \infty \).

Let \( \pi(h)(d\theta) = \frac{\exp[-h(\theta)]}{\int \exp[-h(\theta')] \pi(d\theta')} \pi(d\theta) \).

Direct calculation yields, for any \( \rho \ll \pi \) with \( \int h \rho < \infty \),

\[
\mathcal{K}(\rho, \pi[h]) = \lambda \int h \rho + \mathcal{K}(\rho, \pi) + \log \int \exp(-h) d\pi.
\]

Two well known consequences are

\[
\pi[h] = \arg \min_{\rho \in \mathcal{M}_1(\Theta)} \left\{ \int h \rho + \mathcal{K}(\rho, \pi) \right\},
\]

\[
-\log \int \exp(-h) d\pi = \min_{\rho \in \mathcal{M}_1(\Theta)} \left\{ \int h \rho + \mathcal{K}(\rho, \pi) \right\}.
\]

We will use these inequalities many times in the followings. The most frequent application will be with \( h(\theta) = \lambda r_n(\theta) \) (in this case \( \pi[\lambda r_n] = \hat{\rho}_\lambda \)) or \( h(\theta) = \pm \lambda [r_n(\theta) - R(\theta)] \), the first case leads to

\[
\mathcal{K}(\rho, \hat{\rho}_\lambda) = \lambda \int r_n d\rho + \mathcal{K}(\rho, \pi) + \log \int \exp(-\lambda r_n) d\pi,
\]

\[
\hat{\rho}_\lambda = \arg \min_{\rho \in \mathcal{M}_1(\Theta)} \left\{ \lambda \int r_n d\rho + \mathcal{K}(\rho, \pi) \right\},
\]

\[
-\log \int \exp(-\lambda r_n) d\pi = \min_{\rho \in \mathcal{M}_1(\Theta)} \left\{ \lambda \int r_n d\rho + \mathcal{K}(\rho, \pi) \right\}.
\]

We will use (8), (9) and (10) several times in this appendix.

A.2. Proof of the theorems in Subsection 4.1

Proof of Theorem 4.1. This proof follows the standard PAC-Bayesian approach (see Catoni [2007]). Apply Fubini’s theorem to the first inequality of (1):

\[
\mathbb{E} \int \exp \{ \lambda [R(\theta) - r_n(\theta)] - f(\lambda, n) \} \pi(d\theta) \leq 1
\]

then apply the preliminary remark with \( h(\theta) = \lambda [r_n(\theta) - R(\theta)] \):

\[
\mathbb{E} \exp \left\{ \sup_{\rho \in \mathcal{M}_1(\Theta)} \int \lambda [R(\theta) - r_n(\theta)] \rho(d\theta) - \mathcal{K}(\rho, \pi) - f(\lambda, n) \right\} \leq 1.
\]
Multiply both sides by \( \varepsilon \) and use \( \mathbb{E}[\exp(U)] \geq \mathbb{P}(U > 0) \) for any \( U \) to obtain:

\[
\mathbb{P} \left[ \sup_{\rho \in \mathcal{M}^1_+(\Theta)} \int \lambda [R(\theta) - r_n(\theta)] \rho(d\theta) - K(\rho, \pi) - f(\lambda, n) + \log(\varepsilon) > 0 \right] \leq \varepsilon.
\]

Then consider the complementary event:

\[
\mathbb{P} \left[ \forall \rho \in \mathcal{M}^1_+(\Theta), \quad \lambda \int R d\rho \leq \lambda \int r_n d\rho + f(\lambda, n) + K(\rho, \pi) + \log \left( \frac{1}{\varepsilon} \right) \right] \geq 1 - \varepsilon.
\]

\( \square \)

**Proof of Theorem 4.2.** Using the same calculations as above, we have, with probability at least \( 1 - \varepsilon \), simultaneously for all \( \rho \in \mathcal{M}^1_+(\Theta) \),

\[
\lambda \int R d\rho \leq \lambda \int r_n d\rho + f(\lambda, n) + K(\rho, \pi) + \log \left( \frac{2}{\varepsilon} \right) \quad (11)
\]

\[
\lambda \int r_n d\rho \leq \lambda \int R d\rho + f(\lambda, n) + K(\rho, \pi) + \log \left( \frac{2}{\varepsilon} \right). \quad (12)
\]

We use (11) with \( \hat{\rho}_\lambda = \hat{\rho}_\lambda \) and (9) to get

\[
\lambda \int R d\hat{\rho}_\lambda \leq \inf_{\rho \in \mathcal{M}^1_+(\Theta)} \left\{ \lambda \int r_n d\rho + f(\lambda, n) + K(\rho, \pi) + \log \left( \frac{2}{\varepsilon} \right) \right\}
\]

and plugging (12) into the right-hand side, we obtain

\[
\lambda \int R d\hat{\rho}_\lambda \leq \inf_{\rho \in \mathcal{M}^1_+(\Theta)} \left\{ \lambda \int R d\rho + 2 f(\lambda, n) + 2 K(\rho, \pi) + 2 \log \left( \frac{2}{\varepsilon} \right) \right\}.
\]

Now, we work with \( \tilde{\rho}_\lambda = \arg\min_{\rho \in \mathcal{F}} K(\rho, \hat{\rho}_\lambda) \). Plugging (8) into (11) we get, for any \( \rho \),

\[
\lambda \int R d\rho \leq f(\lambda, n) + K(\rho, \hat{\rho}_\lambda) - \log \int \exp(-\lambda r_n) d\pi + \log \left( \frac{2}{\varepsilon} \right).
\]

