Generalization Bounds for Gradient Methods via Discrete and Continuous Prior

Xuanyuan Luo  
IIIS, Tsinghua University  
xuanyuanluo@google.com

Luo Bei  
Renmin University of China  
rabbit_lb@ruc.edu.cn

Jian Li  
IIIS, Tsinghua University  
lijian83@mail.tsinghua.edu

Abstract

Proving algorithm-dependent generalization error bounds for gradient-type optimization methods has attracted significant attention recently in learning theory. However, most existing trajectory-based analyses require either restrictive assumptions on the learning rate (e.g., fast decreasing learning rate), or continuous injected noise (such as the Gaussian noise in Langevin dynamics). In this paper, we introduce a new discrete data-dependent prior to the PAC-Bayesian framework, and prove high probability generalization bounds of order $O\left(\frac{1}{n} \cdot \sum_{t=1}^{T} \left(\gamma_t / \sigma_t \right)^2 \|g_t\|^2\right)$ for floored GD and SGD (i.e. finite precision versions of GD and SGD with precision level $\varepsilon_t$) where, where $n$ is the number of training samples, $\gamma_t$ is the learning rate at step $t$, $g_t$ is roughly the difference between the average gradient over all samples and that over only prior samples. $\|g_t\|$ is upper bounded by (typically much smaller) than the gradient norm $\|\nabla f(W_t)\|$. We remark that our bounds hold for nonconvex and nonsmooth loss functions. Moreover, our theoretical results provide numerically favorable upper bounds of testing errors (0.026 on MNIST and 0.198 on CIFAR10). Furthermore, we study the generalization bounds for gradient Langevin Dynamics (GLD). Using the same framework with a carefully constructed continuous prior, we show a new high probability generalization bound of order $O\left(\frac{1}{n} + \frac{L^2}{n^2} \sum_{t=1}^{T} (\gamma_t / \sigma_t)^2\right)$ for GLD. The new $1/n^2$ rate is obtained using the concentration of the difference between the gradient of training samples and that of the prior.

1 Introduction

Bounding generalization error of learning algorithms is one of the most important problems in machine learning theory. Formally, for a supervised learning problem, the generalization error is defined as the testing error (or population error) minus the training error (or empirical error). In particular, we denote $R(w, (x, y)) := 1[h_w(x) \neq y]$ as the error of a single data point $(x, y)$, where $h_w(x)$ is the output of a model with parameter $w \in \mathbb{R}^d$. Suppose $S$ is the set of training data, each i.i.d. sampled from the population distribution $D$, and we use $R(w, S) := \frac{1}{|S|} \sum_{z \in S} R(w, z)$ and $R(w, D) := \mathbb{E}_{z \sim D}[R(w, z)]$ to denote the training error and the testing error, respectively. The generalization error of $w$ is formally defined as $\text{err}_\text{gen}(w) = R(w, D) - R(w, S)$.

Proving tighter generalization bounds for general nonconvex learning and particularly deep learning has attracted significant attention recently. While the classical learning theory (uniform convergence theory) which bounds the generalization error by various complexity measures (e.g., the
We first briefly mention some recent work on bounding the generalization error of gradient-based methods, which depends on both the algorithm and data. Recently, learning theorists have tried to understand and explain generalization of deep learning from several other perspectives, such as margin theory [Bartlett et al., 2017, Wei et al., 2019], algorithmic stability [Hardt et al., 2016, Mou et al., 2018, Li et al., 2020, Bousquet et al., 2020], PAC-bayeisan [London, 2017, Bartlett et al., 2017, Neyshabur et al., 2018, Zhou et al., 2019, Yang et al., 2019], neural tangent kernel [Jacot et al., 2018, Du et al., 2019, Arora et al., 2019, Cao and Gu, 2019], information theory [Pensia et al., 2018, Negrea et al., 2019], model compression [Arora et al., 2018, Zhou et al., 2019], differential privacy [Oneto et al., 2017, Wu et al., 2021] and so on.

In this paper, we aim to obtain tighter generalization error bounds that depend on both the training data and the optimization algorithms (a.k.a. gradient-type methods) for general nonconvex learning problems. In particular, we prove algorithm-dependent generalization bounds for several gradient-based optimization algorithms such as certain variants of gradient descent (GD), stochastic gradient descent (SGD) and stochastic gradient Langevin dynamics (SGLD). Our proofs are based on the classic Catoni’s PAC-Bayesian framework [Catoni, 2007] and also have a flavor of algorithmic stability [Bousquet and Elisseeff, 2002]. Several prior works have obtained generalization bounds for SGD and SGLD by analyzing trajectory through either the PAC-Bayesian or the algorithmic stability framework (or closely related information theoretic arguments). However, most existing results based on analyzing the optimization trajectories require either restrictive assumptions on the learning rates, or continuous noise (such as the Gaussian noise in Langevin dynamics) in order to bound the stability or the KL-divergence. In this paper, we resolve the above restrictions by combining the PAC-Bayesian framework with a few simple (yet effective) ideas, so that we can obtain new high probability and non-vacuous generalization bounds for several gradient-based optimization methods with either discrete or continuous noises (in particular certain variants of GD and SGD, either being deterministic or with discrete noise, which cannot be handled by existing techniques).

1.1 Prior work

We first briefly mention some recent work on bounding the generalization error of gradient-based methods. Hardt et al. [2016] first studied the uniform stability (hence the generalization) of stochastic gradient descent (SGD) for both convex and non-convex functions. Their results for non-convex functions requires that the learning rate $\eta_t$ scales with $1/t$. Their work motivates a long line of subsequent work on generalization error bounds of gradient-based optimization methods: Kuzborskij and Lampert [2018], London [2016], Chaudhari et al. [2019], Raginsky et al. [2017], Mou et al. [2018], Chen et al. [2018], Li et al. [2020], Negrea et al. [2019], Wang et al. [2021].

Recently, Simsekli et al. [2020], Hodgkinson et al. [2022] obtained generalization bound of SGD through the perspective of heavy-tailed behaviors and using the notion of Hausdorff dimension $d_H$ which depends on both the algorithm and data.

PAC-Bayesian bounds. The PAC-Bayesian framework [McAllester, 1999] is a powerful method for proving high probability generalization bound [Bartlett et al., 2017, Zhou et al., 2019, Mou et al., 2018]. Roughly speaking, it bounds the generalization error by the KL divergence $\text{KL}(Q \parallel P)$, where $Q$ is the distribution of the learned output and $P$ is a prior distribution which is typically independent of dataset $S$. In this framework, bounding $\text{KL}(Q \parallel P)$ is the most crucial part for obtaining tighter PAC-Bayesian bounds. In order to bound the KL divergence, both the prior $P$ and posterior $Q$ are typically chosen to be continuous distributions (mostly Gaussians so that KL can be computed in closed form). Hence, most prior work either considered gradient methods with continuous noise (such as Gradient Langevin Dynamics) (e.g., [Mou et al., 2018, Li et al., 2020, Negrea et al., 2019]), or injected a Gaussian noise to the final parameter at the end (e.g., [Neyshabur et al., 2018, Zhou et al., 2019]) (so $Q$ is a Gaussian distribution). We also note that designing effective prior $P$ can be also very important. For example, Lever et al. [2013] proposed to use the population distribution to compute the prior. In fact, the prior can even partially depend on the training data [Parrado-Hernández et al., 2012, Negrea et al., 2019], and our Theorem 4.1 is partially inspired by this idea.
1.2 Our contributions

First, we provide high probability generalization bounds for discrete gradient methods. In particular, we study the generalization of Floored Gradient Descent (FGD), which is a variant of GD, and Floored Stochastic Gradient Descent (FSGD), a variant of SGD. We obtain our bound by an interesting construction of discrete priors. Secondly, we consider well studied gradient methods with continuous noise, (stochastic) gradient Langvin dynamics (GLD and SGLD). We show sharper generalization bounds by carefully bounding the concentration of the sample gradients. Now, we summarize our results.

