Stability Based Generalization Bounds for Exponential Family Langevin Dynamics

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Abstract

We study generalization bounds for noisy stochastic mini-batch iterative algorithms based on the notion of stability. Recent years have seen key advances in data-dependent generalization bounds for noisy iterative learning algorithms such as stochastic gradient Langevin dynamics (SGLD) based on stability (Mou et al., 2018; Li et al., 2020) and information theoretic approaches (Xu and Raginsky, 2017; Negrea et al., 2019; Steinke and Zakynthinou, 2020; Haghifam et al., 2020). In this paper, we unify and substantially generalize stability based generalization bounds and make three technical advances. First, we bound the generalization error of general noisy stochastic iterative algorithms (not necessarily gradient descent) in terms of expected (not uniform) stability. The expected stability can in turn be bounded by a Le Cam Style Divergence. Such bounds have a $O(1/n)$ sample dependence unlike many existing bounds with $O(1/\sqrt{n})$ dependence. Second, we introduce Exponential Family Langevin Dynamics (EFLD) which is a substantial generalization of SGLD and which allows exponential family noise to be used with stochastic gradient descent (SGD). We establish data-dependent expected stability based generalization bounds for general EFLD algorithms. Third, we consider an important special case of EFLD: noisy sign-SGD, which extends sign-SGD using Bernoulli noise over $\{-1, +1\}$. Generalization bounds for noisy sign-SGD are implied by that of EFLD and we also establish optimization guarantees for the algorithm. Further, we present empirical results on benchmark datasets to illustrate that our bounds are non-vacuous and quantitatively much sharper than existing bounds.

1 Introduction

Recent years have seen renewed interest and advances in characterizing generalization performance of learning algorithms in terms of stability, which considers change in performance of a learning algorithm based on change of a single training point (Hardt et al., 2016; Bousquet and Elisseeff, 2002; Li et al., 2020; Mou et al, 2018). For stochastic gradient descent (SGD), Hardt et al. (2016) established generalization bounds based on uniform stability (Bousquet and Elisseeff, 2002), although the analysis needed rather small step sizes $\eta_t = 1/t$ which is arguably not useful in practice. While improving the stability analysis for SGD has remained a challenge, advances have been made on noisy SGD algorithms, especially stochastic gradient Langevin dynamics (SGLD) (Welling and Teh, 2011; Mou et al., 2018; Li et al., 2020) which adds Gaussian noise to the stochastic gradients. In parallel, there has been key developments on related information-theoretic generalization bounds applicable to SGLD type algorithms (Negrea et al., 2019; Haghifam et al., 2020; Xu and Raginsky, 2017; Russo and Zou, 2016; Pensia et al., 2018).
While these developments have led to major advances in analyzing generalization of noisy SGD algorithms, they each have certain limitations which leave room for further improvements. Mou et al. (2018) considered SGLD with marginal Gaussian noise variance $\sigma_t$ and step size $\eta_t \leq \sigma_t \ln 2/L$, where $L$ is the global Lipschitz constant for the loss, and established a generalization bound for SGLD of the form $\frac{L}{n} \sqrt{\sum_t \eta_t^2 \sigma_t^2}$ using uniform stability. The bound has a desirable dependency of $O(1/n)$ on the samples, but has an undesirable dependence on $L$, and the step sizes, bounded by $O(\sigma/L)$, are arguably too small. Mou et al. (2018) also presented another bound which addresses some of these issues, but gets an undesirable $O(1/\sqrt{n})$ sample dependence. By building on the developments of Russo and Zou (2016); Xu and Raginsky (2017); Pensia et al. (2018), Negrea et al. (2019) made advances from the information theoretic perspective and established bounds for SGLD which have a desirable dependence on the norm of gradient incoherence, i.e., a suitable difference in gradients over different mini-batches, avoids dependence on Lipschitz constant $L$, and is applicable to unbounded sub-Gaussian losses, but have an undesirable $O(1/\sqrt{n})$ sample dependence. Haghifam et al. (2020) made further advances on the problem from an information theoretic perspective based on the conditional mutual information framework of Steinke and Zakynthinou (2020) and obtained generalization bounds based on gradient incoherence with $O(1/n)$ sample dependence, but their analysis holds for full batch Langevin dynamics, not mini-batch SGLD. Li et al. (2020) made advances on such bounds based on the notion of Bayes-stability, by combining ideas from PAC-Bayes bounds into stability, and established a bound of the form $\frac{\varphi}{n} \sqrt{\sum_t \eta_t^2 g_e(t) / \sigma_t^2}$ for bounded losses, where $g_e(t)$ is the expected gradient norm square at step $t$. While the bound has a desirable sample dependence of $O(1/n)$ and avoids dependence on the Lipschitz constant $K$, the dependence on the gradient norm makes such bounds much weaker than the information theoretic bounds of Negrea et al. (2019); Haghifam et al. (2020) which depend on the norm of gradient incoherence which are typically orders of magnitude smaller. Further, the analysis of Li et al. (2020) still needs small step sizes, bounded by $O(\sigma/\sqrt{n})$.

