ON THE ROLE OF DATA IN PAC-BAYES BOUNDS

GINTARE KAROLINA DZIUGAITE\textsuperscript{1}, KYLE HSU\textsuperscript{2,3}, WASEEM GHARBIEH\textsuperscript{1}, AND DANIEL M. ROY\textsuperscript{2,3}

ABSTRACT. The dominant term in PAC-Bayes bounds is often the Kullback–Leibler divergence between the posterior and prior. For so-called linear PAC-Bayes risk bounds based on the empirical risk of a fixed posterior kernel, it is possible to minimize the expected value of the bound by choosing the prior to be the expected posterior, which we call the oracle prior on the account that it is distribution dependent. In this work, we show that the bound based on the oracle prior can be suboptimal: In some cases, a stronger bound is obtained by using a data-dependent oracle prior, i.e., a conditional expectation of the posterior, given a subset of the training data that is then excluded from the empirical risk term. While using data to learn a prior is a known heuristic, its essential role in optimal bounds is new. In fact, we show that using data can mean the difference between vacuous and nonvacuous bounds. We apply this new principle in the setting of nonconvex learning, simulating data-dependent oracle priors on MNIST and Fashion MNIST with and without held-out data, and demonstrating new nonvacuous bounds in both cases.

1. INTRODUCTION

In this work, we are interested in the application of PAC-Bayes bounds \cite{16, 26} to the problem of understanding the generalization properties of learning algorithms. Our focus will be on supervised learning from i.i.d. data, although PAC-Bayes theory has been generalized far beyond this setting. (Guedj \cite{5} provides a survey.) In our setting, PAC-Bayes bounds control the risk of Gibbs classifiers, i.e., randomized classifiers whose predictions, on each input, are determined by a classifier $h$ sampled according to some distribution $Q$ on the hypothesis space $\mathcal{H}$. The hallmark of a PAC-Bayes bound is a normalized Kullback–Leibler (KL) divergence, $m^{-1}\text{KL}(Q||P)$, defined in terms of a Gibbs classifier $P$ that is called a “prior” because it must be independent of the $m$ data points used to estimate the empirical risk of $Q$.

In applications of PAC-Bayes bounds to generalization error, the contribution of the KL divergence often dominates the bound: In order to have a small KL with a strongly data-dependent posterior, the prior must, in essence, predict the posterior. This is difficult without knowledge of (or access to) the data distribution, and represents a significant statistical barrier to achieving tight bounds. Instead, many PAC-Bayesian analyses rely on generic priors chosen for analytical convenience.

Generic priors, however, are not inherent to the PAC-Bayes framework: every valid prior yields a valid bound. Therefore, if one does not optimize the prior to the data distribution, one may obtain a bound that is loose on the account of ignoring important, favorable properties of the data distribution.

\textsuperscript{1}Element AI, \textsuperscript{2}University of Toronto, \textsuperscript{3}Vector Institute
Langford and Blum [9] were the first to consider the problem of optimizing the prior to minimize the expected value of the high-probability PAC-Bayes bound. In the realizable case, they show that the problem reduces to optimizing the expected value of the KL term. More precisely, they consider a fixed learning rule $S \mapsto Q(S)$, i.e., a fixed posterior kernel, which chooses a posterior, $Q(S)$, based on a training sample, $S$. In the realizable case, the bound depends linearly on the KL term. Then $\mathbb{E}[\text{KL}(Q(S)||P)]$ is minimized by the expected posterior, $P^* = \mathbb{E}[Q(S)]$, i.e., $P^*(B) = \mathbb{E}[Q(S)(B)]$ for measurable $B \subseteq \mathcal{H}$. Both expectations are taken over the unknown distribution of the training sample, $S$. We call $P^*$ the oracle prior. If we introduce an $\mathcal{H}$-valued random variable $H$ satisfying $\mathbb{P}[H|S] = Q(S)$ a.s., we see that its distribution, $\mathbb{P}[H]$, is $P^*$ and thus, the “optimality” of the oracle $P^*$ is an immediate consequence of the identity $I(S;H) = \mathbb{E}[\text{KL}(Q(S)||P^*)] = \inf_{P'} \mathbb{E}[\text{KL}(Q(S)||P')]$, a well-known variational characterization of mutual information in terms of KL divergence.

For so-called linear PAC-Bayes bounds (introduced below), the oracle prior is seen to minimize the bound in expectation, even in the unrealizable setting. In light of this, having settled on a learning rule $S \mapsto Q(S)$, we might seek to achieve the tightest linear PAC-Bayes bound in expectation by attempting to approximate the oracle prior, $P^*$. Indeed, there is a large literature aimed at obtaining localized PAC-Bayes bounds via distribution-dependent priors, whether analytically [2, 12], through data [1, 18], or by way of concentration of measure, privacy, or stability [4, 20, 21, 23].

One of the contributions of this paper is the demonstration that an oracle prior may not yield the tightest linear PAC-Bayes risk bound in expectation. Proposition 3.1 gives conditions on a learning rule for there to exist data-dependent priors that improves the bound based upon the oracle prior. This phenomenon is a hitherto unstated principle of PAC-Bayesian analysis: data-dependent priors are sometimes necessary for tight bounds. Note that, as the prior must be independent of data used to compute the bound a posteriori, if $m$ training data are used to define the prior, only the remaining $n - m$ data should be used to compute the bound (i.e., compute the empirical risk term and divide the KL term). Note that all $n$ training data are used by the learning algorithm. We formalize these subtleties in the body of the paper.

We give an example of a learning problem where Proposition 3.1 implies data-dependent priors dominate. The example is adapted from a simple model of SGD in a linear model by Nagarajan and Kolter [17]. In the example, most input dimensions are noise with no signal and this noise accumulates in the learned weights. In our version, we introduce a learning rate schedule, and so earlier data points have a larger influence on the resulting weights. Even so, there is enough variability in the posterior that the oracle prior yields a vacuous bound. By conditioning on early data points, we reduce the variability and obtain nonvacuous bounds.

The idea of using data-dependent priors to obtain tighter bounds is not new [1, 4, 22, 23]. The idea is also implicit in the luckiness framework [25]. However, the observation that using data can be essential to obtaining a tight bound, even in full knowledge of the true distribution, is new, and brings a new dimension to the problem of constructing data-dependent priors.

In addition to demonstrating the theoretical role of data-dependent priors, we investigate them empirically, by studying generalization in nonconvex learning by stochastic
(sub)gradient methods. As data-dependent oracle priors depend on the unknown distribution, we propose to use held-out data (“ghost sample”) to estimate unknown quantities. Unlike standard held-out test set bounds, this approach relies implicitly on a type of stability demonstrated by SGD. We also propose approximations to data-dependent oracle priors that use no ghost sample, and find, given enough data, the advantage of the ghost sample diminishes significantly. We show that both approaches yield state-of-the-art nonvacuous bounds on MNIST and Fashion-MNIST for posterior Gaussian distributions whose means are clamped to the weights learned by SGD. Our MNIST bound (11%) improves significantly on the best published bound (46%) [28]. Finally, we evaluate minimizing a PAC-Bayes bound with our data-dependent priors as a learning algorithm. We demonstrate significant improvements to both classifier accuracy and bound tightness, compared to optimizing with generic priors.

2. Preliminaries

Let \( Z \) be a space of labeled examples, and write \( \mathcal{M}_1(Z) \) for the space of (probability) distributions on \( Z \). Given a space \( \mathcal{H} \) of classifiers and a bounded loss function \( \ell : \mathcal{H} \times Z \to [0,1] \), the risk of a hypothesis \( w \in \mathcal{H} \) is \( L_{\mathcal{D}}(w) = \mathbb{E}_{z \sim \mathcal{D}}[\ell(w,z)] \). We also consider Gibbs classifiers, i.e., elements \( P \) in the space \( \mathcal{M}_1(\mathcal{H}) \) of distributions on \( \mathcal{H} \), where risk is defined by \( L_{\mathcal{D}}(P) = \mathbb{E}_{w \sim P} L_{\mathcal{D}}(w) \). As \( \mathcal{D} \) is unknown, learning algorithms often work by optimizing an objective that depends on i.i.d. training data \( S \sim \mathcal{D}^n \), such as the empirical risk \( L_S(w) = L_{\mathcal{D}^n}(w) = \frac{1}{n} \sum_{i=1}^n \ell(w,z_i) \), where \( \hat{\mathcal{D}}_n \) is the empirical distribution of \( S \). Writing \( Q(S) \) for a data-dependent Gibbs classifier (i.e., a posterior), our primary focus is its risk, \( L_{\mathcal{D}}(Q(S)) \), and its relationship to empirical estimates, such as \( L_S(Q(S)) \).

We now present a bound within the PAC-Bayes framework [16, 26]. Write \( \text{KL}(Q || P) \) for the KL divergence between distributions \( Q, P \in \mathcal{M}_1(\mathcal{H}) \). (See Appendix A for definitions.) This bound follows from [14, Thm. 2], taking \( \beta = 1 - 1/(2\lambda) \). (See also Catoni [2, Thm. 1.2.6].)