FGD and FSGD. We first study an interesting variant of GD, called Floored GD (FGD) (Algorithm 1). The update rule of FGD is defined as follows:

\[ W_t \leftarrow W_{t-1} - \gamma_t \nabla f(W_{t-1}, S_J) - \varepsilon_t \text{floor}(\gamma_t g_t/\varepsilon_t) , \]

where \( S_J \) is the subset of training dataset \( S \) with size \( m \) indexed by subset \( J \subset [n] \) \((J \) is chosen before training\), \( \nabla f(W_{t-1}, Z) := \frac{1}{|Z|} \sum_{z \in Z} \nabla f(W_{t-1}, z) \) is the average gradient over the dataset \( Z \), \( \gamma_t \) is the learning rate, \( \varepsilon_t \) is the precision level, and \( g_t := \nabla f(W_{t-1}, S) - \nabla f(W_{t-1}, S_J) \) is the gradient difference. The flooring operation is defined by floor \((x) := \text{sign}(x) \times \lfloor |x| \rfloor \) for any real number \( x \). FGD can viewed as GD with given precision limit \( \varepsilon_t \). We can see if we ignore the floor operation or let \( \varepsilon_t \) approaches 0, FGD reduces to GD (see also Appendix A).

We also study a finite precision variant of SGD, called Floored SGD (FSGD) (see Section 5 for its formal definition). Empirically, the optimization and generalization capabilities of FGD and FSGD are very close to those of GD and SGD (see Figure 5 and 6 in Appendix H).

By constructing a discrete data-dependent prior and incorporate it into Catoni’s PAC-Bayesian framework, we prove that the following bound (Theorem 5.2) holds for FGD with high probability:

\[ \mathcal{R}(W_T, D) \leq c_0 \mathcal{R}(W_T, S_J) + O \left( \frac{1}{n-m} + \ln(dT) \right) \left( \frac{\ln(1/T)}{n-m} \sum_{t=1}^{T} \frac{\gamma_t^2}{\varepsilon_t^2} \| g_t \|^2 \right) , \]

where \( d \) is the dimension of parameter space and \( c_0 \) can be chosen to be a small constant. The bound for FSGD is very similar (see Theorem 5.3). Now we make a few remarks about our results.

1. Our result holds for nonconvex and nonsmooth learning problems (replacing the gradients with subgradients for nonsmooth cases). Moreover, there is no additional requirement on the learning rate \( \gamma_t \).

2. The gradient difference \( g_t \) is typically much smaller than the worst case gradient norm. It usually decreases when \( m = |J| \) grows (see Figure 1c in Section 7).

3. We obtain non-vacuous generalization bounds on commonly used datasets. Specifically, our theoretical test error upper bounds on MNIST and CIFAR10 are 0.026 and 0.198, respectively (see Section 7). Both of them are tighter than the best-known MNIST bound (11%) and CIFAR10 bound (23%) reported in Dziugaite et al. [2021]. See Table 1 in Appendix B for more comparisons.

4. In order to bound the KL between \( P \) and the deterministic process of FGD, we construct the prior \( P \) from a discrete random processes. We hope it may inspire future research on handling deterministic optimization algorithms or discrete noise.

Why study FGD/FSGD? We would like to remark that we study FGD/FSGD, not because FGD/FSGD have better performances than GD/SGD or other advantages. Indeed, their performances are almost the same as those of GD/SGD (see Appendix H). We use them as important stepping stones to study generalization bounds for GD and SGD. Note that most existing trajectory-based generalization bounds require either fast decreasing learning rate, or continuous injected noise, such as the Gaussian noise in Langevin dynamics, for general non-convex loss functions. Handling deterministic algorithms (such as GD) or discrete noises (such as SGD) is challenging and beyond the reach of existing techniques. In fact, understanding such discrete noises and their effects on generalization has been an important research topic (see e.g., Li et al. [2020], Zhu et al. [2019], Ziyin et al. [2021]). In particular, Zhu et al. [2019] show that it is insufficient to approximate SGD’s discrete noise by isotropic Gaussian noise. Moreover, proving nontrivial generalization bounds for SGD-like algorithms with discrete noise has also been proposed as an open research direction in Li et al. [2020].
GLD and SGLD. We provide a new generalization bound for Gradient Langevin Dynamics (GLD).

The update rule of GLD is defined as follows.

\[ W_t ← W_{t-1} + γ_t ∇ f(W_{t-1}, S) + σ_t N(0, I_d). \]  

(GLD)

In this paper, we show that the following generalization bound (Theorem 6.2) holds with high probability over the randomness of \( S \sim D^n \) and random subset \( J \subseteq [n] (|J| = m) \):

\[ \mathcal{R}(W_T, D) ≤ c_0 \mathcal{R}(W_T, S_{[n]\setminus J}) + O \left( \frac{1}{n-m} + \frac{1}{m} \right) \mathbb{E} \left[ \sum_{t=1}^{T} \frac{\gamma_t^2}{\sigma_t^2} L(W_{t-1})^2 \right]. \]

where \( L(W_{t-1}) := \max_{z \in S} \| f(W_{t-1}, z) \| \) is the longest gradient norm of any training sample in \( S \) at step \( t \) and \( m \) is the size of \( J \). Since \( W_T \) is independent of the index set \( J \), the first term \( \mathcal{R}(W_T, S_{[n]\setminus J}) \) is upper bounded by \( \mathcal{R}(W_T, S) + O(\frac{1}{\sqrt{m}}) \) with high probability, using standard Hoeffding’s inequality. By setting \( m = n/2 \), our generalization bound has an \( O(\frac{1}{\sqrt{n}} + \frac{1}{n} + \frac{1}{n^2}) \) rate. The new \( 1/n^2 \) rate is obtained using the concentration of the difference between the gradient of training samples and that of the prior (See Lemma 6.1).

We also prove a high probability generalization bound for Stochastic Gradient Langevin Dynamics (SGLD) (see Theorem 6.3):

\[ \mathcal{R}(W_T, D) ≤ c_0 \mathcal{R}(W_T, S_{[n]\setminus J}) + O \left( \frac{1}{n-m} + \frac{1}{m} \right) \mathbb{E} \left[ \sum_{t=1}^{T} \frac{\gamma_t^2}{\sigma_t^2} L(W_{t-1})^2 \right]. \]

We compare our bounds with other GLD/SGLD bounds obtained in [Mou et al., 2018, Negrea et al., 2019, Li et al., 2020] and the details can be found in Appendix B.

CLD. Using the PAC-Bayesian framework, we obtain a new generalization bound for Continuous Langevin Dynamics (CLD), defined by the stochastic differential equation \( dW_t = -∇ F(W_t, S) dt + \sqrt{2β^{-1}} dB_t \). The main term of the generalization bound scales as \( O(1/n^2) \) (by choosing \( m = n/2 \)) and does not grow to infinity as the training time \( T \) increases. See Theorem G.6 for the details.

