De-randomized PAC-Bayes Margin Bounds: Applications to Non-convex and Non-smooth Predictors

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Abstract

In spite of several notable efforts, explaining the generalization of deterministic deep nets, e.g., ReLU-nets, has remained challenging. Existing approaches usually need to bound the Lipschitz constant of such deep nets but such bounds have been shown to increase substantially with the number of training samples yielding vacuous generalization bounds [Nagarajan and Kolter, 2019a]. In this paper, we present new de-randomized PAC-Bayes margin bounds for deterministic non-convex and non-smooth predictors, e.g., ReLU-nets. The bounds depend on a trade-off between the $L_2$-norm of the weights and the effective curvature (‘flatness’) of the predictor, avoids any dependency on the Lipschitz constant, and yield meaningful (decreasing) bounds with increase in training set size. Our analysis first develops a de-randomization argument for non-convex but smooth predictors, e.g., linear deep networks (LDNs). We then consider non-smooth predictors which for any given input realize as a smooth predictor, e.g., ReLU-nets become some LDN for a given input, but the realized smooth predictor can be different for different inputs. For such non-smooth predictors, we introduce a new PAC-Bayes analysis that maintains distributions over the structure as well as parameters of smooth predictors, e.g., LDNs corresponding to ReLU-nets, which after de-randomization yields a bound for the deterministic non-smooth predictor. We present empirical results to illustrate the efficacy of our bounds over changing training set size and randomness in labels.

1 Introduction

Recent years have seen several notable efforts to explain generalization of deterministic deep networks, e.g., ReLU-nets, Res-nets, etc. [Long and Sedghi, 2019, Spencer Frei and Gu, 2019, Golowich et al., 2018, Neyshabur et al., 2018]. The classical approach to generalization bounds are typically based on two terms [Bartlett and Mendelson, 2002, Bartlett et al., 1999, Golowich et al., 2018]: a first term characterizing the empirical performance typically at a certain margin and a second term characterizing the capacity/complexity of the class of functions under consideration. The classical approach has so far struggled to explain the empirical performance of deep nets which perform surprisingly well on the training set even with random labels but is capable of generalizing well on real problems [Zhang et al., 2017]. Such struggles have led to calls for rethinking the classical approach to generalization bounds, including the need to consider the implicit bias of the training algorithms [Neyshabur et al., 2015, Soudry et al., 2018] and concerns regarding the effectiveness of using uniform convergence for such analysis [Nagarajan and Kolter, 2019a].

The current literature has broadly two types of generalization bounds for deep nets: results which apply to the original deterministic network [Nagarajan and Kolter, 2019b, Neyshabur et al., 2018, Bartlett et al., 2017, Li et al., 2018, Golowich et al., 2018] and results which apply to a modified and/or restricted network possibly with suitable restrictions on the learning algorithm [Cao and Gu, 2019a, Arora et al., 2019b]; see Section 2 for details. The focus of the current work is on the first type of bounds. Notable advances have been made for such bounds in recent years including approaches based on bounding the Rademacher complexity [Bartlett et al., 2017, Golowich et al., 2018, Li et al., 2018] or de-randomized PAC-Bayes bounds [Nagarajan and Kolter, 2019b, Neyshabur et al., 2018], among others [Long and Sedghi, 2019]. Getting suitable margin bounds from such approaches require a characterization of the Lipschitz constant of deep nets, which are non-smooth predictors [Neyshabur et al., 2018, Bartlett et al., 2017]. Existing bounds on the Lipschitz constant
are based on product of layer-wise spectral norms which has been shown \cite{Nagarajan2019} to empirically increase substantially with the training set size yielding vacuous bounds. In fact, Nagarajan and Kolter \cite{Nagarajan2019} showed that several prominent existing bounds on the original non-smooth deterministic network increase with the number of training samples whereas the empirical performance on the test set continues to decrease with the number of training samples (Figure 1(a)).

In this paper, we present new margin bounds on the generalization error of deterministic deep nets which avoid the shortcomings of existing bounds, decrease with increase in training set size, and increase with increase in random labels. Our analysis is based on a new de-randomization argument on PAC-Bayes margin bounds and has three key steps. The first step establishes a de-randomized PAC-Bayes margin bound for non-convex but smooth predictors, e.g., linear deep networks (LDNs) with a fixed structure. The analysis is inspired by a classical de-randomization argument for linear predictors \cite{Langford2003, McAllester2003} suitably generalized to smooth non-convex predictors using the Hanson-Wright inequality \cite{Rudelson2013, Hsu2012} among other things.

The second step establishes a bound for non-convex and non-smooth predictors, e.g., ReLU-nets, Res-nets, etc., by utilizing the bound for smooth predictors. The crux of the argument utilizes a self-evident but tricky-to-use fact: for any specific input, a deterministic ReLU net (and many other deep nets) effectively becomes a linear deep net (LDN) with a specific structure where some nodes and next layer connections get dropped because of input activations not crossing the ReLU threshold. Utilizing such realized LDN structures for analysis seems doomed from the start because the realized LDN structures depend on the input and, being discrete objects, are not even continuous functions of the input. Surprisingly, we show that a PAC-Bayes based analysis can be developed which considers distributions with product of two components, one determining the structure of smooth predictors (e.g., LDNs) and the other on the parameters of the network. De-randomizing that PAC-Bayes analysis yields a bound for the deterministic non-smooth predictor. The analysis entirely avoids having to bound the Lipschitz constant of ReLU-nets \cite{Nagarajan2019, Neyshabur2018, Bartlett2017, Golowich2018} and establishes an interesting connection with LDNs \cite{Arora2019, Laurent2018}. Our analysis and results are for non-smooth predictors which realize as a smooth predictor for any given input, e.g., ReLU-nets become some LDN for a given input, and includes commonly used deep nets such as ReLU-nets, Res-nets, and CNNs as special cases.

The third step cuts across both of the earlier steps and establishes de-randomized PAC-Bayes margin bound by considering suitable anisotropic posteriors based on the Hessian of the learned deep net, where the Hessian for non-smooth predictors is in terms of the realized LDNs, is well defined, and easily computable from the training set. In particular, we propose a Gaussian posterior with a diagonal covariance matrix where parameters corresponding to flat directions, i.e., loss is insensitive to changes in these parameters, have the same variance as the prior whereas parameters corresponding to sharp curvature directions, i.e., loss is sensitive...
Further, the margin loss \( \ell_Q \) for a Bayesian predictor, we maintain a distribution without changing the generalization performance, rendering the notion of ‘flatness’ meaningless. Thus, there can be arbitrarily changed through rescaling (“\( \alpha \)-scale transformation” [Dinh et al., 2017]) without changing the generalization performance, rendering the notion of ‘flatness’ meaningless. Thus, there

The bound we propose passes several sanity checks which most existing bounds do not. First, the bounds apply to the original non-smooth deterministic deeps net, e.g., ReLU-net, Rse-net, etc. [Golowich et al., 2018, Neyshabur et al., 2018]. Second, the bound decreases with an increase in the number of training samples. This is in sharp contrast with many existing bounds which increase with an increase in the number of training samples due to their reliance on the product of layer-wise spectral norms to bound the Lipschitz constant of the predictor [Nagarajan and Kolter 2019a, Bartlett et al., 2017, Golowich et al., 2018, Neyshabur et al., 2017]. Third, the bound increases with increase in number of random labels during training [Zhang et al., 2018]. Finally, the bound can take advantage of the recent advances in quantitatively sharpening PAC-Bayes bounds [Yang et al., 2019, Dziugaite and Roy, 2018].

The rest of the paper is organized as follows. We briefly review related work in Section 2. In Section 3 we present bounds for deterministic non-convex but smooth predictors with technical details and proofs in Appendix B. The results use anisotropic posteriors for the PAC-Bayes analysis and we present the isotropic case results in Appendix A. In Section 4 we present bounds for deterministic non-convex and non-smooth predictors with technical details and proofs in Appendix D. We present multi-class extensions of the analysis in Appendix C. We present experimental results in Section 5 and conclude in Section 6.

**Notation.** For ease of exposition, we present most of your results for the 2-class case, then discuss generalizations to the \( k \)-class case. Proofs for all results for both cases are in the Appendix. For 2-class, we denote smooth predictors \( \phi : \mathbb{R}^p \times \mathbb{R}^d \mapsto \mathbb{R} \) with \( \phi(\theta, x) \in \mathbb{R} \). The true labels \( y \in \{-1, +1\} \) and predicted labels \( \hat{y} = \text{sign}(\phi^\theta(x)) \). We denote the training set as \( S \) and true data distribution as \( D \). For any distribution \( W \) on \( \mathcal{X} \times \mathcal{Y} \) and any \( \beta \in \mathbb{R} \), we define the margin loss as \( \ell_\beta(\phi^\theta, W) \triangleq \mathbb{P}_{(x,y) \sim W}[y\phi^\theta(x) \leq \beta] \). For a Bayesian predictor, we maintain a distribution \( \mathcal{Q} \) over the parameters \( \theta \), and the corresponding margin loss is \( \ell_\beta(Q, W) \triangleq \mathbb{P}_{\theta \sim \mathcal{Q}}[\ell_\beta(\phi^\theta, W)] \). For \( k \)-class, with \( \phi : \mathbb{R}^p \times \mathbb{R}^d \mapsto \mathbb{R}^k \), the predictions \( \phi^\theta(x) \in \mathbb{R}^k \). Further, the margin loss \( \ell_\beta(\phi^\theta, W) \triangleq \mathbb{P}_{(x,y) \sim W}[\phi^\theta(x)[y] \leq \max_{\tilde{y} \neq y} \phi^\theta(x)[\tilde{y}] + \beta] \) and, as before, \( \ell_\beta(Q, W) \triangleq \mathbb{P}_{\theta \sim \mathcal{Q}}[\ell_\beta(\phi^\theta, W)] \). We denote non-smooth predictors as \( \psi^\theta(x) \) with the rest of the notation inherited from the smooth case. We use \( c, c_0 \) to denote constants which can change across equations.

## 2 Related work

Since traditional approaches that attribute small generalization error either to properties of the model family or to the regularization techniques fail to explain why large neural networks generalize well in practice [Zhang et al., 2017, Neyshabur et al., 2017]. Several different theories have been suggested to characterize the generalization error of deep nets including PAC-Bayes theory [Langford and Shawe-Taylor 2003, McAllester 1999, 2003], Rademacher complexity [Bartlett and Mendelson 2002], algorithm stability [Bousquet and Elisseeff 2002], and ‘flat minima’ [Dinh et al., 2017, Smith and Le, 2018, Hochreiter and Schmidhuber, 1997, Keskar et al., 2017]. However, for deep nets with positively homogeneous activations, the measure of flatness/sharpness can be arbitrarily changed through rescaling (“\( \alpha \)-scale transformation” [Dinh et al., 2017]) without changing the generalization performance, rendering the notion of ‘flatness’ meaningless. Thus, there

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are some works [Li et al., 2019] exploring scale-invariant generalization bound for the deep network. In the perspective of explaining generalization by Rademacher complexity, [Bartlett et al., 2017, Neyshabur et al., 2015, Golowich et al., 2018] derive bound on the Rademacher complexity of ReLU nets, which depends on the product of the spectral norms of layers. From the viewpoint of PAC-Bayesian theory, [Neyshabur et al., 2018, Nagarajan and Kolter, 2019b] derive generalization bound for deterministic deep nets. Especially, [Neyshabur et al., 2018] gives a similar generalization bound on ReLU as [Bartlett et al., 2017] by using the bound on the Lipschitz constant of such deep nets. However, [Nagarajan and Kolter, 2019a] show that such bounds increase substantially with the number of training samples yielding vacuous generalization bounds.

We acknowledge that besides the aforementioned approaches, recent advances in learning theory aim to explain the generalization performance of neural networks from many other perspectives. Examples include algorithm-dependent approach [Cao and Gu, 2019b, Spencer Frei and Gu, 2019] and data-dependent bound [Du et al., 2019, Arora et al., 2019b].

3 Bounds for Smooth Predictors

We start by considering smooth predictors \( \phi^\theta(x) \) and focus on the 2-class case, and delegate similar analysis for the \( k \)-class case to Appendix C. The smoothness of interest in the context of our analysis is that w.r.t. \( \theta \) rather than \( x \). In particular, for any fixed \( x \in \mathcal{X} \), for any \( \theta_1, \theta_2 \), we assume

\[
\phi^{\theta_1}(x) = \phi^\theta(x) + \langle \theta_1 - \theta_2, \nabla_{\theta_2} \phi^\theta(x) \rangle + \frac{1}{2} (\theta_1 - \theta_2)^T H_\phi^\theta(x)(\theta_1 - \theta_2),
\]

where \( \tilde{\theta} = \tau \theta_1 + (1 - \tau) \theta_2 \) for some \( \tau \in [0, 1] \) and \( H_\phi^\theta(x) = \nabla^2 \phi^\theta(x) \) denotes the Hessian. We will use \( H_\phi^\theta = \frac{1}{n} \sum_{i=1}^n H_\phi^\theta(x_i) \) to denote the Hessian over \( S \).

**Assumption 1** \( \phi^\theta(x) \) is smooth as in (1) such that

\( (\text{NC-1}) \) the gradients have bounded \( L_2 \)-norm, i.e., \( \|\nabla \phi^\theta(x)\|_2^2 \leq G^2 \) for all \( \theta, x \); and

\( (\text{NC-2}) \) the Hessian \( H_\phi^\theta(x) = \nabla^2 \phi^\theta(x) \) is bounded, i.e., \( H_- \preceq H_\phi^\theta(x) \preceq H_+ \), where \( H_+, H_- \) are respectively positive and negative semi-definite with max \( \|H_-\|_F, \|H_+\|_F \leq \eta_F \), max \( \|H_-\|_2, \|H_+\|_2 \leq \eta_2 \), and \( \text{Tr}(H_+) \leq \alpha_+, \text{Tr}(H_-) \geq -\alpha_- \) for \( \alpha_+, \alpha_- > 0 \).

3.1 Bounds for Stochastic vs. Deterministic Predictors

The PAC-Bayes analysis needs suitable choices for prior \( \mathcal{P} \) and posterior \( \mathcal{Q} \). For smooth predictors, we choose \( \mathcal{P} = \mathcal{N}(\theta_0, \sigma^2 \mathbb{I}) \). With \( \theta^\dagger \) denoting the learned parameters after training on \( \mathcal{Z} \), we choose \( \mathcal{Q} = \mathcal{N}(\theta^\dagger, \Sigma_{\theta^\dagger}) \). Choosing \( \Sigma_{\theta^\dagger} = \sigma^2 \mathbb{I} \) leads to a bound which depends on \( \|\theta^\dagger - \theta_0\|_2^2 \) (see Appendix A). For now, we consider \( \Sigma_{\theta^\dagger} \) to be a suitably constructed anisotropic diagonal matrix. With cross-entropy loss for \( \phi^{\theta^\dagger}(x) \) at \((x_i, y_i)\) denoted by \( l(y_i, \phi^{\theta^\dagger}(x_i)) \), we consider the Hessian of the average loss on \( \mathcal{Z} \):

\[
\mathcal{H}^\theta_{l, \phi} = \frac{1}{n} \sum_{i=1}^n \nabla^2 l(y_i, \phi^{\theta^\dagger}(x_i)).
\]

Now, let \( \Sigma_{\theta^\dagger}^{-1} = \text{diag}(\nu_1^2, \ldots, \nu_p^2) \), where

\[
\nu_j^2 = \max \left\{ \mathcal{H}^\theta_{l, \phi}[j, j], \frac{1}{\sigma^2_j} \right\}.
\]

With \( \sigma_j^2 \triangleq 1/\nu_j^2 \), the anisotropy in the posterior can be understood as follows: for parameters \( \theta^\dagger_j \) having high curvature \( H^\theta_{l, \phi}[j, j] \), the posterior variance \( \sigma_j^2 \) is small so that we will not deviate too far in the \( j \)-th component while sampling from the posterior; on the other hand, for parameters \( \theta^\dagger_j \) with small curvature, i.e., ‘flat’ directions, the posterior variance \( \sigma_j^2 = \sigma^2 \), same as the prior. The crux of the de-randomization argument is to relate margin bounds corresponding to the stochastic predictor \( \theta \sim \mathcal{Q} \) and the deterministic predictor with parameter \( \theta^\dagger \). With our choices of \( \mathcal{P} \) and \( \mathcal{Q} \), we have the following result:
Theorem 1  Let $\sigma^2 > 0$ be chosen before seeing the training data. Let $W$ be any distribution on pairs $(x, y)$ with $x \in \mathbb{R}^d$ and $y \in \{-1, +1\}$. For any $\theta^1 \in \mathbb{R}^d$, let $Q$ be a multivariate anisotropic Gaussian distribution with mean $\theta^1$ and covariance $\Sigma_{\theta^1}$, where

$$
\Sigma_{\theta^1}^{-1} = \text{diag}(\nu_1^2, \ldots, \nu_\nu^2), \quad \nu_j^2 \triangleq \max\left\{\mathcal{H}^{\theta^1}_{l, \phi}[j, j], \frac{1}{\sigma^2}\right\},
$$

where $\mathcal{H}^{\theta^1}_{l, \phi}$ is as in (2). Under Assumption [1] for any $\hat{\gamma} > 2$ and any $\beta \in \mathbb{R}$, we have

$$
\ell_{\beta}(Q, W) \leq \ell_{\beta + \sigma^2 \alpha \hat{\gamma}}(\phi^{\theta^1}, W) + 4 \exp(-c \hat{\gamma}) \tag{5}
$$

and,

$$
\ell_{\beta}(\phi^{\theta^1}, W) \leq \ell_{\beta + \sigma^2 \alpha \hat{\gamma}}(Q, W) + 4 \exp(-c \hat{\gamma}) \tag{6}
$$

where $\alpha = \alpha_+ + \alpha_-$, constant $c = c_0 \min\left[\frac{\sigma^2 \alpha_+^2}{\sigma^2}, \frac{\sigma^2 \alpha_-^2}{\sigma^2}, \frac{\alpha_+^2}{\eta_1^2}, \frac{\alpha_-^2}{\eta_2^2}\right]$, $c_0$ is an absolute constant and $G, \alpha_+, \alpha_-, \alpha, \eta_1, \eta_2$ are as in Assumption [1].

We highlight key aspects of the proof, especially the dependence of the analysis on the smoothness of $\phi^{\theta}(x)$ w.r.t. $\theta$ but not the smoothness w.r.t. $x$. While this aspect is not critical for smooth predictors, it will be key when analyzing non-smooth predictors in Section 4.

For establishing (5), we focus on the set

$$
\mathcal{Z}_{\beta + \sigma^2 \alpha \hat{\gamma}}^{(>)}(\theta^1) \triangleq \left\{(x, y) \in \mathcal{X} \times \mathcal{Y} | y \phi^{\theta^1}(x) > \beta + \sigma^2 \alpha \hat{\gamma}\right\}.
$$

For any $z = (x, y) \in \mathcal{Z}_{\beta + \sigma^2 \alpha \hat{\gamma}}^{(>)}(\theta^1)$, we show

$$
\mathbb{P}_{\theta \sim Q} \left[y \phi^{\theta}(x) \leq \beta \middle| z \in \mathcal{Z}_{\beta + \sigma^2 \alpha \hat{\gamma}}^{(>)}(\theta^1)\right] \leq 4 \exp(-c \hat{\gamma}).
$$

In other words, if the deterministic predictor $\phi^{\theta_0}(\cdot)$ has a large margin of at least $(\beta + \sigma^2 \alpha \hat{\gamma})$, then the probability that the stochastic predictor $\phi^{\theta}(x), \theta \sim Q$ will have a small margin of at most $\beta$ is exponentially small, i.e., $4 \exp(-c \hat{\gamma})$. The analysis utilizes the smoothness of $\phi^{\theta}(x)$ w.r.t. $\theta$, but is for a specific $z = (x, y)$.

Further, for $z \notin \mathcal{Z}_{\beta + \sigma^2 \alpha \hat{\gamma}}^{(>)}(\theta^1)$, we simply have

$$
\mathbb{P}_{\theta \sim Q} \left[y \phi^{\theta}(x) \leq \beta \middle| z \notin \mathcal{Z}_{\beta + \sigma^2 \alpha \hat{\gamma}}^{(>)}(\theta^1)\right] \leq 1,
$$

where the result is still for a specific $z = (x, y)$. Taking expectations w.r.t. $z \sim W$ and utilizing the two results above yields (5). The analysis for establishing (6) is similar.

Note that the condition $\hat{\gamma} > 2$ in Theorem 1 is not really restrictive since the result in terms of the un-normalized margin. Predictors such as LDNs are positively homogeneous of degree $q$, where $q$ is the depth of the network, so that for any $\omega > 0$, $\phi^{\omega \theta}(x) = \omega^q \phi^{\theta}(x)$, i.e., the un-normalized margin can be suitably scaled by scaling the parameters.