By definition of \( \hat{\rho}_\lambda \), we have:

\[
\lambda \int R d\hat{\rho}_\lambda \leq \inf_{\rho \in \mathcal{F}} \left\{ f(\lambda, n) + K(\rho, \hat{\rho}_\lambda) - \log \int \exp(-\lambda r_n) d\pi + \log \left( \frac{2}{\varepsilon} \right) \right\}
\]

and, using (8) again, we obtain:

\[
\lambda \int R d\hat{\rho}_\lambda \leq \inf_{\rho \in \mathcal{F}} \left\{ \lambda \int r_n d\rho + f(\lambda, n) + K(\rho, \pi) + \log \left( \frac{2}{\varepsilon} \right) \right\}.
\]

We plug (12) into the right-hand side to obtain:

\[
\lambda \int R d\hat{\rho}_\lambda \leq \inf_{\rho \in \mathcal{F}} \left\{ \lambda \int R d\rho + 2 f(\lambda, n) + 2 K(\rho, \pi) + 2 \log \left( \frac{2}{\varepsilon} \right) \right\}.
\]
This proves the second inequality of the theorem. In order to prove the claim
\[ B_{\lambda}(F) = B_{\lambda}(M_{+}^{1}(\Theta)) + \frac{2}{\lambda} \inf_{\rho \in F} K(\rho, \pi_{\frac{1}{2}}), \]
note that
\[
B_{\lambda}(F) = \inf_{\rho \in F} \left\{ \int R \log \left( \frac{g(\rho, n)}{g(\rho_{\frac{1}{2}})} \right) + K(\rho, \pi_{\frac{1}{2}}) \right\} \\
= \inf_{\rho \in F} \left\{ -\frac{2}{\lambda} \log \int \exp \left( -\frac{\lambda}{2} R \right) d\pi + \frac{2f(\lambda, n)}{\lambda} + \frac{2K(\rho, \pi_{\frac{1}{2}})}{\lambda} + \frac{2 \log \left( \frac{\lambda}{2} \right)}{\lambda} \right\} \\
= -\frac{2}{\lambda} \log \int \exp \left( -\frac{\lambda}{2} R \right) d\pi + \frac{2f(\lambda, n)}{\lambda} + \frac{2 \log \left( \frac{\lambda}{2} \right)}{\lambda} + \frac{2}{\lambda} \inf_{\rho \in F} K(\rho, \pi_{\frac{1}{2}}) \\
= B_{\lambda}(M_{+}^{1}(\Theta)) + \frac{2}{\lambda} \inf_{\rho \in F} K(\rho, \pi_{\frac{1}{2}}).
\]
This ends the proof. □

A.3. Proof of Theorem 4.3 (Subsection 4.2)

Proof of Theorem 4.3. As in the proof of Theorem 4.1, we apply Fubini, then (10) to the first inequality of (2) to obtain
\[
E \exp \left\{ \sup_{\rho} \int [\lambda[R(\theta) - R] - \lambda[r_{n}(\theta) - r_{n}] - g(\lambda, n)[R(\theta) - R]] \right\} \leq 1
\]
and we multiply both sides by \(\varepsilon/2\) to get
\[
\mathbb{P} \left\{ \sup_{\rho} \left[ \lambda - g(\lambda, n) \int R d\rho - \mathbb{R} \right] \geq \lambda \left[ \int r_{n} d\rho - \mathbb{R} \right] + \mathcal{K}(\rho, \pi) + \log \left( \frac{2}{\varepsilon} \right) \right\} \leq \frac{\varepsilon}{2} \quad (13)
\]
We now consider the second inequality in (2):
\[
E \exp \left\{ \lambda[r_{n}(\theta) - r_{n}] - \lambda[R(\theta) - R] - g(\lambda, n)[R(\theta) - R] \right\} \leq 1.
\]
The same derivation leads to
\[
\mathbb{P} \left\{ \sup_{\rho} \left[ \lambda - g(\lambda, n) \int r_{n} d\rho - \mathbb{R} \right] \geq \lambda \left[ \int r_{n} d\rho - \mathbb{R} \right] + \mathcal{K}(\rho, \pi) + \log \left( \frac{2}{\varepsilon} \right) \right\} \leq \frac{\varepsilon}{2} \quad (14)
\]
We combine (13) and (14) by a union bound argument, and we consider the complementary event: with probability at least 1 - \(\varepsilon\), simultaneously for all \(\rho \in M_{+}^{1}(\Theta)\),
\[
[\lambda - g(\lambda, n)] \left[ \int R d\rho - \mathbb{R} \right] \leq \lambda \left[ \int r_{n} d\rho - \mathbb{R} \right] + \mathcal{K}(\rho, \pi) + \log \left( \frac{2}{\varepsilon} \right), \quad (15)
\]
We now derive consequences of these two inequalities (in other words, we focus on the event where these two inequalities are satisfied). Using (9) in (15) yields

\[ \lambda \left[ \int r_n d\rho - \tau_n \right] \leq [\lambda + g(\lambda, n)] \left[ \int Rd\rho - \mathcal{R} \right] + \mathcal{K}(\rho, \pi) + \log \left( \frac{2}{\varepsilon} \right). \]  \hfill (16)