2 Other Related Work

Stochastic Langevin Dynamics Stochastic Langevin dynamics is a popular sampling and optimization method in machine learning [Welling and Teh, 2011]. Zhang et al. [2017], Chen et al. [2020] show a polynomial hitting time (hitting a stationary point) of SGLD in general non-convex setting. Raginsky et al. [2017] study the generalization and excess risk of SGLD in nonconvex settings and their bound depends inversely polynomially on a certain spectral gap parameter, which may be exponential small in the dimension. Continuous Langevin dynamics (SDE) with various noise structure has also been used extensively as approximations of SGD in literature (see e.g., [Li et al., 2017, 2021]). However, in terms of generalization, isotropic Gaussian noise is not a good approximation of the discrete noise in SGD (Zhu et al. [2019]).

Nonvacuous PAC-Bayesian Generalization Bounds. Dziugaite and Roy [2017] first present a nonvacuous PAC-Bayesian generalization bound on MNIST (0.161 for a 1-layer MLP, see column T-600 of Table 1 in their paper). They use a very different training algorithm that explicitly optimizes the PAC-Bayesian bound and the output distribution is a multivariate normal distribution. To computing the closed form of KL, they choose a zero-mean Gaussian distribution as the prior distribution. Zhou et al. [2019] obtain the first non-vacuous generalization bound for ImageNet via a different method. Their method does not require any continuous noise injected but assumes that the network can be significantly compressed (so that the prior distribution is supported over the set of discrete parameters with finite precision). To our best knowledge, it is the only work that utilizes a discrete prior for proving generalization bounds of deep neural networks. Our result for FGD/FSGD has a similar flavor in a high level, that is the optimization method has a finite precision. However, our results do not need any assumption on compressibility of the model and can be applied to nonconvex learning problems other than neural networks.

Generalization bounds via Information theory. Raginsky et al. [2017] first show that the expected generalization error \( \mathbb{E}_{S \sim D^n} [\mathcal{R}(W, D) - \mathcal{R}(W, S)] \) is bounded by \( \sqrt{2I(S; W)/n} \), where \( I(S; W) := \)
KL (P(S, W) || P(S) ⊗ P(W)) is the mutual information between the data set S and the parameter W. This work motivates several subsequent studies [Pensia et al., 2018, Negrea et al., 2019, Bu et al., 2020, Wang et al., 2021]. The main goal in this line of work is to obtain a tight bound on the mutual information I(S; W). This is again reduced to bounding the KL divergence and thus typically requires continuous injected noise (e.g., Wang et al. [2021], Negrea et al. [2019]).

3 Preliminaries

Notations. We assume that the training dataset $S = (z_1, \ldots, z_n)$ is sampled from $\mathcal{D}^n$, where $\mathcal{D}$ is the population distribution over the data domain $\Omega$. The model parameter $w$ is in $\mathbb{R}^d$. The risk function $R : \mathbb{R}^d \times \Omega \rightarrow [0, 1]$ measures the error of a model on a datapoint. The loss function $f : \mathbb{R}^d \times \Omega \rightarrow \mathbb{R}$ is a proxy of the risk. The optimization algorithm minimizes the loss function and we assume we can compute the gradient of the loss function. We note that the loss function may be different from the risk function (e.g., 0/1 risk vs. cross-entropy loss). The empirical risk is $R(w, S) = \frac{1}{|S|} \sum_{z \in S} R(w, z)$ and population risk is $R(w, D) = \mathbb{E}_{z \sim D}[R(w, z)]$. Similarly, we can define the empirical loss $f(w, S)$ and population loss $f(w, D)$. For any $J = (j_1, \ldots, j_m)$, we use $S_J$ to denote the sequence $(S_{j_1}, \ldots, S_{j_m})$. The subsequence $(A_1, A_{i+1}, \ldots, A_j)$ is denoted by $A_i^j$. We use $(A_i^j, B_i^j)$ to denote the merged sequence $(A_1, A_2, \ldots, A_n, B_1, \ldots, B_m)$. When the elements in sequence $J$ are distinct, we also use $J$ to represent the set consisting of all of its elements. We may also slightly abuse the notation of a random variable to denote its distribution. For example, $E_{x \sim X}[f(x)]$ is a shorthand for $E_{z \sim P_X}[f(x)]$, and $KL(X || Y)$ means $KL(P_X || P_Y)$. For a random variable $W$, we define $R(W, S) = E_{w \sim W}[R(w, S)]$ and $R(W, D) = E_{w \sim w}[R(w, D)]$. The set $\{1, 2, \ldots, n\}$ is denoted by $[n]$.

KL-divergence. Let $P$ and $Q$ be two probability distributions. The Kullback–Leibler divergence $KL(P \parallel Q)$ is defined only when $P$ is absolute continuous with respect to $Q$, i.e., for any $x$, $Q(x) = 0$ implies $P(x) = 0$. In particular, if $P$ and $Q$ are discrete distributions, then $KL(P \parallel Q) = \sum_x P(x) \ln \frac{P(x)}{Q(x)}$. Otherwise, if $P$ and $Q$ are continuous distributions, it is defined as $\int P(x) \ln \frac{P(x)}{Q(x)} \, dx$. The following Lemma 3.1 is frequently used in this paper and is a well known property of KL divergence (see Cover [1999, Theorem 2.5.3], Li et al. [2020], Negrea et al. [2019]).

Lemma 3.1 (Chain Rule of KL). Then, the following equation holds (given all KLS are well defined):

$$KL(W \parallel W') = KL(W_0 \parallel W'_0) + \sum_{t=1}^T \mathbb{E}_{w \sim W_0} \left[KL(W_t | W_{t-1}^w = w || W'_t | W_{t-1}^w = w)\right].$$

Here $W_t | W_{t-1}^w = w$ denotes the distribution of $W_t$ conditioning on $W_{t-1}^w = (W_0, \ldots, W_{t-1}) = w$.

PAC-Bayesian. In this paper, we use the PAC-Bayesian bound presented in Catoni [2007] which enjoys a tighter $O(KL(Q \parallel P) / n)$ rate comparing to the traditional $O(\sqrt{KL(Q \parallel P) / n})$ bound, but with a slightly larger constant factor on the empirical error. We restate their bound as follows.

Lemma 3.2 (Catoni’s Bound). (see e.g., Lever et al. [2013]) For any prior distribution $P$ independent of the training set $S$, any $\delta \in (0, 1)$, and any $\eta > 0$, the following bound holds w.p. $\geq 1 - \delta$ over $S \sim \mathcal{D}^n$:

$$\mathbb{E}_{w \sim Q}[R(W, D)] \leq \eta C_\eta \mathbb{E}_{w \sim Q}[R(W, S)] + C_\eta \cdot \frac{KL(Q \parallel P) + \ln(1/\delta)}{n} \quad (\forall Q),$$

where $C_\eta = \frac{1}{1 - e^{-\eta}}$ is an absolute constant.

Concentration inequality. We use the following variant of McDiramid inequality (Lemma 3.3) to prove the concentration of cumulative gradient difference in Section 6. The proof is deferred to Appendix C.

Lemma 3.3. Suppose $\Phi : [n]^m \rightarrow \mathbb{R}^+$ is order-independent$^1$ and $|\Phi(J) - \Phi(J')| \leq c$ holds for any adjacent $J, J' \in [n]^m$ satisfying $|J \cap J'| = m - 1^2$. Let $J$ be $m$ indices sampled uniformly from $[n]$ without replacement. Then $Pr_{J} (\Phi(J) - \mathbb{E}_{J}[\Phi(J)] > \epsilon) \leq \exp\left(\frac{-2\epsilon^2}{mc}\right)$.