3.2 Main Result: Deterministic Smooth Predictors

The two-sided relationships between the stochastic and deterministic predictors in Theorem 1 can now be used to get bounds on the deterministic predictor $\phi^{\theta^1}(x)$. With $\gamma/2 = \sigma^2 \alpha \hat{\gamma}$, respectively choosing $\beta = 0, W = D$ for (5) and $\beta = \gamma/2, W = S$ for (5), we have

$$
\ell_0(\phi^{\theta^1}, D) \leq \ell_{\gamma/2}(Q, D) + 4 \exp(-c \gamma),
$$

$$
\ell_{\gamma/2}(Q, S) \leq \ell_{\gamma}(\phi^{\theta^1}, S) + 4 \exp(-c \gamma).
$$

Footnote: More sophisticated choices of $\sigma^2$ are possible, e.g., based on using differential privacy Dziugaite and Roy [2018], but we do not delve into such directions in the current paper.
With probability at least \((1 - \delta)\), PAC-Bayes gives

\[
KL_B(\ell_{\gamma/2}(Q, S)\|\ell_{\gamma/2}(Q, D)) \leq \frac{KL(Q\|P) + \log \frac{1}{\delta}}{n},
\]

where \(KL_B\) denotes the Bernoulli KL-divergence. For any \(\beta \in (0, 1)\), we unpack \(KL_B\) using the ‘fast-rate’ form \cite{Catoni2007} \cite{Yang2019} to get

\[
\ell_{\gamma/2}(Q, D) \leq \alpha_\beta \ell_{\gamma/2}(Q, S) + \beta_\beta \frac{KL(Q\|P) + \log \frac{1}{\delta}}{n},
\]

where \(\alpha_\beta = \frac{\log(1/\beta)}{1-\beta^2}, \beta_\beta = \frac{1}{1-\beta^2}\) are the same constants in classical regret bounds for online learning \cite{Banerjee2006}. While \(\beta_\beta > 1\), the above form usually yields quantitatively tighter bounds for predictors which have low margin loss \(\ell_{\gamma/2}(Q, S)\) because of the dependence on \(1/n\). Our bounds can also be done with the \(1/\sqrt{n}\) dependence \cite{McAllester2003}. Lining up these bounds yields the following result:

**Theorem 2** Consider any \(\theta_0 \in \mathbb{R}^p, \sigma^2 > 0\) chosen before training, and let \(\theta^\dagger\) be the parameters of the model after training. Let \(\mathcal{H}^\dagger_{\theta, \phi}\) be the Hessian as in \cite{Dziugaite2018}, let \(\nu_j = \max \{ \mathcal{H}^\dagger_{\theta, \phi}[j, j], \frac{1}{\sigma_j^2} \}\), \(\tilde{p} = |\{ j : \mathcal{H}^\dagger_{\theta, \phi}[j, j] > 1/\sigma_j^2 \}|\), and \(\{ \tilde{\nu}_1, \ldots, \tilde{\nu}_p \}\) be the \(\{\tilde{\nu}_1, \ldots, \tilde{\nu}_p\}\) be the subset of values larger than \(1/\sigma^2\). Under Assumption \cite{Liu2019}, with probability at least \(1 - \delta\), for any \(\theta^\dagger, \beta \in (0, 1), \gamma > 4\sigma^2/\alpha\), we have the following scale-invariant bound:

\[
el_0(\theta^\dagger, D) \leq \alpha_\beta \ell_0(\theta^\dagger, S) + \beta_\beta \frac{\sum_{j=1}^{\tilde{p}} \ln \frac{\tilde{\nu}_j}{1/\sigma_j^2} + \frac{\|\theta^\dagger - \theta_0\|^2}{\sigma_j^2} + d_\beta \exp (-c_\gamma) + \beta_\beta \log(\frac{1}{\delta})}{n}, \tag{7}
\]

where \(\alpha_\beta = \frac{\log(1/\beta)}{1-\beta^2}, \beta_\beta = \frac{1}{1-\beta^2}\), \(d_\beta = 4(\alpha_\beta + 1), c = c_0 \min \left[ \frac{\alpha_+^2}{\alpha G^2}, \frac{\alpha_-^2}{\alpha G^2}, \frac{\sigma_+^2}{\sigma^2}, \frac{\sigma_-^2}{\sigma^2}, \frac{\alpha_+^2}{\alpha_+ \sigma^2}, \frac{\alpha_-^2}{\alpha_- \sigma^2} \right], c_0\) is an absolute constant, \(\alpha = \alpha_+ + \alpha_-\) and \(G, \alpha_+, \alpha_-, \eta_F, \eta_2\) are as in Assumption \cite{Liu2019}.

The trade-off between the ‘effective curvature’ term and the ‘\(L_2\) norm’ term in the bound comes because of our use of anisotropic posterior \(Q\). Choosing a higher value for \(\sigma^2\) diminishes the dependency on the ‘\(L_2\) norm’ term and increases the dependency on the ‘effective curvature’ term; and vice versa. There has been recent advances in suitably choosing the prior for PAC-Bayes analysis \cite{Dziugaite2018}, and such advances can be applied here to get quantitatively tighter bounds. We report results for different choices of \(\sigma^2\) in the Appendix \cite{Dinh2017}.

The ‘effective curvature’ term depends on the diagonal elements of the Hessian \(\mathcal{H}^\dagger_{\theta, \phi}\) of the loss. One concern in using the Hessian \(\mathcal{H}^\dagger_{\theta, \phi}\) is its scale dependence \cite{Dinh2017}, but we prove that our bound is scale invariant (Appendix \cite{Dinh2017}). While \(\mathcal{H}^\dagger_{\theta, \phi}\) could have been constructed from the Hessian eigen-values \cite{Li2019}, \cite{Sagun2016}, the resulting bound would have been scale dependent and hence undesirable. Further, the diagonals of the Hessian are much easier to numerically compute compared to the eigen-values. The diagonal elements have an interesting empirical behavior (Section \cite{Dinh2017}): a small number of diagonal elements have relatively high values and most have quite small values. Such behavior aligns well with recent results on the eigen-spectrum of the Hessian \cite{Li2019} \cite{Sagun2016}. Further, all the diagonal elements decrease as more samples are used for training.

The result can be straightforwardly extended to consider an anisotropic prior for the PAC-Bayes analysis. For the bound, this entails choosing \(\sigma_j^2 > 0, j = 1, \ldots, p\) as parameters specific marginal variances. For this setting, the two key terms in the bound become:

\[
\sum_{j=1}^{\tilde{p}} \ln \frac{\mathcal{H}^\dagger_{\theta, \phi}[j, j]}{1/\sigma_j^2} + \sum_{j=1}^{\tilde{p}} \frac{(\theta^\dagger_j - \theta_{0,j})^2}{\sigma_j^2},
\]

\[
\tag{8}
\]
For the effective curvature term, for each parameter \( \theta_j \), if the curvature \( \mathcal{H}_i^{\theta_j}[j,j] > \frac{1}{\sigma_j^2} \), then we get a non-zero contribution from that term. For the \( L_2 \)-norm term, the distance from the initialization is scaled by the marginal variance \( \sigma_j^2 \). Thus, we essentially get the same trade-off between the two terms but now with a fine grained control based on \( \sigma_j^2 \) specific to each term.

4 Bounds for Non-Smooth Predictors

While the bound for the smooth case brings forth a novel trade-off between effective curvature and \( L_2 \)-norm of the weights, the challenge in developing bounds for deterministic deep nets has primarily been for the non-smooth case, which covers popular predictors such as ReLU-nets. We now develop bounds for such non-smooth predictors by utilizing the analysis for the smooth case.

For concreteness, we focus on ReLU-nets, denoted as \( \psi^\theta(x) \). An interesting property of \( \psi^\theta(x) \) is that for a given \( x \), there is a linear deep net (LDN) \( \phi^\xi(x) \) with structure \( \xi \) such that \( \psi^\theta(x) = \phi^\xi(x) \). The structure \( \xi \) depends on \( x \), is a subset of the ReLU-net structure, and is based on certain nodes and next step edges being non-functional because of input activations not crossing thresholds. The tricky bit about using such a property is that the realized structure \( \xi \) depends on \( x \). Our approach is to build a PAC-Bayes analysis which also maintains distributions over such structures \( \xi \) but indirectly, utilize the smooth predictor analysis for any structure \( \xi \), and show that suitable de-randomization gives a margin bound for the deterministic ReLU-net.

4.1 Prior and Posterior Distributions

Let \( \phi^\xi(x) \) denote a LDN with structure \( \xi \) and parameters \( \theta \). Note that the LDN structure \( \xi \) is a subset of the structure \( \Xi \) of the original ReLU-net. Further, while the parameters \( \theta \in \mathbb{R}^p \) correspond to \( \Xi \), \( \phi^\xi(x) \) only considers \( \theta|_\xi \), the components of \( \theta \) included in the LDN structure \( \xi \). For the PAC-Bayes analysis, the prior and posterior will be based on the following generative model:

1. Draw \( \theta_\rho \sim P_\rho \) for a suitable distribution \( P_\rho \) over the parameters \( \theta_\rho \in \mathbb{R}^p \); and
2. Draw \( \theta \sim \mathcal{N}(\mu, \Sigma) \) with mean \( \mu \) and covariance \( \Sigma \).

The distributions \( P_\rho \) and the parameters \( (\mu, \Sigma) \) will be different for the prior and the posterior. Specific draws \( (\theta_\rho, \theta) \) determine a specific hypothesis \( h(\theta_\rho, \theta) : \mathbb{R}^d \to \mathbb{R} \) and the distribution over \( (\theta_\rho, \theta) \) yield distributions over that hypothesis space. The hypotheses of interest are LDNs with structure \( \xi \) determined by \( \theta_\rho \) and parameters \( \theta|_\xi \) determined by \( \theta \). In particular, we consider hypotheses

\[
h(\theta_\rho, \theta)(x) = \phi^\xi(x), \quad \text{where} \quad \xi = S(\psi^\theta_\rho, x),
\]

where \( S(\psi^\theta_\rho, x) \) is the realized structure of the ReLU-net \( \psi^\theta_\rho \) with input \( x \). The specific hypotheses we consider in (9) is arguably the most unusual step in our analysis, and it is worth taking a moment to ensure that these are valid hypotheses, i.e., for a given draw \( (\theta_\rho, \theta) \), we get a deterministic prediction \( h(\theta_\rho, \theta)(x) \) for any input \( x \in \mathcal{X} \).

Now, we specify the prior and posterior for the PAC-Bayes analysis. For the prior,

1. \( \theta_\rho^{\text{prior}} \) is drawn from an isotropic zero mean Gaussian with marginal variance \( \frac{1}{2\pi} \), i.e., \( \theta_\rho^{\text{prior}} \sim \mathcal{N}(0, \frac{1}{2\pi} I) \),
2. \( \theta^{\text{prior}} \) is drawn from an isotropic Gaussian with mean \( \theta_0 \) and marginal variance \( \sigma^2 \), i.e., \( \theta^{\text{prior}} \sim \mathcal{N}(\theta_0, \sigma^2 I) \).

Let \( \theta^1 \) be the parameter of the ReLU network after training. For the posterior, we have

1. \( \theta_\rho^{\text{post}} \) is \( \theta^1 \) almost surely, i.e., \( P(\theta_\rho^{\text{post}} = \theta^1) = 1 \), and
2. \( \theta^{\text{post}} \) is drawn from a Gaussian with mean \( \theta^1 \) and covariance \( \Sigma_{\theta^1} \), i.e., \( \theta^{\text{post}} \sim \mathcal{N}(\theta^1, \Sigma_{\theta^1}) \).
As before, choosing $\Sigma_{\theta^t} = \sigma^2 \mathbb{I}$ leads to a bound which depends on $\|\theta^t - \theta_0\|^2_2$. For the current exposition, we consider $\Sigma_{\theta^t}$ to be an anisotropic diagonal matrix which leads to a bound which illustrates a trade-off between the ‘effective curvature’ term and the ‘L2-norm’ term. Let $\xi_i = S(\psi^{\theta^t}, x_i)$ for $x_i, i = 1, \ldots, n$ in the training set. With $l(y_i, \phi^\theta(x_i))$ denoting the cross-entropy loss, let

$$
\tilde{H}^\theta_{i,\phi} \triangleq \frac{1}{n} \sum_{i=1}^{n} \nabla^2 l (y_i, \phi^\theta(x_i)).
$$

(10)

There is a key difference between $\tilde{H}^\theta_{i,\phi}$ for non-smooth predictors in [10] and $H^\theta_{i,\phi}$ for smooth predictors in [2]. For the non-smooth case, the Hessian is in terms of the LDNs $\phi^\theta(x_i)$ with $\xi_i = S(\psi^{\theta^t}, x_i)$, the realized structure from the original non-smooth predictor $\psi^{\theta^t}(x_i)$. Thus, $\xi_i$ can be potentially different for each $x_i$, but $\tilde{H}^\theta_{i,\phi}$ is well defined and computable based on the training set. Let $\Sigma_{\theta^t}^{-1} = \text{diag}(\nu_1^2, \ldots, \nu_p^2)$, where

$$
\nu_j^2 = \max \left\{ \tilde{H}^\theta_{i,\phi}[j, j], \frac{1}{\sigma^2} \right\}.
$$

(11)

With $\sigma_j^2 = 1/\nu_j^2$, the anisotropy in the posterior is similar to the smooth case: for parameters $\theta^t_j$ which have high ‘curvature’ $\tilde{H}^\theta_{i,\phi}[j, j]$, the posterior variance $\sigma_j^2$ is small so that we will not deviate too far in the $j$-th component while sampling from the posterior; on the other hand, for parameters $\theta^t_j$ with small ‘curvature,’ i.e., flat directions, the posterior variance $\sigma_j^2 = \sigma^2$, same as the prior.

### 4.2 Bounds for Stochastic vs. Deterministic Predictors

Since $\theta^\rho_{\text{post}} = \theta^t$ almost surely, we denote the posterior hypotheses as $h(\theta^t, \theta)$ for convenience and we have $h(\theta^t, \theta)(x) = \phi^\theta_{S(\psi^{\theta^t}, x)}(x)$ from [9]. While our analysis for the non-smooth settings follows that of the smooth setting in Section 3.1, there is a key difference: the structure of LDNs considered $\xi = S(\psi^{\theta^t}, x)$ is potentially different for each input $x$. For the analysis, instead of directly considering the margin loss from the non-smooth predictor $\psi^{\theta^t}$, for any distribution $W$ over the samples and for $h(\theta^t, \theta)(x) = \phi^\theta_{S(\psi^{\theta^t}, x)}(x)$, we consider the surrogate margin loss

$$
\tilde{\ell}_\beta(h(\theta^t, \theta), W) \triangleq \mathbb{E}_{(x, y) \sim W} \left[ y \phi^\theta_{S(\psi^{\theta^t}, x)}(x) \leq \beta \right].
$$

(12)

We refer to the loss as surrogate because although the structure $S(\psi^{\theta^t}, x)$ of the realized LDN is based on $\psi^{\theta^t}$, the parameters $\theta$ could be different and, for the stochastic predictor, will be drawn from the posterior $Q$. Further, note that for $\theta = \theta^t$,

$$
h(\theta^t, \theta^t)(x) = \phi^\theta_{S(\psi^{\theta^t}, x)}(x) = \psi^{\theta^t}(x).
$$

(13)

Our strategy for getting the bound on the deterministic non-smooth predictor is based on [13]: we will de-randomize the stochastic predictors $h(\theta^t, \theta)$, $\theta \sim \mathcal{N}(\theta^t, \Sigma_{\theta^t})$ to get a margin bound on $h(\theta^t, \theta^t)$ which is exactly the deterministic non-smooth predictor $\psi^{\theta^t}$. First, with our choices of $P$ and $Q$, we have the following result:

**Theorem 3** Let $W$ be any distribution on pairs $(x, y)$ with $x \in \mathbb{R}^d$ and $y \in \{-1, +1\}$. For any $\theta^t \in \mathbb{R}^p$, let $Q(\theta^t, \theta) \sim 1[\theta^t = \theta^t]\mathcal{N}(\theta^t, \Sigma_{\theta^t})$ where $\Sigma_{\theta^t}$ is as in [11]. Under Assumption 4 for any $\gamma > 2$ and any $\beta \in \mathbb{R}$, we have

$$
\tilde{\ell}_\beta(Q, W) \leq \tilde{\ell}_{\beta + \gamma^2} (\psi^{\theta^t}, W) + 4 \exp(-c\gamma),
$$

(14)

and

$$
\tilde{\ell}_\beta(\psi^{\theta^t}, W) \leq \tilde{\ell}_{\beta + \gamma^2} (Q, W) + 4 \exp(-c\gamma),
$$

(15)
where $\alpha = \alpha_+ + \alpha_-$, constant $c = c_0 \min \left[ \sigma^2 \alpha^2, \sigma^2 \alpha^2, \alpha^2 \sigma^2, \alpha^2 \eta_2, \alpha^2 \frac{\sigma^2}{\eta_2} \right]$, $c_0$ is an absolute constant and $G$, $\alpha_+, \alpha_-, \alpha, \eta_F, \eta_2$ are as in Assumption 7

For establishing (14), we focus on the set
\[
\mathcal{Z}_{\beta + \sigma^2 \alpha \gamma}(\theta^*) \triangleq \left\{ (x,y) \in \mathcal{X} \times \mathcal{Y} : y_{S(\psi^*,x)}(x) > \beta + \sigma^2 \alpha \gamma \right\}.
\]

For any $z = (x,y) \in \mathcal{Z}_{\beta + \sigma^2 \alpha \gamma}(\theta^*)$, we show
\[
\mathbb{P}_{\theta \sim \mathcal{Q}} \left[ y_{S(\psi^*,x)}(x) \leq \beta | z \in \mathcal{Z}_{\beta + \sigma^2 \alpha \gamma}(\theta^*) \right] \leq 4 \exp(-c \gamma).
\]

In other words, if the deterministic predictor $\psi^*(x) = \phi_{S(\psi^*,x)}^\theta(x)$ has a large margin of at least $(\beta + \sigma^2 \alpha \gamma)$, then the probability that the stochastic predictor $\phi_{S(\psi^*,x)}^\theta(x), \theta \sim \mathcal{N}(\theta^*, \Sigma_{\theta^*})$ will have a small margin of at most $\beta$ is exponentially small, i.e., $4 \exp(-c \gamma)$. Note that here the comparison is between deterministic and stochastic LDNs with the exact same structure $S(\psi^*, x)$ because the input $x$ is the same. Since the structure stays the same, as before, the analysis utilizes the smoothness of $\phi^\theta(x)$ w.r.t. $\theta$ for each specific $z = (x,y)$. Further, for $z \not\in \mathcal{Z}_{\beta + \sigma^2 \alpha \gamma}(\theta^*)$, as before, we simply have
\[
\mathbb{P}_{\theta \sim \mathcal{Q}} \left[ y_{S(\psi^*,x)}(x) \leq \beta | z \not\in \mathcal{Z}_{\beta + \sigma^2 \alpha \gamma}(\theta^*) \right] \leq 1.
\]

While no fancy analysis is needed here, the result is still for a specific $z = (x,y)$. Taking expectations w.r.t. $z \sim \mathcal{W}$ and utilizing the two results above yield (14). The analysis for establishing (15) is similar. The details are in Appendix D.

### 4.3 Bound for Deterministic Non-Smooth Predictors

The two-sided relationships between the stochastic and deterministic predictors in Theorem 3 can now be used to get bounds on the deterministic predictor $\phi_{S(\psi^*,x)}^\theta(x) = \psi^*(x)$. With $\gamma/2 = \sigma^2 \alpha \gamma$, respectively choosing $\beta = 0, W = D$ for (15) and $\beta = \gamma/2, W = S$ for (14), we have
\[
\ell_0(\psi^*, D) \leq \ell_{\gamma/2}(\mathcal{Q}, D) + 4 \exp(-c \gamma)
\]
\[
\ell_{\gamma/2}(\mathcal{Q}, S) \leq \ell_{\gamma}(\psi^*, S) + 4 \exp(-c \gamma),
\]
Then, based on the ‘fast rate’ PAC-Bayes bound as before, we have the following result:

**Theorem 4** Consider any $\theta_0 \in \mathbb{R}^p, \sigma^2 > 0$ chosen before training, and let $\theta^*$ be the parameters of the model after training. Let $\mathcal{H}^\theta_{i,j}$ be the Hessian as in (2), let $\nu_j^2 = \max \left\{ \mathcal{H}^\theta_{i,j}, \frac{1}{\sigma^2} \right\}$, $\tilde{\nu} = \left\{ j : \mathcal{H}^\theta_{i,j} \geq 1/\sigma^2 \right\}$, and $\{ \tilde{\nu}(1), ..., \tilde{\nu}(m) \}$ be the subset of values larger than $1/\sigma^2$. Under Assumption 7 with probability at least $1 - \delta$, for any $\theta^*$, $\beta \in (0,1), \gamma > 4 \sigma^2 \alpha$, we have the following scale-invariant bound:
\[
\hat{\ell}_0(\psi^*, D) \leq a_{\beta} \hat{\ell}_\gamma(\psi^*, S) + \frac{b_{\beta}}{2n} \left( \sum_{t=1}^{\tilde{\nu}} \ln \left( \frac{\tilde{\nu}(t)}{1/\sigma^2} \right) + \frac{(2\pi + 1/\sigma^2)\|\theta^* - \theta_0\|_2^2}{L_2 \text{ norm}} \right) + d_{\beta} \exp(-c \gamma) + b_{\beta} \frac{\log(1/n)}{n},
\]
\[
(16)
\]
where $a_{\beta} = \frac{\log(1/\beta)}{1-\beta}, b_{\beta} = \frac{1}{1-\beta}, d_{\beta} = 4(a_{\beta} + 1), c = c_0 \min \left[ \frac{\alpha_+^2}{\alpha G^2}, \frac{\alpha_-^2}{\alpha G^2}, \frac{\alpha_+^2}{\alpha G^2}, \frac{\alpha_-^2}{\alpha G^2}, \frac{\alpha_+}{\alpha G}, \frac{\alpha_-}{\alpha G} \right]$, $c_0$ is an absolute constant, $\alpha = \alpha_+ + \alpha_-$ and $G, \alpha_+, \alpha_-, \eta_F, \eta_2$ are as in Assumption 7.
(a) Test Error Rate

(b) Diagonal Element of $\tilde{H}_{θ,l,φ}^{α}$.