We plug (16) into the right-hand side to obtain:

\[ \lambda - g(\lambda, n) \left[ \int Rd\hat{\rho}_\lambda - \mathcal{R} \right] \leq \inf_{\rho \in \mathcal{M}_{1}\left(\Theta\right)} \left\{ \lambda \left[ \int r_n d\rho - \tau_n \right] + \mathcal{K}(\rho, \pi) + \log \left( \frac{2}{\varepsilon} \right) \right\}. \]

Now, we work with \( \hat{\rho}_\lambda \). Plugging (8) into (13) we get

\[ \lambda - g(\lambda, n) \left[ \int Rd\hat{\rho} \right] \leq \mathcal{K}(\rho, \hat{\rho}_\lambda) - \log \int \exp[-\lambda(r_n - \tau_n)]d\pi + \log \left( \frac{2}{\varepsilon} \right). \]

By definition of \( \hat{\rho}_\lambda \), we have:

\[ \lambda - g(\lambda, n) \left[ \int Rd\hat{\rho}_\lambda - \mathcal{R} \right] \leq \inf_{\rho \in \mathcal{F}} \left\{ \mathcal{K}(\rho, \hat{\rho}_\lambda) - \log \int \exp[-\lambda(r_n - \tau_n)]d\pi + \log \left( \frac{2}{\varepsilon} \right) \right\}. \]

Then, apply (8) again to get:

\[ \lambda - g(\lambda, n) \left[ \int Rd\hat{\rho}_\lambda - \mathcal{R} \right] \leq \inf_{\rho \in \mathcal{F}} \left\{ \lambda \int (r_n - \tau_n)d\rho + \mathcal{K}(\rho, \pi) + \log \left( \frac{2}{\varepsilon} \right) \right\}. \]

Plug (16) into the right-hand side to get

\[ \lambda - g(\lambda, n) \left[ \int Rd\hat{\rho}_\lambda - \mathcal{R} \right] \leq \inf_{\rho \in \mathcal{F}} \left\{ [\lambda + g(\lambda, n)] \int (R - \mathcal{R})d\rho + 2\mathcal{K}(\rho, \pi) + 2\log \left( \frac{2}{\varepsilon} \right) \right\}. \]

\[ \square \]

**A.4. Proofs of Section 5**

*Proof of Lemma 5.1.* Combine Theorem 2.1 p. 25 and Lemma 2.2 p. 27 in Boucheron et al. 2013. \( \square \)
Proof of Lemma 5.2. Apply Theorem 2.10 in Boucheron et al. [2013], and plug the margin assumption. □

Proof of Corollary 5.4. We remind that thanks to (6) it is enough to prove the claim for $F_1$. We apply Theorem 4.2 to get:

$$B_{\lambda}(F_1) = \inf_{(m, \sigma^2)} \left\{ \int R \Phi_{m, \sigma^2} + \frac{\lambda}{n} + 2 \frac{K(\Phi_{m, \sigma^2}, \pi) + \log \left( \frac{2}{\epsilon} \right)}{\lambda} \right\}$$

$$= \inf_{(m, \sigma^2)} \left\{ \int R \Phi_{m, \sigma^2} + \frac{\lambda}{n} + 2 \frac{d \left[ \frac{1}{2} \log \left( \frac{\sigma^2}{\sigma^2} \right) + \frac{\sigma^2}{\sigma^2} + \frac{\|m\|^2}{\sigma^2} - \frac{d}{2} + \log \left( \frac{2}{\epsilon} \right) \right]}{\lambda} \right\}.$$  

Note that the minimizer of $R$, $\tilde{\theta}$, is not unique (because $f_{\theta}(x)$ does not depend on $\|\theta\|$) and we can chose it in such a way that $\|\tilde{\theta}\| = 1$. Then

$$R(\theta) - R = \mathbb{E} \left[ 1_{(\theta, X)^T Y < 0} - 1_{(\tilde{\theta}, X)^T Y < 0} \right] \leq \mathbb{E} \left[ 1_{(\theta, X)^T \tilde{\theta}, X < 0} \right]$$

$$= \mathbb{P} \left( (\theta, X)^T \tilde{\theta}, X < 0 \right) \leq c \left\| \frac{\theta}{\|\theta\|} - \tilde{\theta} \right\| \leq 2c \|\theta - \tilde{\theta}\|.$$  

So:

$$B_{\lambda}(F_1) \leq R + \inf_{(m, \sigma^2)} \left\{ 2c \int \|\theta - \tilde{\theta}\| \Phi_{m, \sigma^2}(d\theta) \right. \right.$$  

$$+ \frac{\lambda}{n} + \frac{d}{\lambda} \left[ \frac{1}{2} \log \left( \frac{\sigma^2}{\sigma^2} \right) + \frac{\sigma^2}{\sigma^2} + \frac{\|m\|^2}{\sigma^2} - \frac{d}{2} + \log \left( \frac{2}{\epsilon} \right) \right] \left\}.$$  

We now restrict the infimum to distributions $\nu$ such that $m = \tilde{\theta}$:

$$B(F_1) \leq R + \inf_{\sigma^2} \left\{ 2c \sqrt{d} \sigma + \frac{\lambda}{n} + \frac{d \log \left( \frac{\sigma^2}{\sigma^2} \right) + \frac{2 \sigma^2}{\sigma^2} + \frac{\sigma^2}{\sigma^2} - d + 2 \log \left( \frac{2}{\epsilon} \right)}{\lambda} \right\}.$$  