$^1$Order-independent is defined as $\Phi(J) = \Phi(j_1, \ldots, j_m)$ holds for any input $J = (j_1, \ldots, j_m) \in \Omega^m$ and any permutation $\pi \in S_m$.

$^2|J \cap J'| := \{i \in [n] : i \in J \land i \in J'\}.$
4 Data-Dependent PAC-Bayesian Bound

The dominating term in the PAC-Bayesian bound (1) is \( \text{KL}(Q \parallel P) / n \), where \( P \) is a prior distribution independent of the training dataset \( S \). Typically, without knowing any information from \( S \), the best possible bound for \( \text{KL}(Q \parallel P) \) we can hope is at least \( \Theta(1) \) (it should not be a function of \( n \) hence should not decrease with \( n \)). However, if we are allowed to see \( m \) data points from \( S \) when constructing our prior, we may produce better prediction on posterior \( Q_S \). The following theorem enables us to use data-dependent prior in PAC-Bayesian bound. The proof is almost the same as Cantoni’s original proof and we provide a proof for completeness in Appendix D.

**Theorem 4.1 (Data-Dependent PAC-Bayesian).** Suppose \( J \) is a random sequence including \( m \) indices uniformly sampled from \([n]\) without replacement. For any \( \delta \in (0, 1) \) and \( \eta > 0 \), we have w.p. \( 1 - \delta \) over \( S \sim \mathcal{D}^n \) and \( J \):

\[
\mathcal{R}(Q, \mathcal{D}) \leq \eta C_\eta \mathcal{R}(Q, S_J) + C_\eta \cdot \frac{\text{KL}(Q \parallel P(S_j)) + \ln(1/\delta)}{n - m} \quad (\forall Q),
\]

where \( I = [n] \setminus J \) is the set of indices not in \( J \), \( P(S_j) \) is the prior distribution only depending on the information of \( S_J \) (\( S_J \) is the subset of \( S \) indexed by \( J \)), and \( C_\eta := \frac{1}{1-e^{-\eta}} \) is a constant.

**Remarks.** Note that the above bound holds regardless of whether \( Q \) depends on \( S \) or not. Also note that the first term in the right hand side is \( \mathcal{R}(Q, S_J) \), not \( \mathcal{R}(Q, S) \) as in the usual generalization bounds. We remark that for most of our learning algorithms that are independent of \( J \) (i.e., changing \( J \) does not change the output \( Q \)), by standard Chernoff-Hoeffding inequality, \( \mathcal{R}(Q, S_J) \) can be bounded by \( \mathcal{R}(Q, S) + O(1/\sqrt{n - m}) \) with high probability over the randomness of \( J \). For example, the update rules of GLD, SGLD and CLD are independent of \( J \), hence \( \mathcal{R}(Q, S_J) \) can be replaced by \( \mathcal{R}(Q, S) + O(1/\sqrt{n - m}) \) in Theorem 4.1. However, we point out a subtle point that FGD (Algorithm 1) studied in this paper depends on \( J \). It may be the case that by knowing \( J \), FGD extracts more information from \( S_J \) but not much from \( S_J \), unintentionally making \( \mathcal{R}(Q, S_J) \) a validation error, rather than the training error as it should be. However, from our experiment (see Figure 5 and 6 in Appendix H, and Figure 2a), we can see that FGD is very close to GD and the \( S_J \) error \( \mathcal{R}(W_T, S_J) \) is indeed close to the training error \( \mathcal{R}(W_T, S) \) and both are significantly smaller than the testing error \( \mathcal{R}(W_T, D) \). So \( \mathcal{R}(Q, S_J) \) can be considered as a genuine training error in our study of FGD.

5 FGD and FSGD

In this section, we study the generalization error of finite precision variants of gradient descent and stochastic gradient descent: Floored Gradient Descent (FGD) and Floored Stochastic Gradient Descent (FSGD).

First we need to define the “floor” operation which is used in the definitions of FGD and FSGD.

**Definition 5.1 (Floor).** For any vector \( X \in \mathbb{R}^d \), let \( Y = \text{floor}(X) \) defined as:

\[
Y_i = \text{floor}(X_i) = |X_i| \quad \text{if} \quad X_i \geq 0, \quad = -|X_i| \quad \text{if} \quad X_i < 0, \quad \text{for all} \quad i \in [d].
\]

**FGD:** The Floored Gradient Descent algorithm is formally defined in Algorithm 1, where \( (\gamma_t)_{t\geq0} \) and \( (\varepsilon_t)_{t\geq0} \) are the step size and precision sequences, respectively. For a subset \( \mathcal{Z} \subseteq S \), we write

\[
\nabla f(W_{t-1}, \mathcal{Z}) := \frac{1}{|\mathcal{Z}|} \sum_{z \in \mathcal{Z}} \nabla f(W_{t-1}, z).
\]

Note that FGD can be viewed as gradient descent with given precision limit \( \varepsilon_t \). We can see if we ignore the floor operation or let \( \varepsilon_t \) approach 0, FGD reduces to the ordinary GD (see Appendix A). We also study momentum FGD, in which the 5th line of Algorithm 1 is replaced by

\[
W_t \leftarrow W_{t-1} + \alpha \cdot (W_{t-1} - W_{t-2}) - g_2 - \varepsilon_t \cdot \text{floor}(g_1 - g_2)/\varepsilon_t;
\]

Here \( \alpha > 0 \) is a constant. We remark that both FGD and its momentum version are deterministic algorithms. The following theorem provides the generalization error bound for both algorithms.

**Theorem 5.2.** Suppose \( J \) is a random sequence consisting of \( m \) indices uniformly sampled from \([n]\) without replacement. Then for any \( \delta \in (0, 1) \), both FGD (Algorithm 1) and its momentum version satisfy the following generalization bound w.p. at least \( 1 - \delta \) over \( S \sim \mathcal{D}^n \) and \( J \):

\[
\mathcal{R}(W_T, \mathcal{D}) \leq \eta C_\eta \mathcal{R}(W_T, S_J) + C_\eta \cdot \frac{\ln(1/\delta) + 3}{n - m} + \frac{C_\eta \ln(dT)}{n - m} \sum_{t=1}^{T} \left( \frac{\varepsilon_t^2}{\varepsilon_t^2} \|g_t\|^2 \right),
\]
Algorithm 1: Floored Gradient Descent (FGD)

**Input:** Training dataset $S = (z_1, ..., z_n)$. Index set $J$.

**Result:** Parameter $W_T \in \mathbb{R}^d$.

1. Initialize $W_0 \leftarrow w_0$;
2. for $t : 1 \rightarrow T$ do
   3. $g_1 \leftarrow \gamma_t \nabla f(W_{t-1}, S)$;
   4. $g_2 \leftarrow \gamma_t \nabla f(W_{t-1}, S_J)$;
   5. $W_t \leftarrow W_{t-1} - g_2 - \varepsilon_t \cdot \text{floor}(g_1 - g_2)/\varepsilon_t$;
end

where $d$ is the dimension of parameter space, $I = [n] \backslash J$ is the set of indices not in $J$, $C_n := \frac{1}{1 - e^{-\eta}}$ is a constant, and $g_t := \nabla f(W_{t-1}, S) - \nabla f(W_{t-1}, S_J)$.