(c) Effective Curvature.

(d) $L_2$ Norm.

(e) Margin Loss.

(f) Scale-invariant Generalization Bound.

Figure 2: Results for ReLU-nets trained on MNIST, distributions over 20 runs (a) test set error rate; (b) diagonal elements (mean) of $\tilde{H}_{θ,l,φ}^{α}$; (c) effective curvature; d) $L_2$ norm of $θ^α$; (e) margin loss with margin $γ = 6.5$; (f) generalization bound with $β = 0.1$ and $σ^2 = 100$. With increasing percentage of random labels, the generalization bound as well as the components (effective curvature, $L_2$ norm, margin loss) increase, and the bound in (f) stays valid for the test error rate in (a).

The result above for non-smooth predictors is essentially the same as Theorem 2 for smooth predictors with an additional term involving $π$ times the $L_2$ norm term and an effective curvature based on a Hessian defined using the realized LDNs. Multi-class versions of the bounds can be developed using a similar approach (see Appendix D). Further, these results can be straightforwardly extended to consider anisotropic priors to get bounds with terms of the form $\mathcal{S}$.

5 Experimental Results

We discuss a variety of experiments based on training ReLU-nets on MNIST. Details of the setup is in Appendix E.

5.1 Bounds with Changing Random Labels

Figure 2 plots the change in test set error rate, the bound, and different components of the bound as the percentage of random labels is increased. Figure 2(a) shows the test set error rate which understandably increases with increase in random labels. Figure 2(b) plots the diagonal elements of $\tilde{H}_{θ,l,φ}^{α}$ and shows that $\tilde{H}_{θ,l,φ}^{α}[j,j]$ increases with increase in random labels. The plot implies that the loss surface for $θ^α$ learned from randomly labeled data has more curvature compared to the one learned from true labeled data. Figure 2(c) shows that the effective curvature increases with randomly labeled data, in line with the observations in 2(b). While $\tilde{H}_{θ,l,φ}^{α}[j,j]$ can change based on $α$-scaling [Dinh et al. 2017], the effective curvature is scale invariant. Figure 2(d) plots the $L_2$ norm $\|θ^α\|_2/σ^2$ (with $θ_0 = 0$) and shows that $θ^α$ learned with more random labels has a larger $L_2$ norm. Figure 2(e) shows that the empirical margin loss distribution shifts to a higher value with increase in random labels. Figure 2(f) plots the proposed bound as $a_β \ell_γ(θ^α, S) + b_β (\sum_{ℓ=1}^β \ln \frac{ρ_2}{1/σ^2} + \frac{\|θ^α - θ_0\|^2}{σ^2})$.
Figure 3: Results for ReLU-nets on MNIST with change in training set size $n$ (20 runs for each): (a) test set error rate; (b) diagonal elements (mean) of $\tilde{H}_{t,\phi}$; (c) effective curvature; (d) $L_2$ norm of $\theta^t$; (e) margin loss; (f) generalization bound. The bound and all its components decrease with increase in $n$ from 50 to 50,000.

with $\beta = 0.1$ and $\sigma^2 = 100$. We omit the $d_\beta \exp(-c_\gamma) + b_\beta \log(\frac{1}{\delta})$ term since it does not change with change in random labels. Figure 2(f) shows that with the randomness in labels increasing from 0% to 100%, the generalization error shifts to a higher value and bounds the test set error rate in Figure 2(a).

5.2 Bounds with Changing Training Set Size

We study the behavior of the bound with increase in training set size, and also take a closer look at how the product of spectral norms, which recur in several recent bounds [Nagarajan and Kolter 2019b, Neyshabur et al. 2018, Golowich et al. 2018, Bartlett et al. 2017], behave relative to the $L_2$ norm with increase in training set size.

Figure 3 shows the change in test set error rate, the bound, and different components of the bound with increase in training set size $n$. Figure 3(a) shows that the test set error rate decreases with increase in the training set size $n$ [Nagarajan and Kolter 2019a]. We observe in Figure 3(b) that the diagonal elements of $\tilde{H}_{t,\phi}$ decrease with increase in $n$. As a consequence, the effective curvature decreases with increase in $n$ as shown in Figure 3(c). Recall that the effective curvature is scale invariant and hence does not change based on $\alpha$-scaling. Figure 3(d) shows that the weighted $L_2$ norm divided by sample $\|\theta^t\|_2/(n\sigma^2)$ also decreases with increase in $n$. The behavior of the $L_2$ norm has been studied closely in recent literature [Nagarajan and Kolter 2019a] and we revisit this shortly in the sequel. Figure 3(e) shows that the empirical margin loss $\ell_S(\hat{\theta}^t, S)$ also decreases with increase in $n$. Figure 3(f) plots the proposed generalization bound with $\beta = 0.1$ and $\sigma^2 = 100$, and shows that with $n$ increasing from 50 to 50000, the generalization error decreases, which is consistent with the test set error rate in Figure 3(a) and unlike bounds from several other recent bounds [Nagarajan and Kolter 2019a].

We now take a closer look at the relative behavior of the product of spectral norms often used in existing bounds and the $L_2$ norm in our bound. We observe in Figure 4(a) that both these quantities grow with training sample size $n$, but the $L_2$ norm (red line) grows far slower than the product of the spectral norms (blue line). Figure 4(b) shows the same quantities but divided by the number of samples. Note that both seem to decrease with increase in $n$, with $L_2$ norm having a tiny edge at higher $n$. Figure 4(c) shows both the

Figure 4: Comparison of $L_2$ norm and product of spectral norms with increase in training set size $n$: (a)-(b) original MNIST, and (c)-(d) MNIST with 5% random labels. $L_2$ norm grows far slower than product of spectral norms.

quantities where we have a little bit randomness in the labels (5% randomness) and the high level behavior seem similar to Figure 4(a). However, the magnitude of the increases in the product of the spectral norms is significant for the 5% randomness setting, e.g., look at the y-axis scale. Figure 4(d) shows the same quantities divided by the number of samples for data with 5% random labels. The product of the spectral norms scaled by $n$ starts increasing after 5000 samples whereas the scaled $L_2$ norm keeps decreasing.

Additional results are in Appendix E including how the bound varies with the margin $\gamma$ and the prior variance $\sigma^2$.

6 Conclusions

Explaining the generalization of deterministic deep nets has remained challenging. Recent work has shown that most existing bounds are not quantitatively tight, and often display unusual empirical behavior, e.g., increases with increase in training set size. A technical challenge in existing bounds have been the need to handle the non-smoothness of deep nets. In this paper, we have presented new bounds for non-smooth deep nets based on a de-randomization argument on PAC-Bayes. The bound demonstrates a trade-off between effective curvature and $L_2$ norm of the learned weights. Further, the bounds are quantitatively meaningful even without optimization and display correct qualitative behavior with change in training set size and random labels. The empirical results look promising and will inspire future work on quantitative sharpening of the bound.

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A De-randomized Margin Bound: Smooth Predictors and PAC-Bayes with Isotropic Posterior

We consider the case where $\phi^\theta(x_i)$ is a smooth function of $\theta$, and provide detailed proofs of the technical results corresponding to PAC-Bayes with isotropic posteriors briefly mentioned in Section 3. We start by recalling the Assumption 1 which will be used for the analysis:

**Assumption 1** $\phi^\theta(x)$ is smooth as in (1) such that

1. the gradients have bounded $L_2$-norm, i.e., $\|\nabla\phi^\theta(x)\|_2^2 \leq G^2$ for all $\theta, x$; and
2. the Hessian $H^\theta(x) = \nabla_2^2 \phi^\theta(x)$ is bounded, i.e., $H_- \preceq H^\theta(x) \preceq H_+$, where $H_+, H_-$ are respectively positive and negative semi-definite with $\max \{\|H_-\|_F, \|H_+\|_F\} \leq \eta_F$, $\max \{\|H_-\|_2, \|H_+\|_2\} \leq \eta_2$, and $\text{Tr}(H_+) \leq \alpha_+$, $\text{Tr}(H_-) \geq -\alpha_-$ for $\alpha_+, \alpha_- > 0$. 

A.1 Bounds for Stochastic vs. Deterministic Predictors

For analyzing smooth predictors using PAC-Bayes with isotropic posterior, we first establish the following bound relating the performance of deterministic and stochastic predictors:

**Theorem 5** Let \( W \) be any distribution on pairs \((x, y)\) with \( x \in \mathbb{R}^d \) and \( y \in \{-1, +1\} \). For any \( \theta^i \in \mathbb{R}^d \), let \( Q \) be a multivariate Gaussian distribution with mean \( \theta^i \) and covariance \( \sigma^2 I_p \). Under Assumption 1 for \( \gamma > 2 \) and any \( \beta \in R \), we have

\[
\ell_{\beta}(Q, W) \leq \ell_{\beta+\sigma^2\alpha\gamma}(\phi^{\theta^i}, W) + 4 \exp(-c\gamma),
\]

and,

\[
\ell_{\beta}(\phi^{\theta^i}, W) \leq \ell_{\beta+\sigma^2\alpha\gamma}(Q, W) + 4 \exp(-c\gamma),
\]

where \( \alpha = \alpha_+ + \alpha_-, \) constant \( c = c_0 \min \left[ \frac{\sigma^2(\gamma - 1)^2}{\eta_F^2}, \frac{\alpha_+(\gamma - 1)}{\eta_2} \right], \) \( c_0 \) is an absolute constant and \( G, \alpha_+, \alpha_-, \alpha, \eta_F, \eta_2 \) are as in Assumption 1.

We need the following result for the proofs:

**Lemma 1** For \( \delta \sim N(0, \sigma^2 I_p) \), respectively positive and negative semi-definite matrices \( H_+, H_- \) with \(-\alpha_- \leq \text{Tr}(H_-) \) and \( \text{Tr}(H_+) \leq \alpha_+ \), and \( \max \|H_-\|_F, \|H_+\|_F \leq \eta_F, \max \|H_-\|_2, \|H_+\|_2 \leq \eta_2 \), we have the following upper bound and lower bound:

\[
P[\delta^T H_- \delta < -\sigma^2\alpha_-\gamma] \leq \exp \left( -c_0 \min \left[ \frac{\alpha_-^2(\gamma - 1)^2}{\eta_F^2}, \frac{\alpha_-(\gamma - 1)}{\eta_2} \right] \right),
\]

and

\[
P[\delta^T H_+ \delta > \sigma^2\alpha_+\gamma] \leq \exp \left( -c_0 \min \left[ \frac{\alpha_+^2(\gamma - 1)^2}{\eta_F^2}, \frac{\alpha_+(\gamma - 1)}{\eta_2} \right] \right),
\]

where \( \gamma > 1 \) and \( c_0 \) is an absolute constant.

**Proof:** From Hanson-Wright inequality and the fact that \( \mathbb{E} [\delta^T H_+ \delta] = \mathbb{E} [\text{Tr}(H_+ \delta \delta^T)] = \sigma^2 \text{Tr}(H_+) \leq \sigma^2 \alpha_+ \), and \( \max \|\delta_i\|_{\psi_2} \leq c_0 \sigma \),

we have

\[
P[\delta^T H_+ \delta - \sigma^2\alpha_+ \geq t] \leq \exp \left( -c_0 \min \left[ \frac{t^2}{\sigma^4 \|H_+\|_F^2}, \frac{t}{\sigma^2 \|H_+\|_2} \right] \right)
\]

\[
\leq \exp \left( -c_0 \min \left[ \frac{t^2}{\sigma^4 \eta_F^2}, \frac{t}{\sigma^2 \eta_2} \right] \right).
\]

By taking \( t = \gamma \sigma^2\alpha_+ \) (\( > 0 \)), we have:

\[
P[\delta^T H_+ \delta \geq (\gamma + 1)\sigma^2\alpha_+] \leq \exp \left( -c_0 \min \left[ \frac{\alpha_+ \gamma^2}{\eta_F^2}, \frac{\alpha_+ \gamma}{\eta_2} \right] \right).
\]

Similarly,

\[
P[\delta^T H_- \delta - \sigma^2(-\alpha_-) \leq -t] \leq \exp \left( -c_0 \min \left[ \frac{t^2}{\sigma^4 \|H_-\|_F^2}, \frac{t}{\sigma^2 \|H_-\|_2} \right] \right)
\]

\[
\leq \exp \left( -c_0 \min \left[ \frac{t^2}{\sigma^4 \eta_F^2}, \frac{t}{\sigma^2 \eta_2} \right] \right).
\]
Taking $t = \sigma^2\alpha_\gamma(>0)$:

$$
\mathbb{P} \left[ \delta^T H^\theta_\gamma(x) \delta \leq -(\gamma + 1)\sigma^2\alpha_\gamma \right] \leq \exp \left( -c_0 \min \left[ \frac{\alpha_\gamma^2}{\eta_F^2}, -\gamma \right] \right).
$$

Denoting $\gamma + 1$ as $\tilde{\gamma}$ completes the proof. □

**Proof of Theorem 5.** Since $\phi$ is twice differentiable, for some suitable (random) $\tilde{\theta} = (1 - \tau)\theta^i + \tau\theta = \theta^i + \tau(\theta - \theta^i)$ where $\tau \in [0, 1)$, we have

$$
\phi^\theta(x_i) = \phi^{\theta^i}(x_i) + \langle \theta - \theta^i, \nabla\phi^{\theta^i}(x_i) \rangle + (\theta - \theta^i)^T H^\theta_\phi(x_i)(\theta - \theta^i).
$$

Now consider the following set where $\theta^i$ achieves a margin greater than $(\beta + \sigma^2\alpha_\gamma)$:

$$
Z^{(\gamma)}_{\beta^i + \sigma^2\alpha_\gamma}(\theta^i) = \left\{ (x, y) \in \mathcal{X} \times \mathcal{Y} \mid y\phi^{\theta^i}(x) > \beta + \sigma^2\alpha_\gamma \right\},
$$

where $\alpha = \alpha_\gamma + \alpha_+$. Let $P = N(0, \sigma^2\mathbb{I}_p)$ be a multivariate distribution with mean 0 and covariance $\sigma^2\mathbb{I}_p$. Now, for $z \in Z^{(\gamma)}_{\beta^i + \sigma^2\alpha_\gamma}(\theta^i)$, we have

$$
\mathbb{P}_{\theta \sim Q} \left[ y\phi^\theta(x) \leq \beta \mid z \in Z^{(\gamma)}_{\beta^i + \sigma^2\alpha_\gamma}(\theta^i) \right] = \mathbb{P}_{\theta \sim P} \left[ y\phi^{\theta^i}(x) \leq \beta \mid z \in Z^{(\gamma)}_{\beta^i + \sigma^2\alpha_\gamma}(\theta^i) \right].
$$

Now we first present the proof of [17], where we bound the loss on stochastic predictors with the theoretical loss on deterministic predictor.

Conditioned on $y = +1$, we have

$$
\mathbb{P}_{\delta \sim P} \left[ \phi^{\theta^i + \delta}(x) \leq \beta \mid z \in Z^{(\gamma)}_{\beta^i + \sigma^2\alpha_\gamma}(\theta^i), y = +1 \right]
$$

$$
= \mathbb{P}_{\delta \sim P} \left[ \phi^{\theta^i}(x) + \langle \delta, \nabla\phi^{\theta^i}(x) \rangle + \delta^T H^\theta_\phi(x)\delta \leq \beta \mid z \in Z^{(\gamma)}_{\beta^i + \sigma^2\alpha_\gamma}(\theta^i), y = +1 \right]
$$

$$
\leq \mathbb{P}_{\delta \sim P} \left[ \langle \delta, \nabla\phi^{\theta^i}(x) \rangle + \delta^T H_{\theta^i} \delta \leq \beta - \phi^{\theta^i}(x) \mid z \in Z^{(\gamma)}_{\beta^i + \sigma^2\alpha_\gamma}(\theta^i), y = +1 \right]
$$

(a) $$\leq \mathbb{P}_{\delta \sim P} \left[ \langle \delta, \nabla\phi^{\theta^i}(x) \rangle + \delta^T H_{\theta^i} \delta \leq -\sigma^2\tilde{\gamma}(\alpha_\gamma + \alpha_+) \mid z \in Z^{(\gamma)}_{\beta^i + \sigma^2\alpha_\gamma}(\theta^i), y = +1 \right] + \mathbb{P}_{\delta \sim P} \left[ \delta^T H_{\theta^i} \delta \leq -\sigma^2\tilde{\gamma} \right]
$$

(b) $$\leq \exp \left( -c_0 \sigma^2 \frac{\tilde{\gamma}}{G^2} \right) + \exp \left( -c_0 \min \left[ \frac{\alpha_\gamma^2}{\eta_F^2}, -\gamma \right] \right),
$$

where (a) follows since for $(x, y) \in Z^{(\gamma)}_{\beta^i + \sigma^2\alpha_\gamma}(\theta^i)$ and $y = +1$ we have $\phi^{\theta^i}(x) > \beta + \sigma^2\alpha_\gamma$; (b) follows since $\mathbb{P}[x+y \leq a+b] \leq \mathbb{P}[x \leq a] + \mathbb{P}[y \leq b]$; (c) is from Hoeffding’s inequality with $||\nabla\phi^{\theta^i}(x)||^2 \leq G^2$, $\max_i ||\delta_i||_2 \leq c_0\sigma$, and Lemma [1].
Similarly, conditioned in \( y = -1 \), we have

\[
\mathbb{P}_{\delta \sim P} \left[ -\phi^{\theta^1}(x) \leq \beta \mid z \in Z^{(>)}_{\beta + \sigma^2 \alpha \gamma}(\theta^1), y = -1 \right] = \mathbb{P}_{\delta \sim P} \left[ -\phi^{\theta^1}(x) - \delta + \delta^T H^\delta(x) \delta - \delta^T H^\delta(x) \delta \leq \beta \mid z \in Z^{(>)}_{\beta + \sigma^2 \alpha \gamma}(\theta^1), y = -1 \right]
\]

\[
\leq \mathbb{P}_{\delta \sim P} \left[ -\delta, \nabla \phi^{\theta^1}(x) - \delta^T H_+ \delta - \delta + \phi^{\theta^1}(x) \mid z \in Z^{(>)}_{\beta + \sigma^2 \alpha \gamma}(\theta^1), y = -1 \right]
\]

\[
\leq \mathbb{P}_{\delta \sim P} \left[ -\delta, \nabla \phi^{\theta^1}(x) - \delta^T H_+ \delta \mid z \in Z^{(>)}_{\beta + \sigma^2 \alpha \gamma}(\theta^1), y = -1 \right] + \mathbb{P}_{\delta \sim P} \left[ -\delta^T H_+ \delta \leq -\sigma^2 \alpha \gamma \right]
\]

\[
\leq \exp \left(-c_0 \frac{\sigma^2 \alpha \gamma}{G^2} \right) + \exp \left(-c_0 \min \left[ \frac{\alpha^2_\gamma (\bar{\gamma} - 1)^2}{\eta_1^2}, \frac{\alpha_\gamma (\bar{\gamma} - 1)}{\eta_2} \right] \right)
\]

where (a) follows since for \( (x, y) \in Z^{(>)}_{\beta + \sigma^2 \alpha \gamma}(\theta^1) \) and \( y = -1 \) we have \(-\phi^{\theta^1}(x) > \beta + \sigma^2 \alpha \gamma\); (b) follows since \( \mathbb{P}[x+y \leq a+b] \leq \mathbb{P}[x \leq a]+\mathbb{P}[y \leq b] \); (c) is from Hoeffding’s inequality with \( \| \nabla \phi^{\theta^1}(x) \|_2^2 \leq G^2 \), \( \max_i \| \delta_i \|_{\psi_2} \leq c_0 \sigma \), and Lemma \[1\].