**Theorem 2.1** (Linear PAC-Bayes bound). Let \( \beta, \delta \in (0,1) \), \( n \in \mathbb{N} \), \( \mathcal{D} \in \mathcal{M}_1(Z) \), and \( P \in \mathcal{M}_1(\mathcal{H}) \). With probability at least \( 1 - \delta \) over \( S \sim \mathcal{D}^n \), for all \( Q \in \mathcal{M}_1(\mathcal{H}) \),

\[
L_{\mathcal{D}}(Q) \leq \Psi_{\beta, \delta}(Q;P;S) \overset{\text{def}}{=} \frac{1}{\beta} L_S(Q) + \frac{\text{KL}(Q || P) + \log \frac{1}{\delta}}{2\beta(1-\beta)|S|}.
\]

We call \( P \) the **prior**. Since the bound is valid for all priors independent from \( S \), we can choose \( P \) by optimizing, e.g., the risk bound in expectation, as first proposed by Langford and Blum [9]:

**Theorem 2.2.** Let \( n \in \mathbb{N} \) and fix a probability kernel \( Q : Z^n \to \mathcal{M}_1(\mathcal{H}) \). For all \( \beta, \delta \in (0,1) \) and \( \mathcal{D} \in \mathcal{M}_1(Z) \), \( \mathbb{E}_{S \sim \mathcal{D}^n} \Psi_{\beta, \delta}(Q(S);P;S) \) is minimized by the “oracle” prior \( P^* = \mathbb{E}_{S \sim \mathcal{D}^n}[Q(S)] \).
3. Data-dependent oracle priors

Here we demonstrate that, for linear PAC-Bayes bounds, one may obtain a stronger bound using a “data-dependent oracle” prior, rather than the usual (data-independent) oracle prior. Further, using a data-dependent oracle prior may mean the difference between a vacuous and nonvacuous bound.

A typical PAC-Bayes generalization bound for a posterior kernel \( S \rightarrow Q(S) \) is based on the empirical risk \( L_S(Q(S)) \) computed from the same data fed to the kernel. Instead, let \( J \) be a (possibly random) subset of \([n]\) of size \( m < n \), independent from \( S \), let \( S_J \) denote the subsequence of data with indices in \( J \), and let \( S \setminus S_J \) denote the complementary subsequence. Consider now the PAC-Bayes bound based on the estimate \( \hat{L} \) of \( L \).

Here we demonstrate that, for linear PAC-Bayes bounds, one may obtain a stronger bound using a “data-dependent oracle” prior, rather than the usual (data-independent) oracle prior. Further, using a data-dependent oracle prior may mean the difference between a vacuous and nonvacuous bound.

Letting \( \hat{h} \) be a random element in \( \mathcal{H} \) satisfying \( \mathbb{P}[\hat{h}|S,J] = Q(S) \) a.s., the value of Eq. (2) is the conditional mutual information \( I(\hat{h};S|S_J) \). Define the information rate gain (from using \( S_J \) to choose the prior) and the excess bias (from using \( S \setminus S_J \) to estimate the risk) to be, respectively,

\[
R(\hat{h};S|S_J) = \frac{I(\hat{h};S)}{|S|} - \frac{I(\hat{h};S|S_J)}{|S \setminus S_J|}
\]

and

\[
B(\hat{h};S|S_J) = \mathbb{E}[L_{S,J}(\hat{h}) - L_S(\hat{h})].
\]

Note that, if \( J \) is chosen uniformly at random, then \( B(\hat{h};S|S_J) = 0 \). Using these two quantities, we can characterize whether a data-dependent prior can outperform the oracle prior.

Proposition 3.1. Let \( \beta, \delta \in (0,1) \), \( n \in \mathbb{N} \), and \( \mathcal{D} \in \mathcal{M}_1(Z) \). Fix \( Q : Z^n \rightarrow \mathcal{M}_1(\mathcal{H}) \) and let \( J \subseteq [n] \) be a (possibly random) subset of nonrandom cardinality \( m < n \), independent from \( S \sim \mathcal{D}^n \). Conditional on \( S \) and \( J \), let \( \hat{h} \) have distribution \( Q(S) \). Then

\[
\mathbb{E}_\mathcal{D}[\mathbb{E}_{S \sim \mathcal{D}^n} \Psi_{\beta,\delta}(Q(S),P^*(S_J);S \setminus S_J)] \leq \mathbb{E}_{S \sim \mathcal{D}^n} \Psi_{\beta,\delta}(Q(S),P^*;S)
\]

if and only if

\[
R(\hat{h};S|S_J) > 2(1 - \beta) B(\hat{h};S|S_J) + \frac{\log \frac{\delta}{\delta}}{n} \left( \frac{m}{n - m} \right).
\]

(Proof in Appendix B.) To interpret the proposition, consider \( \beta = 1/2 \): if the information rate gain is larger than the excess bias and a term that accounts for excess variance, then a data-dependent prior yields a tighter bound. It is reasonable to ask whether such situations arise. The following demonstration modifies a linear classification problem presented by Nagarajan and Kolter [17]. Their example was originally constructed to demonstrate potential roadblocks to studying generalization in SGD using uniform convergence arguments. Here, we modify the learning algorithm to have a decreasing step size, which causes earlier data points to have more influence. We exploit this property to achieve much tighter bounds.
using data-dependent oracle priors. Indeed, we will obtain nonvacuous bounds, while the optimal data-independent oracle prior yields a vacuous bound.

Example 3.2. Consider the hypothesis class $\mathcal{H} = \mathbb{R}^d$, interpreted as linear classifiers

$$\mathbf{x} \mapsto \text{sign}(\langle \mathbf{x}, \mathbf{w} \rangle) : \mathbb{R}^d \to \{-1, 0, 1\}, \quad \text{for } \mathbf{w} \in \mathbb{R}^d. \quad (7)$$

Assume that $d = K + D$, with $D \gg K$, and decompose each input $\mathbf{x} \in \mathbb{R}^d$ as $\mathbf{x} = (\mathbf{x}_1, \mathbf{x}_2)$, where $\mathbf{x}_1 \in \mathbb{R}^K$ and $\mathbf{x}_2 \in \mathbb{R}^D$. (We will decompose the weights similarly.) Labels $y$ take values in $\{\pm 1\}$ and so a prediction of 0 (i.e., on the decision boundary) is a mistake.

Consider the following $n$ i.i.d. training data: Let $\mathbf{u} \in \mathbb{R}^K$ be a nonrandom vector and, for each $i = 1, \ldots, n$, choose $y_i$ uniformly at random in $\{\pm 1\}$, let $\mathbf{x}_{i,1} = y_i \mathbf{u}$, and let $\mathbf{x}_{i,2}$ be multivariate normal with mean 0 and covariance $(\sigma^2/D) I_D$, where $I_D$ is the $D \times D$ identity matrix. Let $\mathcal{D}$ denote the common marginal distribution of each training example $(y_i, \mathbf{x}_i)$.

Consider the following one-pass learning algorithm: Let $\mathbf{w}_0 = 0$, then, for $t = 1, \ldots, n$ and $\eta_t = 1/t$, put $\mathbf{w}_t = \mathbf{w}_{t-1} + \eta_t y_i \mathbf{x}_i$. Then define the final weights to be $\mathbf{W} = \mathbf{w}_n + (0, \xi)$, where $\xi$ is an independent, zero-mean multivariate Gaussian with covariance $\kappa I_D$. Note that $\mathbf{w}_n = (\mathbf{w}_{n,1}, \mathbf{w}_{n,2})$ where $\mathbf{w}_{n,1} = (\sum_{i=1}^n \eta_i) \mathbf{u}$ and $\mathbf{w}_{n,2} = \sum_{i=1}^n \eta_i y_i \mathbf{x}_{i,2}$.

We will compare bounds based on oracle priors with those based on data-dependent oracle priors. To that end, let $S = \{(y_i, \mathbf{x}_i)\}_{i=1}^n$ and define $Q$ by $\mathbb{P}[W|S] = Q(S)$ a.s. Let $[n] = \{1, \ldots, n\}$. For a subset $J \subseteq [n]$, let $S_J$ be the corresponding subset of the data $S$ and let $S \setminus S_J$ be the complement.

Lemma 3.3. There are constants $n, D, \sigma, \kappa, \delta, u$ such that the infimum

$$\inf_{J \subseteq [n]} \inf_{\beta \in (0,1)} \inf_{P \in \mathbb{Z}^{|J|} \rightarrow \mathcal{H}_1(\mathcal{H})} \mathbb{E}\left[|\Psi_{\beta, \delta}(Q(S), P(S_J); S \setminus S_J)|\right], \quad (8)$$

is achieved by a nonempty set $J$. In particular, the optimal prior is data dependent.

Lower and upper bounds on the objective (Eq. (8)) for $J$ of the form $\{1, \ldots, \lfloor 100\alpha \rfloor\}$, for $\alpha \in [0, 1]$, are visualized in Fig. 1. Using a data-dependent prior in this scenario is critical for obtaining a nonvacuous bound. The derivation of these bounds as well as a sketch of the proof and a complete rigorous proof, can be found in Appendix C.
4. Data-dependent priors for SGD

As the theoretical results in the previous section demonstrate, data-dependent oracle priors can lead to dramatically tighter bounds. In this section, we take the first steps towards understanding whether data-dependent priors can aid us in the study of stochastic gradient descent (SGD).

In Section 3, we studied a posterior that depended more heavily on some data points than others. This property was introduced intentionally in order to serve as a toy model for SGD. Unlike the toy model, however, we know of no representations of the marginal distribution of the parameters learned by SGD that would allow us to optimize or compute a PAC-Bayes bound with respect to a data-dependent oracle prior. As a result, we are forced to make approximations.