In this paper, we build on the core strengths of such existing approaches, most notably (a) the $O(1/n)$ sample dependence of stability based bounds (Mou et al. 2018; Li et al. 2020), (b) the dependence on the norm of gradient incoherence rather than the norm of gradient for information theoretic bounds (Negrea et al. 2019; Haghifam et al. 2020), and (c) no dependence on the global Lipschitz constant $K$, and develop a framework (Section 3) for establishing generalization bounds for noisy stochastic iterative algorithms. Our framework considers generalization based on the concept of expected stability, rather than uniform stability (Hardt et al. 2016; Bousquet and Elisseeff 2002; Bousquet et al. 2020; Mou et al. 2018), and yields distribution dependent generalization bounds which avoid the worst-case setting of uniform stability. Recall that for any data domain $Z$ and a distribution $D$ over the domain, uniform stability considers the worst case difference in loss over two datasets $S_n, S'_n \in Z^n$ of size $n$ which differ by one point, i.e., over $\sup_{S_n, S'_n, |S_n \Delta S'_n|=1} \cdots$. (Bousquet and Elisseeff 2002; Hardt et al. 2016). In Section 3 we show that one gets a valid generalization bound by replacing the supremum $\sup$ by and expectation $E_{S_n, S'_n}$, where $S_n \sim D^n$ and, without loss of generality, $S'_n$ shares the first $(n - 1)$ samples with $S_n$ with the $n$-th sample $z'_n \sim D$. Replacing $\sup$ by $E$ makes the bound distribution dependent, avoids the worst case analysis associated with uniform stability, and can arguably lead to quantitatively sharper bounds will less assumptions. Building on some analyses in [Li et al. 2020], we show that expected stability of general noisy mini-batch stochastic iterative algorithms, not just noisy SGD, can be bounded by the expectation of a Le Cam Style Divergence (LSD) over distributions over parameters obtained from $S_n$ and $S'_n$. Thus, getting an expected stability based generalization bound for a specific algorithm reduces to that of bounding the expected LSD.

In Section 3 we introduce Exponential Family Langevin Dynamics (EFLD), a family of noisy stochastic gradient descent algorithms based on exponential family noise. Special cases of EFLD include SGLD and
noisy versions of Sign-SGD or quantized SGD algorithms widely used in practice (Bernstein et al., 2018a,b; Jin et al., 2020; Alistarh et al., 2017). Our main result provides an expected stability based generalization bound applicable to any EFLD algorithm with several desirable properties: (a) a $O(1/n)$ sample dependence, (b) a dependence on the norm of gradient discrepancy, a variant of gradient incoherence (Negrea et al., 2019), rather than a dependence on the norm of gradients, (c) no dependence on the global Lipschitz constant $K$, and (d) step sizes $\eta_t$ need not be tiny, i.e., $\eta_t = O(1/K)$ is not necessary. Existing generalization bounds for SGLD (Li et al., 2020; Negrea et al., 2019) usually use properties of the Gaussian distribution, and do not generalize to EFLD. Our proof technique is new, and uses properties of exponential family distributions. We also consider optimization guarantees for EFLD, establish convergence results for SGLD based on Gaussian noise and for noisy Sign-SGD based on Bernoulli noise over $\{-1,+1\}$ where the Bernoulli noise parameters depend on the stochastic gradients. The analysis for SGLD is a variant of existing analyses whereas the analysis for noisy sign-SGD based on gradient dependent Bernoulli noise is new.

In Section 5 we present experiment results on benchmark datasets and illustrate that our bounds for SGLD are non-vacuous and quantitatively tighter than existing bounds (Li et al., 2020; Negrea et al., 2019) due to the desirable dependence on sample size and gradient discrepancy norms, which are empirically shown to be orders of magnitude smaller than gradient norms. We also present results for noisy Sign-SGD on benchmark datasets and illustrate that our bounds give a quantitatively tight upper bound to the empirical test error across epochs and the optimization performance is comparable to that of sign-SGD.

2 Related Work

Uniform stability. Uniform stability is a classical approach for bounding generalization error (Bousquet and Elisseeff, 2002; Hardt et al., 2016; Bousquet et al., 2020; Shalev-Shwartz et al., 2009; Feldman and Vondrak, 2018, 2019), pioneered by Rogers and Wagner (1978); Devroye and Wagner (1979). Recently, uniform stability has been used in analyzing the stability of stochastic gradient descent (SGD) (Hardt et al., 2016). Mou et al. (2018) prove the uniform stability of SGLD (Welling and Teh, 2011; Raginsky et al., 2017) by showing that uniform stability can be bounded by the squared Hellinger distance, and further they establish discretized Fokker-Planck equations for analyzing the squared Hellinger distance. Then they provide uniform stability based generalization bounds for SGLD as $\frac{L}{n} \sqrt{\sum_t \eta_t^2 / \sigma_t^2}$ which depends on $L$, the global Lipschitz constant for gradients, and the step size $\eta_t \leq \sigma_t \ln 2$. Mou et al. (2018) followed up on Mou et al. (2018) and derived a data-dependent bound based on Bayes-stability, and got a bound of the form $\frac{\sigma}{d} \sqrt{\sum_t \eta_t^2 g_e(t) / \sigma_t^2}$, where $g_e(t)$ is the expected gradient norm square at step $t$. Their bound improves the Lipschitz constant $L$ to the expected gradient norm square. Recently, Bassily et al. (2019) analyze the uniform stability of differentially private SGD (DP-SGD) for convex optimization by showing the gradient update is a non-expansive operation, which is the key fact in proving the stability of SGD (Hardt et al., 2016). The approach in Hardt et al. (2016) can extend to non-convex setting as well, however it requires fast decaying in step size as $\eta_t = O(1/t)$. Bassily et al. (2020) provide stability analysis of SGD for convex and non-smooth functions.