We put $\sigma = \frac{1}{2\lambda}$ and substitute $\frac{1}{\sqrt{d}}$ for $\tilde{\theta}$ to get

$$B(F_1) \leq R + \frac{\lambda}{n} + \frac{c \sqrt{d} + d \log \left( \frac{4 \lambda^2}{\sigma^2} \right) + \frac{\sigma^2}{2\lambda^2} + d + 2 \log \left( \frac{2}{\epsilon} \right)}{\lambda}.$$  

Substitute $\sqrt{nd}$ for $\lambda$ to get the desired result. □

Proof of Corollary 5.5. We apply Theorem 4.3

$$\int (R - \bar{R}) d\tilde{\rho}_\lambda$$

$$\leq \inf_{m, \sigma^2} \left\{ \frac{\lambda + g(\lambda, n)}{\lambda - g(\lambda, n)} \int (R - \bar{R}) d\Phi_{m, \sigma^2} + \frac{1}{\lambda - g(\lambda, n)} \left( 2K(\Phi_{m, \sigma^2}, \pi) + 2 \log \left( \frac{2}{\epsilon} \right) \right) \right\}.$$  

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where $\lambda < \frac{2n}{c+1}$. Computations similar to those in the the proof of Corollary 5.4 lead to

$$\int Rd\bar{\rho}_\lambda \leq R + \inf_{m,\sigma^2}\left\{2c\frac{\lambda + g(\lambda, n)}{\lambda - g(\lambda, n)} \int \frac{||\theta - \bar{\theta}||\Phi_{m,\sigma^2}(d\theta)}{\lambda - g(\lambda, n)} \right\} + 2\sum_{j=1}^{d} \left[ \frac{1}{2} \log \left( \frac{\sigma^2}{\sigma^2} \right) + \frac{m_j^2}{\sigma^2} - \frac{d}{2} + \log \left( \frac{2}{\epsilon} \right) \right].$$

taking $m = \bar{\theta}$ and $\lambda = \frac{2n}{c+2}$, we get the result. □

**A.5. Proofs of Section 6**

**Proof of Lemma [b.1]** For fixed $\theta$ we can upper bound the individual risk such that:

$$0 \leq \max(0, 1 - \theta, X_i > Y_i) \leq 1 + |\theta, X_i > |$$

such that we can apply Hoeffding’s inequality conditionally on $X_i$ and fixed $\theta$. We get,

$$E\left[ \exp \left( \lambda(RH - r_H^m) \right) | X_1, \cdots, X_n \right] \leq \exp \left\{ \frac{\lambda^2}{8n^2} \sum_{i=1}^{n} (1 + |\theta, X_i > |)^2 \right\} \leq \exp \left\{ \frac{\lambda^2}{4n} + \frac{\lambda^2 c_x^2}{4n} \|\theta\|^2 \right\}$$

where the last inequality stems from the fact that $(a + b)^2 \leq 2(a^2 + b^2)$ and the fact that we have supposed the $X_i$ to be bounded. We can take the expectation of this term with respect to the $X_i$’s and with respect to our Gaussian prior.

$$\pi\left\{ E\left[ \exp \left( \lambda(RH - r_H^m) \right) \right] \right\} \leq \exp \left( \frac{\lambda^2}{4n} \right) \int \exp \left( \frac{\lambda^2 c_x^2}{4n} \|\theta\|^2 - \frac{1}{2\sigma^2} \|\theta\|^2 \right) d\theta \leq \exp \left( \frac{\lambda^2}{4n} \right) \int \exp \left( -\frac{1}{2} \left[ \frac{1}{\sigma^2} - \frac{\lambda^2 c_x^2}{4n} \right] \|\theta\|^2 \right) d\theta$$

The integral is a properly defined Gaussian integral under the hypothesis that $\frac{1}{\sigma^2} - \frac{\lambda^2 c_x^2}{4n} > 0$ hence $\lambda < \frac{2}{c_x} \sqrt{n^2}$. The integral is proportional to a Gaussian and we can directly write:

$$\pi\left\{ E\left[ \exp \left( \lambda(RH - r_H^m) \right) \right] \right\} \leq \frac{\exp \left( \frac{\lambda^2}{4n} \right)}{\sqrt{1 - \sigma^2 \lambda^2 c_x^2}}$$

writing everything in the exponential gives the desired result. □
Proof of Corollary 6.2. We apply Theorem 4.2 to get:

\[ B\lambda(F_1) = \inf_{m, \sigma^2} \left\{ \int R^H d\Phi_{m, \sigma^2} + \frac{\lambda}{2n} - \frac{1}{\lambda} \log \left( 1 - \frac{\theta^2 \lambda^2 \sigma^2}{4n} \right) + \frac{1}{\lambda} K(\Phi_{m, \sigma^2}, \pi) + \log \left( \frac{2}{\lambda} \right) \right\} \]

\[ = \inf_{m, \sigma^2} \left\{ \int R^H d\Phi_{m, \sigma^2} + \frac{\lambda}{2n} - \frac{1}{\lambda} \log \left( 1 - \frac{\theta^2 \lambda^2 \sigma^2}{4n} \right) \right. \]

\[ + \left. 2 \sum_{j=1}^{d} \left[ \frac{1}{2} \log \left( \frac{2^j}{\sigma^2} \right) + \frac{\sigma^2}{\sigma^2} \right] + \|m\|^2 \right\}. \]