Issues of tractability aside, another obstacle to using a data-dependent oracle prior is its dependence on the unknown data distribution. Ostensibly, this statistical barrier can be surmounted with extra data, although this would not make sense in a standard model-selection or self-bounded learning setup. In these more traditional learning scenarios, one has a training data set S and wants to exploit this data set to the maximum extent possible. Using some of this data to estimate or approximate (functionals of) the unknown distribution means that this data is not available to the learning algorithm or the PAC-Bayes bound. Indeed, if our goal is simply to obtain the tightest possible bound on the risk of our classifier, we ought to use most of this extra data to learn a better classifier, leaving out a small fraction to get a tight Hoeffding-style estimate of our risk.

However, if our goal is to understand the generalization properties of some posterior kernel Q (and indirectly an algorithm like SGD), we do not simply want a tight estimate of risk. Indeed, a held-out test set bound is useless for understanding as it merely certifies that a learned classifier generalizes. If a classifier generalizes due to favorable properties of the data distribution, then we must necessarily capture these properties in our bound. These properties may be natural side products of the learning algorithm (such as weight norms) or functionals of the unknown distribution that we must estimate (such as data-dependent oracle priors or functionals thereof). In this case, it makes sense to exploit held out data to gain insight.

We begin by optimizing a prior over a restricted family. In particular, we consider Gaussian priors when the posterior kernel chooses Gaussian posteriors. Based on empirical findings on SGD in the literature, we propose an approximation to the data-dependent oracle prior.

4.1. Optimal isotropic Gaussian priors. Let $(\Omega, \mathcal{F}, \nu)$ be a probability space representing the distribution of a source of randomness. Our focus here is on kernels $Q : \Omega \times \mathbb{Z}^n \rightarrow \mathcal{M}_1(\mathcal{H})$ where $Q(U, S) = \mathcal{N}(w_S, \Sigma)$ is a multivariate normal, centered at the weights $w_S \in \mathbb{R}^p$ learned by SGD (using randomness $U$, which we may assume without loss of generality encodes both the random initialization and the sequence of minibatches) on the full data set, $S$. Such posteriors underlie several recent approaches to obtaining PAC-Bayes bounds for SGD. In these bounds, the covariance matrix $\Sigma$ is chosen to be diagonal and the scales are chosen to allow one to derive the bound on a deterministic classifier from the bound on a randomized classifier $Q$. For example, Neyshabur et al. [19] derive deterministic
classifier bounds from a PAC-Bayes bound based on (an estimate of) the Lipschitz constant of the network.

Fix some nonnegative integer \( m \leq n \) and let \( \alpha = m/n \). Let \( S_\alpha \) denote the size \( m \) subset of \( S \) corresponding to the first \( m \) indices processed by SGD. (Note that these indices are encoded in \( U \).) Writing \( E_{S_\alpha,U}[\cdot] \) for the conditional expectation operator given \( S_\alpha,U \), Theorem 2.2 implies that the tightest (linear PAC-Bayes) bound in expectation is obtained by minimizing \( E_{S_\alpha,U}[\text{KL}(Q(U,S)||P)] \) in terms of \( P \), which yields the data-dependent oracle prior \( P = E_{S_\alpha,U}[Q(U,S)] \). (We are permitted to condition on \( U \) because \( U \) is independent from \( S \).)

As this prior is assumed to be intractable and the data distribution is unknown, we consider choosing the prior from the family of multivariate Gaussians. Specifically, consider the problem of finding an isotropic Gaussian prior \( P = \mathcal{N}(w_\alpha, \sigma_P I) \) that minimizes \( E_{S_\alpha,U}[\text{KL}(Q(U,S)||P)] \). (We will revisit this simplification in Section 6.3, where we consider priors and posteriors with non-isotropic diagonal covariance matrices.) For a fixed \( \alpha \), the problem reduces to

\[
\arg\min_{w_\alpha} E_{S_\alpha,U}[||w_S - w_\alpha||^2].
\]

It follows that the (Gaussian) oracle prior mean is conditional expectation \( E_{S_\alpha,U}[w_S] \) of weights learned by SGD. Under this choice, the contribution of the mean component to the bound is the trace of the conditional covariance of \( w_S \) given \( S_\alpha,U \). For the remainder of the section we will focus on the problem of approximating the oracle prior mean. The optimal choice of \( \sigma_P \) depends on the distribution of \( \Sigma \). One approach, which assumes that we build separate bounds for different values of \( \sigma_P \) that we combine via a union bound argument, is outlined in Appendix D.

4.2. **Ghost samples.** In the setting above, the optimal Gaussian prior mean is given by the conditional expectation \( E_{S_\alpha,U}[w_S] \). Although the distribution \( S \) is presumed to be unknown, there is a natural statistical estimate for \( E_{S_\alpha,U}[w_S] \). Namely, consider a ghost sample, \( S^G \), independent from and equal in distribution to \( S \). Let \( S^G_\alpha \) be the data set obtained by combining \( S_\alpha \) with a \( 1 - \alpha \) fraction of \( S^G \). (We can do so by matching the position of \( S_\alpha \) within \( S \) and within \( S^G_\alpha \).) Note that \( S^G_\alpha \) is also equal in distribution to \( S \). We may then take \( w^G_\alpha \) to be the mean of \( Q(U,S^G_\alpha) \), i.e., the weights produced by SGD on the data set \( S^G_\alpha \) using the randomness \( U \).

By design, SGD acting on \( S^G_\alpha \) and randomness \( U \) will process \( S_\alpha \) first and then start processing the data from the ghost sample. Crucially, the initial \( \alpha \) fraction of the first epoch in both runs will be identical. By design, \( w^G_\alpha \) and \( w_S \) are equal in distribution when conditioned on \( S_\alpha \) and \( U \), and so \( w^G_\alpha \) is an unbiased estimator for \( E_{S_\alpha,U}[w_S] \). \(^1\)

4.3. **Terminology.** We call the run of SGD on data \( S_\alpha \) the \( \alpha \)-prefix run. The run of SGD on the full data is called the base run. A prior is constructed from the \( \alpha \)-prefix run by centering a Gaussian at the parameters obtained after \( T \) steps of optimization. Prefix stopping time \( T \) is chosen from a discrete set of values to minimize \( L^2 \) distance to posterior mean. \(^2\) Note, that for \( \alpha = 0 \), \( w_\alpha = w_0 \), i.e., the prior is centered at random initialization as it has no access

---

1 We can minimize the variance of the KL term by producing conditionally i.i.d. copies of \( w^G_\alpha \) and averaging, although each such copy requires an independent \( n - m \)-sized ghost sample.

2 We account for these data-dependent choices via a union bound, which produces a negligible contribution.
to data. This is equivalent to the approach taken by Dziugaite and Roy [3]. When the prior has access to data $S^G_\alpha$, we call an SGD run training on $S^G_\alpha$ an $\alpha$-prefix+ghost run, obtaining parameters $w^G_\alpha$.

The procedure of running the $\alpha$-prefix and base runs together for the first $\alpha$-fraction of a base run epoch using shared information $U$ (storing the data order) is an example of a coupling. This coupling is simple and does not attempt to match base and $\alpha$-prefix runs beyond the first $m/b$ iterations (where $b$ is the batch size, which we presume divides $m$ evenly for simplicity). It exploits the fact that the final weights have an outsized dependence on the first few iterations of SGD. More advanced coupling methods can be constructed. Such methods might attempt to couple beyond the first $\alpha$-fraction of the first epoch.

As argued above, it is reasonable to use held-out data to probe the implications of a data-dependent prior as it may give us insight into the generalization properties of $Q$. At the same time, we may be interested in approximations to the data-dependent oracle that do not use a ghost sample. Ordinarily, we would expect two independent runs of SGD, even on the same dataset, to produce potentially quite different weights (measured, e.g., by their $L^2$ distance) [17]. Fig. 2 shows that, when we condition on an initial prefix of data, we dramatically decrease the variability of the learned weights.

This experiment shows that we can predict fairly well the final weights of SGD on the full data set using only a fraction of the data set, implying that most of the variability in SGD comes in the beginning of training. Crucially, the two runs are coupled in the same manner as the ghost-sample runs: the first $\alpha$-fraction of first epoch is identical. When only a fraction of the data is available, SGD treats this data as the entire data set, starting its second epoch immediately.

5. METHODOLOGY FOR EMPIRICAL EVALUATION

Section 3 shows that a data-oracle priors can yield tighter generalization bounds than an oracle prior. In this section, we describe the experimental methodology we use to evaluate this phenomenon in neural networks trained by stochastic gradient descent (SGD).

5.1. Pseudocode. Algorithm 2 (right) describes the procedure for obtaining a PAC-Bayes risk bound on a network trained by SGD.\footnote{Algorithm 2 (right) uses a fixed learning rate and a vanilla SGD for simplicity, but the algorithm can be adapted to any variants of SGD with different learning rate schedules.} Note that the steps outlined in Lines 1–3 do not
change with $\sigma_P$ and therefore the best $\sigma_P$ can be chosen efficiently without re-running the optimization. If ghost data is not used, $S^G_\alpha$ should be replaced with $S_\alpha$.

To avoid choosing $\tilde{b}$, we use a variational KL bound, described in Appendix E, which allows us to optimize $\tilde{b}$ a posteriori for a small penalty. This PAC-Bayes bound on risk, denoted $\Psi^*_\delta(Q,P,S \setminus S_\alpha)$, is evaluated with $\delta = 0.05$ confidence level in all of our experiments during evaluation/optimization.