**Proof.** We use Theorem 4.1 to prove our theorem for the momentum version. The ordinary FGD is a special case of the momentum version with $\alpha = 0$. The key is to construct the prior distribution $P(S_J)$ such that $\text{KL}(W_T \mid P(S_J))$ is tractable. Let $p$ be any real number in $(0, 1/3)$. We first define a stochastic process $\{W_0', ..., W_T\}$, by the following update rule ($W_0' := w_0$):

$$W_t' \leftarrow W_{t-1}' + \alpha \cdot (W_{t-1}' - W_{t-2}') - \gamma_t \nabla f(W_{t-1}', S_J) - \varepsilon_t \cdot \xi_t,$$

where $\xi_t$ is a discrete random variable such that for all $(a_1, ..., a_d) \in \mathbb{Z}^d$:

$$\text{Pr}[\xi_t = (a_1, ..., a_d)^T] := \left( \sum_{i=-\infty}^{\infty} p^2 \right)^{-d} \exp \left( -\frac{d}{\ln(1/p)} a_k^2 \right).$$

It is easy to verify that the sum of the probabilities ($\sum_{a \in \mathbb{Z}^d} \text{Pr}[\xi_t = a]$) equals to 1. Note that $W_t'$ only depends on $S_J$. We define $P(S_J)$ as the distribution of $W_T'$.

Recall that $W_0' = (W_0, ..., W_t)$ is the parameter sequence of FGD (Algorithm 1). Applying the chain rule of KL-divergence (Lemma 3.1), we have:

$$\text{KL}(W_T \mid P(S_J)) = \text{KL}(W_T \mid W_T') \leq \text{KL}(W_0' \mid W_0').$$

(2)

The last equation holds because FGD is deterministic. Let $w = W_0'^{-1}$. The distribution of $W_1 | W_0' = w$ (where $w = (w_0, ..., w_{T-1})$) is a point mass on $w_{t-1} + \alpha \cdot (w_{t-1} - w_{t-2}) - \gamma_t \nabla f(w_{t-1}, S_J) - \varepsilon_t \cdot \text{floor} \left( \gamma_t \frac{\nabla f(w_{t-1}, S) - \nabla f(w_{t-1}, S_J)}{\varepsilon_t} \right).$

Let vector $a = (a_1, ..., a_d) = \text{floor}(\frac{2}{\varepsilon_t} (\nabla f(w_{t-1}, S) - \nabla f(w_{t-1}, S_J)))$. By the definition of $W_t'$, we have

$$\text{KL}(W_t' \mid W_0' = w) = 1 \cdot \ln(1/\text{Pr}[\xi_t = a])$$

$$= \ln \left( \sum_{i=-\infty}^{\infty} p^2 \right) + \sum_{k=1}^{d} \ln(1/p) \cdot a_k^2.$$

Since $|i| \leq i^2$ and $p \in (0, 1/3)$, we have $\ln \left( \sum_{i=-\infty}^{\infty} p^2 \right)$ is at most $d \ln (1 + 2 \sum_{i=1}^{\infty} p^2)$. It can be further bounded by $d \ln (1 + 3p)$. Moreover, it can be bounded by $3dp$ as $\ln(1 + x) \leq x$. Thus, the above KL-divergence can be bounded by $3dp + \sum_{k=1}^{d} \ln(1/p) a_k^2$. Recall that the
We conclude our proof by plugging it into Theorem 5.3.

where randomness of sequence independent of $W$

Here the gradient as follows:

\[ \nabla f(w_{t-1}, S) - \nabla f(w_{t-1}, S_j) \]

Therefore, we have

\[
\text{KL} \left( W_t | W_0^{t-1} = w \right) \leq 3dp + \frac{\ln(1/p)\gamma_t^2}{\epsilon_t^2} \| \nabla f(w_{t-1}, S) - \nabla f(w_{t-1}, S_j) \|_2^2.
\]

Plugging the above inequality into (2), we have

\[
\text{KL} \left( W_T \mid P(S_j) \right) \leq \sum_{t=1}^{T} \left( 3dp + \frac{\ln(1/p)\gamma_t^2}{\epsilon_t^2} \| \nabla f(W_{t-1}, S) - \nabla f(W_{t-1}, S_j) \|_2^2 \right).
\]

We conclude our proof by plugging it into Theorem 4.1 (setting $p = 1/(Td)$).

**FSGD:** We can use a similar approach to prove a generalization bound for Floored Stochastic Gradient Descent (FSGD). Formally, FSGD is identical to Algorithm 1 except for the definitions of $g_1$ and $g_2$ replaced with:

\[
g_1 \leftarrow \nabla f(W_{t-1}, S_{B_t}), \quad g_2 \leftarrow \nabla f(W_{t-1}, S_{B_t \cap J}),
\]

where $B_t \subseteq [n]$ is a random batch independent of $S, J$ and $W_0^{t-1}$. Formally, each $B_t$ is a set including $b$ indices uniformly sampled from $[n]$ without replacement. The following theorem provides a generalization bound for FSGD. The proof can be found in Appendix E.

**Theorem 5.3.** Suppose $J$ is a random sequence consisting of $m$ indices uniformly sampled from $[n]$ without replacement. Then for any $\delta \in (0, 1), \epsilon \in (0, 1)$, FSGD satisfies the following generalization bound: w.p. at least $1 - \delta$ over $S \sim \mathcal{D}^n$ and $J$:

\[
\mathcal{R}(W_T, \mathcal{D}) \leq \eta C_\eta \mathcal{R}(W_T, S_I) + C_\eta \cdot \frac{\ln(1/\delta) + 3}{n - m} + \frac{C_\eta \ln(dT)}{n - m} + \frac{1}{T} \mathbb{E}_{B_t} \left[ \sum_{t=1}^{T} \frac{\gamma_t^2}{\epsilon_t^2} \| g_t \|_2^2 \right],
\]

where $d$ is the dimension of parameter space, $I = [n] \setminus J, C_\eta := \frac{1}{1 - e^{-\eta}}$ is a constant, and $g_t := f(W_{t-1}, S_{B_t}) - \nabla f(W_{t-1}, S_{J \cap B_t})$.

## 6 Gradient Langevin Dynamics

In this section, we present new generalization bounds for Gradient Langevin Dynamics (GLD) and Stochastic Gradient Langevin Dynamics (SGLD) based on Theorem 4.1.

**Gradient Langevin Dynamics (GLD):** The GLD algorithm can be viewed as gradient descent plus a Gaussian noise. Formally, for a given training set $S \sim \mathcal{D}^n$, the update rule of GLD is defined as follows:

\[
W_{t+1} \leftarrow W_t - \frac{\gamma_{t+1}}{n} \sum_{z \in S} \nabla f(W_t, z) + \sigma_{t+1} \mathcal{N}(0, I_d),
\]

(GLD)

Here the gradient $\nabla f(W_t, z)$ can be replaced with any gradient-like vector such as a clipped gradient. The output of GLD is the last step parameter $W_T$ or some function of the whole training trajectory $W_0^T$ (e.g., the average of the suffix $\frac{1}{K} \sum_{t=T-K}^{T} W_t$).

We still use the data-dependent PAC-Bayesian framework (Theorem 4.1) to prove the generalization bound. Unlike FGD (Algorithm 1), GLD is independent of the prior indices $J$, which enables us to prove the following concentration bound (Lemma 6.1) for the gradient difference. The proof is based on Lemma 3.3, which is postponed to Appendix F.