We use the fact that the hinge loss is Lipschitz and that the \( (X_i) \) are uniformly bounded \( \|X\|_\infty < c_x \). We get \( R^H(\theta) \leq R^H + c_x \sqrt{d}\|\theta - \bar{\theta}\| \) and restrict the infemum to distributions \( \nu \) such that \( m = \bar{\theta} \):

\[ B(F_1) \leq R^H + \inf_{\sigma^2} \left\{ c_x \sigma^2 + \frac{\lambda}{2n} - \frac{1}{\lambda} \log \left( 1 - \frac{\theta^2 \lambda^2 \sigma^2}{4n} \right) + \frac{\lambda}{2n} \log \left( \frac{2^j}{\sigma^2} \right) + \frac{\sigma^2}{\sigma^2} \right\}. \]

We specify \( \sigma^2 = \frac{1}{\sqrt{dn}} \) and \( \lambda = c_x \sqrt{\frac{d}{n}} \) such that we get:

\[ B(F_1) \leq R^H + c_x \sqrt{\frac{d}{n}} \frac{\sqrt{\theta^2}}{2c_x \sqrt{n}} - c_x \frac{1}{\sqrt{dn}} \log \left( 1 - \frac{1}{4} \right) + \frac{c_x}{\sqrt{d}} \log \left( \frac{\theta^2 \sqrt{n\theta}}{\theta^2 \sqrt{n\theta}} \right) + c_x \frac{2d}{\sqrt{d}} \frac{1}{\sqrt{d}} - d + 2 \log \left( \frac{2}{\lambda} \right). \]

To get the correct rate we take the prior variance to be \( \theta^2 = \frac{1}{\theta} \) by replacing in the above equation we get the desired result.

\[ \square \]

Proof of Theorem 6.3. From [Nesterov 2004] (th. 3.2.2) we have the following bound on the objective function minimized by VB, (the objective is not uniformly Lipschitz)

\[ \rho^k(n, \frac{1}{\lambda} K(\rho^k, \pi) - \inf_{\rho \in F_1} \left\{ \rho(n^H, \frac{1}{\lambda} K(\rho, \pi) \right\} \leq \frac{LM}{\sqrt{1 + k}}. \] (17)

We have from equation (11) specified for measures \( \rho^k \) probability \( 1 - \varepsilon \),

\[ \lambda \int n^H d\rho^k \leq \lambda \int R^H d\rho^k + f(\lambda, n) + K(\rho^k, \pi) + \log \left( \frac{1}{\varepsilon} \right) \]

Combining the two equations yields,

\[ \int R^H d\rho^k \leq \frac{LM}{\sqrt{1 + k}} + \frac{1}{\lambda} f(n, \lambda) + \inf_{\rho \in F_1} \left\{ \rho(n^H, \frac{1}{\lambda} K(\rho, \pi) \right\} + \frac{1}{\lambda} \log \left( \frac{1}{\varepsilon} \right) \]

We can therefore write for any \( \rho \in F_1 \),

\[ \int R^H d\rho^k \leq \frac{LM}{\sqrt{1 + k}} + \frac{1}{\lambda} f(n, \lambda) + \rho(n^H, \frac{1}{\lambda} K(\rho, \pi) + \frac{1}{\lambda} \log \left( \frac{1}{\varepsilon} \right) \]
Using equation (11) a second time we get with probability $1 - \varepsilon$

$$\int R^H d\rho^k \leq \frac{LM}{\sqrt{1 + k}} +\frac{2}{\lambda} f(n, \lambda) + \rho(R^H) + \frac{2}{\lambda} \mathcal{K}(\rho, \pi) + \frac{2}{\lambda} \log \frac{2}{\varepsilon}$$

Because this is true for any $\rho \in \mathcal{F}_1$ in $1 - \varepsilon$ we can write the bound for the smallest measure in $\mathcal{F}_1$.

$$\int R^H d\rho^k \leq \frac{LM}{\sqrt{1 + k}} +\frac{2}{\lambda} f(n, \lambda) + \inf_{\rho \in \mathcal{F}_1} \left\{ \rho(R^H) + \frac{2}{\lambda} \mathcal{K}(\rho, \pi) \right\} + \frac{2}{\lambda} \log \frac{2}{\varepsilon}$$

By taking the Gaussian measure with variance $\frac{1}{n}$ and mean $\bar{\theta}$ in the infemum and taking $\lambda = \frac{1}{\sqrt{n}}$ and $\theta = \frac{1}{n}$, we can use the results of Corrolary 6.2 to get the result. 

A.6. Proofs of Section 7

Proof of Lemma 7.1. The idea of the proof is to use Hoeffding’s decomposition of U-statistics combined with Hoeffding’s inequality for iid random variables. This was done in ranking by Clémencçon et al. [2008], and later in Robbiano [2013], Ridgway et al. [2014] for ranking via aggregation and Bayesian statistics. The proof is as follows: we define

$$q_{i,j}^\theta = 1(Y_i - Y_j)(f_0(X_i) - f_0(X_j)) < 0 - R(\theta)$$

so that

$$U_n := \frac{1}{n(n - 1)} \sum_{i,j} q_{i,j}^\theta = r_n(\theta) - R(\Theta).$$

From Hoeffding [1948] we have

$$U_n = \frac{1}{n!} \sum_{\pi} \left[ \frac{1}{n} \sum_{i=1}^{[\frac{n}{2}]} \sum_{\pi(i), \pi(i + [\frac{n}{2}])} q_{i,j}^\theta \right]$$

where the sum is taken over all the permutations $\pi$ of $\{1, \ldots, n\}$. Jensen’s inequality leads to

$$\mathbb{E} \exp[\lambda U_n] = \mathbb{E} \exp \left[ \frac{1}{n} \sum_{\pi} \left[ \frac{1}{n} \sum_{i=1}^{[\frac{n}{2}]} \sum_{\pi(i), \pi(i + [\frac{n}{2}])} q_{i,j}^\theta \right] \right]$$

$$\leq \frac{1}{n} \sum_{\pi} \mathbb{E} \exp \left[ \frac{\lambda}{\left[\frac{n}{2}\right]} \sum_{i=1}^{[\frac{n}{2}]} q_{i,j}^\theta \right].$$