5.2. Datasets and Architectures. We use three datasets: MNIST, Fashion-MNIST and CIFAR-10. See Appendix F for more details. The architectures used are described in detail in Appendix G. For the details of the training procedure, see Appendix H.

5.3. Stopping criteria. We terminate SGD optimization in the base run once the empirical error ($L^{b-1}$ in Algorithms 1 and 2) measured on all of $S$ fell below some desired value $\varepsilon$, which we refer to as the stopping criteria. We evaluate the results for different stopping criteria.

6. Empirical study of SGD-trained networks

6.1. Evaluating data-dependent priors. A PAC-Bayes risk bound trades off empirical risk and the contribution coming from the KL term. For isotropic Gaussian priors and posteriors, the mean component in the KL is proportional to the squared difference in means normalized by the effective number of training samples not seen by the prior, i.e.,

$$d(\alpha, S_\alpha) := \frac{\|w_\alpha - \mu_\alpha\|^2}{|T - \alpha|S_\alpha^2}.$$  

This scaled squared L2 distance term determines the tightness of the bound when the prior variance and the posterior $Q$ and data $S$ are fixed, as the bound grows with $d(\alpha, S_\alpha)$. In this section we empirically evaluate how $d(\alpha, S_\alpha)$ and $d(\alpha, S^G_\alpha)$ vary with different values of $\alpha$.

Our goal is to evaluate whether, on standard vision datasets and architectures, a data-dependent oracle prior can be superior to an oracle prior. Since we do not have access to

Algorithm 2 PAC-Bayes bound computation (right) and optimization (left). Given: Data $S$, ghost data $S^G$ (if $\alpha$-prefix+ghost), batch size $b$. Hyperparameters: stopping criteria $\varepsilon$, prefix fraction $\alpha$, prefix stopping time $T$, prior variance $\sigma_P$.

```plaintext
function BOUND-OPT($\alpha, \sigma_P, T, \eta$)
    $S_\alpha \leftarrow \{z_{1, \ldots, z_{|S|}} \} \subset S$  // Select $\alpha$-prefix
    $w_\alpha^0 \leftarrow \text{SGD}(w_0, S_\alpha, b, \frac{|S_\alpha|}{b})$  // Coupling
    $w_S^0 \leftarrow \text{SGD}(w_0^0, S, b, \infty, 0)$  // $\alpha$-prefix
    $P \leftarrow \mathcal{N}(w_\alpha^0, \sigma_P I_P)$
    $\theta_Q \leftarrow (w_\alpha^0, \sigma_P)$  // $Q$ trainable params
    $\triangleright$ Let $Q(\theta_Q) = \mathcal{N}(w_\alpha^0, \sigma_P I_P)$
    for $i \leftarrow 1$ to $T$
        Sample minibatch $S' \in S \setminus S_\alpha$, $|S'| = b$.
        $\theta_Q \leftarrow \theta_Q - \eta \nabla_{\theta_Q} \Psi^*_\delta(Q(\theta_Q), P; S \setminus S_\alpha)$
    Bound $\leftarrow \Psi^*_\delta(Q(\theta_Q), P; S \setminus S_\alpha)$
    return Bound

function GET-BOUND($\varepsilon, \alpha, T, \sigma_P$)
    $S_\alpha \leftarrow \{z_{1, \ldots, z_{|S|}} \} \subset S$
    $w_\alpha^0 \leftarrow \text{SGD}(w_0, S_\alpha, b, \frac{|S_\alpha|}{b})$
    $\triangleright$ Perform base run
    $w_S^0 \leftarrow \text{SGD}(w_0^0, S, b, \infty, \varepsilon)$
    $\triangleright$ Perform $\alpha$-prefix+ghost run
    $w_S^G \leftarrow \text{SGD}(w_0^0, S^G_\alpha, b, T, \cdot)$
    $P \leftarrow \mathcal{N}(w_S^G, \sigma_P I_P)$
    $Q \leftarrow \mathcal{N}(w_S^G, \sigma_P I_P)$
    Bound $\leftarrow \Psi^*_\delta(Q, P; S \setminus S_\alpha)$
    return Bound
```

an oracle prior, we approximate it by using a ghost sample $S^G_\alpha$ with $\alpha = 0$, as described in Section 4.2. Data-dependent oracle priors are approximated by using a combination of training samples and ghost samples.

Our experimental results on MNIST and Fashion-MNIST appear in Fig. 3, where we plot $d(\alpha, S_\alpha)$ and $d(\alpha, S^G_\alpha)$. The results suggest that the value of $\alpha$ minimizing $d(\alpha, S^G_\alpha)$ is data- and architecture-dependent. The optimal prefix size for MNIST, FC minimizing $d(\alpha, S_\alpha)$ is $\alpha > 0.2$. For MNIST, LeNet-5 and Fashion-MNIST, LeNet-5, the optimal $\alpha$ is between 0 and 0.1. We found that batch size affects the optimal $\alpha$, whether on $\alpha$-prefix or ghost data. As one might expect, the best $\alpha$ is larger for smaller batch sizes. We hypothesize that this is due to increased stochasticity of SGD.

Interestingly, at larger values of $\alpha$ we observe that the gap between $d(\alpha, S_\alpha)$ and $d(\alpha, S^G_\alpha)$ closes. This happens in all three experimental setups by $\alpha = 0.4$: we observe that the prior mean obtained with $S_\alpha$ training data alone is as close to final SGD weights as the prior mean obtained with $S^G_\alpha$.

6.2. Generalization bounds for SGD-trained networks. We apply data-dependent priors to obtain tighter PAC-Bayes risk bounds for SGD-trained networks. We do not use ghost data in these experiments, as oracle priors are inaccessible in practice. Thus the prior mean is obtained by the $\alpha$-prefix run on prefix data alone. See Algorithm 2 (right) and Section 5 for the details of the experiment.

From the data in Fig. 4, it is apparent that $\alpha$ has a significant impact on the size of the bound. In all of the three networks tested, the best results are achieved for $\alpha > 0$.

One of the clearest relationships to emerge from the data is the dependence of the bound on the stopping criterion: The smaller the error at which the base run was terminated, the looser the bound. This suggests that the extra optimization introduces variability into the weights that we are not able to predict well.

6.3. Optimal prior variance. We use oracle bounds to quantify limits on how much tighter these generalization bounds could be, were we able to optimize a diagonal prior variance.

Our data-dependent priors do not attempt to minimize the variance component of the KL bound. For a fixed $\Sigma_P$, the variance component in Eq. (39) (see Appendix D) increases if posterior variance $\Sigma$ deviates from $\Sigma_P$. When the prior is isotropic, our empirical study shows that the optimized posterior variance is also close to isotropic. However, an isotropic
ON THE ROLE OF DATA IN PAC-BAYES BOUNDS

Figure 4. Columns left to right: MNIST, LeNet-5; Fashion-MNIST, LeNet-5; MNIST, FC. y-axis: error-rate; x-axis: fraction $\alpha$ of the data used by the $\alpha$-prefix run of SGD to predict the weights produced by the base run of SGD, $w_S$, where the prior $P$ is centered; dashed lines: test error; solid lines: error bound for a Gaussian Gibbs classifier $Q$, with mean $w_S$ isotropic covariance minimizing a PAC-Bayes risk bound; legend: training error used as the stopping criterion for the base run of SGD. Top row: Gaussian prior $P$ with isotropic covariance matrix. The best error bound on MNIST ($\approx 11\%$) is significantly better than the 46% bound by Zhou et al. [28]. Bottom row: Gaussian prior $P$ with diagonal (non-isotropic) covariance matrix set to optimal. The improvement on the bound is seen only for low $\alpha$ values. At higher $\alpha$ values, the bounds are similar to the ones obtained with isotropic prior variance.

structure may not describe the local minima found by SGD well. We are thus also interested in a hypothetical experiment, where we allow the prior variance to be optimal for any given diagonal Gaussian $Q$. While this produces an invalid bound, it reveals the contribution to the risk bound due to the prior variance. Optimizing Eq. (39) w.r.t. diagonal $\Sigma_P$ yields a prior $P^{\Sigma}_\alpha$ with optimal variance, and $\text{KL}(Q||P^{\Sigma}_\alpha)$ expression reduces to

$$\frac{1}{2} \sum_{i=1}^{p} \log(1 + (w'_i - w^i_\alpha)/\sigma^2_i),$$

where $\sigma^2_i$ is the $i$th entry of the diagonal of $\Sigma$.

Computing the bounds with $P^{\Sigma}_\alpha$ as a prior, requires some minor modifications to Algorithm 2 (right). As in Algorithm 2 (right), the posterior is set to $Q = \mathcal{N}(w_S, \Sigma)$, with a diagonal covariance matrix $\Sigma$ that is initialized to $\sigma^2_P I_P$. The prior $P$ is centered at $w^0_\alpha$, and the variance is automatically determined by the posterior variance. The KL then takes the form stated in Eq. (10). The $\alpha$-prefix run in Algorithm 2 (right) is followed by another SGD run minimizing $\Psi^*_\delta(Q(\theta_Q), P; S \setminus S_\alpha)$ with respect to a diagonal covariance $\Sigma$.