**Lemma 6.1.** Let $S = (z_1, \ldots, z_n)$ be any fixed training set. $J$ is a random sequence including $m$ indices uniformly sampled from $[n]$ without replacement, and $W = (W_0, \ldots, W_T)$ is any random sequence independent of $J$. Then the following bound holds with probability at least $1 - \delta$ over the randomness of $J$:

\[
\mathbb{E}_W \left[ \sum_{t=1}^{T} \frac{\gamma_t^2}{\epsilon_t^2} \| \nabla f(W_{t-1}, S) - \nabla f(W_{t-1}, S_j) \|_2^2 \right] \leq \frac{C_\delta}{m} \mathbb{E}_W \left[ \sum_{t=1}^{T} \frac{\gamma_t^2}{\epsilon_t^2} L(W_{t-1})^2 \right],
\]

where $C_\delta = 4 + 2\ln(1/\delta) + 5.66\sqrt{\ln(1/\delta)}$, and $L(w) = \max_{z \in [n]} \| \nabla f(w, z) \|$.  

8
Now we are ready to present our main results. The proofs can be found in Appendix F.

**Theorem 6.2.** Suppose $J$ is a random sequence consisting of $m$ indices uniformly sampled from $[n]$ without replacement. Let $W_T$ be the output of GLD. Then for any $\delta \in (0, \frac{1}{2})$ and $\eta > 0$, we have w.p. $1 - 2\delta$ over $S \sim \mathcal{D}^n$ and $J$, the following holds ($L(w) := \max_{z \in S} \|f(w, z)\|$):

$$
\mathcal{R}(W_T, D) \leq \eta C_\eta \mathcal{R}(W_T, S_I) + \frac{C_\eta \ln(1/\delta)}{n-m} + \frac{C_\eta C_\delta}{2(n-m)m} E_{W^T_0} \left[ \sum_{t=1}^{T} \frac{\gamma_t^2}{\sigma_t^2} L(W_{t-1})^2 \right],
$$

where $C_\delta = 4 + 2 \ln(1/\delta) + 5.66 \sqrt{\ln(1/\delta)}$, $I = [n] \setminus J$ and $C_\eta = \frac{1}{1-e^{-\eta}}$.

**Stochastic Gradient Langevin Dynamics (SGLD):** For a given training data set $S$, the update rule of SGLD is defined as:

$$
W_{t+1} \leftarrow W_t - \gamma_{t+1} \nabla f(W_t, S_{B_t}) + \sigma_{t+1} N(0, I_d),
$$

where $B_t \sim \text{uniform}([n])$ is the mini-batch of size $b$ at step $t$. Note that $B_t$ is a sequence instead of a set, thus it may include duplicate elements. Similar to the analysis of GLD, we can prove the following bound for SGLD.

**Theorem 6.3.** Let $W_T$ be the output of SGLD when the training set is $S$, and $J$ be a random sequence with $m$ indices uniformly sampled from $[n]$ without replacement. For any $\delta \in (0, 1)$ and $m \geq 1$, we have w.p. $1 - 2\delta$ over $S \sim \mathcal{D}^n$ and $J$, the following holds:

$$
\mathcal{R}(W_T, D) \leq \eta C_\eta \mathcal{R}(W_T, S_I) + \frac{C_\eta \ln(1/\delta)}{n-m} + \frac{C_\eta}{b} + \frac{C_\delta}{2m} E_{W^T_0} \left[ \sum_{t=1}^{T} \frac{\gamma_t^2}{\sigma_t^2} L(W_{t-1})^2 \right],
$$

where $L(w) := \max_{z \in S} \|f(w, z)\|$, $C_\delta = 4 + 2 \ln(1/\delta) + 5.66 \sqrt{\ln(1/\delta)}$, $C_\eta = \frac{1}{1-e^{-\eta}}$, $b$ is the batch size, and $I = [n] \setminus J$.

**Remark 6.4.** If the gradient norm is bounded\(^3\) and we use a decaying learning rate schedule such as $\gamma_t \propto O(1/t)$, then the summation in our bound converges. Hence, under such a learning rate schedule, Theorem 6.2 and 6.3 imply the following test error bound for GLD or SGLD: $\mathcal{R}(W_T, D) \leq \eta C_\eta \mathcal{R}(W_T, S_I) + O\left(\frac{1}{n-m}\right)$ which is independent of $T$, where $O$ hides some logarithmic factors.

7 Experiment

In this section, we conduct experiments for FGD and FSGD on MNIST [LeCun et al., 1998] and CIFAR10 [Krizhevsky et al., 2009] to investigate the the optimization and generalization properties of FGD and FSGD, and the numerical closeness between our theoretical bounds and true test errors. Due to space limit, the detailed experimental setting and some additional experimental results can be found in Appendix H.

**FGD/FSGD vs GD/SGD.** We first demonstrate that the training and testing curves of FGD and GD are nearly identical (we choose precision level $\varepsilon = 0.005$ or 0.004). We also show that the same is true for FSGD vs SGD. Due to space limit, the figures are presented in Appendix H (Figure 5 and 6).

\(^3\) $\|\nabla f(w, z)\| \leq L$ holds for all $w, z$
we train a SimpleNet \( (\text{the size of}) \) Theorem 5.3 with \( \eta = 2, \delta = 0.1 \). The red part corresponds to the first term of our bound (the empirical risk) and the green part corresponds to the rest. The last step test error and our bound are 0.18 and 0.198, respectively. In (c), we show how cumulative gradient difference decreases as \( m \) (the size of \( J \)) increases.

**Non-vacuous bounds.** For MNIST, we train a CNN \( (d = 1.4 \cdot 10^6) \) by FGD with \( \gamma_t = 0.005 \cdot 0.9^t \) and \( \varepsilon_t = 0.005 \) and momentum \( \alpha = 0.9 \). The size \( m = |J| \) is set to \( n/2 = 30000 \). As shown in Figure 1a and 1b, our bound (Theorem 5.2 with \( \eta = 1.5, \delta = 0.1 \)) tracks the testing error closely. At step \( T = 990 \), our bound is 0.026 while the testing error is 0.011. This is non-vacuous and tighter than best known 11\% MNIST bound reported in Dziugaite et al. [2021]. For CIFAR10, we train a SimpleNet [Hasanpour et al., 2016] without BatchNorm and Dropout. The number of parameters \( d \) is nearly \( 18 \cdot 10^6 \). We use FSGD to train our model. The learning rate \( \gamma_t \) is set to \( 0.001 \cdot 0.9^{(t/200)} \), the precision \( \varepsilon_t \) is set to 0.004, and the momentum \( \alpha \) is set to 0.99. The batch size is 2000. \( m = |J| \) is set to \( n/5 = 10000 \). The result is shown in Figure 2b. We stop training at step \( t = 8000 \) when the testing error is and 0.18. At that time, our testing error bound is 0.198 which is non-vacuous and tighter than best known 0.23 CIFAR10 bound reported in Dziugaite et al. [2021].

**Decrease of the gradient difference.** Intuitively, the cumulative squared norm of gradient difference \( g_t := \nabla f(W_t, S) - \nabla f(W_t, S_T) \) should decrease as \( m = |J| \) increases. Although we cannot prove a concentration like Lemma 6.1 (i.e., \( \|g_t\|^2 \) scales as \( O(1/m) \)), we can still observe that \( \|g_t\|^2 \) decreases when \( m \) increases. The results are depicted in Figure 1c and Figure 2c.

**Random labels.** We conduct the random label experiment designed in Zhang et al. [2017]. Our theoretical bounds can distinguish the datasets with different portion \( (p) \) of random labels. See Appendix H.