Then, we have

\[
\mathbb{P}_{\theta \sim Q} \left[ y\phi^\theta(x) \leq \beta \mid z \in Z^{(>)}_{\beta + \sigma^2 \alpha \gamma}(\theta^1) \right] = \mathbb{P}_{\delta \sim P} \left[ y\phi^{\theta^1}(x) \leq \beta \mid z \in Z^{(>)}_{\beta + \sigma^2 \alpha \gamma}(\theta^1) \right]
\]

\[
\leq \mathbb{P} \left[ y\phi^{\theta^1}(x) \leq \beta \mid z \in Z^{(>)}_{\beta + \sigma^2 \alpha \gamma}(\theta^1), y = +1 \right] + \mathbb{P} \left[ y\phi^{\theta^1}(x) \leq \beta \mid z \in Z^{(>)}_{\beta + \sigma^2 \alpha \gamma}(\theta^1), y = -1 \right]
\]

\[
\leq \exp \left(-c_0 \frac{\sigma^2 \alpha \gamma}{G^2} \right) + \exp \left(-c_0 \min \left[ \frac{\alpha^2_\gamma (\bar{\gamma} - 1)^2}{\eta_1^2}, \frac{\alpha_\gamma (\bar{\gamma} - 1)}{\eta_2} \right] \right)
\]

\[
+ \exp \left(-c_0 \frac{\sigma^2 \alpha \gamma}{G^2} \right) + \exp \left(-c_0 \min \left[ \frac{\alpha^2_\gamma (\bar{\gamma} - 1)^2}{\eta_1^2}, \frac{\alpha_\gamma (\bar{\gamma} - 1)}{\eta_2} \right] \right).
\]

(26)

For \( z \notin Z^{(>)}_{\beta + \sigma^2 \alpha \gamma}(\theta^1) \), we have

\[
\mathbb{P}_{\theta \sim Q} \left[ y\phi^\theta(x) \leq \beta \mid z \notin Z^{(>)}_{\beta + \sigma^2 \alpha \gamma}(\theta^1) \right] \leq \mathbb{P} \left[ y\phi^\theta(x) \leq \beta + \sigma^2 \alpha \gamma \mid z \notin Z^{(>)}_{\beta + \sigma^2 \alpha \gamma}(\theta^1) \right].
\]

where the right hand side considers the indicator of the event \([y\phi^\theta(x) \leq \beta + \sigma^2 \alpha \gamma]\) conditioned on \( z \notin Z^{(>)}_{\beta + \sigma^2 \alpha \gamma}(\theta^1) \). Note that the inequality is true since for \( z \notin Z^{(>)}_{\beta + \sigma^2 \alpha \gamma}(\theta^1) \), by definition, \( y\phi^\theta(x) \leq \beta + \sigma^2 \alpha \gamma \), so that the conditional indicator is 1, and hence upper bounds the conditional probability on the left hand side.
By definition, we have

\[
\ell_\beta(Q, W) = P_{\theta \sim Q \given z \sim W} \left[ y \phi^\theta(x) \leq \beta \right] = P_{\theta \sim Q \given z \sim W} \left[ y \phi^\theta(x) \leq \beta \mid z \notin Z_{\beta + \sigma^2 \alpha \tilde{\gamma}}^{(\geq)}(\theta^\dagger) \right] + P_{\theta \sim Q \given z \sim W} \left[ y \phi^\theta(x) \leq \beta \mid z \in Z_{\beta + \sigma^2 \alpha \tilde{\gamma}}^{(\geq)}(\theta^\dagger) \right]
\]

\[
\leq P_{z \sim W} \left[ 1 \left[ y \phi^\theta(x) \leq \beta + \sigma^2 \alpha \tilde{\gamma} \mid z \notin Z_{\beta + \sigma^2 \alpha \tilde{\gamma}}^{(\geq)}(\theta^\dagger) \right] \right] + \exp \left( -c_0 \sigma^2 \alpha \tilde{\gamma}^2 G^2 \right) + \exp \left( -c_0 \sigma^2 \alpha \tilde{\gamma}^2 G^2 \right)
\]

which establishes (17).

Now we first present the proof of (18), where we bound the the loss on deterministic predictor with the loss on stochastic predictors.

Consider the following set where \( \theta^\dagger \) achieves a margin of at most \( \beta \):

\[
Z_{\beta}^{(\geq)}(\theta^\dagger) = \left\{ (x, y) \in \mathcal{X} \times \mathcal{Y} \mid y \phi^\theta(x) \leq \beta \right\} .
\]

Let \( P = N(0, \sigma^2 I_p) \) be a multivariate distribution with mean 0 and covariance \( \sigma^2 I_p \). Now, for \( z \in Z_{\beta}^{(\geq)}(\theta^\dagger) \), we have

\[
P_{\theta \sim Q} \left[ y \phi^\theta(x) > \beta + \sigma^2 \alpha \tilde{\gamma} \mid z \in Z_{\beta}^{(\geq)}(\theta^\dagger) \right] = P_{\delta \sim P} \left[ y \phi^{\theta + \delta}(x) > \beta + \sigma^2 \alpha \tilde{\gamma} \mid z \in Z_{\beta}^{(\geq)}(\theta^\dagger) \right].
\]

Now, conditioned in \( y = +1 \), we have

\[
P_{\delta \sim P} \left[ \phi^{\theta + \delta}(x) > \beta + \sigma^2 \alpha \tilde{\gamma} \mid z \in Z_{\beta}^{(\geq)}(\theta^\dagger), y = +1 \right]
\]

\[
= P_{\delta \sim P} \left[ \phi^\theta(x) + \langle \delta, \nabla \phi^\theta(x) \rangle + \delta^T H_\delta^\theta(x) \delta > \beta + \sigma^2 \alpha \tilde{\gamma} \mid z \in Z_{\beta}^{(\geq)}(\theta^\dagger), y = +1 \right]
\]

\[
\leq P_{\delta \sim P} \left[ \langle \delta, \nabla \phi^\theta(x) \rangle + \delta^T H_\delta \delta > \beta + \sigma^2 \alpha \tilde{\gamma} - \phi^\theta(x) \mid z \in Z_{\beta}^{(\geq)}(\theta^\dagger), y = +1 \right]
\]

\[
\leq P_{\delta \sim P} \left[ \langle \delta, \nabla \phi^\theta(x) \rangle + \delta^T H_\delta \delta > \sigma^2 \alpha \tilde{\gamma} \mid z \in Z_{\beta}^{(\geq)}(\theta^\dagger), y = +1 \right] + P_{\delta \sim P} \left[ \delta^T H_\delta \delta \geq \sigma \alpha \tilde{\gamma} \right]
\]

\[
\leq \exp \left( -c_0 \sigma^2 \alpha \tilde{\gamma}^2 G^2 \right) + \exp \left( -c_0 \min \left[ \frac{(\tilde{\gamma} - 1)^2}{\eta_2^2}, \frac{(\tilde{\gamma} - 1)}{\eta_2} \right] \right),
\]

(28)
\[ \begin{align*}
\text{where (a) follows since for } (x, y) \in Z_\beta^{(\leq)}(\theta^t) \text{ and } y = +1 \text{ we have } \phi^{\theta^t}(x) & \leq \beta \Rightarrow \beta - \phi^{\theta^t}(x) \geq 0; \text{ (b) follows since } P[x + y \leq a + b] \leq P[x \leq a] + P[y \leq b]; \text{ (c) is from Hoeffding’s inequality with } \|\nabla \phi^{\theta^t}(x)\|_2^2 \leq G^2, \text{ max}_t \|\delta_i\|_{\psi_2} \leq c_0 \sigma, \text{ and Lemma I.} \\
\text{Similarly, conditioned on } y = -1, \text{ we have}
\end{align*}\]
By definition, we have
\[
1 - \ell_{\beta + \sigma^2 \alpha \hat{\gamma}}(Q, W) \\
= \mathbb{P}_{\theta \sim Q, z \sim W} \left[ y_{\phi^0}(x) > \beta + \sigma^2 \alpha \hat{\gamma} \right] \\
\leq \mathbb{P}_{\theta \sim Q, z \sim W} \left[ y_{\phi^0}(x) > \beta + \sigma^2 \alpha \hat{\gamma} \mid z \notin \mathcal{Z}^{(\leq)}(\theta^1) \right] + \mathbb{P}_{\theta \sim Q, z \sim W} \left[ y_{\phi^0}(x) > \beta + \sigma^2 \alpha \hat{\gamma} \mid z \in \mathcal{Z}^{(\leq)}(\theta^1) \right] \\
\leq \mathbb{P}_{z \sim W} \left[ 1 \left[ y_{\phi^0}(x) > \beta \mid z \notin \mathcal{Z}^{(\leq)}(\theta^1) \right] \right] + \exp \left( -c_0 \frac{\sigma^2 \alpha^2 \hat{\gamma}^2}{G^2} \right) + \exp \left( -c_0 \frac{\sigma^2 \alpha^2 \hat{\gamma}^2}{G^2} \right) \\
+ \exp \left( -c_0 \min \left[ \frac{\alpha^2 (\hat{\gamma} - 1)^2}{\eta_F^2}, \frac{\alpha^2 (\hat{\gamma} - 1)}{\eta_2} \right] \right) \right) + \exp \left( -c_0 \min \left[ \frac{\alpha^2 (\hat{\gamma} - 1)^2}{\eta_F^2}, \frac{\alpha^2 (\hat{\gamma} - 1)}{\eta_2} \right] \right) \right),
\] (31)

which implies
\[
\ell_{\beta}(\phi^0, W) \leq \ell_{\beta + \sigma^2 \alpha \hat{\gamma}}(Q, W) + \exp \left( -c_0 \frac{\sigma^2 \alpha^2 \hat{\gamma}^2}{G^2} \right) + \exp \left( -c_0 \frac{\sigma^2 \alpha^2 \hat{\gamma}^2}{G^2} \right) \\
+ \exp \left( -c_0 \min \left[ \frac{\alpha^2 (\hat{\gamma} - 1)^2}{\eta_F^2}, \frac{\alpha^2 (\hat{\gamma} - 1)}{\eta_2} \right] \right) \right) + \exp \left( -c_0 \min \left[ \frac{\alpha^2 (\hat{\gamma} - 1)^2}{\eta_F^2}, \frac{\alpha^2 (\hat{\gamma} - 1)}{\eta_2} \right] \right) \right).
\] (32)

By choosing \( \hat{\gamma} > 2 \), we have \( \hat{\gamma}^2 > \hat{\gamma} \), \( (\hat{\gamma} - 1)^2 > \hat{\gamma} - 1 > \frac{1}{2} \hat{\gamma} \). Therefore, taking a constant \( c = c_0 \min \left[ \frac{\alpha^2}{G^2}, \frac{\alpha^2}{\eta_F^2}, \frac{\alpha^2}{\eta_2}, \frac{\alpha^2}{\eta_2}, \frac{\alpha^2}{\eta_2}, \frac{\alpha^2}{\eta_2} \right] \) completes the proof.

A.2 Deterministic Margin Bounds with Fast Rates

With the above de-randomization, another piece we need to derive a deterministic margin bound is the fast rate PAC-Bayes bound in \cite{Catoni2007, Yang2019}, which is formally stated as below:

\textbf{Theorem 6} (Fast-Rate \textit{PAC-Bayes} \cite[Theorem 1.2.6]{Yang2019}) For any prior distribution \( P \), for any \( \delta \in (0, 1) \) and \( \beta \in (0, 1) \), with probability at least \( 1 - \delta \) over the draw of \( n \) samples \( S \sim D^n \), for any \( Q \) we have
\[
\ell(Q, D) \leq \frac{\log(1/\beta)}{1 - \beta} \ell(Q, S) + \frac{1}{1 - \beta} \frac{KL(Q\|P) + \log(\frac{1}{\beta})}{n},
\] (33)

where \( \ell(Q, D), \ell(Q, S) \) are true and empirical losses.

Recall that these multiplicative factors are exactly the ones which appear in classical algorithms such as the Weighted Majority \cite{Littlerstone1994} and the connections between online regret bounds and PAC-Bayes bounds are well known \cite{Banerjee2006}. For settings where the empirical loss \( \ell(Q, S) \) is small, e.g., (margin) loss with deep nets on the training set, one can choose relatively smaller values of \( \beta \) to get quantitatively tighter bounds. Denoting \( a_\beta = \log(1/\beta) \) and \( b_\beta = \frac{1}{1 - \beta} \), Table 1 illustrates the trade-off between the empirical loss and the KL-divergence terms.

Utilizing the fast rate PAC-Bayes bound, we have the following bound for the deterministic predictor:
Then, the absolute constant, $\alpha = \alpha_+ + \alpha_-$ and $G$, $\alpha_+$, $\alpha_-$, $\eta_F$, $\eta_2$ are as in Assumption 7.

Proof: To get to a de-randomized margin bound, we utilize the results in Theorem 5. First, with $\beta = 0$, $\sigma^2\gamma_0 = \frac{\gamma}{2}$ and $W = D$ in Theorem 5 we have

$$\ell_0(\phi^0, D) \leq a_\beta \ell_\gamma(\phi^0, S) + \frac{b_\beta}{2n} \frac{\|\theta^0 - \theta_0\|^2}{\sigma^2} + d_\beta \exp \left(-c_\gamma\right) + b_\beta \log \left(\frac{\gamma}{n}\right),$$  

(34)

where $a_\beta = \frac{\log(1/\beta)}{1-\beta}, b_\beta = \frac{1}{1-\beta}, d_\beta = 4(a_\beta + 1), c = c_0 \min \left[\frac{\alpha^2_+}{\alpha^2_+ - \alpha^2_0}, \frac{\alpha^2_+}{\alpha^2_+ + \sigma^2_0}, \frac{\alpha^2_-}{\alpha^2_- - \sigma^2_0}, \frac{\alpha^2_-}{\alpha^2_- + \sigma^2_0}\right], c_0$ is an absolute constant, $\alpha = \alpha_+ + \alpha_-$ and $G$, $\alpha_+$, $\alpha_-$, $\eta_F$, $\eta_2$ are as in Assumption 7.

Similarly, with $\beta = \gamma/2$ and $W = S$ in Theorem we have

$$\ell_{\gamma/2}(Q, S) \leq \ell_\gamma(\phi^0, S) + 4 \exp \left(-c_\gamma\right).$$  

(36)

Now, from the Fast Rate PAC-Bayesian bound [34], with probability at least $(1 - \delta)$ over the draw of $n$ samples $S \sim D^n$, for any $\beta \in (0, 1)$ and for any $Q$ we have

$$\ell_{\gamma/2}(Q, D) \leq \frac{\log(1/\beta)}{1-\beta} \ell_{\gamma/2}(Q, S) + \frac{1}{1-\beta} \frac{KL(Q\|P) + \log(\frac{1}{\delta})}{n},$$  

(37)

Using (35) and (36), and noting that $KL(Q\|P) = \frac{\|\theta^0 - \theta_0\|^2}{2\sigma^2}$, we have

$$\ell_0(\phi^0, D) \leq \frac{\log(1/\beta)}{1-\beta} \ell_\gamma(\phi^0, S) + \frac{1}{1-\beta} \frac{\|\theta^0 - \theta_0\|^2}{2\sigma^2 n} + \frac{1}{1-\beta} \frac{\log(\frac{1}{\delta})}{n} + 4 \left(\frac{\log(1/\beta)}{1-\beta} + 1\right) \exp \left(-c_\gamma\right).$$  

(38)

To show that our bound is scale-invariant, we use the property of KL-divergence between any continuous distributions $Q$ and $P$ such that the KL-divergence between $Q$ and $P$ remains invariant under $\alpha$-scale transformation [Kleeman 2011], i.e.,

$$KL(Q'\|P') = KL(Q\|P),$$  

(39)

where $Q'$ and $P'$ are the distributions after $\alpha$-scale transformation corresponding to $Q$ and $P$ respectively. Thus, the $KL(Q\|P)$ in (37) remains invariant under $\alpha$-scale transformation. Note that the other terms apart from the $KL(Q\|P)$ in (37) do not change by $\alpha$-scale transformation since the functions represented by the networks are the same.

Thus, our bound is scale-invariant.

That completes the proof. □

Recent work [Dinh et al. 2017] show that $\alpha$-scale transformation can arbitrarily change the flatness of the loss landscape for deep networks with positively homogeneous activation without changing the functions represented by the networks, which invalid many flatness-based generalization bound.

Our generalization bound remains invariant under $\alpha$-scale transformation since the KL-divergence between two continuous distributions remains invariant under invertible transformations, such as $\alpha$-scale transformation.
A.3 Normalized Margin

Assume that the predictor \( \phi^\theta(x) \) is positively homogeneous of degree \( k \) so that \( \phi(\alpha \theta, x) = \alpha^k \phi^\theta(x) \). Note that commonly used deep networks do satisfy the property. For such predictors, the margin \( \gamma \) used in our analysis is the un-normalized margin in the sense that the margin can be changed by just changing \( \|\theta^\dagger\|_2 \) without changing the direction of \( \theta^\dagger \). Consider the normalized margin

\[
\bar{\gamma} \equiv y \phi^{\theta^\dagger}(x) \quad \text{such that} \quad \|\theta^\dagger\|_2 = 1. \tag{40}
\]

For the general setting, with \( \theta^\dagger = \alpha \theta^\dagger_1 \), we have \( \|\theta^\dagger\|_2 = \alpha \|\theta^\dagger_1\|_2 = \alpha \), and the un-normalized margin

\[
\gamma = y \phi^{\theta^\dagger}(x) = \alpha^k y \phi^{\theta^\dagger_1}(x) = \alpha^k \bar{\gamma} = \|\theta^\dagger\|_2^k \bar{\gamma}. \tag{41}
\]

Then, for \( \theta_0 = 0 \), we choose

\[
\|\theta^\dagger\|_2 = \left( \log(n \bar{\gamma}) / c \tilde{\gamma} \right)^{\frac{1}{k}}, \tag{42}
\]

Then,

\[
\frac{\|\theta^\dagger - \theta_0\|_2^2}{n} = \frac{1}{n} \left( \log(n \bar{\gamma}) / c \tilde{\gamma} \right)^{\frac{1}{k}} = \frac{\log(n \bar{\gamma})^2}{nc^{\frac{k}{2}} \bar{\gamma}^2}. \tag{43}
\]

Further, note that

\[
\gamma = \|\theta^\dagger\|_2 \bar{\gamma} = \log(n \bar{\gamma}) / c, \tag{44}
\]

Then,

\[
\exp(-c \gamma) = \exp(-\log(n \bar{\gamma})) = \frac{1}{n \bar{\gamma}}. \tag{45}
\]

As a result, both terms can be made to scale as \( O(\frac{1}{n}) \) by suitably choosing \( \|\theta^\dagger\|_2 \) and the constants improve if the normalized margin \( \bar{\gamma} \) is large.

B De-randomized Margin Bound: Smooth Predictors and PAC-Bayes with Anisotropic Posterior

We consider the case where \( \phi^\theta(x) \) is a smooth function of \( \theta \), and provide detailed proofs of the technical results corresponding to PAC-Bayes with anisotropic posteriors briefly mentioned in Section 3.

B.1 Bounds for Stochastic vs. Deterministic Predictors

Recall Theorem 1 which establishes the relationship between stochastic and deterministic predictors in the main paper:

\begin{theorem}
Let \( \sigma^2 > 0 \) be chosen before seeing the training data\footnote{More sophisticated choices of \( \sigma^2 \) are possible, e.g., based on using differential privacy \cite{dziugaite2018}, but we do not delve into such directions in the current paper.}. Let \( W \) be any distribution on pairs \((x, y)\) with \( x \in \mathbb{R}^d \) and \( y \in \{-1, +1\} \). For any \( \theta^\dagger \in \mathbb{R}^d \), let \( Q \) be a multivariate anisotropic Gaussian distribution with mean \( \theta^\dagger \) and covariance \( \Sigma_{\theta^\dagger} \), where

\[
\Sigma_{\theta^\dagger}^{-1} = \text{diag}(\nu_1^2, \ldots, \nu_p^2), \quad \nu_j^2 \triangleq \max \left\{ \mathcal{H}_{\theta^\dagger, \phi}[j, j], \frac{1}{\sigma^2} \right\}, \tag{4}
\]

where \( \mathcal{H}_{\theta^\dagger, \phi} \) is as in \cite{dziugaite2018}. Under Assumption 2 for any \( \bar{\gamma} > 2 \) and any \( \beta \in \mathbb{R} \), we have

\[
\ell_\beta(Q, W) \leq \ell_{\beta + \sigma^2 \alpha \bar{\gamma}}(\phi^\theta, W) + 4 \exp(-c \bar{\gamma}), \tag{5}
\]
\end{theorem}

and,

\[ \ell_\beta(\phi^q, W) \leq \ell_{\beta + \sigma^2\gamma}(\mathcal{Q}, W) + 4 \exp(-c\gamma), \]  

where \( \alpha = \alpha_+ + \alpha_- \), constant \( c = c_0 \min \left[ \frac{\alpha_+^2}{G^2}, \frac{\alpha_-^2}{G^2}, \frac{\alpha_+^2}{\eta_2^2}, \frac{\alpha_-^2}{\eta_2^2} \right] \), \( c_0 \) is an absolute constant and \( G \), \( \alpha_+, \alpha_-, \gamma, \eta_F, \eta_2 \) are as in Assumption [2].

First we prove the following result for anisotropic covariance \( \delta \sim \mathcal{N}(0, \Sigma_\beta) \) similar to Lemma [1] for isotropic covariance \( \delta \sim \mathcal{N}(0, \sigma^2 I) \), which turns out to have the same bound:

**Lemma 2** For \( \delta \sim \mathcal{N}(0, \Sigma_\beta) \) and matrices \( H_+, H_- \) are respectively positive and negative semi-definite with \( \max \|H_+\|_F, \|H_+\|_F \leq \eta_F, \max \|H_-\|_2, \|H_-\|_2 \leq \eta_2 \), and \( \text{Tr}(H_+) \leq \alpha_+, \text{Tr}(H_-) \geq -\alpha_- \) for \( \alpha_+, \alpha_- > 0 \). We have the following upper bound and lower bound

\[ \mathbb{P} [\delta^T H_- \delta < -\sigma^2 \alpha_- \gamma] \leq \exp \left( -c_0 \min \left[ \frac{\alpha_+^2(\gamma - 1)^2}{\eta_F^2}, \frac{\alpha_-^2(\gamma - 1)^2}{\eta_2^2} \right] \right), \]  

and

\[ \mathbb{P} [\delta^T H_+ \delta > \sigma^2 \alpha_+ \gamma] \leq \exp \left( -c_0 \min \left[ \frac{\alpha_+^2(\gamma - 1)^2}{\eta_F^2}, \frac{\alpha_-^2(\gamma - 1)^2}{\eta_2^2} \right] \right), \]

where \( \gamma > 1 \) and \( c_0 \) is an absolute constant.