We present the results in Fig. 4, second row. At $\alpha = 0$, the optimal prior variance decreases the bound substantially. However, at larger values of $\alpha$, the effect diminishes. In particular, at the values of $\alpha$ that produce the lowest risk bound with a fixed isotropic prior variance, optimal prior variance makes little to no improvement. Interestingly, the
optimized posterior variance remains close to isotropic. Overall, the results suggest that a diagonal prior offers little advantage over an isotropic prior.

7. **DIRECT RISK BOUND MINIMIZATION.**

One of the dominant approaches to training Gaussian neural networks is to minimize the evidence lower bound (ELBO), which essentially takes the same form as Eq. (1), but with a different relative weight on the KL term. Here, we optimize a PAC-Bayes bound using our data-dependent prior methodology which can be related to empirical Bayes approaches. The details of the algorithm are outlined in Algorithm 2, left, where $\Psi_{\delta}(Q, P; S \setminus S_{\alpha})$ denotes a PAC-Bayes bound computed with differentiable surrogate loss. We perform experiments on 3 different datasets and architectures (see Appendix I for further details).

Fig. 5 presents the error of the posterior $Q$ (dashed line) optimized using Algorithm 2 with different values of $\alpha$. It is apparent from the figure that for all the networks and datasets tested, the error of $Q$ drops dramatically as $\alpha$ increases, all the way up to around $\alpha = 0.9$. Note that $Q$ with the optimal $\alpha$ achieves very high performance even compared to state-of-the-art networks and at the same time comes with a valid guarantee on error. For example, ResNet20 (without data augmentation and weight decay) trained on CIFAR10 achieved error of around 0.16, and the best-performing $Q$ in Fig. 5 gets an average error of $\approx 0.2$ with a bound $\approx 0.23$ that holds with 0.95 probability.

**Acknowledgments.** The authors would like to thank Mufan Li, Jeffrey Negrea, Alexandre Drouin, and Blair Bilodeau for feedback on drafts. DMR was supported, in part, by an NSERC Discovery Grant, Ontario Early Researcher Award, and a stipend provided by the Charles Simonyi Endowment. This research was carried out in part during the Foundations of Deep Learning program at the Simons Institute for the Theory of Computing, and during the Special Year on Optimization, Statistics, and Theoretical Machine Learning at the Institute of Advanced Studies.
REFERENCES

[1] A. Ambroladze, E. Parrado-Hernández, and J. Shawe-Taylor. “Tighter PAC-Bayes bounds”. In: Adv. Neural Information Processing Systems. 2007, pp. 9–16.
[2] O. Catoni. PAC-Bayesian supervised classification: the thermodynamics of statistical learning. Vol. 56. Lecture Notes-Monograph Series. IMS. 2007. arXiv: 0712.0248.
[3] G. K. Dziugaite and D. M. Roy. “Computing Nonvacuous Generalization Bounds for Deep (Stochastic) Neural Networks with Many More Parameters than Training Data”. In: Proc. 33rd Ann. Conf. Uncertainty in Artificial Intelligence (UAI). 2017. arXiv: 1703.11088.
[4] G. K. Dziugaite and D. M. Roy. “Data-dependent PAC-Bayes priors via differential privacy”. In: Adv. Neural Information Processing Systems. 2018. arXiv: 1802.09583.
[5] B. Guedj, “A Primer on PAC-Bayesian Learning”. In: Proceedings of the 2nd Congress of the Société Mathématique de France. 2019, pp. 391–414. arXiv: 1901.05353.
[6] K. He, X. Zhang, S. Ren, and J. Sun. “Deep residual learning for image recognition”. In: Proc. IEEE Conf. Computer Vision and Pattern Recognition (CVPR). 2016, pp. 770–778.
[7] A. Krizhevsky, “Learning multiple layers of features from tiny images” (2009).
[8] J. Langford. “Quantitatively tight sample complexity bounds”. PhD thesis. Carnegie Mellon University, 2002.
[9] J. Langford and A. Blum. “Microchoice bounds and self bounding learning algorithms”. Machine Learning 51.2 (2003), pp. 165–179.
[10] J. Langford and M. Seeger. Bounds for Averaging Classifiers. Tech. rep. CMU-CS-01-102. Carnegie Mellon University, 2001.
[11] Y. LeCun, C. Cortes, and C. J. C. Burges. MNIST handwritten digit database. 1998.
[12] G. Lever, F. Laviolette, and J. Shawe-Taylor. “Distribution-dependent PAC-Bayes priors”. In: Proc. Int. Conf. Algorithmic Learning Theory (ALT). Springer. 2010, pp. 119–133.
[13] A. Maurer. A note on the PAC-Bayesian theorem. 2004. arXiv: cs/0411099.
[14] D. A. McAllester. A PAC-Bayesian Tutorial with A Dropout Bound. 2013. arXiv: 1307.2118.
[15] D. A. McAllester. “PAC-Bayesian Model Averaging”. In: Proc. 12th Ann. Conf. Computational Learning Theory. COLT’99. Santa Cruz, California, USA: ACM, 1999, pp. 164–170.
[16] D. A. McAllester. “Some PAC-Bayesian Theorems”. Machine Learning 37.3 (Dec. 1999), pp. 355–363.
[17] V. Nagarajan and J. Z. Kolter. “Uniform convergence may be unable to explain generalization in deep learning”. In: Adv. Neural Information Processing Systems. 2019.
[18] J. Negrea, M. Haghifam, G. K. Dziugaite, A. Khisti, and D. M. Roy. “Information-Theoretic Generalization Bounds for SGLD via Data-Dependent Estimates”. In: Adv. Neural Information Processing Systems. 2019, pp. 11013–11023.
[19] B. Neyshabur, S. Bhojanapalli, D. McAllester, and N. Srebro. “A PAC-Bayesian approach to spectrally-normalized margin bounds for neural networks”. In: Int. Conf. Learning Representations (ICLR), 2018.
[20] L. Oneto, D. Anguita, and S. Ridella. “PAC-bayesian analysis of distribution dependent priors: Tighter risk bounds and stability analysis”. Pattern Recognition Letters 80 (2016), pp. 200–207.
[21] L. Oneto, S. Ridella, and D. Anguita. “Differential privacy and generalization: Sharper bounds with applications”. *Pattern Recognition Letters* 89 (2017), pp. 31–38.

[22] E. Parrado-Hernández, A. Ambroladze, J. Shawe-Taylor, and S. Sun. “PAC-Bayes bounds with data dependent priors”. *J. Machine Learning Research* 13.Dec (2012), pp. 3507–3531.

[23] O. Rivasplata, E. Parrado-Hernandez, J. Shawe-Taylor, S. Sun, and C. Szepesvari. “PAC-Bayes bounds for stable algorithms with instance-dependent priors”. In: *Adv. Neural Information Processing Systems*. 2018.

[24] O. Rivasplata, V. M. Tankasali, and C. Szepesvari. *PAC-Bayes with Backprop*. 2019. arXiv: 1908.07380.

[25] J. Shawe-Taylor, P. L. Bartlett, R. C. Williamson, and M. Anthony. “A framework for structural risk minimisation”. In: *Proc. 9th Ann. Conf. Computational Learning Theory (COLT)*. 1996, pp. 68–76.

[26] J. Shawe-Taylor and R. C. Williamson. “A PAC analysis of a Bayesian estimator”. In: *Proc. 10th Ann. Conf. Computational Learning Theory (COLT)*. ACM. 1997, pp. 2–9.

[27] H. Xiao, K. Rasul, and R. Vollgraf. *Fashion-MNIST: a Novel Image Dataset for Benchmarking Machine Learning Algorithms*. Aug. 28, 2017. arXiv: 1708.07747.

[28] W. Zhou, V. Veitch, M. Austern, R. P. Adams, and P. Orbanz. “Non-vacuous Generalization Bounds at the ImageNet Scale: a PAC-Bayesian Compression Approach”. In: *Proc. Int. Conf. Learning Representations (ICLR)*. 2019. arXiv: 1804.05862.
This material is adapted from [3].

Let $Q, P \in \mathcal{M}(\mathcal{H})$ be probability measures defined on a common measurable space $\mathcal{H}$. When $Q$ is absolutely continuous with respect to $P$, written $Q \ll P$, we write $\frac{dQ}{dP} : \mathcal{H} \to \mathbb{R}_+ \cup \{\infty\}$ for some Radon–Nikodym derivative (aka, density) of $Q$ with respect to $P$. The Kullback–Liebler (KL) divergence from $Q$ to $P$ is $\text{KL}(Q||P) = \int \ln \frac{dQ}{dP} \, dQ$ if $Q \ll P$ and $\infty$ otherwise.

Assume $Q$ and $P$ admit densities $q$ and $p$, respectively, w.r.t. some sigma-finite measure $\nu \in \mathcal{M}(\mathcal{H})$. In this case, the definition of the KL divergence satisfies

$$\text{KL}(Q||P) = \int \log \frac{q(x)}{p(x)} \, q(x) \, d\nu(x).$$

### B. Proof of Proposition 3.1

The proof follows essentially from definitions. Note that we do not require $J$ to have any particular distribution and so, e.g., $J$ could be uniformly distributed among subsets of cardinality $\alpha n$ or could be a.s. nonrandom and equal to $[m]$. Note that the statement that $\mathbb{P}[\hat{h}|J] = Q(S)$ a.s. implies that $\mathbb{P}[\hat{h}|S] = Q(S)$ a.s. and that $\hat{h}$ is independent of $J$, both marginally and conditionally on $S$. Informally, any randomness in $J$ plays no role in the determination of $\hat{h}$. Let $\bar{J} = [n] \setminus J$.