### 8 Conclusion

In this paper, we prove new generalization bounds for several gradient-based methods with either discrete or continuous noises based on carefully constructed data-dependent priors. Recall that FGD requires to compute the gradient difference for technical reasons. It would be more natural and desirable if we only need to compute the full gradient and rounded to the nearest grid point. An intriguing future direction is to free FGD/FSGD from the dependence of the prior subset \( J \) so that we can apply the concentration on the gradient difference to obtain a tighter bound. Of course, a major further direction is to obtain similar generalization bounds for vanilla GD and SGD, which remains to be an important open problem in this line of work. Our technique can be useful for handling deterministic algorithms and discrete noises, but it seems that new technical ideas or assumptions are needed for tackling GD or SGD.

### 9 Acknowledgements

The authors would like to thank the anonymous reviewers for their constructive comments. The authors are supported in part by the National Natural Science Foundation of China Grant 62161146004, Turing AI Institute of Nanjing and Xi’an Institute for Interdisciplinary Information Core Technology.
References
Sanjeev Arora, Rong Ge, Behnam Neyshabur, and Yi Zhang. Stronger generalization bounds for deep nets via a compression approach. In International Conference on Machine Learning, pages 254–263. PMLR, 2018.
Sanjeev Arora, Simon Du, Wei Hu, Zhiyuan Li, and Ruosong Wang. Fine-grained analysis of optimization and generalization for overparameterized two-layer neural networks. In International Conference on Machine Learning, pages 322–332. PMLR, 2019.
Peter L Bartlett, Dylan J Foster, and Matus J Telgarsky. Spectrally-normalized margin bounds for neural networks. Advances in neural information processing systems, 30, 2017.
Olivier Bousquet and André Elisseeff. Stability and generalization. The Journal of Machine Learning Research, 2:499–526, 2002.
Olivier Bousquet, Yegor Klochkov, and Nikita Zhivotovskiy. Sharper bounds for uniformly stable algorithms. In Conference on Learning Theory, pages 610–626. PMLR, 2020.
Yuheng Bu, Shao Feng Zou, and Venugopal V Veeravalli. Tightening mutual information-based bounds on generalization error. IEEE Journal on Selected Areas in Information Theory, 1(1):121–130, 2020.
Yuan Cao and Quanquan Gu. Generalization bounds of stochastic gradient descent for wide and deep neural networks. Advances in neural information processing systems, 32, 2019.
Olivier Catoni. Pac-bayesian supervised classification: the thermodynamics of statistical learning. IMS Lecture Notes Monograph Series, 56:1–163, 2007. doi: 10.1214/074921707000000391.
Pratik Chaudhari, Anna Choromanska, Stefano Soatto, Yann LeCun, Carlo Baldassi, Christian Borgs, Jennifer Chayes, Levent Sagun, and Riccardo Zecchina. Entropy-sgd: Biasing gradient descent into wide valleys. Journal of Statistical Mechanics: Theory and Experiment, 2019(12):124018, 2019.
Xi Chen, Simon S Du, and Xin T Tong. On stationary-point hitting time and ergodicity of stochastic gradient langevin dynamics. Journal of Machine Learning Research, 2020.
Yuansi Chen, Chi Jin, and Bin Yu. Stability and convergence trade-off of iterative optimization algorithms. CoRR, 2018.
Thomas M Cover. Elements of information theory. John Wiley & Sons, 1999.
Monroe D Donsker and SR Srinivasa Varadhan. Asymptotic evaluation of certain markov process expectations for large time. iv. Communications on pure and applied mathematics, 36(2):183–212, 1983.
Simon Du, Jason Lee, Haochuan Li, Liwei Wang, and Xiyu Zhai. Gradient descent finds global minima of deep neural networks. In International conference on machine learning, pages 1675–1685. PMLR, 2019.
Devdatt P. Dubhashi and Alessandro Panconesi. Concentration of Measure for the Analysis of Randomized Algorithms. Cambridge University Press, 2009. ISBN 978-0-521-88427-3.
John Duchi. Derivations for linear algebra and optimization. Berkeley, California, 3(1):2325–5870, 2007.
Gintare Karolina Dziugaite and Daniel M Roy. Computing nonvacuous generalization bounds for deep (stochastic) neural networks with many more parameters than training data. UAI, 2017.
Gintare Karolina Dziugaite, Kyle Hsu, Waseem Gharbieh, Gabriel Arpino, and Daniel Roy. On the role of data in pac-bayes bounds. In International Conference on Artificial Intelligence and Statistics, pages 604–612. PMLR, 2021.
Vitaly Feldman and Jan Vondrak. High probability generalization bounds for uniformly stable algorithms with nearly optimal rate. In Conference on Learning Theory, pages 1270–1279. PMLR, 2019.
Noah Golowich, Alexander Rakhlin, and Ohad Shamir. Size-independent sample complexity of neural networks. In *Conference On Learning Theory*, pages 297–299. PMLR, 2018.

Mahdi Haghifam, Jeffrey Negrea, Ashish Khisti, Daniel M Roy, and Gintare Karolina Dziugaite. Sharpened generalization bounds based on conditional mutual information and an application to noisy, iterative algorithms. *Advances in Neural Information Processing Systems*, 33:9925–9935, 2020.

Moritz Hardt, Ben Recht, and Yoram Singer. Train faster, generalize better: Stability of stochastic gradient descent. In *International conference on machine learning*, pages 1225–1234. PMLR, 2016.

Nick Harvey, Christopher Liaw, and Abbas Mehrabian. Nearly-tight vc-dimension bounds for piecewise linear neural networks. In *Conference on learning theory*, pages 1064–1068. PMLR, 2017.

Seyyed Hossein Hasanpour, Mohammad Rouhani, Mohsen Fayyaz, and Mohammad Sabokrou. Lets keep it simple, using simple architectures to outperform deeper and more complex architectures. *CoRR*, 2016.

Liam Hodgkinson, Umut Simsekli, Rajiv Khanna, and Michael Mahoney. Generalization bounds using lower tail exponents in stochastic optimizers. In *International Conference on Machine Learning*, pages 8774–8795. PMLR, 2022.

Arthur Jacot, Franck Gabriel, and Clément Hongler. Neural tangent kernel: Convergence and generalization in neural networks. *Advances in neural information processing systems*, 31, 2018.

Alex Krizhevsky, Geoffrey Hinton, et al. Learning multiple layers of features from tiny images. *Master’s thesis, University of Tront*, 2009.

Ilja Kuzborskij and Christoph Lampert. Data-dependent stability of stochastic gradient descent. In *International Conference on Machine Learning*, pages 2815–2824. PMLR, 2018.

Yann LeCun, Léon Bottou, Yoshua Bengio, and Patrick Haffner. Gradient-based learning applied to document recognition. *Proceedings of the IEEE*, 86(11):2278–2324, 1998.

Guy Lever, François Laviolette, and John Shawe-Taylor. Tighter pac-bayes bounds through distribution-dependent priors. *Theoretical Computer Science*, 473:4–28, 2013.

Jian Li, Xuanyuan Luo, and Mingda Qiao. On generalization error bounds of noisy gradient methods for non-convex learning. In *International Conference on Learning Representations*, 2020.

Qianxiao Li, Cheng Tai, and E Weinan. Stochastic modified equations and adaptive stochastic gradient algorithms. In *International Conference on Machine Learning*, pages 2101–2110. PMLR, 2017.