Information-theoretic bounds. Besides the works mentioned above, other theories of deriving generalization bounds for noisy iterative algorithms have been proposed via information-theoretic approaches (Russo and Zou, 2016; Xu and Raginsky, 2017). Such results show that the generalization error of any learning algorithm can be bounded as $O(\sqrt{I(S; W)/n})$, where $I(S; W)$ is the mutual information between the algorithm input $S$ and the algorithm output $W$. Recent work following this approach focus on bounding
the mutual information for a broad class of iterative algorithms, including SGLD to obtain an $O(\sqrt{\log T/n})$ generalization bound by choosing $\eta_t = O(1/t)$, where $T$ is the total number of iterations (Pensia et al., 2018; Bu et al., 2019). Subsequent improvements to this technique were made by Negrea et al. (2019); Haghifam et al. (2020); Rodríguez-Gálvez et al. (2021) to prove data-dependent generalization bounds that do not depend on the Lipschitz constant of the loss function and obtain $\sum_t \eta_t/n$ bounds. Especially, Haghifam et al. (2020); Zhou et al. (2021) introduce generalization bounds based on conditional mutual information inspired by Steinke and Zakynthinou (2020), leading to tighter bounds than those based on mutual information. Recently, Rodríguez-Gálvez et al. (2021) extend the result of Haghifam et al. (2020) from full-batch gradient to stochastic setting. Neu et al. (2021) extend this information-theoretic approach to derive generalization bound for vanilla SGD. Hellström and Durisi (2021) provide a fast-rate bound for bounded loss functions based via Conditional Information Measures (Grünwald et al., 2021; Hellström and Durisi, 2020), which also provides a unified view of some of the above results.

Noisy iterative algorithms. Introducing additional noise in the stochastic gradient has been popular in training deep nets. Noisy iterative methods have proven to be useful for machine learning applications, especially for deep neural networks in terms of escaping from saddle points (Jin et al., 2017, 2019), preserving privacy (Bassily et al. 2020; Wang and Xu, 2019), boosting generalization and stability (Mou et al. 2018; Li et al. 2020). SGLD (Welling and Teh, 2011) has been one of the most popular noisy iterative algorithms for non-convex learning problems, where an isotropic Gaussian noise is added to the stochastic gradient. There has been some work (Wang et al., 2015; Li et al., 2019) connecting SGLD with differentially private SGD algorithm (DP-SGD) (Bassily et al. 2020; Wang and Xu, 2019) which usually adds noise with constant variance to the stochastic gradient. Uniform stability has also been popular in the differential privacy literature for analyzing the generalization error bound of DP-SGD algorithms. Recently, noise has been proven to be useful in Sign-SGD (Bernstein et al., 2018a,b; Chen et al. 2019) which has gained popularity as it reduces communication cost in distributed learning. Existing versions of noisy sign-SGD first adds symmetric noise to the stochastic gradient, then take the sign of the noisy stochastic gradient to update the parameters (Chen et al. 2019; Jin et al. 2020). Bernstein et al. (2018b); Chen et al. (2019); Jin et al. (2020) have shown that when noise is unimodal and symmetric, sign-SGD can guarantee convergence to stationary point.

3 Generalization Bounds with Expected Stability

In the setting of statistical learning, there is an instance space $\mathcal{Z}$, a hypothesis space $\mathcal{W}$, and a loss function $\ell : \mathcal{W} \times \mathcal{Z} \mapsto \mathbb{R}_+$. Let $D$ be an unknown distribution of $\mathcal{Z}$ and let $S_n \sim D^n$ be $n$ i.i.d. draws from $D$. For any specific hypothesis $w \in \mathcal{W}$, the population and empirical loss are respectively given by $L_D(w) \triangleq \mathbb{E}_{z \sim D}[\ell(w, z)]$, and $L_S(w) \triangleq \frac{1}{n} \sum_{i=1}^{n} \ell(w, z_i)$. For any distribution $P$ over the hypothesis space, we respectively denote the expected population and empirical loss as

$$L_D(P) \triangleq \mathbb{E}_{z \sim D}\mathbb{E}_{w \sim P}[\ell(w, z)], \quad \text{and} \quad L_S(P) \triangleq \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_{w \sim P}[\ell(w, z_i)].$$

Consider a randomized algorithm $A$ which works with $S_n = \{z_1, \ldots, z_n\} \sim D^n$ and creates a distribution over the hypothesis space $\mathcal{W}$. For convenience, we will denote the distribution as $A(S_n)$. The focus of our analysis is to bound the generalization error of $A$ defined as:

$$\operatorname{gen}(A(S_n)) \triangleq L_D(A(S_n)) - L_S(A(S_n)) .$$
We consider a general family of noisy stochastic iterative (NSI) algorithms. Given expected stability, we start our analysis by noting that the expected generalization error can be upper bounded by

$$\mathbb{E}_{S_n}[L_D(A(S_n)) - L_S(A(S_n))]$$

and discuss high-probability bounds in the Appendix. All technical proofs for results in this section are in Appendix A.