**Proof:** Since \( H_+ \) is positive semi-definite, the diagonals of \( H_+ \) must be non-negative, then we have,

\[ \mathbb{E} [\delta^T H_+ \delta] = \mathbb{E} [\text{Tr}(H_+ \delta \delta^T)] = \text{Tr}(H_+ \Sigma_\beta) = \sum_i \min \left( \sigma^2, \frac{1}{\mathcal{H}_{1,0}^{\beta^1} [i, i]} \right) H_+[i, i] \]

\[ = \sigma^2 \sum_i \min \left( 1, \frac{1}{\sigma^2 \mathcal{H}_{1,0}^{\beta^1} [i, i]} \right) H_+[i, i] \]

\[ \leq \sigma^2 \sum_i H_+[i, i] = \sigma^2 \text{Tr}(H_+) \leq \sigma^2 \alpha_+ , \]

Similarly, we have

\[ \mathbb{E} [\delta^T H_- \delta] = \mathbb{E} [\text{Tr}(H_- \delta \delta^T)] = \text{Tr}(H_- \Sigma_\beta) = \sum_i \min \left( \sigma^2, \frac{1}{\mathcal{H}_{1,0}^{\beta^1} [i, i]} \right) H_-[i, i] \]

\[ = \sigma^2 \sum_i \min \left( 1, \frac{1}{\sigma^2 \mathcal{H}_{1,0}^{\beta^1} [i, i]} \right) H_-[i, i] \]

\[ \geq \sigma^2 \sum_i H_-[i, i] = \sigma^2 \text{Tr}(H_-) \geq -\sigma^2 \alpha_- . \]

We have

\[ \kappa := \max_i \|\delta_i\|_{\psi_2} \leq c_0 \max_i \left( \sigma, \frac{1}{\sqrt{\mathcal{H}_{1,0}^{\beta^1} [i, i]}} \right) \leq c_0 \sigma. \]

Therefore, from Hanson-Wright inequality we have

\[ \mathbb{P} [\delta^T H_+ \delta - \sigma^2 \alpha_+ \geq t] \leq \exp \left( -c_0 \min \left[ \frac{t^2}{\kappa^4 \|H_+\|_F^2}, \frac{t}{\kappa^2 \|H_+\|_2^2} \right] \right) \]

\[ \leq \exp \left( -c_0 \min \left[ \frac{t^2}{\kappa^4 \eta_F^2}, \frac{t}{\kappa^2 \eta_2^2} \right] \right). \]
By taking $t = \gamma \sigma^2 \alpha_+ (> 0)$, we have

$$
\mathbb{P}[\delta^T H_+ \delta \geq (\gamma + 1)\sigma^2 \alpha_+] \leq \exp \left(-c_0 \min \left[ \frac{\sigma^2 \alpha_+ \hat{\beta}^2}{\kappa^4 \eta_F^2}, \frac{\sigma^2 \alpha_+ \hat{\beta}}{\kappa^2 \eta_2} \right] \right)
$$

$$
\leq \exp \left(-c_0 \min \left[ \frac{\alpha_+ \hat{\beta}^2}{\eta_F^2}, \frac{\alpha_+ \hat{\beta}}{\eta_2} \right] \right).
$$

Similarly, from Hanson-Wright inequality, we have

$$
\mathbb{P} \left[ \delta^T H_- \delta - \sigma^2 (-\alpha_-) \leq -t \right] \leq \exp \left(-c_0 \min \left[ \frac{t^2}{\kappa^4 \|H_\cdot\|_F^2}, \frac{t}{\kappa^2 \|H_\cdot\|_2} \right] \right)
$$

$$
\leq \exp \left(-c_0 \min \left[ \frac{t^2}{\kappa^4 \eta_F^2}, \frac{t}{\kappa^2 \eta_2} \right] \right).
$$

Taking $t = \sigma^2 \alpha_- \gamma (> 0)$, we have

$$
\mathbb{P} \left[ \delta^T H_- \delta \leq -(\gamma + 1)\sigma^2 \alpha_- \right] \leq \exp \left(-c_0 \min \left[ \frac{\sigma^2 \alpha_- \hat{\beta}^2}{\kappa^4 \eta_F^2}, \frac{\sigma^2 \alpha_- \hat{\beta}}{\kappa^2 \eta_2} \right] \right)
$$

$$
\leq \exp \left(-c_0 \min \left[ \frac{\alpha_- \hat{\beta}^2}{\eta_F^2}, \frac{\alpha_- \hat{\beta}}{\eta_2} \right] \right).
$$

Denote $\hat{\gamma} + 1$ as $\hat{\gamma}$ completes the proof.

**Proof of Theorem 4** Since $\phi$ is twice differentiable, for some suitable (random) $\hat{\theta} = (1 - \tau)\theta_1 + \tau \theta = \theta_1 + \tau (\theta - \theta_1)$ where $\tau \in [0, 1]$, we have

$$
\phi^\dagger(x_1) = \phi^\dagger(x_i) + \langle \theta - \theta_1, \nabla \phi^\dagger(x_i) \rangle + (\theta - \theta_1)^T H_{\phi^\dagger}(x_i)(\theta - \theta_1).
$$

Consider the following set where $\theta^\dagger$ achieves a margin greater than $(\beta + \sigma^2 \alpha \hat{\gamma})$

$$
\mathcal{Z}_{\beta + \sigma^2 \alpha \hat{\gamma}}(\theta^\dagger) = \left\{ (x, y) \in \mathcal{X} \times \mathcal{Y} \mid y \phi^{\dagger}(x) > \beta + \sigma^2 \alpha \hat{\gamma} \right\},
$$

where $\alpha = \alpha_- + \alpha_+$. Let $P = \mathcal{N}(0, \Sigma_{\theta^\dagger})$ be a multivariate distribution with mean 0 and covariance $\Sigma_{\theta^\dagger}$, where $\Sigma_{\theta^\dagger}$ is defined as $[\Pi]$. Now, for $z \in \mathcal{Z}_{\beta + \sigma^2 \alpha \hat{\gamma}}(\theta^\dagger)$, we have

$$
\mathbb{P}_{\theta \sim \mathcal{Q}} \left[ y \phi^\dagger(x) \leq \beta \mid z \in \mathcal{Z}_{\beta + \sigma^2 \alpha \hat{\gamma}}(\theta^\dagger) \right] = \mathbb{P}_{\delta \sim P} \left[ y \phi^{\dagger + \delta}(x) \leq \beta \mid z \in \mathcal{Z}_{\beta + \sigma^2 \alpha \hat{\gamma}}(\theta^\dagger) \right].
$$

Now, conditioned on $y = +1$, we have

$$
\mathbb{P}_{\delta \sim P} \left[ \phi^{\dagger + \delta}(x) \leq \beta \mid z \in \mathcal{Z}_{\beta + \sigma^2 \alpha \hat{\gamma}}(\theta^\dagger), y = +1 \right]
$$

$$
= \mathbb{P}_{\delta \sim P} \left[ \phi^\dagger(x) + \langle \delta, \nabla \phi^\dagger(x) \rangle + \delta^T H_{\phi^\dagger}(x) \delta \leq \beta \mid z \in \mathcal{Z}_{\beta + \sigma^2 \alpha \hat{\gamma}}(\theta^\dagger), y = +1 \right]
$$

$$
\leq \mathbb{P}_{\delta \sim P} \left[ \langle \delta, \nabla \phi^\dagger(x) \rangle + \delta^T H_- \delta \leq \beta - \phi^\dagger(x) \mid z \in \mathcal{Z}_{\beta + \sigma^2 \alpha \hat{\gamma}}(\theta^\dagger), y = +1 \right]
$$

$$
\leq \mathbb{P}_{\delta \sim P} \left[ \langle \delta, \nabla \phi^\dagger(x) \rangle + \delta^T H_- \delta \leq -\sigma^2 \hat{\gamma}(\alpha_- + \alpha_+) \mid z \in \mathcal{Z}_{\beta + \sigma^2 \alpha \hat{\gamma}}(\theta^\dagger), y = +1 \right]
$$

$$
\leq \mathbb{P}_{\delta \sim P} \left[ \langle \delta, \nabla \phi^\dagger(x) \rangle \leq -\sigma^2 \alpha_- \hat{\gamma} \mid z \in \mathcal{Z}_{\beta + \sigma^2 \alpha \hat{\gamma}}(\theta^\dagger), y = +1 \right] + \mathbb{P}_{\delta \sim P} \left[ \delta^T H_- \delta \leq -\sigma^2 \alpha_- \hat{\gamma} \right]
$$

$$
\leq \exp \left(-c_0 \frac{\sigma^2 \alpha_+ \tilde{\beta}^2}{G^2} \right) + \exp \left(-c_0 \min \left[ \frac{\sigma^2 \alpha_- \tilde{\beta}^2}{\eta_F^2}, \frac{\alpha_- (\tilde{\gamma} - 1)}{\eta_2} \right] \right).
$$
where (a) follows since for \((x, y) \in \mathcal{Z}^{(>)}_{\beta + \sigma^2 \alpha \gamma}(\theta^1)\) and \(y = +1\) we have \(\phi^{\theta^1}(x) > \beta + \sigma^2 \alpha \gamma\); (b) follows since \(P[x+y \leq a+b] \leq P[x \leq a] + P[y \leq b]\); (c) is from Hoeffding’s inequality with \(\|\nabla \phi^{\theta^1}(x)\|_2^2 \leq G^2\), \(\max_i \|\delta_i\|_{\psi_2} \leq c_0 \sigma\), and Lemma \[2\].

Similarly, conditioned in \(y = -1\), we have

\[
\mathbb{P}_{\delta \sim P} \left[ -\phi^{\theta^1+\delta}(x) \leq \beta \mid z \in \mathcal{Z}^{(>)}_{\beta + \sigma^2 \alpha \gamma}(\theta^1), y = -1 \right] = \mathbb{P}_{\delta \sim P} \left[ -\phi^{\theta^1}(x) - \langle \delta, \nabla \phi^{\theta^1}(x) \rangle - \delta^T H^\delta(x) \delta \leq \beta \mid z \in \mathcal{Z}^{(>)}_{\beta + \sigma^2 \alpha \gamma}(\theta^1), y = -1 \right] \leq \mathbb{P}_{\delta \sim P} \left[ -\langle \delta, \nabla \phi^{\theta^1}(x) \rangle - \delta^T H^\delta \leq \beta + \phi^{\theta^1}(x) \mid z \in \mathcal{Z}^{(>)}_{\beta + \sigma^2 \alpha \gamma}(\theta^1), y = -1 \right] \leq \mathbb{P}_{\delta \sim P} \left[ -\langle \delta, \nabla \phi^{\theta^1}(x) \rangle - \delta^T H^\delta \leq -\sigma^2(\alpha_+ \gamma) \mid z \in \mathcal{Z}^{(>)}_{\beta + \sigma^2 \alpha \gamma}(\theta^1), y = -1 \right] + \mathbb{P}_{\delta \sim P} \left[ -\delta^T H^\delta \leq -\sigma^2 \alpha_+ \gamma \right] \leq \exp \left( -c_0 \frac{\sigma^2 \alpha_+ \gamma^2}{G^2} \right) + \exp \left( -c_0 \min \left[ \frac{\alpha_+^2(\gamma - 1)^2}{\eta_P^2}, \frac{\alpha_-^2(\gamma - 1)^2}{\eta_2} \right] \right),
\]

where (a) follows since for \((x, y) \in \mathcal{Z}^{(>)}_{\beta + \sigma^2 \alpha \gamma}(\theta^1)\) and \(y = -1\) we have \(-\phi^{\theta^1}(x) > \beta + \sigma^2 \alpha \gamma\); (b) follows since \(P[x+y \leq a+b] \leq P[x \leq a] + P[y \leq b]\); (c) is from Hoeffding’s inequality with \(\|\nabla \phi^{\theta^1}(x)\|_2^2 \leq G^2\), \(\max_i \|\delta_i\|_{\psi_2} \leq c_0 \sigma\), and Lemma \[2\].

Then, we have

\[
\mathbb{P}_{\theta \sim Q} \left[ y \phi^{\theta^1}(x) \leq \beta \mid z \in \mathcal{Z}^{(>)}_{\beta + \sigma^2 \alpha \gamma}(\theta^1) \right] = \mathbb{P}_{\delta \sim P} \left[ y \phi^{\theta^1+\delta}(x) \leq \beta \mid z \in \mathcal{Z}^{(>)}_{\beta + \sigma^2 \alpha \gamma}(\theta^1) \right] \leq \mathbb{P} \left[ y \phi^{\theta^1+\delta}(x) \leq \beta \mid z \in \mathcal{Z}^{(>)}_{\beta + \sigma^2 \alpha \gamma}(\theta^1), y = +1 \right] + \mathbb{P} \left[ y \phi^{\theta^1+\delta}(x) \leq \beta \mid z \in \mathcal{Z}^{(>)}_{\beta + \sigma^2 \alpha \gamma}(\theta^1), y = -1 \right] \leq \exp \left( -c_0 \frac{\sigma^2 \alpha_+ \gamma^2}{G^2} \right) + \exp \left( -c_0 \min \left[ \frac{\alpha_+^2(\gamma - 1)^2}{\eta_P^2}, \frac{\alpha_-^2(\gamma - 1)^2}{\eta_2} \right] \right) + \exp \left( -c_0 \frac{\sigma^2 \alpha_+ \gamma^2}{G^2} \right) + \exp \left( -c_0 \min \left[ \frac{\alpha_+^2(\gamma - 1)^2}{\eta_P^2}, \frac{\alpha_-^2(\gamma - 1)^2}{\eta_2} \right] \right).
\]

For \(z \not\in \mathcal{Z}^{(>)}_{\beta + \sigma^2 \alpha \gamma}(\theta^1)\), we have

\[
\mathbb{P}_{\theta \sim Q} \left[ y \phi^{\theta^1}(x) \leq \beta \mid z \not\in \mathcal{Z}^{(>)}_{\beta + \sigma^2 \alpha \gamma}(\theta^1) \right] \leq \mathbb{P} \left[ y \phi^{\theta^1}(x) \leq \beta + \sigma^2 \alpha \gamma \mid z \not\in \mathcal{Z}^{(>)}_{\beta + \sigma^2 \alpha \gamma}(\theta^1) \right],
\]

where the right hand side considers the indicator of the event \([y \phi^{\theta^1}(x) \leq \beta + \sigma^2 \alpha \gamma]\) conditioned on \(z \not\in \mathcal{Z}^{(>)}_{\beta + \sigma^2 \alpha \gamma}(\theta^1)\). Note that the inequality is true since for \(z \not\in \mathcal{Z}^{(>)}_{\beta + \sigma^2 \alpha \gamma}(\theta^1)\), by definition, \(y \phi^{\theta^1}(x) \leq \beta + \sigma^2 \alpha \gamma\), so that the conditional indicator is 1, and hence upper bounds the conditional probability on the left hand side.
By definition, we have

$$\ell_\beta(Q, W) = \mathbb{P}_{\theta \sim Q} \left[ y \phi^\theta(x) \leq \beta \right]$$

$$= \mathbb{P}_{\theta \sim Q} \left[ y \phi^\theta(x) \leq \beta \mid z \notin Z_{\beta + \sigma^2 \alpha \hat{\gamma}}^{(\geq)}(\theta^\dagger) \right] + \mathbb{P}_{\theta \sim Q} \left[ y \phi^\theta(x) \leq \beta \mid z \in Z_{\beta + \sigma^2 \alpha \hat{\gamma}}^{(\geq)}(\theta^\dagger) \right]$$

$$\leq \mathbb{P}_{z \sim W} \left[ \mathbb{1} \left[ y \phi^\theta(x) \leq \beta + \sigma^2 \alpha \hat{\gamma} \mid z \notin Z_{\beta + \sigma^2 \alpha \hat{\gamma}}^{(\geq)}(\theta^\dagger) \right] \right] + \exp \left( -c_0 \frac{\sigma^2 \alpha^2 \gamma^2}{G^2} \right) + \exp \left( -c_0 \frac{\sigma^2 \alpha^2 \gamma^2}{G^2} \right)$$

$$+ \exp \left( -c_0 \min \left[ \frac{\alpha^2 \gamma^2}{\eta_F^2}, \frac{\alpha \gamma - 1}{\eta_2} \right] \right) + \exp \left( -c_0 \min \left[ \frac{\alpha^2 \gamma^2}{\eta_F^2}, \frac{\alpha \gamma - 1}{\eta_2} \right] \right)$$

$$\leq \mathbb{P}_{z \sim W} \left[ y \phi^\theta(x) \leq \beta + \sigma^2 \alpha \hat{\gamma} \right] + \exp \left( -c_0 \frac{\sigma^2 \alpha^2 \gamma^2}{G^2} \right) + \exp \left( -c_0 \frac{\sigma^2 \alpha^2 \gamma^2}{G^2} \right)$$

$$+ \exp \left( -c_0 \min \left[ \frac{\alpha^2 \gamma^2}{\eta_F^2}, \frac{\alpha \gamma - 1}{\eta_2} \right] \right) + \exp \left( -c_0 \min \left[ \frac{\alpha^2 \gamma^2}{\eta_F^2}, \frac{\alpha \gamma - 1}{\eta_2} \right] \right)$$

$$= \ell_{\beta + \sigma^2 \alpha \hat{\gamma}}(\phi^\theta, W) + \exp \left( -c_0 \frac{\sigma^2 \alpha^2 \gamma^2}{G^2} \right) + \exp \left( -c_0 \frac{\sigma^2 \alpha^2 \gamma^2}{G^2} \right)$$

$$+ \exp \left( -c_0 \min \left[ \frac{\alpha^2 \gamma^2}{\eta_F^2}, \frac{\alpha \gamma - 1}{\eta_2} \right] \right) + \exp \left( -c_0 \min \left[ \frac{\alpha^2 \gamma^2}{\eta_F^2}, \frac{\alpha \gamma - 1}{\eta_2} \right] \right)$$

(55)

which establishes (6).