We now use, for each of the terms in the sum we use the same argument as in the proof of Lemma 5.1 to get

$$\mathbb{E} \exp[\lambda U_n] \leq \frac{1}{n} \sum_{\pi} \exp \left[ \frac{\lambda^2}{2\left[\frac{n}{2}\right]} \right] \leq \exp \left[ \frac{\lambda^2}{n - 1} \right]$$

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(in the last step, we used \( \lfloor \frac{d}{2} \rfloor \geq (n-1)/2 \)). We proceed in the same way to upper bound \( \mathbb{E} \exp[-\lambda U_n] \). □

**Proof of Lemma 7.2.** As already done above, we use Bernstein inequality and Hoeffding decomposition. Fix \( \theta \). We define this time

\[
q_{i,j}^\theta = 1\{\langle \theta, X_i - X_j \rangle (Y_i - Y_j) < 0\} - 1\{[\sigma(X_i) - \sigma(X_j)](Y_i - Y_j) < 0\} - R(\theta) + \bar{R}
\]

so that

\[
U_n := r_n(\theta) - \bar{r}_n - R(\theta) + \bar{R} = \frac{1}{n(n-1)} \sum_{i\neq j} q_{i,j}^\theta.
\]

Then,

\[
U_n = \frac{1}{n!} \sum_{\pi} \frac{1}{\lfloor \frac{n}{2} \rfloor} \sum_{i=1}^{\lfloor \frac{n}{2} \rfloor} q_{\pi(i),\pi(i+\lfloor \frac{n}{2} \rfloor)}^\theta.
\]

Jensen’s inequality:

\[
\mathbb{E} \exp[\lambda U_n] = \mathbb{E} \exp \left[ \lambda \frac{1}{n!} \sum_{\pi} \frac{1}{\lfloor \frac{n}{2} \rfloor} \sum_{i=1}^{\lfloor \frac{n}{2} \rfloor} q_{\pi(i),\pi(i+\lfloor \frac{n}{2} \rfloor)}^\theta \right]
\]

\[
\leq \frac{1}{n!} \sum_{\pi} \mathbb{E} \exp \left[ \lambda \frac{1}{\lfloor \frac{n}{2} \rfloor} \sum_{i=1}^{\lfloor \frac{n}{2} \rfloor} q_{\pi(i),\pi(i+\lfloor \frac{n}{2} \rfloor)}^\theta \right].
\]

Then, for each of the terms in the sum, use Bernstein’s inequality:

\[
\mathbb{E} \exp \left[ \lambda \frac{1}{\lfloor \frac{n}{2} \rfloor} \sum_{i=1}^{\lfloor \frac{n}{2} \rfloor} q_{\pi(i),\pi(i+\lfloor \frac{n}{2} \rfloor)}^\theta \right] \leq \exp \left[ \frac{\mathbb{E}((q_{\pi(1),\pi(1+\lfloor \frac{n}{2} \rfloor)}^\theta)^2) \lambda^2}{2 \left( 1 - 2 \left( \frac{\lambda}{\lfloor \frac{n}{2} \rfloor} \right) \right)} \right].
\]

We use again \( \lfloor \frac{n}{2} \rfloor \geq (n-1)/2 \). Then, as the pairs \((X_i, Y_i)\) are iid, we have \( \mathbb{E}((q_{\pi(1),\pi(1+\lfloor \frac{n}{2} \rfloor)}^\theta)^2) = \mathbb{E}((q_{1,2}^\theta)^2) \) and then \( \mathbb{E}((q_{1,2}^\theta)^2) \leq C[R(\theta) - \bar{R}] \) thanks to the margin assumption. So

\[
\mathbb{E} \exp \left[ \lambda \frac{1}{\lfloor \frac{n}{2} \rfloor} \sum_{i=1}^{\lfloor \frac{n}{2} \rfloor} q_{\pi(i),\pi(i+\lfloor \frac{n}{2} \rfloor)}^\theta \right] \leq \exp \left[ \frac{C[R(\theta) - \bar{R}] \lambda^2}{\left( 1 - \frac{4\lambda}{n-1} \right)} \right].
\]

This ends the proof of the proposition. □

**Proof of Corollary 7.4.** The calculations are similar to the ones in the proof of Corollary 5.4 so we don’t give the details. Note that when we reach

\[
B_\lambda(F_1) \leq \bar{R} + \frac{2\lambda}{n-1} + \frac{c\sqrt{d} + d \log(2\lambda) + 2 \log \left( \frac{2\lambda}{\delta} \right)}{\lambda},
\]

an approximate minimization with respect to \( \lambda \) leads to the choice \( \lambda = \sqrt{\frac{d(n-1)}{2}} \). □
A.7. Proofs of Section 8

Proof. First, note that, for any \( \rho \),

\[
\mathcal{K}(\rho, \pi) = \beta \int (R - \overline{R})d\rho + \mathcal{K}(\rho, \pi) + \log \int \exp \left[ -\beta (R - \overline{R}) \right] d\pi \leq \beta \int (R - \overline{R})d\rho + \mathcal{K}(\rho, \pi).
\]

Now, we define a subset of \( \mathcal{F} \) that will be used for the calculation of the bound. We define for \( \delta > 0 \) the probability distribution \( \rho_{U,V,\delta}(d\theta) \) as \( \pi \) conditioned to \( \theta = \mu \nu^T \) with \( \mu \) is uniform on \{\forall (i, \ell), |\mu_{i, \ell} - U_{i, \ell}| \leq \delta \} \) and \( \nu \) is uniform on \{\forall (j, \ell), |\nu_{i, \ell} - V_{j, \ell}| \leq \delta \}.