### 3.1 Bounds based on Expected Stability

We start our analysis by noting that the expected generalization error can be upper bounded by expected stability based on the Hellinger divergence $H(P || P')$ between two distributions given by (Sason and Verdú, 2016; Li et al., 2020):

$$H^2(P || P') = \frac{1}{2} \int_w (\sqrt{p(w)} - \sqrt{p'(w)})^2 dw.$$

**Proposition 1.** Let $S_n \sim D^n$ and let $S_n'$ be a dataset obtained by replacing $z_n \in S_n$ with $z_n' \sim D$. Let $A(S_n), A(S_n')$ respectively denote the distributions over the hypothesis space $W$ obtained by running randomized algorithm $A$ on $S_n, S_n'$. Assume that for all $S_n \in \mathbb{Z}^n, z \in \mathcal{Z}$, $E_{W \sim A(S_n)}[\ell^2(W, z)] \leq c_0^2/4$ for some constant $c_0 > 0$. With $H(\cdot, \cdot)$ denoting the Hellinger divergence, we have

$$\|\mathbb{E}_{S_n \sim D^n}[L_D(A(S_n)) - L_S(A(S_n))]\| \leq c_0 \mathbb{E}_{S_n \sim D^n} \mathbb{E}_{z_n' \sim D} \sqrt{2H^2(A(S_n), A(S_n'))}.$$  \hspace{1cm} (3)

**Remark 3.1.** Proposition 1 does not need bounded losses. Just the second moment of $\ell(W, z), W \sim A(S_n)$ need to be bounded. The assumption is satisfied by bounded losses. It is instructive to compare the assumption to that in recent information theoretic bounds (Haghifam et al., 2020; Xu and Raginsky, 2017), where one assumes $\ell(w, Z), Z \sim D, \forall w \in W$ to be sub-Gaussian.

**Remark 3.2.** The bound in Proposition 1 is in terms of expected stability where we consider $\mathbb{E}_{S_n \sim D^n} \mathbb{E}_{z_n' \sim D} [\cdots]$, an important departure from bounds based on uniform stability (Elisseeff et al., 2005; Bousquet and Elisseeff, 2002; Mou et al., 2018; Bousquet et al., 2020; Feldman and Vondrak, 2018, 2019) where one considers $\sup_{S, S' \in Z^n, |S \Delta S'| = 1} \cdots$. Replacing $\sup$ by $\mathbb{E}$ makes the bounds distribution dependent, avoids the worst case analysis associated with uniform stability, and arguably leads to quantitatively tighter bounds.

Note that the Hellinger divergence can be bounded by the KL divergence, and our analysis in the sequel will focus on bounding the KL divergence.

**Proposition 2.** For any distributions $P$ and $P'$, $2H^2(P, P') \leq \min \{ KL(P, P'), \sqrt{\frac{1}{2} KL(P, P')} \}$.

**Remark 3.3.** While our analysis in the sequel focuses on bounding the KL-divergence, in certain settings one may be able to directly bound the Hellinger divergence possibly leading to sharper bounds. Further, the Hellinger divergence can be upper bounded by the Total Variation (TV) divergence (e.g., used in proof of Proposition 2) which may also lead to sharp bounds. An analysis based on KL-divergence needs $P$ to be absolutely continuous w.r.t. $P'$ which is not necessary when working with Hellinger or TV divergences.

### 3.2 Expected Stability of Noisy Stochastic Iterative Algorithms

We consider a general family of noisy stochastic iterative (NSI) algorithms. Given $S_n \sim D^n$, such iterative algorithms have two additional sources of randomness in each iteration $t$: (a) a stochastic mini-batch of samples $S_{B_t}$, with $|S_{B_t}| = b$, drawn uniformly at random with replacement from $S_n$; and (b) noise $\xi_t$ suitably...
We will often drop the conditioning $w$ to avoid clutter in the sequel.

Let $P_{0: (t-1)}$ denote the joint distribution over $W_{0:(t-1)} = (W_0, \ldots, W_{t-1})$, and let $P_{t} := P_{B_t, \xi_t|w_{0:(t-1)}}$ compactly denote the conditional distribution on $W_t$ conditioned on the trajectory $W_{0:(t-1)} = w_{0:t-1}$. Further, let $P_T, P_T'$ denote the marginal distributions over hypotheses $w \in W$ after $T$ steps of the algorithm based on $S_n, S'_n$ respectively, where $S'_n$ is as discussed in Proposition [1] i.e., obtained from $S_n$ by replacing $z_n \in S_n \sim D^n$ by $z'_n \sim D$. Following (Pensia et al., 2018; Negrea et al., 2019; Haghifam et al., 2020), we use the following chain rule to bound the KL-divergence between $P_T$ and $P_T'$:

$$KL(P_T \| P_T') \leq KL(P_{0:T} \| P'_{0:T}) = \sum_{t=1}^{T} \mathbb{E}_{P_{0:(t-1)}} KL(P_t \| P'_t).$$