Consider the linear PAC-Bayes bound based on $L_S(Q(S))$. It is optimized, in expectation, by choosing an oracle prior:

$$\inf_{P \in \mathcal{M}(\mathcal{H})} \mathbb{E}_{S \sim \mathcal{D}^n \mathcal{Y}} \mathcal{Y}_{\beta, \delta}(Q(S), P; S) = \mathbb{E}[\beta^{-1} L_S(Q(S))] + \inf_{P \in \mathcal{M}(\mathcal{H})} \mathbb{E}[\text{KL}(Q(S)||P)] + \log \frac{1}{\delta}$$

$$= \mathbb{E}[\beta^{-1} L_S(Q(S))] + \frac{\mathbb{E}[\text{KL}(Q(S)||\mathbb{E}(Q(S)))] + \log \frac{1}{\delta}}{2}\frac{1}{\beta(1-\beta)n}$$

For $\bar{J} = [n] \setminus J$.

$$\mathbb{E}[\beta^{-1} L_{\bar{J}}(Q(S))] + \frac{1}{2}\frac{1}{\beta(1-\beta)n}.$$

In contrast, the linear PAC-Bayes bound based on $L_{S_J}(Q(S))$ is optimized, in expectation, by choosing a data-dependent oracle prior:

$$\inf_{P \in \mathcal{Z} \sim D^n \mathcal{H}(\mathcal{H})} \mathbb{E}_{J} \mathbb{E}_{S \sim \mathcal{D}^n \mathcal{Y}} \mathcal{Y}_{\beta, \delta}(Q(S), P(S_J); S \setminus S_J)$$

$$= \mathbb{E}[\beta^{-1} L_{S_J}(Q(S))] + \inf_{P \in \mathcal{Z} \sim D^n \mathcal{H}(\mathcal{H})} \mathbb{E}[\text{KL}(Q(S)||P(S_J))] + \log \frac{1}{\delta}$$

$$= \mathbb{E}[\beta^{-1} L_{S_J}(Q(S))] + \frac{\mathbb{E}[\text{KL}(Q(S)||\mathbb{E}(Q(S)|S_J))] + \log \frac{1}{\delta}}{2}\frac{1}{\beta(1-\beta)(1-\alpha)n}$$

$$= \mathbb{E}[\beta^{-1} L_{S_J}(Q(S))] + \frac{1}{2}\frac{1}{\beta(1-\beta)(1-\alpha)n}.$$
It follows that the data-dependent risk bound is tighter, in expectation, when

\[(1 - \beta) \mathbb{E}[L_S(Q(S))] + \frac{I(\hat{h}; S) + \log \frac{1}{\alpha}}{2n} > (1 - \beta) \mathbb{E}[L_{S_j}(Q(S))] + \frac{I(\hat{h}; S|S_j) + \log \frac{1}{\alpha}}{2(1 - \alpha)n}.
\]

Equivalently,

\[\frac{I(\hat{h}; S) + \log \frac{1}{\alpha}}{2n} - \frac{I(\hat{h}; S|S_j) + \log \frac{1}{\alpha}}{2(1 - \alpha)n} > (1 - \beta) \mathbb{E}[L_{S_j}(Q(S)) - L_S(Q(S))].
\]

Rewriting the left-hand side,

\[\frac{I(\hat{h}; S) + \log \frac{1}{\alpha}}{2n} - \frac{I(\hat{h}; S|S_j) + \log \frac{1}{\alpha}}{2(1 - \alpha)n} = \frac{1}{2} \left( \frac{I(\hat{h}; S)}{n} - \frac{I(\hat{h}; S|S_j)}{(1 - \alpha)n} \right) - \log \frac{1}{\alpha} \left( \frac{\alpha}{1 - \alpha} \right).
\]

Therefore, we prefer a data-dependent prior based on \(J\) when

\[\left( \frac{I(\hat{h}; S)}{n} - \frac{I(\hat{h}; S|S_j)}{(1 - \alpha)n} \right) > 2(1 - \beta) \mathbb{E}[L_{S_j}(Q(S)) - L_S(Q(S))] + \frac{\log \frac{1}{\alpha}}{n} \left( \frac{\alpha}{1 - \alpha} \right).
\]

The result follows by the definition of the information rate gain and excess bias.

C. Proof of Lemma 3.3

We begin with a proof sketch.

**Proof sketch.** With \(J\) and \(\beta\) fixed, the minimization over \(P(S_j)\) meets the hypotheses of Theorem 2.2 and so we may simplify the objective by taking \(P(S_j) = \mathbb{E}[Q(S)|S_j] = \mathbb{P}[W|S_j]\). The KL term then becomes a conditional mutual information \(I(W; S_j|S_j)\). Due to linearity of expectation, we may then optimize \(\beta\) explicitly, leaving only a minimization over subsets \(J\).

\[\inf_{J \subseteq [n]} \left( \Phi(J) := R(J) + C(J) + \sqrt{2R(J)C(J) + C^2(J)} \right)
\]

where \(R(J) = \mathbb{E}[L_{S\setminus S_j}(Q)]\) and \(C(J) = I(W; S\setminus S_j|S_j) + \log \frac{1}{\alpha})/|S\setminus S_j|\).

One can show that \(I(W; S\setminus S_j|S_j) = \frac{D}{\tau} \ln \phi \kappa,\) where \(\phi\) is the variance contribution from \(S\setminus S_j\) and \(\xi\). Using sub-Gaussian and sub-exponential tail bounds, one can establish that \(R(J) \leq R = \exp \{-D/16\} + \exp \{-\tau^2/(4\phi_0^2\sigma^2)\}\), where \(\phi_0^2\) is due to variance in \(S, \xi, \) and \(\tau = (\sum_{i=1}^n \eta_i)||u||^2\).

Choosing \(n = 100, D = 1000, \sigma = 8, \kappa = 4, \tau = 64,\) and \(\delta = 0.05,\) we obtain \(\Phi(\emptyset) \geq 2C(\emptyset) \approx 1.1,\) while \(\min_J \Phi(J) \leq 0.15,\) our upper bound is achieved by \(J = [24],\) i.e., by using the initial 24 data points to obtain a data-dependent (oracle) prior.

C.1. Complete proof and bounds on the objective. We now provide a complete rigorous proof. For subsets \(J\) (of \([n]\)), let \(J = [n] \setminus J\) and \(\eta_j^p = \sum_{i \in j} \eta_i^p\) for \(p \in \{1, 2\}\); let \(\phi_J = \sum_{i \in j} \eta_i^2 \sigma^2 / D + \kappa;\) and let \(\phi_{-i} = \phi_{[n]\setminus \{i\}}\).

By Theorem 2.2 and linearity of expectation, for every subset \(J\) and \(\beta \in (0, 1),\) Theorem 2.2 implies that the optimal prior is \(P_J(S_j) = \mathbb{P}[W|S_j]\), and so we can simplify Eq. (8) by choosing this prior. In particular, now \(\mathbb{E}[K_L(Q||P_J(S_j))] = I(W; S_j|S_j)\).
Define $R(J) = \mathbb{E}[L_{S_J}(Q)]$ and $C(J) = (I(W; S_J|S_J) + \log \frac{1}{\delta})/|S_J|$. By linearity of expectation, we can remove the infimum over $\beta \in (0, 1)$ by explicit minimization. As a result, we see that Eq. (8) is equivalent to

$$\inf_{J \subseteq [n]} R(J) + C(J) + \sqrt{2R(J)C(J) + C^2(J)}.$$  

(22)

Pick some $J \subseteq [n]$. Then the optimal prior conditioned on $S_J$ is

$$P_J(S_J) = \mathbb{E}[Q(S)|S_J] = \delta_{\eta^{1}_{|i|}} u \otimes N_J,$$

(23)

where $N_J = \mathcal{N}(\sum_{i \in J} \eta_{i} y_{i} x_{i,2}, \phi_J I_D)$. Let $\psi(r) = r - 1 - \ln r$ for $r > 0$. Then

$$\text{KL}(Q(S)||P_J(S_J)) = D\psi(\kappa/\phi_J)/2 + \frac{1}{2\phi_J} \sum_{j \in J} (\sum_{i \in J} \eta_i y_i x_{i,j,2})^2.$$  

(24)

Taking expectations,

$$I(W; S_J|S_J) = \mathbb{E}[\text{KL}(Q(S)||P_J(S_J))] = \frac{D}{2} \left( \psi(\kappa/\phi_J) + \frac{\sigma^2 \eta_0^2 / D}{\phi_J} \right),$$

(25)

$$= \frac{D}{2} \left( \psi(\kappa/\phi_J) + (1 - \kappa/\phi_J) \right),$$

(26)

$$= \frac{D}{2} \ln \phi_J/\kappa.$$  

(27)

It remains to control the empirical risk term. To that end, pick $i \in [n]$ and let $\tau = \eta^{1}_{|i|} \|u\|^2$. Then

$$\mathbb{E}\ell(W, z_i) = \mathbb{P}[y_i \langle W, x_i \rangle \leq 0] = \mathbb{P}[\tau + y_i \langle w_{n,2}, x_{i,2} \rangle + y_i \langle \xi, x_{i,2} \rangle \leq 0],$$

(28)

where

$$y_i \langle w_{n,2}, x_{i,2} \rangle = \eta_i \|x_{i,2}\|^2 + \sum_{j \neq i} \eta_j y_j \langle x_{j,2}, x_{i,2} \rangle.$$  

(29)

Rearranging and exploiting the chain rule of conditional expectation and symmetry of the normal distribution,

$$\mathbb{E}\ell(W, z_i) = \mathbb{E}\mathbb{P}^\mathbb{P}_{z_{i,2}} \left[ \sum_{j \neq i} \langle \eta_j x_{j,2}, x_{i,2} \rangle + \langle \xi, x_{i,2} \rangle \geq \tau + \eta_i \|x_{i,2}\|^2, \right]$$

where the conditional probability is a tail bound on a univariate Gaussian with mean zero and variance $\|x_{i,2}\|^2/\phi_{-i}$.