Note that

\[
\int (R - \overline{R})d\rho_{M,N,\delta} = \int \mathbb{E}((\theta_X - M_X)^2)\rho_{U,V,\delta}(d\theta) \leq \int 3\mathbb{E}((UV^T)_X - M_X)^2)\rho_{U,V,\delta}(d(\mu, \nu)) + 3 \int \mathbb{E}((\nu^T)_X - (UV^T)_X)^2)\rho_{U,V,\delta}(d(\mu, \nu)) + 3 \int \mathbb{E}((\mu^T)_X - (UV^T)_X)^2)\rho_{U,V,\delta}(d(\mu, \nu)).
\]

By definition, the first term is = 0. Moreover:

\[
\int \mathbb{E}((UV^T)_X - (UV^T)_X)^2)\rho_{U,V,\delta}(d(\mu, \nu)) = \int \frac{1}{m_1m_2} \sum_{i,j} \left[ \sum_k U_{i,k}(\nu_{j,k} - V_{j,k}) \right]^2 \rho_{U,V,\delta}(d(\mu, \nu)) \leq \int \frac{1}{m_1m_2} \sum_{i,j} \left[ \sum_k U_{i,k}^2 \left[ \sum_k (\nu_{j,k} - V_{j,k})^2 \right] \right] \rho_{U,V,\delta}(d(\mu, \nu)) \leq KrC^2\delta^2.
\]

In the same way,

\[
\int \mathbb{E}((\mu^T)_X - (UV^T)_X)^2)\rho_{U,V,\delta}(d(\mu, \nu)) \leq \int ||\mu - U||_F^2 ||\nu||_F^2 \rho_{U,V,\delta}(d(\mu, \nu)) \leq Kr(C + \delta)^2\delta^2.
\]

So:

\[
\int (R - \overline{R})d\rho_{M,N,\delta} \leq 2Kr\delta^2(C + \delta^2).
\]

Now, let us consider the term \( \mathcal{K}(\rho_{U,V,\delta}, \pi) \). An explicit calculation is possible but tedious. Instead, we might just introduce the set \( \mathcal{G}_\delta = \{\theta = \mu \nu^T, ||\mu - U||_F \leq \delta, ||\nu - V||_F \leq \delta\} \).
and note that $\mathcal{K}(\rho_{U,V,\delta}, \pi) \leq \log \frac{1}{\pi(m_1)}$. An upper bound for $\mathcal{G}_t$ is calculated page 317-320 in [Alquier 2014] and the result is given by (10) in this reference:

$$\mathcal{K}(\rho_{U,V,\delta}, \pi) \leq 4\delta^2 + 2\|U\|_F^2 + 2\|N\|_F^2 + 2 \log(2) + (m_1 + m_2) r \log \left( \frac{1}{\delta} \sqrt{\frac{3\pi(m_1 \vee m_2)K}{4}} \right) + 2K \log \left( \frac{\Gamma(a)3^{a+1}\exp(2)}{b^{a+1/2}} \right)$$

as soon as the restriction $b \leq \frac{\delta^2}{2m_1K \log(2m_1K)}, \frac{\delta^2}{2m_2K \log(2m_2K)}$ is satisfied. So we obtain:

$$\mathcal{K}(\rho_{U,V,\delta}, \pi_\beta) \leq \beta 2K r \delta^2(C + \delta^2) + 4\delta^2 + 2\|U\|_F^2 + 2\|N\|_F^2 + 2 \log(2) + (m_1 + m_2) r \log \left( \frac{1}{\delta} \sqrt{\frac{3\pi(m_1 \vee m_2)K}{4}} \right) + 2K \log \left( \frac{\Gamma(a)3^{a+1}\exp(2)}{b^{a+1/2}} \right).$$

Note that $\|U\|_F^2 \leq C^2 r m_1, \|V\|_F^2 \leq C^2 r m_2$ and $K \leq m_1 + m_2$ so it is clear that the choice $\delta = \sqrt{\frac{b}{2}}$ and $b \leq \frac{1}{2\beta(m_1 \vee m_2) \log(2K(m_1 \vee m_2))}$ leads to the existence of a constant $C(a, C)$ such that

$$\mathcal{K}(\rho_{U,V,\delta}, \pi_\beta) \leq C(a, C) \left\{ r(m_1 + m_2) \log [\beta b(m_1 + m_2)K] + \frac{1}{\beta} \right\}.$$

\[\Box\]

\section*{B. Implementation details}

\subsection*{B.1. Sequential Monte Carlo}

Tempering SMC approximates iteratively a sequence of distribution $\rho_{\lambda_t}$, with

$$\rho_{\lambda_t}(d\theta) = \frac{1}{Z_t} \exp \left( -\lambda_t r_n(\theta) \right) \pi(d\theta),$$

and temperature ladder $\lambda_0 = 0 < \ldots < \lambda_T = \lambda$. The pseudo code below is given for an adaptive sequence of temperatures.
Algorithm 1 Tempering SMC

Input $N$ (number of particles), $\tau \in (0,1)$ (ESS threshold), $\kappa > 0$ (random walk tuning parameter)

Init. Sample $\theta_i^0 \sim \pi_0(\theta)$ for $i = 1$ to $N$, set $t \leftarrow 1$, $\lambda_0 = 0$, $Z_0 = 1$.