Let $\bar{S}_{n+1} \sim D^{n+1}$ with $\bar{S}_{n+1} = \{z_1, \ldots, z_{n+1}\}$ so that $S_n, S'_n$ are size $n$ subsets of $\bar{S}_{n+1}$ with $S_n = \{z_1, \ldots, z_{n-1}, z_n\}$ and $S'_n = \{z_1, \ldots, z_{n-1}, z'_n\}$, where $z'_n = z_{n+1}$. Let $S_0 = \{z_1, \ldots, z_{n-1}\}$. The algorithms we consider use a mini-batch of size $b$ in each iteration uniformly sampled from $n$ samples in $S_n$ or $S'_n$. Let the set of all mini-batch index sets be denoted by $G$. Let the set of all mini-batch index sets $A$ drawn from $S_0$ be denoted by $G_0$. Note that $|G_0| = \binom{n-1}{b}$. Let $G_1$ denote the set of all mini-batch index sets $B$ which includes the last sample, viz. $z_n$ for $S_n$ and $z'_n$ for $S'_n$. Note that $|G_1| = \binom{n-1}{b-1}$. Also note that $|G_0| + |G_1| = \binom{n-1}{b} + \binom{n-1}{b-1} = \binom{n}{b} = |G|$.

Following Li et al. (2020), we can bound their conditional KL-divergences $KL(P_t \| P'_t)$ in the right-hand-side of (5) in terms of a Le Cam Style Divergence (LSD). While the classical Le Cam divergence (Sason and Verdu, 2016) is $LCD(P \| P') \triangleq \frac{1}{2} \int \frac{(dP - dP')^2}{dP + dP'}$ (where $dP$ denotes the density), our bounds are in terms of

$$LSD(P_{t} \| P'_{t}) \triangleq \mathbb{E}_{B_t \in G_1} \mathbb{E}_{A_t \in G_0} \left[ \int_{\xi_t} \frac{(dP_{B_t, \xi_t} - dP'_{B_t, \xi_t})^2}{dP_{A_t, \xi_t}} d\xi_t \right],$$

where $B_t \in G_1, A_t \in G_0$. Note that $P_{B_t, \xi_t}$ and $P'_{B_t, \xi_t}$ represent the conditional distribution of $W_t$ for $S_n$ and $S'_n$ respectively since the mini-batch $S_{B_t}$ of $S_n$ and $S'_n$ differs in the $n$-th sample. Bounding the KL-divergences in (5) with LSDs, we have the following expected LSD based generalization bound.

**Lemma 1.** Consider a noisy stochastic iterative algorithms of the form (4) with mini-batch size $b \leq n/2$. Then, with $c_1 = \sqrt{2\epsilon_0}$ (with $c_0$ as in Proposition [1]), we have

$$\mathbb{E}_{S_n}[L_D(A(S_n)) - L_S(A(S_n))] \leq c_1 \frac{b}{n} \mathbb{E}_{S_n} \mathbb{E}_{z'_n} \sum_{t=1}^{T} \mathbb{E}_{W_{0:(t-1)}} \mathbb{E}_{B_t \in G_1} \mathbb{E}_{A_t \in G_0} \left[ \int_{\xi_t} \frac{(dP_{B_t, \xi_t} - dP'_{B_t, \xi_t})^2}{dP_{A_t, \xi_t}} d\xi_t \right].$$

(7)

**Remark 3.4.** Though not stated explicitly, Li et al. (2020) essentially has this result for SGLD and inspired our work. Our proofs are significantly simpler, does not make any additional assumptions, and illustrates applicability to general noisy iterative algorithms of the form (4), not just SGLD with Gaussian noise as in Li et al. (2020).
Remark 3.5. Note that the bound depends on expectations over samples $S_{\alpha}$, $\tau'$, trajectories $W_{0(t-1)}$, and mini-batches $B_t$, $A_t$. Unlike uniform stability and other worst case analysis, there is no sup over samples, trajectories, or mini-batches. Further, the bound depends on the distribution discrepancy as captured by the expected LSD.

Remark 3.6. The bound seems to worsen with $b$, the size of the mini-batch. As we shown in Section 4, the expected LSD terms have a $\frac{1}{n^2}$ dependence for the Exponential Family Langevin dynamics (EFLD) models we introduce, so the leading $b$ is neutralized.

4 Exponential Family Langevin Dynamics

In recent years, considerable advances have been made in establishing generalization bounds for stochastic gradient Langevin dynamics (SGLD) (Li et al., 2020; Pensia et al., 2018; Negrea et al., 2019; Haghifam et al., 2020). As an example of a noisy stochastic iterative algorithm of the form (4), SGLD adds isotropic Gaussian noise at every step of SGD: $w_{t+1} = w_t - \eta_t \nabla \ell(w_t, S_{B_t}) + \mathcal{N}(0, \sigma_t^2 I)$, where $\nabla \ell(w_t, S_{B_t})$ is the stochastic gradient on mini-batch $B_t$, $\eta_t$ is the step size, and $\sigma_t^2$ is noise variance.