Applying the standard (sub-)Gaussian tail bound,

$$\mathbb{E}\ell(W, z_i) \leq \mathbb{E} \exp \left\{ - \frac{1}{2} \left( \tau + \eta_i \|x_{i,2}\|^2 \right)^2 \right\} \leq \mathbb{E} \exp \left\{ - \frac{\tau^2}{2\|x_{i,2}\|^2/\phi_{-i}} \right\},$$

(30)

where the last inequality is crude, but suffices for our application. Note that $D\|x_{i,2}\|^2/\sigma^2$ is a chi-squared random variable with $D$ degrees of freedom, hence sub-exponential. Indeed, with probability at least $1-c$,

$$D\|x_{i,2}\|^2/\sigma^2 \leq D + 2\sqrt{D\log(1/c)} + 2\log(1/c).$$  

(31)
Rearranging,
\[
\| x_i \|_2^2 \leq \frac{\sigma^2}{D} (D + 2 \sqrt{D \log(1/c)} + 2 \log(1/c))
\]
\[
\leq \sigma^2 (1 + 4/\log(1/c)/D) =: B(c),
\]
where the second inequality holds assuming \( c \geq \exp\{-D\} \), which we will ensure from this point on. So
\[
\mathbb{E}[\ell(W, z_i)] \leq \inf_{c \geq e^{D}} \left\{ \frac{1}{c} + \left( 1 - \frac{1}{c} \right) \exp\{-r^2/(2\phi_i B(c))\} \right\}.
\]
Taking \( c = \exp\{-D/16\} \), we have \( B(c) = 2\sigma^2 \). Then, using \( \phi_i \leq \phi[n] \),
\[
\mathbb{E}[\ell(W, z_i)] \leq \exp\{-D/16\} + \exp\{-r^2/(4\phi[n] \sigma^2)\}.
\]
We may now obtain a bound
\[
R(J) = \mathbb{E}[\ell_S(J(Q))] = \frac{1}{n - |J|} \sum_{i \not\in J} \mathbb{E}[\ell(W, z_i)] \leq \max_{i \not\in J} \mathbb{E}[\ell(W, z_i)] = \overline{R}.
\]
Thus
\[
\Phi(J) \leq \overline{R} + C(J) + \sqrt{2\overline{R}C(J) + C(J)^2}
\]
At the same time, we have \( \Phi(J) \geq 2C(J) \) for all \( J \subseteq [n] \). (Note that these two bounds are used to produce Fig. 1.)

In particular, noting \( \log 1/\delta > 0 \),
\[
\Phi(\emptyset) \geq \frac{D}{m} \ln \frac{\sigma^2 \eta^2[\emptyset]}{D + \kappa}.
\]
The result can be seen to follow from these bounds by evaluation using the particular values. In particular, one can see that taking \( J \) to be a nonempty initial segment of \([n]\), we have \( \Phi(J) < 2C(\emptyset) \leq \Phi(\emptyset) \).

D. Analytic Form of the KL for an Approximate Data-Dependent Oracle Bound

In this section, we explore one possible analytic bound for a KL term for a PAC-Bayes bound, based on the setup in Section 4. We assume \( \text{tr}(\Sigma) \) and \( \det(\Sigma) \) are nonrandom. In an application, one would have to cover a set of possible values to handle the random case.

The KL divergence between Gaussians \( Q(U, S) = \mathcal{N}((, w_S), \Sigma) \) and \( P = \mathcal{N}((, w_\alpha), \Sigma_\alpha) \) takes the form
\[
2\text{KL}(Q(U, S) || P) = \|w_S - w_\alpha\|_2^2 + \text{tr}(\Sigma^{-1}(\Sigma)) - p + \ln \frac{\det(\Sigma_\alpha)}{\det(\Sigma)}.
\]
Specializing to an isotropic prior, i.e., $\Sigma = \sigma I$, we obtain

$$2KL(Q(U,S) || P) = \frac{1}{\sigma P} \| w_S - w_\alpha \|^2 + \frac{1}{\sigma P} \text{tr}(\Sigma) - p + p \ln \sigma P - \ln \det \Sigma.$$ 

Note that

$$\text{tr}(\text{cov}^{S_\alpha,U}(w_S)) = \inf_{w_\alpha} \mathbb{E}^{S_\alpha,U}[\| w_S - w_\alpha \|^2].$$ 

Consider

$$\sigma P = \frac{1}{p} (\text{tr}(\text{cov}^{S_\alpha,U}(w_S)) + \text{tr}(\Sigma)).$$ 

Substituting above, for some random variable $Z$ such that $\mathbb{E}^{S_\alpha,U}[Z] = 1$,

$$2KL(Q(U,S) || P) = Zp - p + p \ln \left\{ \frac{\frac{1}{p} \text{tr}(\text{cov}^{S_\alpha,U}(w_S)) + \frac{1}{p} \text{tr}(\Sigma)}{\det \Sigma} \right\} \leq Zp - p + p \frac{\frac{1}{p} \text{tr}(\text{cov}^{S_\alpha,U}(w_S)) + \frac{1}{p} \text{tr}(\Sigma) - (\det \Sigma)^{1/p}}{\det \Sigma}. $$

Taking expectations, conditional on $S_\alpha, U$,

$$2\mathbb{E}^{S_\alpha,U}[KL(Q(U,S) || P)] \leq \frac{\text{tr}(\text{cov}^{S_\alpha,U}(w_S))}{\det \Sigma} + p \frac{\frac{1}{p} \text{tr}(\Sigma) - (\det \Sigma)^{1/p}}{\det \Sigma}. $$

Further, if we assume $\Sigma = \sigma I$, then

$$\mathbb{E}^{S_\alpha,U}[KL(Q(U,S) || P)] \leq \frac{1}{2\sigma} \text{tr}(\text{cov}^{S_\alpha,U}(w_S)).$$

### E. Variational KL Bound

The linear PAC-Bayes bound requires one to specify a value of $\beta$. For a particular posterior kernel $Q$, the optimal value of $\beta$ depends on the likely value of the empirical risk term. However, the value of $\beta$ must be chosen independently of the data used to evaluate the bound.

In the proof of Lemma 3.3 in Appendix C, the linear PAC-Bayes bound is optimized, in expectation. Since the expected value of the bound is independent of the data, and since the constant $\beta$ can be pulled outside the expectations, we can choose the value of beta that minimizes the bound in expectation. The result is Eq. (22), with $C(J)$ defined in terms of an expected KL, as the mutual information appears only when the prior is chosen to be the oracle prior.

In this section, we describe how the bound due to Maurer [13] can be approximated to reveal a high-probability tail bound with the same form as if we optimized $\beta$. The cost is a $O(\log \sqrt{m}/m)$ term.

Let $\mathcal{B}_p$ denote the Bernoulli distribution on $\{0, 1\}$ with mean $p$. For $p, q \in [0, 1]$, we abuse notation and define

$$\text{kl}(q || p) \overset{\text{def}}{=} KL(\mathcal{B}_q || \mathcal{B}_p) = q \ln \frac{q}{p} + (1 - q) \ln \frac{1 - q}{1 - p}.$$
The following PAC-Bayes bound for bounded loss is due to Maurer [13]. The same result for 0–1 loss was first established by Langford and Seeger [10], building off the seminal work of McAllester [15]. See also [8] and [2].

**Theorem E.1 (PAC-Bayes; [13, Thm. 5]).** Under bounded loss \( \ell \in [0, 1] \), for every \( \delta > 0 \), \( m \in \mathbb{N} \), distribution \( D \) on \( Z \), and distribution \( P \) on \( \mathcal{H} \),

\[
P \left( \forall Q \right) \left( \text{kl} \left( L_S(Q) || L_{\varnothing}(Q) \right) \leq \frac{\text{KL}(Q||P) + \ln \frac{2\sqrt{m}}{\delta}}{m} \right) \geq 1 - \delta.
\]

One can recover the bound by McAllester [15] via Pinsker’s inequality, resulting in a (looser) bound on \( |L_S(Q) - L_{\varnothing}(Q)| \). Maurer’s bound behaves like the bound in Theorem 2.1, except that it holds for all \( \beta \) simultaneously, at the cost of a \( \frac{1}{m} \log \sqrt{m} \) term.

E.1. Inverting the KL bound. Here we derive a novel PAC-Bayes bound that is an upper bound on the inverted KL bound (Theorem E.1) and that is used during optimization in our empirical work. The bound is the piecewise combination of two bounds. In independent work, Rivasplata, Tankasali, and Szepesvari [24] derive the first of the two parts, which they call a “quad bound”. The second part is a consequence of Pinsker’s inequality.