Loop

a. Solve in $\lambda_t$ the equation

$$\frac{\{\sum_{i=1}^N w_t(\theta_{t-1}^i)\}^2}{\sum_{i=1}^N \{w_t(\theta_{t-1}^i)\}^2} = \tau N, \quad w_t(\theta) = \exp\left[-(\lambda_t - \lambda_{t-1})r_n(\theta)\right]$$

(18)

using bisection search. If $\lambda_t \geq \lambda_T$, set $Z_T = Z_{t-1} \times \left\{ \frac{1}{N} \sum_{i=1}^N w_t(\theta_{t-1}^i) \right\}$, and stop.

b. Resample: for $i = 1$ to $N$, draw $A_i^t$ in $1, \ldots, N$ so that $P(A_i^t = j) = w_t(\theta_{t-1}^j)/\sum_{k=1}^N w_t(\theta_{t-1}^k)$; see Algorithm 2 in the appendix.

c. Sample $\theta_t^i \sim M_t(\theta_{t-1}^A_i, d\theta)$ for $i = 1$ to $N$ where $M_t$ is a MCMC kernel that leaves invariant $\pi_t$; see comments below.

d. Set $Z_t = Z_{t-1} \times \left\{ \frac{1}{N} \sum_{i=1}^N w_t(\theta_{t-1}^i) \right\}$.

The algorithm outputs a weighted sample $(w_T^i, \theta_T^i)$ approximately distributed as target posterior, and an unbiased estimator of the normalizing constant $Z_T$.

Step b. of algorithm 1 depends of a resampling algorithm. We choose to use Systematic resampling, described in Algorithm 2.
Algorithm 2 Systematic resampling

Input: Normalised weights $W^j_t := w_t(\theta^j_{t-1}) / \sum_{i=1}^{N} w_t(\theta^i_{t-1})$.

Output: indices $A^i \in \{1, \ldots, N\}$, for $i = 1, \ldots, N$.

a. Sample $U \sim \mathcal{U}([0, 1])$.

b. Compute cumulative weights as $C^n = \sum_{m=1}^{n} NW^m$.

c. Set $s \leftarrow U$, $m \leftarrow 1$.

d. For $n = 1 : N$

   While $C^m < s$ do $m \leftarrow m + 1$.

   $A^n \leftarrow m$, and $s \leftarrow s + 1$.

End For

For the MCMC step, we used a Gaussian random-walk Metropolis kernel, with a covariance matrix for the random step that is proportional to the empirical covariance matrix of the current set of simulations.

B.2. Optimizing the bound

A natural idea to find a global optimum of the objective is to try to solve a sequence of local optimization problems with increasing temperatures. For $\gamma = 0$ the problem can be solved exactly (as a KL divergence between two Gaussians). Then, for two consecutive temperatures, the corresponding solutions should be close enough.

This idea has been coined under several names. It has a long history in variational algorithm under the name deterministic annealing. Yuille [2010] uses it on mean field on Gibbs distribution for Markov random fields. In addition the intermediate results can be of interest in our case for selecting the temperature. One can compute the bound at almost no additional cost as a function of the current risk. In turns this can be used to monitor the bound.
Algorithm 3 Deterministic annealing

**Input** \((\lambda_t)_{t \in [0,T]}\) a sequence of temperature

**Init.** Set \(m = 0\) and \(\Sigma = \vartheta I_d\), the values minimizing KL-divergence for \(\lambda = 0\)

**Loop** \(t = 1, \ldots, T\)

a. \(m^{\lambda_t}, \Sigma^{\lambda_t} = \text{Minimize} \mathcal{L}^{\lambda_t}(m, \Sigma)\) using some local optimization routine with initial points \(m^{\lambda_{t-1}}, \Sigma^{\lambda_{t-1}}\)

b. Break if the empirical bound increases.

**End Loop**

---

Figure 2: Deterministic annealing on a Pima Indians with one covariate and full model resp.
The right panel gives the empirical bound obtained for the DA method (in red) and the dot are direct global optimization based on L-BFGS algorithms from starting values drawn from the prior. Each optimization problem is repeated 20 times.

---

We find that using a deterministic annealing algorithm with a limited amount of steps helps in finding a high enough optimum. On the left panel of Figure 2, we can see the one dimensional case where the initial problem \(\gamma = 0\) corresponds to a convex minimization problem and where the increasing temperature gradually complexifies the optimization problem. Figure 2 shows that the solution given by DA is in average lower than randomly
C. Stochastic gradient descent

The stochastic gradient descent algorithm used in Section ?? is described as Algorithm 4.

Algorithm 4 Stochastic Gradient Descent

Input $B$ a batch size, an unbiased estimator of the gradient $\hat{\nabla} B f$, $\eta \in (0, 1)$ and $c$

While ~converged
  a. $x_{t+1} = x_t - \lambda_t \hat{\nabla} B f(x_t)$
  b. Update $\lambda_{t+1} = \frac{1}{(t+c)\eta}$

End Loop

In all our experiment we take $c = 1$ and $\eta = 0.9$. 

initialized optimization.