In this paper, we introduce a substantial generalization of SGLD called Exponential Family Langevin Dynamics (EFLD) which uses general exponential family noise in noisy iterative updates of the form (4). In addition to being a mathematical generalization of the popular SGLD, the proposed EFLD provides flexibility to use noisy gradient algorithms with different representation of the gradient, e.g., Bernoulli noise for Sign-SGD, discrete distribution for quantized or finite precision SGD, etc. (Canonne et al., 2020; Alistarh et al., 2017; Jiang and Agrawal, 2018; Yang et al., 2019).

4.1 Exponential Family Langevin Dynamics (EFLD)

Exponential families (Barndorff-Nielsen, 2014; Brown, 1986; Wainwright and Jordan, 2008) constitute a large family of parametric distributions which include Gaussian, Bernoulli, gamma, Poisson, Dirichlet, etc., as special cases. Exponential families are typically represented in terms of natural parameters $\theta$, and we consider component-wise independent distributions with scaled natural parameter $\theta_\alpha = \theta / \alpha$ with scaling $\alpha > 0$, i.e.,

$$p_\psi(\xi, \theta_\alpha) = \exp(\langle \xi, \theta_\alpha \rangle - \psi(\theta_\alpha)) \pi_{0,\alpha}(\xi) = \prod_{j=1}^p \exp(\xi_j \theta_{j\alpha} - \psi_j(\theta_{j\alpha})) \pi_{0,\alpha}(\xi_j),$$

where $\xi \in \mathbb{R}^p$ is the sufficient statistic, $\psi(\theta_\alpha) = \sum_{j=1}^p \psi_j(\theta_{j\alpha})$ is the log-partition function, and $\pi_{0,\alpha}(\xi) = \prod_{j=1}^p \pi_{0,\alpha}(\xi_j)$ is the base measure. Note that $\alpha = 1$ gives the canonical form of the exponential family distributions. For general scaling $\alpha > 0$, for certain distributions the base measure $\pi_0$ may depend on the scaling, i.e., $\pi_{0,\alpha}$. A scaling $\alpha > 0$ is valid as long as $\exp(\langle \xi, \theta_0 \rangle)$ is integrable, i.e., $\int_\xi \exp(\langle \xi, \theta_0 \rangle) \pi_{0,\alpha}(\xi) d\xi < \infty$. Further, $\psi$ is a smooth function by construction (Barndorff-Nielsen, 2014; Banerjee et al., 2005; Wainwright and Jordan, 2008) and the smoothness of $\psi$ implies $\nabla^2_{\theta_0} \psi(\theta_\alpha) \leq c_2 I$ for some constant $c_2 > 0$.

Exponential family Langevin dynamics (EFLD) uses noisy stochastic gradient updates similar to SGLD, but using exponential family noise rather than Gaussian noise as in SGLD. In particular, for mini-batch $S_{B_t}$, EFLD updates are as follows: with step size $\rho_t > 0$

$$w_t = w_{t-1} - \rho_t \xi_t, \quad \xi_t \sim p_\psi(\xi; \theta_{B_t, \alpha_t}),$$

(8)
where
\[
p_\psi(\xi; \theta_{Bt,\alpha t}) = \exp(\langle \xi, \theta_{Bt,\alpha t} \rangle - \psi(\theta_{Bt,\alpha t})) \pi_{0,\alpha}(\xi), \quad \theta_{Bt,\alpha t} \triangleq \frac{\theta_{Bt}}{\alpha_t} = \frac{\nabla \ell(w_{t-1}, S_{Bt})}{\alpha_t}. \tag{9}
\]

For EFLD, the natural parameter \(\theta_{Bt,\alpha t}\) at step \(t\) is simply a scaled version of the mini-batch gradient \(\nabla \ell(w_{t-1}, S_{Bt})\). We first show that EFLD becomes SGLD when the exponential family is Gaussian, and becomes a noisy version of sign-SGD (Bernstein et al., 2018a,b) when the exponential family is Bernoulli over \{-1, +1\}. More details and examples are in Appendix B.1.

**Example 4.1 (SGLD).** SGLD uses scaled Gaussian noise with \(\psi(\theta) = \|\theta\|_2^2/2, \alpha_t = \sigma_t/\eta_t, \pi_{0,\alpha}(\xi) = \frac{1}{\sqrt{(2\pi)^p\alpha_t^p}} \exp(-\|\xi\|_2^2/2\alpha_t^2)\) so that \(p_\psi(\xi; \theta_{Bt,\alpha t}) = N(\theta_{Bt,\alpha t}^2 \mathbb{I}_d)\). By taking \(\rho_t = \eta_t\), the update (8) based on \(\rho_t \xi_t\) is distributed as \(N(\eta_t \theta_{Bt,\alpha t}^2 \mathbb{I}_d) = N(\eta_t \nabla \ell(w_{t-1}, S_{Bt}), \sigma_t^2 \mathbb{I}_d)\). Thus the EFLD update reduces to the SGLD update: \(w_t = w_{t-1} - \eta_t \nabla \ell(w_{t-1}, S_{Bt}) + \mathcal{N}(0, \sigma_t^2 \mathbb{I}_d)\).