Now we turn to the proof of (6). Consider the following set where $\theta^\dagger$ achieves a margin of at most $\beta$:

$$Z_{\beta}^{(\leq)}(\theta^\dagger) = \left\{ (x, y) \in X \times Y \mid y \phi^\theta(x) \leq \beta \right\}.$$

Let $P = N(0, \Sigma_{\theta^\dagger})$ be a multivariate distribution with mean 0 and covariance $\Sigma_{\theta^\dagger}$, where $\Sigma_{\theta^\dagger}$ is defined as (4). Now, for $z \in Z_{\beta}^{(\leq)}(\theta^\dagger)$, we have

$$\mathbb{P}_{\theta \sim Q} \left[ y \phi^\theta(x) > \beta + \sigma^2 \alpha \hat{\gamma} \mid z \in Z_{\beta}^{(\leq)}(\theta^\dagger) \right] = \mathbb{P}_{\delta \sim P} \left[ y \phi^\theta(x) > \beta + \sigma^2 \alpha \hat{\gamma} \mid z \in Z_{\beta}^{(\leq)}(\theta^\dagger) \right].$$

Now, conditioned in $y = +1$, we have

$$\mathbb{P}_{\delta \sim P} \left[ y \phi^\theta(x) > \beta + \sigma^2 \alpha \hat{\gamma} \mid z \in Z_{\beta}^{(\leq)}(\theta^\dagger), y = +1 \right]$$

$$= \mathbb{P}_{\delta \sim P} \left[ y \phi^\theta(x) > \beta + \sigma^2 \alpha \hat{\gamma} \mid z \in Z_{\beta}^{(\leq)}(\theta^\dagger), y = +1 \right]$$

$$\leq \mathbb{P}_{\delta \sim P} \left[ (\delta, \nabla \phi^\theta(x)) + \delta^T H_{\phi^\theta}(x) \delta > \beta + \sigma^2 \alpha \hat{\gamma} \mid z \in Z_{\beta}^{(\leq)}(\theta^\dagger), y = +1 \right]$$

$$\leq \mathbb{P}_{\delta \sim P} \left[ (\delta, \nabla \phi^\theta(x)) + \delta^T H_{\phi^\theta}(x) \delta > \beta + \sigma^2 \alpha \hat{\gamma} \mid z \in Z_{\beta}^{(\leq)}(\theta^\dagger), y = +1 \right]$$

$$\leq \exp \left( -c_0 \frac{\sigma^2 \alpha^2 \gamma^2}{G^2} \right) + \exp \left( -c_0 \min \left[ \frac{\alpha^2 \gamma^2}{\eta_F^2}, \frac{\alpha \gamma - 1}{\eta_2} \right] \right),$$

where (a) follows since for $(x, y) \in Z_{\beta}^{(\leq)}(\theta^\dagger)$ and $y = +1$ we have $\phi^\theta(x) \leq \beta \Rightarrow \beta - \phi^\theta(x) \geq 0$; (b) follows since $P(\delta) = \mathbb{P}(\delta) \leq a+b \leq \mathbb{P}(\delta \leq a)+\mathbb{P}(\delta \leq b)$; (c) is from Hoeffding’s inequality with $||\nabla \phi^\theta(x)||_2^2 \leq G^2$, max $||\delta||_2 \leq c_0 \sigma$, and Lemma 2.
Similarly, conditioned on \( y = -1 \), we have

\[
\mathbb{P}_{\delta \sim P} \left[ -\phi^{\theta + \delta}(x) > \beta + \sigma^2 \alpha \tilde{\gamma} \mid z \in \mathcal{Z}_{\beta}^{(\leq)}(\theta^1), y = -1 \right]
\]

\[
= \mathbb{P}_{\delta \sim P} \left[ -\phi^{\theta}(x) - \langle \delta, \nabla \phi^{\theta}(x) \rangle - \delta^T H_{\theta}^\delta(x) \delta > \beta + \sigma^2 \alpha \tilde{\gamma} \mid z \in \mathcal{Z}_{\beta}^{(\leq)}(\theta^1), y = -1 \right]
\]

\[
\leq \mathbb{P}_{\delta \sim P} \left[ -\langle \delta, \nabla \phi^{\theta}(x) \rangle - \delta^T H_{-\delta} \delta > \beta + \sigma^2 \alpha \tilde{\gamma} + \phi^{\theta}(x) \mid z \in \mathcal{Z}_{\beta}^{(\leq)}(\theta^1), y = -1 \right]
\]

\[
\leq \mathbb{P}_{\delta \sim P} \left[ -\langle \delta, \nabla \phi^{\theta}(x) \rangle - \delta^T H_{-\delta} \delta > \sigma^2 \alpha \tilde{\gamma} \mid z \in \mathcal{Z}_{\beta}^{(\leq)}(\theta^1), y = -1 \right]
\]

\[
\leq \mathbb{P}_{\delta \sim P} \left[ -\langle \delta, \nabla \phi^{\theta}(x) \rangle > \sigma^2 \alpha \tilde{\gamma} \mid z \in \mathcal{Z}_{\beta}^{(\leq)}(\theta^1), y = -1 \right] + \mathbb{P}_{\delta \sim P} \left[ -\delta^T H_{-\delta} \delta \geq \sigma^2 \alpha - \tilde{\gamma} \right]
\]

\[
\leq \exp \left( -c_0 \frac{\sigma^2 \alpha \tilde{\gamma}^2}{G^2} \right) + \exp \left( -c_0 \min \left[ \frac{\alpha_+^2 (\tilde{\gamma} - 1)^2}{\eta_F^2}, \frac{\alpha_- (\tilde{\gamma} - 1)}{\eta_2} \right] \right),
\]

where (a) follows since for \((x, y) \in \mathcal{Z}_{\beta}^{(\leq)}(\theta^1)\) and \(y = -1\) we have \(-\phi(\theta^1) \leq \beta \Rightarrow \beta + \phi(\theta^1) \geq 0\); (b) follows since \(\mathbb{P}[x+y \leq a+b] = \mathbb{P}[x=a]+\mathbb{P}[y \leq b]\); (c) is from Hoeffding’s inequality with \(\|\nabla \phi^{\theta}(x)\|^2 \leq G^2\), \(\max_i \|\delta_i\|_{\psi_2} \leq c_0 \sigma\), and Lemma [2].

Then, we have

\[
\mathbb{P}_{\theta \sim \mathcal{Q}} \left[ y \phi^{\theta}(x) > \beta + \sigma^2 \alpha \tilde{\gamma} \mid z \in \mathcal{Z}_{\beta}^{(\leq)}(\theta^1) \right]
\]

\[
= \mathbb{P}_{\delta \sim P} \left[ y \phi^{\theta + \delta}(x) > \beta + \sigma^2 \alpha \tilde{\gamma} \mid z \in \mathcal{Z}_{\beta}^{(\leq)}(\theta^1) \right]
\]

\[
\leq \mathbb{P} \left[ y \phi^{\theta + \delta}(x) > \beta + \sigma^2 \alpha \tilde{\gamma} \mid z \in \mathcal{Z}_{\beta}^{(\leq)}(\theta^1), y = +1 \right] + \mathbb{P} \left[ y \phi^{\theta + \delta}(x) > \beta + \sigma^2 \alpha \tilde{\gamma} \mid z \in \mathcal{Z}_{\beta}^{(\leq)}(\theta^1), y = -1 \right]
\]

\[
\leq \exp \left( -c_0 \frac{\sigma^2 \alpha \tilde{\gamma}^2}{G^2} \right) + \exp \left( -c_0 \min \left[ \frac{\alpha_+^2 (\tilde{\gamma} - 1)^2}{\eta_F^2}, \frac{\alpha_- (\tilde{\gamma} - 1)}{\eta_2} \right] \right) + \exp \left( -c_0 \min \left[ \frac{\alpha_+^2 (\tilde{\gamma} - 1)^2}{\eta_F^2}, \frac{\alpha_- (\tilde{\gamma} - 1)}{\eta_2} \right] \right) \cdot (57)
\]

For \(z \notin \mathcal{Z}_{\beta}^{(\leq)}(\theta^1)\), we have

\[
\mathbb{P}_{\theta \sim \mathcal{Q}} \left[ y \phi^{\theta}(x) > \beta + \sigma^2 \alpha \tilde{\gamma} \mid z \notin \mathcal{Z}_{\beta}^{(\leq)}(\theta^1) \right] \leq 1 \left[ y \phi^{\theta}(x) > \beta \mid z \notin \mathcal{Z}_{\beta}^{(\leq)}(\theta^1) \right], \quad (58)
\]

where the right hand side considers the indicator of the event \([y \phi^{\theta}(x) > \beta]\) conditioned on \(z \notin \mathcal{Z}_{\beta}^{(\leq)}(\theta^1)\).

Note that the inequality is true since for \(z \notin \mathcal{Z}_{\beta}^{(\leq)}(\theta^1)\), by definition, \(y \phi^{\theta}(x) > \beta\), so that the conditional indicator is 1, and hence upper bounds the conditional probability on the left hand side.
By definition, we have

$$1 - \ell_{\beta + \sigma^2 \tilde{\alpha} \tilde{\gamma}}(Q, W)$$

$$= \mathbb{P}_{\theta \sim Q, z \sim W} [y \phi^\theta(x) > \beta + \sigma^2 \alpha \tilde{\gamma} ]$$

$$\leq \mathbb{P}_{\theta \sim Q, z \sim W} [y \phi^\theta(x) > \beta + \sigma^2 \alpha \tilde{\gamma} | z \notin Z_{\beta}^{(\leq)}(\theta^\dagger)] + \mathbb{P}_{\theta \sim Q, z \sim W} [y \phi^\theta(x) > \beta + \sigma^2 \alpha \tilde{\gamma} | z \in Z_{\beta}^{(\leq)}(\theta^\dagger) ]$$

$$\leq \mathbb{P}_{z \sim W} \left[ 1 \left[ y \phi^\theta(x) > \beta \ | z \notin Z_{\beta}^{(\leq)}(\theta^\dagger) \right] \right] + \exp \left( -c_0 \frac{\sigma^2 \alpha \gamma^2}{G^2} \right) + \exp \left( -c_0 \frac{\sigma^2 \alpha \gamma^2}{G^2} \right)$$

$$+ \exp \left( -c_0 \min \left[ \frac{\alpha^2 (\tilde{\gamma} - 1)^2}{\eta_{F}^2}, \frac{\alpha (\tilde{\gamma} - \tilde{\gamma})}{\eta_{2}} \right] \right) + \exp \left( -c_0 \min \left[ \frac{\alpha^2 (\tilde{\gamma} - 1)^2}{\eta_{F}^2}, \frac{\alpha (\tilde{\gamma} - \tilde{\gamma})}{\eta_{2}} \right] \right)$$

$$= 1 - \ell_{\beta}(\phi^\theta, W) + \exp \left( -c_0 \frac{\sigma^2 \alpha \gamma^2}{G^2} \right) + \exp \left( -c_0 \frac{\sigma^2 \alpha \gamma^2}{G^2} \right)$$

$$+ \exp \left( -c_0 \min \left[ \frac{\alpha^2 (\tilde{\gamma} - 1)^2}{\eta_{F}^2}, \frac{\alpha (\tilde{\gamma} - \tilde{\gamma})}{\eta_{2}} \right] \right) + \exp \left( -c_0 \min \left[ \frac{\alpha^2 (\tilde{\gamma} - 1)^2}{\eta_{F}^2}, \frac{\alpha (\tilde{\gamma} - \tilde{\gamma})}{\eta_{2}} \right] \right)$$

which implies

$$\ell_{\beta}(\phi^\theta, W) \leq \ell_{\beta + \sigma^2 \alpha \tilde{\gamma}}(Q, W) \leq \ell_{\beta + \sigma^2 \alpha \tilde{\gamma}}(Q, W) + \exp \left( -c_0 \frac{\sigma^2 \alpha \gamma^2}{G^2} \right) + \exp \left( -c_0 \frac{\sigma^2 \alpha \gamma^2}{G^2} \right)$$

$$+ \exp \left( -c_0 \min \left[ \frac{\alpha^2 (\tilde{\gamma} - 1)^2}{\eta_{F}^2}, \frac{\alpha (\tilde{\gamma} - \tilde{\gamma})}{\eta_{2}} \right] \right) + \exp \left( -c_0 \min \left[ \frac{\alpha^2 (\tilde{\gamma} - 1)^2}{\eta_{F}^2}, \frac{\alpha (\tilde{\gamma} - \tilde{\gamma})}{\eta_{2}} \right] \right) .$$

By choosing \( \tilde{\gamma} > 2 \), we have \( \tilde{\gamma}^2 > \tilde{\gamma}, (\tilde{\gamma} - 1)^2 > \tilde{\gamma} - 1 > \frac{1}{2} \tilde{\gamma} \). Therefore, taking a constant \( c = c_0 \min \left[ \frac{\alpha^2}{\sigma^2}, \frac{\alpha^2}{\sigma^2}, \frac{\alpha^2}{\sigma^2}, \frac{\alpha^2}{\sigma^2}, \frac{\alpha^2}{\sigma^2}, \frac{\alpha^2}{\sigma^2} \right] \) completes the proof.

**B.2 Deterministic Margin Bounds**

Recall Theorem 2 which establishes the margin bound for deterministic smooth predictors in the main paper:

**Theorem 2** Consider any \( \theta_0 \in \mathbb{R}^p \), \( \sigma^2 > 0 \) chosen before training, and let \( \theta^\dagger \) be the parameters of the model after training. Let \( \mathcal{H}_{\beta, \phi} \) be the Hessian as in [2], let \( \nu_j^2 = \max \left\{ \mathcal{H}_{\beta, \phi}[j, j], \frac{1}{\sigma^2} \right\} \), \( \tilde{\nu} = \{ j : \mathcal{H}_{\beta, \phi}[j, j] > 1/\sigma^2 \} \), and \( \{ \tilde{\nu}(1), \ldots, \tilde{\nu}(\tilde{\nu}) \} \) be the subset of values larger than \( 1/\sigma^2 \). Under Assumption 7, with probability at least \( 1 - \delta \), for any \( \theta^\dagger, \beta \in (0, 1), \gamma > 4\sigma^2 \alpha \), we have the following scale-invariant bound:

$$\ell_{\beta}(\phi^\theta, D) \leq a_{\beta} \ell_{\gamma}(\phi^\theta, S) + \frac{b_{\beta}}{2n} \left( \sum_{i=1}^{\tilde{\nu}} \ln \frac{\tilde{\nu}(i)}{1/\sigma^2} \right) + \frac{\| \theta^\dagger - \theta_0 \|^2}{\frac{\sigma^2}{L_{2 \text{norm}}} \text{effective curvature}} + d_{\beta} \exp (-c_\gamma) + b_{\beta} \frac{\log(\frac{1}{\delta})}{n} ,$$

where \( a_{\beta} = \log(\frac{1}{1-\beta}) \), \( b_{\beta} = \frac{1}{1-\beta} \), \( d_{\beta} = 4(a_{\beta} + 1) \), \( c = c_0 \min \left[ \frac{\alpha^2}{\sigma^2}, \frac{\alpha^2}{\sigma^2}, \frac{\alpha^2}{\sigma^2}, \frac{\alpha^2}{\sigma^2}, \frac{\alpha^2}{\sigma^2}, \frac{\alpha^2}{\sigma^2} \right] \), \( c_0 \) is an absolute constant, \( \alpha = \alpha_+ + \alpha_- \) and \( G, \alpha_+, \alpha_- \), \( \eta_F, \eta_2 \) are as in Assumption 7.
Proof: To get to a de-randomized margin bound, we utilize the results in Theorem 1. First, with $\beta = 0$, $\sigma^2\gamma\alpha = \frac{1}{2}$ and $W = D$ in Theorem 1, we have
\[
\ell_0(\phi^0, D) \leq \ell_{\gamma/2}(Q, D) + 4 \exp \left( -c \frac{\gamma}{\sigma^2\alpha} \right).
\]
Similarly, with $\beta = \gamma/2$ and $W = S$ in Theorem 1, we have
\[
\ell_{\gamma/2}(Q, S) \leq \ell_{\gamma}(\phi^0, S) + 4 \exp \left( -c \frac{\gamma}{\sigma^2\alpha} \right).
\]
From the Fast Rate PAC-Bayesian bound (33), with probability at least $(1 - \delta)$ over the draw of $n$ samples $S \sim D^n$, for any $\beta \in (0, 1)$ and for any $Q$ we have
\[
\ell_{\gamma/2}(Q, D) \leq \frac{\log(1/\beta)}{1 - \beta} \ell_{\gamma/2}(Q, S) + \frac{1}{1 - \beta} K L(Q || P) + \log(\frac{1}{\beta}) + 4 \exp \left( -c \frac{\gamma}{\sigma^2\alpha} \right).
\]
Noting that
\[
2 K L(Q || P) = \sum_{j=1}^{p} \frac{1}{\sigma^2\nu_j} - 1 + \sum_{j=1}^{p} \frac{\|\theta[j] - \theta_0[j]\|^2}{\sigma^2} + \sum_{i=1}^{p} \ln \frac{\nu_j}{1/\sigma^2}
\]
we have
\[
\ell_0(\phi^0, D) \leq \frac{\log(1/\beta)}{1 - \beta} \ell_{\gamma}(\phi^0, S) + \frac{1}{2(1 - \beta)} \left( \sum_{i=1}^{p} \ln \frac{\nu_j}{1/\sigma^2} + \frac{\|\theta^i - \theta_0\|^2}{\sigma^2} \right)
\]
\[
+ 4 \left( \frac{\log(1/\beta)}{1 - \beta} + 1 \right) \exp \left( -c \frac{\gamma}{\sigma^2\alpha} \right) + \frac{1}{1 - \beta} \frac{\log(\frac{1}{\beta})}{n}.
\]
Using the argument in the proof of Theorem 1, we know that the $K L(Q || P)$ in the PAC-Bayes bound (63) remains invariant under $\alpha$-scale transformation [Kleeman 2011], i.e.,
\[
K L(Q' || P') = K L(Q || P),
\]
where $Q'$ and $P'$ are the distributions after $\alpha$-scale transformation corresponding to $Q$ and $P$ respectively. Note that the other terms apart from the $K L(Q || P)$ in (63) do not change by $\alpha$-scale transformation since the functions represented by the networks are the same. Thus, our generalization bound is scale-invariant.

Our generalization bound in Theorem 2 captures the information of local curvature by using the Hessian $\mathcal{H}_{l,\phi}$ at the parameter $\theta^l$. Recent work [Dinh et al. 2017] show that the Hessian $\mathcal{H}_{l,\phi}$ can be modified by a certain $\alpha$-scale transformation which scales the weights by non-negative coefficients but does not change the function. Thus, $\alpha$-scale transformation invalidates certain recently proposed flatness based generalization bounds [Hochreiter and Schmidhuber 1997, Keskar et al. 2017] by arbitrarily changing the flatness of the loss landscape for deep networks. However, we show that our generalization bound which measure the generalization by the KL divergence or differential relative entropy between the posterior and the prior distribution remains invariant, although the although the local structure such as the Hessian $\mathcal{H}_{l,\phi}$ get modified by the $\alpha$-scale transformation.

C De-randomized Margin Bound: Multi-class Classification with Smooth Predictors

In this section, we focus on constructing the fast-rate deterministic bound using the anisotropic posterior case for multi-class problem, with a similar de-randomization. Results for isotropic case shall be essentially the same.
Let \( \phi : \mathbb{R}^p \times \mathbb{R}^d \mapsto \mathbb{R}^k \) be the output \( \phi^\theta(x_i) \in \mathbb{R}^k \) of a deep net with parameter \( \theta \) and input \( x_i \). For a sample point \( (x_i, y_i) \in \mathcal{X} \times \mathcal{Y} \), where \( \mathcal{X}, \mathcal{Y} \) denotes the input and output space respectively, \( \phi^\theta(x_i)[y_i] \) denotes the score corresponding to class \( y_i \), and in general, \( \phi^\theta(x_i)[h] \) denotes the score corresponding to class \( h \). Note that the classification is correct when

\[
\phi^\theta(x_i)[y_i] > \phi^\theta(x_i)[h], \quad \forall h \neq y_i .
\]  

(67)

We define margin loss for a specific \( z = (x, y) \) as

\[
\ell_\beta(\theta, z) \triangleq \mathbb{I}[\phi^\theta(x)[y] \leq \beta + \phi^\theta(x)[h], \forall h \neq y] ,
\]

(68)

where \( \mathbb{I}[a] = 1 \) if \( a \) is true, and 0 otherwise. For a Bayesian predictor, we maintain a distribution \( Q \) over the parameters \( \theta \), and the corresponding margin loss

\[
\ell_\beta(Q, z) \triangleq \mathbb{P}_{\theta \sim Q}[\phi^\theta(x)[y] \leq \beta + \phi^\theta(x)[h], \forall h \neq y] .
\]

(69)

For any distribution \( W \) on \( \mathcal{X} \times \mathcal{Y} \), and parameter \( \theta \), we define the margin loss as

\[
\ell_\beta(\theta, W) \triangleq \mathbb{P}_{(x,y) \sim W}[\phi^\theta(x)[y] \leq \beta + \phi^\theta(x)[h], \forall h \neq y] .
\]

(70)

Further, for any distribution \( W \) on \( \mathcal{X} \times \mathcal{Y} \), and any distribution over parameter \( \theta \), we define the margin loss as

\[
\ell_\beta(Q, W) \triangleq \mathbb{E}_{\theta \sim Q}[\ell_\beta(\theta, W)] = \mathbb{E}_{(x,y) \sim W}[\phi^\theta(x)[y] \leq \beta + \phi^\theta(x)[h], \forall h \neq y] .
\]

(71)

We assume the Assumption \( \square \) holds for functions on each class \( h \in [k] \), the proof idea is essentially the same as in the 2-class case, with constants changed.

C.1 Bounds for Stochastic vs. Deterministic Predictors for Multi-class

We first establishes the relationship between stochastic and deterministic predictors:

**Theorem 8** For \( k \)-class classification problem, let \( \sigma^2 > 0 \) be chosen before seeing the training data. Let \( W \) be any distribution on pairs \( (x, y) \) with \( x \in \mathbb{R}^d, y \in \mathbb{R}^k \). For any \( \theta^0 \in \mathbb{R}^d \), let \( Q \) be a multivariate anisotropic Gaussian distribution with mean \( \theta^0 \) and covariance \( \Sigma_{\theta^0} \), where

\[
\Sigma_{\theta^0}^{-1} = \text{diag}(\nu_1^2, \ldots, \nu_p^2) , \quad \nu_j^2 \triangleq \max \left\{ \mathcal{H}^{\theta^0}_{i,\phi}[j, j], \frac{1}{\sigma^2} \right\} , \quad (72)
\]

where \( \mathcal{H}^{\theta^0}_{i,\phi} \) is as in [2]. Suppose Assumption \( \square \) holds for prediction function on each class \( h \in [k] \), for any \( \gamma > 2 \) and any \( \beta \in \mathbb{R} \), we have

\[
\ell_\beta(Q, W) \leq \ell_{\beta + 2\sigma^2\alpha_2}(\phi^{\theta^0}, W) + k \exp(-c\gamma) ,
\]

(73)

and

\[
\ell_{\beta}(\phi^{\theta^0}, W) \leq \ell_{\beta + 2\sigma^2\alpha_2}(Q, W) + k \exp(-c\gamma) ,
\]

(74)

where \( \alpha = \alpha_+ + \alpha_- \), constant \( c = c_0 \min \left[ \frac{\sigma^2\alpha_2^2}{G^2}, \frac{\alpha_2^2}{\eta_F^2}, \frac{\alpha_2^2}{\eta_2} \right] \), \( c_0 \) is an absolute constant and \( G, \alpha_+, \alpha_-, \alpha, \eta_F, \eta_2 \) are as in Assumption \( \square \).