**Theorem E.2 (Variational KL bound).** With probability at least \( 1 - \delta \) over \( S \),

\[
L_{\varnothing}(Q) \leq \min \left\{ L_S(Q) + B + \sqrt{B(B + 2L_S(Q))}, L_S(Q) + \sqrt{\frac{B}{2}} \right\},
\]

where

\[
B = \frac{\text{KL}(Q||P) + \log \frac{2\sqrt{m}}{\delta}}{|S|}.
\]

The variational KL bound takes the minimum value of the moment bound (top) and the Pinsker bound (bottom).

**Proof.** Let \( \text{kl}(L_S(Q)||L_{\varnothing}(Q)) \) be KL between two Bernoulli random variables with success probabilities \( L_S(Q) \) and \( L_{\varnothing}(Q) \), respectively. Then by Theorem E.1, with probability greater than \( 1 - \delta \),

\[
\text{kl}(L_S(Q)||L_{\varnothing}(Q)) \leq \frac{\text{KL}(Q||P) + \log \frac{2\sqrt{|S|}}{\delta}}{|S|}.
\]

Let \( B \) denote the right hand side of the inequality. By Donsker–Varadhan we get

\[
\text{kl}(L_S(Q)||L_{\varnothing}(Q)) \geq \lambda L_S(Q) - \log \mathbb{E}_{x \sim \text{Ber}(L_{\varnothing}(Q))} [e^{\lambda x}]
\]

for any \( \lambda \). The final term is the moment generating function of a Bernoulli random variable and so

\[
\text{kl}(L_S(Q)||L_{\varnothing}(Q)) \geq \lambda L_S(Q) - \log (1 - L_S(Q) + L_S(Q)e^\lambda).
\]

We can use this lower bound on \( \text{kl}(L_S(Q)||L_{\varnothing}(Q)) \) in Eq. (50). After rearranging, we obtain

\[
-L_{\varnothing}(Q)(1 - e^\lambda) \geq e^{\lambda L_S(Q) - B} - 1.
\]
Take $\lambda \leq 0$. Then

\begin{equation}
L_D(Q) \leq \frac{1 - e^{\lambda L_S(Q)} - B}{1 - e^\lambda}.
\end{equation}

Using the inequality $1 - e^{-x} \leq -x$ in the numerator of Eq. (54), we finally arrive at

\begin{equation}
L_D(Q) \leq L_S(Q) + B + \sqrt{B(B + 2L_S(Q))}.
\end{equation}

Also, note that by Pinsker’s inequality,

\begin{equation}
\text{kl}(L_S(Q) || L_D(Q)) \geq 2(L_S(Q) - L_D(Q))^2,
\end{equation}

and so

\begin{equation}
L_D(Q) \leq L_S(Q) + \frac{B}{2}.
\end{equation}

Both Eq. (57) and Eq. (55) are upper bounds on risk obtained from the inverted kl bound. Taking the minimum of the two bounds gives us the final result.

The inverted KL bound is visualized in Fig. 6. We see that depending on the empirical risk and KL, either the moment or the Pinsker bound is tighter. The inverted KL bound is the minimum of the two and so is tight in both regimes. By taking the minimum of two bounds, we obtain a bound this is tighter over a wider range of values for the empirical risk and KL terms.

\section*{F. Experimental details: datasets}

We use three datasets in our experiments: 1) The MNIST dataset [11], which consists of $28 \times 28$ grayscale images of handwritten decimal digits. 2) The Fashion-MNIST dataset [27], which consists of $28 \times 28$ grayscale images each associated with one of 10 categories (clothing and accessories). 3) The CIFAR-10 dataset [7], which consists of $32 \times 32$ RGB images each associated with one of ten categories (airplane, automobile, bird, etc.). For all datasets we use the standard training and test splits. This results in 60,000 training data for MNIST and Fashion-MNIST, 50,000 training data for CIFAR-10, and 10,000 test data for all three datasets. For CIFAR-10 we standardize all images according to the training split’s statistics.
G. EXPERIMENTAL DETAILS: ARCHITECTURES

We use fully connected feed-forward multilayer perceptrons with ReLU activations for MNIST. We study networks with architecture 784–600–600–10 (featuring two hidden layers) in order to compare to Rivasplata, Tankasali, and Szepesvari [24]. Such a network has 837,610 parameters.

We also borrow the modified LeNet-5 architecture used by Zhou et al. [28] in order to compare our bounds on SGD-trained classifiers. The network has 431,080 parameters. We use this architecture for MNIST and Fashion-MNIST.

We use the ResNet-20 architecture [6] for CIFAR-10. It has 269,722 parameters. For consistency with the other experiments, we use neither data augmentation nor weight decay.

H. EXPERIMENTAL DETAILS: TRAINING DETAILS

The bounds are evaluated on the 0–1 loss, which is not differentiable. To enable gradient-based optimization, we replace this with the cross entropy loss divided by the log number of classes, which gives a tight upper bound on the 0–1 loss.

We use SGD with momentum as the optimizer. We use one learning rate for the \( \alpha \)-prefix and base runs and another, lower learning rate for the bound optimization. For experiments on MNIST and Fashion-MNIST, the momentum is 0.95 and the batch size is 256. For MNIST, the learning rate for the \( \alpha \)-prefix and base runs is 0.003 and the learning rate for bound optimization is 0.0003; for Fashion-MNIST, they are respectively 0.01 and 0.003. We sweep over the prior variance \( \sigma_P \in \{3 \times 10^{-8}, 1 \times 10^{-7}, 3 \times 10^{-7}, \ldots, 1 \times 10^{-2}\} \). Via a union bound argument, our hyperparameter sweeps contribute a negligible amount to the bounds.

For the best hyperparameter setting, Algorithm 2 (right) was repeated 50 times with different data-orders and \( w_0 \). In all figures any shaded area corresponds to 2 standard deviations around the mean as computed from the 50 runs.

I. MORE DETAILS ON DIRECT RISK BOUND MINIMIZATION

We evaluated the performance of a learning algorithm based on optimizing a PAC-Bayes bound based on a data-dependent prior. Our proposed algorithm gets nearly state-of-the-art performance and produces a valid and tight PAC-Bayes bound on risk.

Let \( Q = \mathcal{N}(w, \Sigma) \) and \( P = \mathcal{N}(w_\alpha, \Sigma_\alpha) \). The algorithm starts with the coupling and \( \alpha \)-prefix runs as before. Then the base run is replaced with SGD minimizing the PAC-Bayes bounds \( \Psi^*_{\delta}(Q(\theta_Q), P; S \setminus S_\alpha) \) with respect to the posterior mean \( w \). Here \( \Psi^*_\delta(Q(\theta_Q), P; S \setminus S_\alpha) \) is the same bound as \( \Psi^*_{\delta}(Q(\theta_Q), P; S \setminus S_\alpha) \) but with risk evaluate on a differentiable surrogate loss. The procedure is outlined in Algorithm 2 (left).

Similarly as before, for each \( \alpha \) we choose the learning rate and prior variance that yield the tightest bounds. For a fixed set of hyperparameters, we repeat the optimization 50 times.

The results on 4 different networks and 3 different datasets appear in Fig. 5. The risk bounds and test errors drop dramatically with \( \alpha \) up to \( \alpha \approx 0.9 \) for all the networks tested. For MNIST and Fashion-MNIST, the momentum and batch size is the same as above. For CIFAR-10, the momentum is 0.9 and the batch size is 128. For MNIST and Fashion-MNIST, the \( \alpha \)-prefix run learning rate is 0.01; for CIFAR-10 it is 0.03. For all datasets, we
Figure 7. **Top row:** MNIST, LeNet-5; **bottom row:** MNIST, FC; **y-axis:** error-rate; **x-axis:** fraction $\alpha$ of the data used by the $\alpha$-prefix run of SGD to predict the weights produced by the base run of SGD; **left column:** test error and PAC-Bayes error bounds with isotropic prior covariance using half of MNIST data; **right column:** data and oracle prior bounds, where the prior is an isotropic Gaussian. The oracle prior is approximated by using ghost samples. When using ghost samples, some improvement on the bounds is seen for small values of $\alpha$ (below 0.2). For large values of $\alpha$ (at around 0.9) and some stopping times, the bound with a data and oracle dependent prior is worse than with a data-dependent prior.

sweep the direct bound optimization learning rate over $\{1 \times 10^{-6}, 3 \times 10^{-6}, 1 \times 10^{-5}, \ldots, 3 \times 10^{-3}\}$ and the prior variance over $\{1 \times 10^{-9}, 3 \times 10^{-9}, 1 \times 10^{-8}, \ldots, 3 \times 10^{-3}\}$.

**I.1. Comparison to PAC-Bayes by Backprop.** When $\alpha = 0$, the setting of our direct bound optimization experiments aligns closely to that considered by Rivasplata, Tankasali, and Szepesvari [24]: evaluating a PAC-Bayes bound-based learning algorithm using a prior centered at random initialization. This work reports a test error of 0.014 and a risk bound of 0.023 on MNIST with a 784–600–600–10 fully-connected network architecture, a Gaussian prior, and a PAC-Bayes bound expression similar to ours. Despite correspondence with the authors, we were unable to reproduce these results. For direct comparison, our $\alpha = 0$ baseline results with the same network architecture are a mean test error of 0.116 and a mean risk bound of 0.303 over 10 random seeds. Using a data-dependent prior learnt with proportion $\alpha = 0.7$ of the training data, this improves to a mean test error of 0.022 and a mean risk bound of 0.031 over 10 random seeds.