**Example 4.2 (Noisy Sign-SGD).** By taking \(\rho_t = \eta_t\) and componentwise \(\xi_j \in \{-1, 1\}\), \(\pi_{0,\alpha}(\xi_j) = 1, \psi(\theta) = \log(\exp(-\theta) + \exp(\theta))\) in exponential family update equation (8), the \(j\)-th component of exponential family distribution \(p_\psi(\xi_j; \theta_{Bt,\alpha t})\) becomes \(p_\psi(\xi_j; \theta_{Bt,\alpha t}) = \frac{\exp(\xi_j \theta_{Bt,\alpha t})}{\exp(\xi_j \theta_{Bt,\alpha t}) + \exp(\theta_{Bt,\alpha t})}\). Thus, the EFLD update reduces to a noisy version of Sign-SGD: \(w_t = w_{t-1} - \eta_t \xi_t, j \sim p(\xi_j, \theta_{Bt,\alpha t}), j \in [p]\), where \(\theta_{Bt,\alpha t} = \nabla \ell(w_{t-1}, S_{Bt})/\alpha_t\) is the scaled mini-batch gradient.

### 4.2 Expected Stability of Exponential Family Langevin Dynamics

From Lemma 1, conditioned on a trajectory \(W_0\{t\} = w_0\{t\}\), mini-batches \(S_{Bt}, S_{At}\), we can get an expected stability based generalization bound by suitably bounding the Le Cam Style Divergence (LSD) given by:

\[
I_{At,Bt} = \int \frac{\left( dP_{Bt,\xi_t} - dP'_{Bt,\xi_t} \right)^2}{dP_{A,\xi_t}} d\xi_t. \tag{10}
\]

For EFLD, the density functions \(dP_{Bt,\xi_t}, dP'_{Bt,\xi_t}\) are exponential family densities \(p_\psi(\xi; \theta_{Bt,\alpha t}), p_\psi(\xi; \theta'_{Bt,\alpha t})\) as in (8)-(9), and we have the following bound on the per step LSD in (10).

**Theorem 1.** For a given set \(\tilde{S}_{n+1} \sim D^{n+1}\) and \(w_{t-1}\) at iteration \((t-1)\), let \(\Delta_t|_{w_{t-1}}(\tilde{S}_{n+1}) = \max_{z, z' \in \tilde{S}_{n+1}} \|\nabla \ell(w_{t-1}, z) - \nabla \ell(w_{t-1}, z')\|_2\). Further, for a \(c_2\)-smooth log-partition function \(\psi\), let the scaling \(\alpha_t|_{w_{t-1}}\) be data-dependent such that \(\alpha_t^2|_{w_{t-1}} \geq 8c_2\Delta_t^2|_{w_{t-1}}(\tilde{S}_{n+1})\). Then, we have

\[
I_{At,Bt} \leq 5c_2\|\theta_{Bt,\alpha t} - \theta'_{Bt,\alpha t}\|^2_2 = \frac{5c_2}{2\alpha_t^2|_{w_{t-1}}} \left[ \|\nabla \ell(w_{t-1}, S_{Bt}) - \nabla \ell(w_{t-1}, S'_{Bt})\|_2^2 \right]. \tag{11}
\]

**Remark 4.1.** Theorem 1 shows that per step LSD can be bounded by a scaled version of the mini-batch gradient discrepancy. The result holds for all exponential family Langevin dynamics algorithms of the form (8)-(9), not just Gaussian noise based SGLD.

**Remark 4.2.** Recall that for \(\tilde{S}_{n+1} \sim D^{n+1}\) with \(\tilde{S}_{n+1} = \{z_1, \ldots, z_{n+1}\}\), \(S_{Bt}, S'_{Bt}\) are respectively drawn from \(S_n, S'_n\) which are size \(n\) subsets of \(\tilde{S}_{n+1}\) with \(S_n = \{z_1, \ldots, z_{n-1}, z_n\}\) and \(S'_n = \{z_1, \ldots, z_{n-1}, z'_n\}\), where \(z'_n = z_{n+1}\) so that \(S_{Bt}\) and \(S'_{Bt}\) only differ at samples \(z_n\) and \(z'_n\). As a result \(\nabla \ell(w_{t-1}, S_{Bt}) - \nabla \ell(w_{t-1}, S'_{Bt}) = \frac{1}{b} \sum_{z \in S_{Bt}} \nabla \ell(w_{t-1}, z) - \frac{1}{b} \sum_{z' \in S'_{Bt}} \nabla \ell(w_{t-1}, z') = \frac{1}{b} (\nabla \ell(w_{t-1}, z_n) - \nabla \ell(w_{t-1}, z'_n))\).

The \(1/b\) scale factor neutralizes the leading \(b\) term in Lemma 1.
The bound in Theorem 1 can now be directly applied to Lemma 1 to get expected stability based generalization bounds for any EFLD algorithm.