We need the following result for the proofs:
Lemma 3 For $\delta \sim N(0, \Sigma_{\theta^\dagger})$, respectively positive and negative semi-definite matrices $H_+, H_-$ with $-\alpha_- \leq \text{Tr}(H_-)$ and $\text{Tr}(H_+) \leq \alpha_+$, and $\max \{\|H_-\|_F, \|H_+\|_F\} \leq \eta_F$, $\max \{\|H_-\|_2, \|H_+\|_2\} \leq \eta_2$, we have the following bound:

$$\mathbb{P}[\delta^T (H_+ - H_-)\delta \geq \sigma^2 \alpha \tilde{\gamma}] \leq \exp \left( -c_0 \min \left[ \frac{\alpha^2 (\tilde{\gamma} - 1)^2}{\eta_F^2}, \frac{\alpha (\tilde{\gamma} - 1)}{\eta_2} \right] \right).$$

(75)

where $\alpha = \alpha_+ + \alpha_-, \tilde{\gamma} > 1$ and $c_0$ is an absolute constant.

Proof: From the Hanson-Wright inequality, and the fact that $\mathbb{E}[\delta^T (H_+ - H_-)\delta] = \mathbb{E}[\delta^T H_+ \delta] - \mathbb{E}[\delta^T H_- \delta] \leq \sigma^2 \alpha \tilde{\gamma}$, and $\max \|\delta_i\|_{\psi_2} \leq c_0 \sigma$ as in Lemma 2, we have:

$$\mathbb{P}[\delta^T (H_+ - H_-)\delta - \sigma^2 \alpha \tilde{\gamma} \geq t] \leq \exp \left( -c_0 \min \left[ \frac{t^2}{\sigma^4 \|H_+ - H_-\|_F^2}, \frac{t}{\sigma^2 \|H_+ - H_-\|_2} \right] \right)$$

$$\leq \exp \left( -c_0 \min \left[ \frac{t^2}{\sigma^4 \eta_F^2}, \frac{t}{\sigma \eta_2} \right] \right)$$

By taking $t = \sigma^2 \alpha \tilde{\gamma} (> 0)$, we have:

$$\mathbb{P}[\delta^T (H_+ - H_-)\delta \geq \sigma^2 \alpha (\tilde{\gamma} + 1)] \leq \exp \left( -c_0 \min \left[ \frac{\alpha^2 \tilde{\gamma}^2}{\eta_F^2}, \frac{\alpha \tilde{\gamma}}{\eta_2} \right] \right)$$

$$\leq \exp \left( -c_0 \min \left[ \frac{\alpha^2 \tilde{\gamma}^2}{\eta_F^2}, \frac{\alpha \tilde{\gamma}}{\eta_2} \right] \right)$$

Denoting $\tilde{\gamma} + 1$ as $\tilde{\gamma}$ completes the proof.

Proof of Theorem 8 Since $\phi^{\theta}(h) \mid \theta$ is twice differentiable, for some suitable (random) $\tilde{\theta} = (1 - \tau) \theta^\dagger + \tau \theta = \theta^\dagger + \tau (\theta - \theta^\dagger)$ where $\tau \in [0, 1]$, we have

$$\phi^{\tilde{\theta}}(x) = \phi^{\theta^\dagger}(x) \mid h + \langle \theta - \theta^\dagger, \nabla \phi^{\theta^\dagger}(x) \mid h \rangle + (\theta - \theta^\dagger)^T H^{\tilde{\theta}}(x) \mid h \rangle\theta - \theta^\dagger \rangle$$.

(76)

Consider the following set where $\theta^\dagger$ achieves a margin greater than $(\beta + 2 \sigma^2 \alpha \tilde{\gamma})$:

$$Z^{(\geq)}_{\beta + 2 \sigma^2 \alpha \tilde{\gamma}}(\theta^\dagger) = \left\{ (x, y) \in \mathcal{X} \times \mathcal{Y} \mid \phi^{\theta^\dagger}(x) \mid y - \phi^{\theta^\dagger}(x) \mid h > \beta + 2 \sigma^2 \alpha \tilde{\gamma}, \forall h \neq y \right\}.$$

(77)

Let $P = \mathcal{N}(0, \Sigma_{\theta^\dagger})$ be a multivariate distribution with mean 0 and covariance $\Sigma_{\theta^\dagger}$, where $\Sigma_{\theta^\dagger}$ is defined as
Similarly, consider the following set:

$$Z_{\tilde{\beta}+2\sigma^2\alpha\gamma}(\theta^t) = \{ (x, y) \in \mathcal{X} \times \mathcal{Y} \mid \phi^{\theta^t}(x)_y - \phi^{\theta^t}(x)_h \leq \beta, \forall h \neq y \} .$$

(80)
Now, for $z \in \mathcal{Z}_{\beta}^{(\leq)}(\theta^t)$, we have

$$
P_{z \sim P} \left[ \phi_{\theta^t + \delta}(x)[y] - \phi_{\theta^t + \delta}(x)[h] > \beta + 2\sigma^2 \alpha \tilde{\gamma}, \forall h \neq y \ | \ z \in \mathcal{Z}_{\beta}^{(\leq)}(\theta^t) \right]
$$

$$
= P_{z \sim P} \left[ \phi_{\theta^t}(x)[y] + \langle \delta, \nabla \phi_{\theta^t}(x)[y] \rangle + \delta^T H_{\theta^t}(x)[y] \delta - \left( \phi_{\theta^t}(x)[h] + \langle \delta, \nabla \phi_{\theta^t}(x)[h] \rangle + \delta^T H_{\theta^t}(x)[h] \delta \right) > \beta + 2\sigma^2 \alpha \tilde{\gamma}, \forall h \neq y \ | \ z \in \mathcal{Z}_{\beta}^{(\leq)}(\theta^t) \right]
$$

$$
> \beta + 2\sigma^2 \alpha \tilde{\gamma}, \forall h \neq y \ | \ z \in \mathcal{Z}_{\beta}^{(\leq)}(\theta^t)
$$

$$
\leq P_{z \sim P} \left[ \langle \delta, \nabla \phi_{\theta^t}(x)[y] - \nabla \phi_{\theta^t}(x)[h] \rangle + \delta^T (H_+ - H_-) \delta > \beta + 2\sigma^2 \alpha \tilde{\gamma} - \phi_{\theta^t}(x)[y] + \phi_{\theta^t}(x)[h],
\forall h \neq y \ | \ z \in \mathcal{Z}_{\beta}^{(\leq)}(\theta^t) \right]
$$

$$
\leq P_{z \sim P} \left[ \langle \delta, \nabla \phi_{\theta^t}(x)[y] - \nabla \phi_{\theta^t}(x)[h] \rangle + \delta^T (H_+ - H_-) \delta > \beta + 2\sigma^2 \alpha \tilde{\gamma}, \forall h \neq y \ | \ z \in \mathcal{Z}_{\beta}^{(\leq)}(\theta^t) \right] + P_{z \sim P} \left[ \delta^T (H_+ - H_-) \delta \leq -\sigma^2 \alpha \tilde{\gamma} \right]
$$

$$
\leq (k - 1) \exp \left( -c_0 \frac{\sigma^2 \alpha \tilde{\gamma}^2}{G^2} \right) + \exp \left( -c_0 \min \left[ \frac{\alpha^2 (\tilde{\gamma} - 1)^2}{\eta_2^2}, \frac{\alpha (\tilde{\gamma} - 1)}{\eta_2} \right] \right),
$$

where the last step is from Hoeffding’s inequality with $\|\nabla \phi_{\theta^t}(x)[y] - \phi_{\theta^t}(x)[h]\|_2^2 \leq 2\|\nabla \phi_{\theta^t}(x)[y]\|_2^2 + 2\|\phi_{\theta^t}(x)[h]\|_2^2 \leq 4G^2$, max, $\|\delta_1\|_{\psi_2} \leq c_0 \sigma$, and taking union bound over all $h \neq y$; and Lemma 3.

$$
1 - \ell_{\beta + 2\sigma^2 \alpha \tilde{\gamma}}(Q, W)
$$

$$
= P_{\theta \sim W} \left[ \phi_{\theta^t}(x) > \beta + 2\sigma^2 \alpha \tilde{\gamma}, \forall h \neq y \right]
$$

$$
\leq P_{\theta \sim W} \left[ \phi_{\theta^t + \delta}(x)[y] - \phi_{\theta^t + \delta}(x)[h] > \beta + 2\sigma^2 \alpha \tilde{\gamma}, \forall h \neq y \ | \ z \notin \mathcal{Z}_{\beta}^{(\leq)}(\theta^t) \right]
$$

$$
+ P_{\theta \sim W} \left[ \phi_{\theta^t + \delta}(x)[y] - \phi_{\theta^t + \delta}(x)[h] > \beta + 2\sigma^2 \alpha \tilde{\gamma}, \forall h \neq y \ | \ z \in \mathcal{Z}_{\beta}^{(\leq)}(\theta^t) \right]
$$

$$
\leq P_{z \sim W} \left[ \phi_{\theta^t + \delta}(x)[y] - \phi_{\theta^t + \delta}(x)[h] > \beta, h \neq y \ | \ z \notin \mathcal{Z}_{\beta}^{(\leq)}(\theta^t) \right]
$$

$$
+ (k - 1) \exp \left( -c_0 \frac{\sigma^2 \alpha \tilde{\gamma}^2}{G^2} \right) + \exp \left( -c_0 \min \left[ \frac{\alpha^2 (\tilde{\gamma} - 1)^2}{\eta_2^2}, \frac{\alpha (\tilde{\gamma} - 1)}{\eta_2} \right] \right)
$$

$$
= 1 - \ell_{\beta}(\phi_{\theta^t}, W) + (k - 1) \exp \left( -c_0 \frac{\sigma^2 \alpha \tilde{\gamma}^2}{G^2} \right) + \exp \left( -c_0 \min \left[ \frac{\alpha^2 (\tilde{\gamma} - 1)^2}{\eta_2^2}, \frac{\alpha (\tilde{\gamma} - 1)}{\eta_2} \right] \right),
$$

which implies

$$
\ell_{\beta}(\phi_{\theta^t}, W) \leq \ell_{\beta + 2\sigma^2 \alpha \tilde{\gamma}}(Q, W) + (k - 1) \exp \left( -c_0 \frac{\sigma^2 \alpha \tilde{\gamma}^2}{G^2} \right) + \exp \left( -c_0 \min \left[ \frac{\alpha^2 (\tilde{\gamma} - 1)^2}{\eta_2^2}, \frac{\alpha (\tilde{\gamma} - 1)}{\eta_2} \right] \right) .
$$

Choosing $\tilde{\gamma} > 2$, we have $\tilde{\gamma}^2 > \tilde{\gamma}$, $\tilde{\gamma} - 1 > 2 > \frac{1}{3}\tilde{\gamma}$. Therefore, taking a constant $c = c_0 \min \left[ \frac{\sigma^2 \alpha \tilde{\gamma}^2}{G^2}, \frac{\alpha^2}{\eta_2^2}, \frac{\alpha}{\eta_2} \right]$ completes the proof.

### C.2 Deterministic Margin Bound for Multi-class

With Theorem 3, we can construct the deterministic margin bound for multi-class problem.
Suppose Assumption 1 holds for prediction function on every classes $h$, we remark that the term $KL_{\alpha}$. For $k$-class classification problem, consider any $h$ and define $\nu_j = \max\{H_k^{\theta}[j, j], 1/\sigma_j^2\}$, $\hat{\nu}_i = \{j : H_k^{\theta}[j, j] > 1/\sigma_j^2\}$, $\nu(\hat{\nu})$ be the subset of values larger than $1/\sigma^2$. Suppose Assumption 7 holds for prediction function on every classes $h \in [k]$, then with probability at least $1 - \delta$, for any $\theta^1, \beta \in (0, 1), \gamma > 4\sigma^2\alpha$, we have the following scale-invariant bound:

\[
\ell_0(\theta^0, D) \leq a_\beta \ell_\gamma(\theta^0, S) + \frac{b_\beta}{2n} \left( \sum_{\ell=1}^{\bar{p}} \ln \frac{\hat{\nu}^2_{(\ell)}}{1/\sigma^{2_{(\ell)}}} + \frac{\|\theta^0 - \theta_0\|^2}{\sigma^2} \right) + d_\beta \exp(-c_\gamma) + b_\gamma \frac{\log(\frac{1}{n})}{n},
\]

where $a_\beta = \frac{\log(1/\beta)}{1 - \beta}$, $b_\beta = \frac{1}{1 - \beta}$, $d_\beta = k(a_\beta + 1)$, $c = c_0 \min \{\alpha_{\gamma^2}, \frac{\alpha_{\gamma^2}}{\sigma_{\gamma^2}^2}, \frac{1}{\sigma_{\gamma^2}^2}\}$, $c_0$ is an absolute constant, $\alpha = \alpha_+ + \alpha_-$ and $G, \alpha_+, \alpha_-, \eta_F, \eta_{\gamma}$ are as in Assumption 7.

**Proof:** To get to a de-randomized margin bound, we utilize the results in Theorem 8. First, with $\beta = 0, \sigma^2\alpha\gamma = \frac{\sigma^2}{\gamma}$ and $W = D$ in Theorem 8 we have

\[
\ell_0(\theta^0, D) \leq \ell_\gamma(Q, D) + k \exp \left( -c_\gamma \frac{\gamma}{\sigma^2 \alpha} \right).
\]

Similarly, with $\beta = \gamma/2$ and $W = S$ in Theorem 8 we have

\[
\ell_\gamma(Q, S) \leq \ell_\gamma(\theta^0, S) + k \exp \left( -c_\gamma \frac{\gamma}{\sigma^2 \alpha} \right).
\]

From the Fast Rate PAC-Bayesian bound (33), with probability at least $1 - \delta$ over the draw of $n$ samples $S \sim D^n$, for any $\beta \in (0, 1)$ and for any $Q$ we have

\[
\ell_\gamma(Q, D) \leq \frac{\log(1/\beta)}{1 - \beta} \ell_\gamma(Q, S) + \frac{1}{1 - \beta} \frac{KL(Q||P) + \log(\frac{1}{n})}{n},
\]

Noting that

\[
2KL(Q||P) = \sum_{j=1}^{p} \frac{1}{\sigma^2_{\nu_j}} - 1 + \sum_{j=1}^{p} \frac{[\theta[j] - \theta_0[j]]^2}{\sigma^2} + \sum_{i=1}^{p} \ln \frac{\nu_j}{\sigma^2} \leq \sum_{i=1}^{\bar{p}} \ln \frac{\hat{\nu}^2_{(\ell)}}{1/\sigma^{2_{(\ell)}}} + \frac{\|\theta^0 - \theta_0\|^2}{\sigma^2},
\]

we have

\[
\ell_0(\theta^0, D) \leq \frac{\log(1/\beta)}{1 - \beta} \ell_\gamma(\theta^0, S) + \frac{1}{2(1 - \beta)} \left( \sum_{\ell=1}^{\bar{p}} \ln \frac{\hat{\nu}^2_{(\ell)}}{1/\sigma^{2_{(\ell)}}} + \frac{\|\theta^0 - \theta_0\|^2}{\sigma^2} \right) + k \left( \frac{\log(1/\beta)}{1 - \beta} + 1 \right) \exp(-c_\gamma) + \frac{1}{1 - \beta} \frac{\log(\frac{1}{n})}{n},
\]

Using the same argument in the proof of Theorem 7, we know that the $KL(Q||P)$ in the PAC-Bayes bound (37) remains invariant under $\alpha$-scale transformation (Kleeman 2011), i.e.,

\[
KL(Q'||P') = KL(Q||P),
\]

where $Q'$ and $P'$ are the distributions after $\alpha$-scale transformation corresponding to $Q$ and $P$ respectively. Note that the other terms apart from the $KL(Q||P)$ in (37) does not change by $\alpha$-scale transformation since the functions represented by the networks are the same.

Thus, our generalization bound is scale-invariant.

We remark that the term $d_\beta \exp(-c_\gamma)$ appears in the bound is not significantly large since we can do normalized margin as mentioned in Appendix A.
D De-randomized Margin Bound: Non-Smooth Predictor

We will focus on non-smooth functions $\psi^\theta(x)$ which has a smooth surrogate. In particular, given any $\theta, x$, we assume the existence of a linear deep net(LDN) $\phi_{\xi}^\theta(x)$ such that

$$\psi^\theta(x) = \phi_{\xi}^\theta(x),$$

where the structure $\xi$ depends on $x$, is a subset of the ReLU-net structure, and is based on certain nodes and next step edges being non-functional because of input activations not crossing thresholds.

D.1 Bounds for Stochastic vs. Deterministic Predictors

Recall Theorem 3 which establishes the relationship between stochastic and deterministic predictors in the main paper:

**Theorem 3** Let $W$ be any distribution on pairs $(x, y)$ with $x \in \mathbb{R}^d$ and $y \in \{-1, +1\}$. For any $\theta^* \in \mathbb{R}^p$, let $Q(\theta, \theta^*) \sim I[\theta_\rho = \theta^*]N(\theta^*, \Sigma_{\theta^*})$ where $\Sigma_{\theta^*}$ is as in (11). Under Assumption 1, for any $\gamma > 0$ and $\beta \in \mathbb{R}$, we have

$$\hat{\ell}_\beta(Q, W) \leq \hat{\ell}_{\beta+\sigma^2\alpha}\gamma(\psi^\theta, W) + 4 \exp(-c_\gamma),$$

and

$$\hat{\ell}_{\beta}(\psi^\theta, W) \leq \hat{\ell}_{\beta+\sigma^2\alpha}\gamma(\psi^\theta, W) + 4 \exp(-c_\gamma),$$

where $\alpha = \alpha_+ + \alpha_-$, constant $c = c_0 \min \left[\frac{\sigma^2\alpha_+^2}{\gamma^2}, \frac{\sigma^2\alpha_-^2}{\gamma^2}, \frac{\sigma^2}{\gamma^2}, \frac{\sigma^2}{\gamma^2}, \frac{\alpha_+}{\gamma^2}, \frac{\alpha_-}{\gamma^2}\right]$, $c_0$ is an absolute constant and $G$, $\alpha_+, \alpha_-, \alpha, \eta_F, \eta_2$ are as in Assumption 1.

**Proof:** The proof of Theorem 3 follows the proof of Theorem 1 such that we have the Taylor expansion for some suitable (random) $\tilde{\theta} = (1 - \tau)\theta^* + \tau\theta = \theta^* + \tau(\theta - \theta^*)$ where $\tau \in [0, 1]$,

$$\phi_{S(\psi^\theta, x)}(x_i) = \phi_{S(\psi^\theta, x)}(x_i) + \langle \theta - \theta^*, \nabla \phi_{S(\psi^\theta, x)}(x_i) \rangle + (\theta - \theta^*)^T H_{S(\psi^\theta, x)}(x_i)(\theta - \theta^*).$$

Then we consider the following set

$$\tilde{Z}_{\beta+\sigma^2\alpha}\gamma(\theta^*) \triangleq \{(x, y) \in \mathcal{X} \times \mathcal{Y} | y\phi_{S(\psi^\theta, x)}(x) > \beta + \sigma^2\alpha \gamma\}.$$  

Let $P = \mathcal{N}(0, \Sigma_{\theta^*})$ be a multivariate distribution with mean 0 and covariance $\Sigma_{\theta^*}$, where $\Sigma_{\theta^*}$ is defined as (11). Now, for $z \in \tilde{Z}_{\beta+\sigma^2\alpha}\gamma(\theta^*)$, we bound

$$\mathbb{P}_{\theta \sim Q}[y\phi_{S(\psi^\theta, x)}(x) \leq \beta | z \in \tilde{Z}_{\beta+\sigma^2\alpha}\gamma(\theta^*)] = \mathbb{P}_{\delta \sim P}[y\phi_{S(\psi^\theta, x)}(x) \leq \beta | z \in \tilde{Z}_{\beta+\sigma^2\alpha}\gamma(\theta^*)],$$

by considering the case $y = +1$ and $y = -1$. Following the proof of Theorem 1 we can obtain

$$\hat{\ell}_\beta(Q, W) \leq \hat{\ell}_{\beta+\sigma^2\alpha}\gamma(\phi_{S(\psi^\theta, x)}(x), W) + 4 \exp(-c_\gamma),$$

Similarly, considering the set

$$\tilde{Z}_{\beta+\sigma^2\alpha}\gamma(\theta^*) \triangleq \{(x, y) \in \mathcal{X} \times \mathcal{Y} | y\phi_{S(\psi^\theta, x)}(x) > \beta + \sigma^2\alpha \gamma\}.$$
We bound the
\[ \mathbb{P}_{\theta \sim Q} \left[ y^{\theta}_{S(\psi^{\theta},z)}(x) \leq \beta \mid z \in \tilde{Z}^{(\gamma)}_{\alpha}(\theta) \right] = \mathbb{P}_{\hat{\theta} \sim \hat{\pi}} \left[ y^{\hat{\theta}}_{S(\psi^{\hat{\theta}},z)}(x) \leq \beta \mid z \in \tilde{Z}^{(\gamma)}_{\alpha}(\theta) \right]. \]
by considering the case \( y = +1 \) and \( y = -1 \). Following the proof of Theorem 1 we can obtain
\[ \hat{\ell}_{\hat{\beta}}(\psi^{\hat{\beta}}, W) = \hat{\ell}_{\hat{\beta}}(\hat{\theta}^{\hat{\psi}}_{S(\psi^{\hat{\theta}}, z)}, W) \leq \hat{\ell}_{\hat{\beta} + \sigma^2 \alpha^2}(Q, W) + 4 \exp(-c\hat{\gamma}) \] 
(96)
By choosing \( \hat{\gamma} > 2 \), we have \( \hat{\gamma}^2 > \hat{\gamma} \), \( (\hat{\gamma} - 1)^2 > \frac{1}{2} \hat{\gamma} \). Therefore, taking a constant \( c = c_0 \min \left[ \frac{\alpha^2}{\sigma^2}, \frac{\sigma^2}{\sigma^2}, \frac{\alpha^2}{\sigma^2}, \frac{\alpha^2}{\sigma^2}, \frac{\alpha^2}{\sigma^2}, \frac{\alpha^2}{\sigma^2}, \frac{\alpha^2}{\sigma^2}, \frac{\alpha^2}{\sigma^2} \right] \) completes the proof.