Zhiyuan Li, Sadhika Malladi, and Sanjeev Arora. On the validity of modeling sgd with stochastic differential equations (sdes). *Advances in Neural Information Processing Systems*, 34, 2021.

Ben London. Generalization bounds for randomized learning with application to stochastic gradient descent. In *NIPS Workshop on Optimizing the Optimizers*, 2016.

Ben London. A pac-bayesian analysis of randomized learning with application to stochastic gradient descent. *Advances in Neural Information Processing Systems*, 30, 2017.

David A McAllester. Some pac-bayesian theorems. *Machine Learning*, 37(3):355–363, 1999.

Wenlong Mou, Liwei Wang, Xiyu Zhai, and Kai Zheng. Generalization bounds of sgld for non-convex learning: Two theoretical viewpoints. In *Conference on Learning Theory*, pages 605–638. PMLR, 2018.

Vaishnavh Nagarajan and J Zico Kolter. Generalization in deep networks: The role of distance from initialization. *NeurIPS*, 2017.
Vaishnavh Nagarajan and J Zico Kolter. Uniform convergence may be unable to explain generalization in deep learning. *Advances in Neural Information Processing Systems*, 32, 2019.

Jeffrey Negrea, Mahdi Haghifam, Gintare Karolina Dziugaite, Ashish Khisti, and Daniel M Roy. Information-theoretic generalization bounds for sgld via data-dependent estimates. *Advances in Neural Information Processing Systems*, 32, 2019.

Behnam Neyshabur, Srinadh Bhojanapalli, and Nathan Srebro. A pac-bayesian approach to spectrally-normalized margin bounds for neural networks. In *International Conference on Learning Representations*, 2018.

Luca Oneto, Sandro Ridella, and Davide Anguita. Differential privacy and generalization: Sharper bounds with applications. *Pattern Recognition Letters*, 89:31–38, 2017.

Emilio Parrado-Hernández, Amiran Ambroladze, John Shawe-Taylor, and Shiliang Sun. Pac-bayes bounds with data dependent priors. *The Journal of Machine Learning Research*, 13(1):3507–3531, 2012.

Ankit Pensia, Varun Jog, and Po-Ling Loh. Generalization error bounds for noisy, iterative algorithms. In *2018 IEEE International Symposium on Information Theory (ISIT)*, pages 546–550. IEEE, 2018.

Maxim Raginsky, Alexander Rakhlin, and Matus Telgarsky. Non-convex learning via stochastic gradient langevin dynamics: a nonasymptotic analysis. In *Conference on Learning Theory*, pages 1674–1703. PMLR, 2017.

Hannes Risken. Fokker-planck equation. In *The Fokker-Planck Equation*, pages 63–95. Springer, 1996.

Umut Simsekli, Ozan Sener, George Deligiannidis, and Murat A Erdogdu. Hausdorff dimension, heavy tails, and generalization in neural networks. *Advances in Neural Information Processing Systems*, 33:5138–5151, 2020.

Hao Wang, Yizhe Huang, Rui Gao, and Flavio Calmon. Analyzing the generalization capability of sgld using properties of gaussian channels. *Advances in Neural Information Processing Systems*, 34, 2021.

Colin Wei, Jason D Lee, Qiang Liu, and Tengyu Ma. Regularization matters: Generalization and optimization of neural nets vs their induced kernel. *Advances in Neural Information Processing Systems*, 32, 2019.

Max Welling and Yee W Teh. Bayesian learning via stochastic gradient langevin dynamics. In *Proceedings of the 28th international conference on machine learning (ICML-11)*, pages 681–688. Citeseer, 2011.

Bingzhe Wu, Zhicong Liang, Yatao Bian, ChaoChao Chen, Junzhou Huang, and Yuan Yao. Generalization bounds for stochastic gradient langevin dynamics: A unified view via information leakage analysis. *CoRR*, 2021.

Jun Yang, Shengyang Sun, and Daniel M Roy. Fast-rate pac-bayes generalization bounds via shifted rademacher processes. *Advances in Neural Information Processing Systems*, 32, 2019.

Valentina Zantedeschi, Paul Viallard, Emilie Morvant, Rémi Emonet, Amaury Habrard, Pascal Germain, and Benjamin Guedj. Learning stochastic majority votes by minimizing a pac-bayes generalization bound. *Advances in Neural Information Processing Systems*, 34:455–467, 2021.

Chiyuan Zhang, Samy Bengio, Moritz Hardt, Benjamin Recht, and Oriol Vinyals. Understanding deep learning requires rethinking generalization. In *5th International Conference on Learning Representations, ICLR 2017, Toulon, France, April 24-26, 2017, Conference Track Proceedings*. OpenReview.net, 2017.

Yuchen Zhang, Percy Liang, and Moses Charikar. A hitting time analysis of stochastic gradient langevin dynamics. In *Conference on Learning Theory*, pages 1980–2022. PMLR, 2017.
Wenda Zhou, Victor Veitch, Morgane Austern, Ryan P. Adams, and Peter Orbanz. Non-vacuous
generalization bounds at the imagenet scale: a pac-bayesian compression approach. In 7th
International Conference on Learning Representations, ICLR 2019, New Orleans, LA, USA, May
6-9, 2019. OpenReview.net, 2019.

Zhanxing Zhu, Jingfeng Wu, Bing Yu, Lei Wu, and Jinwen Ma. The anisotropic noise in stochastic
gradient descent: Its behavior of escaping from sharp minima and regularization effects. In
International Conference on Machine Learning, pages 7654–7663. PMLR, 2019.

Liu Ziyin, Kangqiao Liu, Takashi Mori, and Masahito Ueda. Strength of minibatch noise in sgd. In
International Conference on Learning Representations, 2021.

Checklist

The checklist follows the references. Please read the checklist guidelines carefully for information on
how to answer these questions. For each question, change the default [TODO] to [Yes], [No], or
[N/A]. You are strongly encouraged to include a justification to your answer, either by referencing
the appropriate section of your paper or providing a brief inline description. For example:

• Did you include the license to the code and datasets? [Yes]
• Did you include the license to the code and datasets? [No] The code and the data are
proprietary.
• Did you include the license to the code and datasets? [N/A]

Please do not modify the questions and only use the provided macros for your answers. Note that the
Checklist section does not count towards the page limit. In your paper, please delete this instructions
block and only keep the Checklist section heading above along with the questions/answers below.

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper’s
       contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes] See the conclusion section.
   (c) Did you discuss any potential negative societal impacts of your work? [N/A]
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to
       them? [Yes]

2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes]
   (b) Did you include complete proofs of all theoretical results? [Yes]

3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experi-
       mental results (either in the supplemental material or as a URL)? [Yes]
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they
       were chosen)? [Yes]
   (c) Did you report error bars (e.g., with respect to the random seed after running experi-
       ments multiple times)? [Yes]
   (d) Did you include the total amount of compute and the type of resources used (e.g., type
       of GPUs, internal cluster, or cloud provider)? [Yes] It can be found in our supplemental
       material.

4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
   (a) If your work uses existing assets, did you cite the creators? [Yes]
   (b) Did you mention the license of the assets? [N/A]
   (c) Did you include any new assets either in the supplemental material or as a URL? [N/A]
   (d) Did you discuss whether and how consent was obtained from people whose data you’re
       using/curating? [N/A]
(c) Did you discuss whether the data you are using/curating contains personally identifiable information or offensive content? [N/A] We only use the standard MNIST and CIFAR10 datasets.

5. If you used crowdsourcing or conducted research with human subjects...

   (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]

   (b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A]

   (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]