D.2 Deterministic Margin Bounds

Recall Theorem 4 which establishes the margin bound for deterministic predictors in the main paper:

**Theorem 4** Consider any \( \theta_0 \in \mathbb{R}^p, \sigma^2 > 0 \) chosen before training, and let \( \theta^1 \) be the parameters of the model after training. Let \( H_{i,\phi}^{\theta} \) be the Hessian as in (2), let \( \bar{\nu} = \max \left\{ H_{i,\phi}^{\theta}[j, j], \frac{1}{\sigma^2} \right\} \), \( \hat{\nu} = \| (j : H_{i,\phi}^{\theta}[j, j] > 1/\sigma^2) \|, \) and \( \{ \hat{\nu}(1), \ldots, \hat{\nu}(\hat{\theta}) \} \) be the set of values larger than \( 1/\sigma^2 \). Under Assumption 7 with probability at least \( 1 - \delta \), for any \( \theta^1, \beta \in (0, 1), \gamma > 4\sigma^2 \alpha \), we have the following scale-invariant bound:

\[ \tilde{\ell}_0(\psi^{\theta^1}, D) \leq a_{\beta} \tilde{\ell}_0(\psi^{\theta^1}, S) + \frac{b_{\beta}}{2\pi} \left( \sum_{\ell=1}^p \ln \frac{\tilde{\nu}^2(\ell)}{1/\sigma^2} + (2\pi + \frac{1}{\sigma^2}) \| \theta^1 \|_2 \right) + d_{\beta} \exp(-c\gamma) + b_{\beta} \log(\frac{1}{\delta}) \]
(16)
where \( a_{\beta} = \frac{\log(1/\beta)}{1 - \beta} \), \( b_{\beta} = \frac{1}{1 - \beta} \), \( d_{\beta} = 4(a_{\beta} + 1) \), \( c = c_0 \min \left[ \frac{\alpha^2}{\sigma^2}, \frac{\sigma^2}{\sigma^2}, \frac{\alpha^2}{\sigma^2}, \frac{\alpha^2}{\sigma^2}, \frac{\alpha^2}{\sigma^2}, \frac{\alpha^2}{\sigma^2}, \frac{\alpha^2}{\sigma^2}, \frac{\alpha^2}{\sigma^2} \right] \), \( c_0 \) is an absolute constant, \( \alpha = \alpha_+ + \alpha_- \) and \( G, \alpha_+, \alpha_-, \eta_F, \eta_2 \) are as in Assumption 7.

**Proof:** To get to a de-randomized margin bound, we utilize the results in Theorem 3. First, with \( \beta = 0 \), \( \sigma^2 \hat{\gamma} \alpha = \frac{\gamma}{2} \) and \( W = D \) in Theorem 3 we have
\[ \tilde{\ell}_0(\psi^{\theta^1}, D) \leq \tilde{\ell}_{\gamma/2}(Q, D) + 4 \exp \left( -\frac{c\gamma}{\sigma^2 \alpha} \right) . \]
(97)
Further, with \( \beta = \gamma/2 \) and \( W = S \) in Theorem 4 we have
\[ \tilde{\ell}_{\gamma/2}(Q, S) \leq \tilde{\ell}_0(\psi^{\theta^1}, S) + 4 \exp \left( -\frac{c\gamma}{\sigma^2 \alpha} \right) . \]
(98)
Now, from the Fast Rate PAC-Bayesian bound [33], with probability at least \( 1 - \delta \) over the draw of \( n \) samples \( S \sim D^n \), for any \( \beta \in (0, 1) \) and for any \( Q \) we have
\[ \tilde{\ell}_{\gamma/2}(Q, D) \leq \frac{\log(1/\beta)}{1 - \beta} \tilde{\ell}_{\gamma/2}(Q, S) + \frac{1}{1 - \beta} KL(Q\|P) + \log(\frac{1}{\delta}) \],
(99)
Noting that
\[ KL(Q\|P) = \mathbb{E}_{\theta_{\rho} \sim \rho[\theta = \theta^1], \theta_{\alpha} \sim N(\theta^1, \sigma^2I)} \left[ \log \frac{1[\theta_{\rho} = \theta^1]}{(2\pi)^{\frac{1}{2}d}\Sigma_{\alpha}^{-1}} \exp \left( -\frac{1}{2} (\theta_{\rho} - \theta^1)^T \Sigma_{\alpha}^{-1} (\theta_{\rho} - \theta^1) \right) \frac{1}{(2\pi)^{\frac{1}{2}d}\Sigma_{\alpha}^{\frac{1}{2}}} \exp \left( -\frac{1}{2\sigma^2} \| \theta_{\rho} - \theta^1 \|_2^2 \right) \right] 
= \frac{1}{2} \sum_{\ell=1}^p \ln \frac{\tilde{\nu}^2(\ell)}{1/\sigma^2} + (\pi + \frac{1}{2\sigma^2}) \| \theta_{\rho} - \theta^1 \|_2^2 . \]
we have
\[
\hat{\ell}_0(\psi^{\theta^l}, D) \leq \frac{\log(1/\beta)}{1-\beta} \hat{\ell}_r(\psi^{\theta^l}, S) + \frac{1}{2(1-\beta)} \left( \sum_{\ell=1}^{\hat{p}} \ln \frac{\hat{v}^2_{(\ell)}}{1/\sigma^2} + (2\pi + \frac{1}{\sigma^2}) \|\theta^l - \theta_0\|_2^2 \right) + \frac{1}{1-\beta} \frac{\log(\frac{1}{\beta})}{n} \tag{100}
\]
\[+ 4 \left( \frac{\log(1/\beta)}{1-\beta} + 1 \right) \exp(-c\gamma).\]

Using the argument in the proof of Theorem 7, we know that the \( KL(Q||P) \) in the PAC-Bayes bound \( \text{(99)} \) remains invariant under \( \alpha \)-scale transformation \( [\text{Kleeman, 2011}] \), i.e.,
\[
KL(Q'||P') = KL(Q||P),
\]
where \( Q' \) and \( P' \) are the distributions after \( \alpha \)-scale transformation corresponding to \( Q \) and \( P \) respectively.

Note that the other terms apart from the \( KL(Q||P) \) in \( \text{(99)} \) does not change by \( \alpha \)-scale transformation since the functions represented by the networks are the same.

Thus, our generalization bound is scale-invariant.

The scale-invariant property also applies to the non-smooth predictors, i.e., the generalization bound in Theorem 4. Although the posterior distribution relies on the Hessian \( H_{l,\varphi}^{\theta_e} \) which get modified by a certain \( \alpha \)-scale transformation, the bound in Theorem 4 remains invariant. Similar result holds for multi-class problem, with slight change of constants, which is formally stated as the following:

**Theorem 10** Consider any \( \theta_0 \in \mathbb{R}^p, \sigma^2 > 0 \) chosen before training, and let \( \theta^\dagger \) be the parameters of the model after training. Let \( H_{l,\varphi}^{\theta_e} \) be the Hessian as in \( \text{(2)} \), let \( \nu_j^2 = \max_{j} \{ H_{l,\varphi}^{\theta_e}[j,j], \frac{1}{\sigma^2} \} \), \( \hat{p} = |\{ j : H_{l,\varphi}^{\theta_e}[j,j] > 1/\sigma_j^2 \}| \), and \( \{ \tilde{v}_1, \ldots, \tilde{v}_{\hat{p}} \} \) be the subset of values larger than \( 1/\sigma^2 \). Suppose Assumption 7 holds for prediction function on each class \( h \in [k] \), then with probability at least \( 1-\delta \), for any \( \theta^l, \beta \in (0,1), \gamma > 4\sigma^2\alpha \), we have the following scale-invariant bound:
\[
\hat{\ell}_0(\psi^{\theta^l}, D) \leq a_\beta \hat{\ell}_r(\psi^{\theta^l}, S) + \frac{b_\beta}{2n} \left( \sum_{\ell=1}^{\hat{p}} \ln \frac{\tilde{v}^2_{(\ell)}}{1/\sigma^2} + (2\pi + \frac{1}{\sigma^2}) \|\theta^l - \theta_0\|_2^2 \right) + d_\beta \exp(-c\gamma) + b_\beta \frac{\log(\frac{1}{\beta})}{n},
\]
where
\[
a_\beta = \frac{\log(1/\beta)}{1-\beta}, \quad b_\beta = \frac{1}{1-\beta}, \quad d_\beta = k(a_\beta + 1), \quad c = c_0 \min \left[ \frac{a}{\sigma^2}, \frac{a}{\sigma^2 \eta_F}, \frac{1}{\sigma^2 \eta_2} \right], \quad c_0 \text{ is an absolute constant},
\]
\[\alpha = \alpha_+ + \alpha_- \text{ and } G, \alpha_+, \alpha_-, \eta_F, \eta_2 \text{ are as in Assumption 7}.
\]

The proof is essential the same as Theorem 4 with union bound over all function class in the step of applying Hoeffding’s inequality (See final step of Equation \( \text{(77)} \) and \( \text{(81)} \)), which incurs constants change in the final result, compared to Theorem 4 for 2-class problem.

### E Experimental Results

In this section, we experimentally evaluate our generalization bound on the fully connected feed-forward network with ReLU activation for image classification problems. In practice, it has been empirically observed that 1) the generalization error (test error rate) decreases as the training sample size increases \( [\text{Nagarajan and Kolter, 2019a}] \), and 2) the generalization error increases when the randomness in the label increases \( [\text{Zhang et al., 2017}] \). To examine whether our bound efficiently capture the above observations, we divide our experiments into two sets to address questions: (i) How does our bound behave as we increase the number of random labels? (ii) How does our bound behave with an increase in the number of training samples? After discussing the experimental setup in Section \( \text{E.1} \), we evaluate these questions empirically in Sections \( \text{E.2} \) and \( \text{E.3} \) respectively.
E.1 Experimental Setup

Network Architecture and Datasets: We focus on fully connected networks with ReLU activation of 2 hidden layers, width [64, 128] trained on MNIST. The MNIST dataset contains 60,000 black and white training images, representing handwritten digits 0 to 9. Each image of size $28 \times 28$ is normalized by subtracting the mean and dividing the standard deviation of the training set and converted into a vector of size 784. The Relu network has 59648 parameters. For the random label experiment, We use a subsample of size 1000 from the original MNIST training set, with an equal number of samples from each class. Then we introduce different levels of randomness $r$ in labels Zhang et al. [2017]. In our context, $r$ is the portion of labels for each class that has been replaced by random labels uniformly chosen from $k$ classes. $r = 0$ denotes the original dataset with no corruption, and $r = 1$ means a dataset with completely random labels.

Training and Evaluation: We use Adam with learning rate $0.001$ to minimize cross-entropy loss until convergence. For the random label experiment, i.e., question (i), due to the different degrees of training difficulties introduced by different levels of randomness in the labels, the number of epochs required to convergence is different; we present the details in Table 2. For the sample size experiment, i.e., question (ii), we train the ReLU network with sample size $n \in \{50, 100, 500, 1000, 5000, 10000, 50000\}$ for 100 epochs. The details of the setting are presented in Table 2 and Table 3 respectively for these two questions. To evaluate the proposed generalization bound, we first report the test error rate for each set of experiments. Note that our bound is composed of several key terms: empirical margin loss, $L_2$ norm of the weights, and effective curvature. We report these metrics and the value of the bound to check if the behaviors of our bound are aligned with those of the test error rate. We repeat each experiment for 20 times and report the distribution of the above measurement, and the mean and standard deviation.

| Data      | Input Dimension: | 784 | 784 | 784 | 784 | 784 |
|-----------|------------------|-----|-----|-----|-----|-----|
| No. of Classes k: | 10 | 10 | 10 | 10 | 10 |
| Sample size: | 1000 | 1000 | 1000 | 1000 | 1000 |
| Random Labels: | 0 | 25% | 50% | 75% | 100% |
| Learning Rate $\eta$: | 0.001 | 0.001 | 0.001 | 0.001 | 0.001 |
| Batch Size: | 128 | 128 | 128 | 128 | 128 |
| Epochs: | 100 | 150 | 200 | 250 | 300 |

| Data      | Input Dimension: | 784 | 784 | 784 | 784 | 784 | 784 | 784 |
|-----------|------------------|-----|-----|-----|-----|-----|-----|-----|
| No. of Classes k: | 10 | 10 | 10 | 10 | 10 | 10 | 10 |
| Training set size: | 50 | 100 | 500 | 1000 | 5000 | 10000 | 50000 |
| Random Labels: | 0% | 0% | 0% | 0% | 0% | 0% | 0% |
| Learning Rate $\eta$: | 0.001 | 0.001 | 0.001 | 0.001 | 0.001 | 0.001 | 0.001 |
| Batch Size: | 32 | 32 | 32 | 32 | 32 | 32 | 32 |
| Epochs: | 100 | 100 | 100 | 100 | 100 | 100 | 100 |

E.2 Randomness and Generalization Bound

In the first set of experiments, we validate the theoretical promise of our bound with different level of randomness by reporting the key factors i.e., empirical margin loss $\ell_{\gamma}(\theta^1, S)$, $L_2$ norm of the weights $\|\theta^1 - \theta_0\|_2^2$, and effective curvature $\sum_{\ell=1}^{\tilde{\nu}} \ln \frac{\sigma^2(\ell)}{1/\sigma^2}$, in our generalization bound. With the level of randomness increases,
Figure 5: Results for ReLU-nets trained on MNIST, distributions over 20 runs (a) test set error rate; (b) diagonal elements (mean) of $\tilde{H}_{\theta_t}^{\phi}$; (c) effective curvature; d) $L_2$ norm of $\theta_\dagger$; (e) margin loss with margin $\gamma = 6.5$; (f) generalization bound with $\beta = 0.1$ and $\sigma^2 = 100$. With increasing percentage of random labels, the generalization bound as well as the components (effective curvature, $L_2$ norm, margin loss) increase, and the bound in (f) stays valid for the test error rate in (a).

we observe in in Figure 5 (a) that the test error rate also increases Zhang et al. [2017].

The bound grows with level of randomness. Figure 5 (b) plots the diagonal elements of $H_{\theta_t}^{\phi}$ (mean over 20 runs) and indicates that the value of $H_{\theta_t}^{\phi}[j,j]$ increases as the level of the randomness increase. The large diagonal elements of the Hessian on the random labeled data also implies that the loss surface of the parameter learned from random labeled data is sharper than the one learned from true labeled data. Note that the spectrum of the diagonal elements of $H_{\theta_t}^{\phi}$ can change by $\alpha$-scale transformation. However the ratio of the diagonal elements to the corresponding precision does not change, since the scaling on both terms gets canceled. Figure 5 (c) presents the effective curvature increases as the random labeled data increases, in line with the observations in 5 (b) that more $H_{\theta_t}^{\phi}[j,j]$ cross 1/$\sigma^2$ for more randomness in the label. Figure 5 (d) plots the weighted $L_2$ norm: $\|\theta\|_2/\sigma^2$, which implies that the parameter learned with more random labels has a larger $L_2$ norm corresponding to a larger generalization error. Figure 5 (e) shows that the margin loss distribution shifts to a higher value when the randomness increases. Figure 5 (f) plots the proposed generalization bound as $a_\beta \ell_\gamma (\theta_\dagger, S) + b_\beta \ln(\frac{1}{n}) + \sum_{\ell=1}^n \frac{\rho^2(\ell)}{1/\sigma^2} + \|\theta_\dagger - \theta_0\|^2_2/\sigma^2$ with $\beta = 0.1$ and $\sigma^2 = 100$. We omit the term $d_\beta \exp(-c\gamma) + b_\beta \ln(\frac{1}{n})$ since it stays the same for different level of randomness in the labels. Figure 5 (f) shows that with the randomness increased from 0% to 100%, the generalization error shifts to a higher value, which is consistent with the observations in Figure 5 (a) that random labeled data has larger generalization error. Note that Figure 5 (b), (c) (d) and (e) are scale-invariant.

Margin loss grows with margin $\gamma$. Note that the empirical margin loss plays a role in the generalization bound. The choice of the margin $\gamma$ affects the empirical margin loss $\ell_\gamma (\theta_t, S)$ and the terms $d_\beta \exp(-c\gamma)$ in our bound. Increasing the value of $\gamma$ will increase the empirical margin loss $\ell_\gamma (\theta_t, S)$, but the term $d_\beta \exp(-c\gamma)$ will decrease. Figure 6 illustrates how the margin loss changes $\ell_\gamma (\theta_t, S)$ with different choice of $\gamma$, i.e., $\gamma = 6$ in Figure 6 (a); $\gamma = 6.5$ in Figure 6 (b); and $\gamma = 7$ in Figure 6 (c). We can see that with the margin $\gamma$ increases, the margin loss distribution shifts to a higher value, implying the increases in the margin loss term.
Figure 6: (a) and (b): Margin loss distribution with different $\gamma$. (c): Generalization bound with different $\sigma^2$.  

E.3 Sample Size and Generalization Bound

To evaluate how the generalization bound behaves when the training set size increases, we report the key factors i.e., empirical margin loss $\ell_{\gamma}(\theta^1, S)$, $L_2$ norm of the weights $\|\theta^1 - \theta_0\|^2_2$, and effective curvature $\sum_{\ell=1}^\beta \ln \frac{\ell^2(\ell)}{1/\sigma^2}$ in the bound for different size $n \in \{50, 100, 500, 1000, 5000, 10000, 50000\}$ of the training set. It has recently been observed that certain norms of the weights grow with training set size $n$ [Nagarajan and Kolter, 2019a]. Before we examine the overall generalization bound, we first focus on Product of Spectral Norms that recur in the numerator of many recent bounds [Nagarajan and Kolter, 2019b, Bartlett et al., 2017, Golowich et al., 2018], and $L_2$ norm which recurs in our bound.

$L_2$ norm increases far slower than the product of the spectral norms with training sample size $n$. We observe in Figure 7 (a) that both these quantities grow with training sample size $n$, but the $L_2$ norm (red line) grows far slower than the product of the spectral norms (blue line). The same observation happens in Figure 7 (c), where we increase little bit randomness in the label (5% randomness). But the magnitude of the increases in the product of the spectral norms is significant for 5% randomness. Since the norm term in the bound is scaled by the sample size $n$, we also observe in Figure 7 (b) that both norms scaled by the sample decrease as the sample increases for 0 % random label. However, Figure 7 (d) shows that, even when we add 5% randomness to the label, the product of the spectral norms scaled by sample get increases after 5000 samples. But the scaled $L_2$ norm keeps decreasing.

The bound decrease with training sample size $n$. We now turn to evaluating our bound by reporting the key terms in the bound as the sample size increases in Figure 8. Figure 8 (a) shows the test error rate decreases as the training sample size grows. We observe in Figure 8 (b) that the diagonal elements of $H_{\ell,\phi}$ decreases as more training sample $n$ are used to train the model. In consequence, the effective curvature decreases as the training set size $n$ as shown in Figure 8 (c). Figure 8 (d) and (e) show that the weighted $L_2$ norm divided by sample $\|\theta\|^2_2/(n\sigma^2)$ and empirical the margin loss $\ell_{\gamma}(\theta^1, S)$ decreases as the sample increases. Figure 8 (f) plots the proposed generalization bound with measurement in Section E.2 ($\beta = 0.1$ and $\sigma^2 = 100$). It shows that with sample size increased from 50 to 50000, the generalization error decreases, which is consistent with the observations in Figure 8 (a) and existing work [Nagarajan and Kolter, 2019a].
Optimal \( \sigma \). Note that the choice of variance \( \sigma^2 \) of the prior distribution also plays a role in the generalization bound: \( \sum_{\ell=1}^{\tilde{p}} \ln \frac{\tilde{p}^2(t)}{1/\sigma^2} + \frac{\|\theta^\dagger - \theta_0\|^2}{\sigma^2} \). The dependence on the prior covariance in the two terms illustrates a trade-off, i.e., a large \( \sigma \) diminishes the dependence on \( \|\theta^\dagger - \theta_0\|^2 \), but increases the dependence on the effective curvature, and vice versa. To illustrate how the value of \( \sigma \) affects the bound, we choose \( \sigma^2 \in \{1, 10, 25, 50, 100\} \), and present the corresponding bound in Figure 8 (c). It shows that the optimal value of \( \sigma^2 \) may locate in (10, 25). This observation suggests that optimizing the covariance \( \sigma \) of the PAC-Bayes prior distribution, which is data-independent can lead to a sharper bound. We consider such analysis as our future work.