**Theorem 2.** Consider an exponential family Langevin dynamics (EFLD) algorithm of the form (8)–(9) with a $c_2$-smooth log-partition function $\psi$. Then, for mini-batch size $b \leq n/2$, with $c = c_0 \sqrt{5c_2}$ (with $c_0$ as in Proposition 7) and $\alpha_i^2 \geq 8c_2 \Delta_i^2(S_{n+1})$ (as in Theorem 1) with the conditioning on $w_{t-1}$ hidden to avoid clutter), we have

$$\mathbb{E}_S[|L_D(A(S)) - L_S(A(S))|] \leq \frac{C}{n} \sum_{S_n+1} \sum_{t=1}^T \frac{1}{\alpha_i^2} \left[ \left\| \nabla \ell(w_{t-1}, z_n) - \nabla \ell(w_{t-1}, z'_n) \right\|^2_2 \right].$$

(12)

**Remark 4.3.** Theorem 2 establishes generalization bounds for all exponential family Langevin dynamics algorithms. The key term in the bound is the expected gradient discrepancy only on the sample $z_n, z'_n$ where $S_n, S'_n$ differ. Further, the only dependence on the specific exponential family is through the constant $c_2$, the smoothness of the corresponding log-partition function.

**Remark 4.4.** Since SGLD is a special case of EFLD, Theorem 2 gives a generalization bound for SGLD. The bound has effectively the same dependence on $n$ and $T$ as the bound in Li et al. (2020). However, the bound is quantitatively much sharper since the gradient norm term $\frac{1}{n} \sum_{z \in S} \left\| \nabla \ell(w_t, z) \right\|^2$ in Li et al. (2020) gets replaced by the gradient discrepancy term $\left\| \nabla \ell(w_t, z) - \nabla \ell(w_t, z') \right\|^2$. As illustrated in our experiments (Section 5), the gradient discrepancy is orders of magnitude smaller than the gradient norm. The bound in Negrea et al. (2019) depends on a related gradient incoherence which we found to be empirically smaller than gradient discrepancy in our experiments (Section 5). However, their bound has a $1/\sqrt{n}$ sample dependence, which is worse than the $1/n$ dependence in our bound.

**Remark 4.5.** EFLD can be extended to work with anisotropic noise by using $\theta_{B,\alpha} t = \nabla \ell(w_{t-1}, S_{B_t}) \otimes \alpha_t$ in (9) where $\alpha_t \in \mathbb{R}^p$ determines different scaling for each dimension and $\otimes$ denotes Hadamard division. Theorems 1 and 2 can be extended to such anisotropic noise by using $\alpha$-scaled norms for the gradient discrepancy, i.e., $\|g - g'\|_{2, \alpha}^2 = \sum_j (g_j - g'_j)^2 / \alpha_j^2$.

**Remark 4.6.** The lower bound on $\alpha_t$ in Theorem 2 is a data-dependent quantity $\Delta_t(S_{n+1})$ which can be computed during training. From Example 4.1, since $\alpha_t = \sigma_t / \eta_t$, the lower bound $\alpha_t \geq c_3 \Delta_t(S_{n+1})$ for a constant $c_3$ implies an upper bound on the step size: $\eta_t \leq \sigma_t / c_3 \Delta_t(S_{n+1})$. The upper bound is a much more benign (and computable) condition on the step size compared to those in the related work. Mou et al. (2018); Li et al. (2020); Hardt et al. (2016) (Mou et al., 2018; Li et al., 2020, Hardt et al. 2016) which require step size being bounded by $\sigma_t / K$, where $K$ is the global Lipschitz constant for the loss $\ell$. Note that $\Delta_t(S_{n+1}) \ll K$ because global Lipschitz constant $K$ is a uniform bound on the entire space, and $\Delta_t(S_{n+1})$ is computable data-dependent measure based on gradient discrepancy. Further, $\Delta_t(S_{n+1})$ is expected to decrease over iterations, i.e., as $t$ increases, and gradients get smaller.

**4.3 Proof Sketches of Main Results: Theorems 1 and 2**

We focus on Theorem 1. To avoid clutter, we drop the subscript $t$ for the analysis and note that the analysis holds for any step $t$. When the densities $dP_{B, \xi} = p_\psi(\xi; \theta_{B, \alpha})$ and $dP'_{B, \xi} = p_\psi(\xi; \theta'_{B, \alpha})$, i.e., densities in the same exponential family but with different parameters $\theta_{B, \alpha}$ and $\theta'_{B, \alpha}$ because of the difference in the mini-batches, by mean-value theorem, for each $\xi$, we have

$$p_\psi(\xi; \theta_{B, \alpha}) - p_\psi(\xi; \theta'_{B, \alpha}) = (\theta_{B, \alpha} - \theta'_{B, \alpha}, \nabla \theta_{B, \alpha} p_\psi(\xi; \theta_{B, \alpha})),$$  

(13)
for some $\tilde{\theta}_{B,\alpha} = \gamma_\xi \theta_{B,\alpha} + (1 - \gamma_\xi) \theta'_{B,\alpha}$ where $\gamma_\xi \in [0,1]$ with the subscript $\xi$ illustrating dependence on $\xi$. Then,

$$I_{A,B} = \int_{\xi} \frac{(p_\psi(\xi; \theta_{B,\alpha}) - p_\psi(\xi; \theta'_{B,\alpha}))^2}{p_\psi(\xi; \theta_{A,\alpha})} d\xi = \int_{\xi} \frac{\langle \theta_{B,\alpha} - \theta'_{B,\alpha}, \nabla \theta_{B,\alpha} p_\psi(\xi; \tilde{\theta}_{B,\alpha}) \rangle^2}{p_\psi(\xi; \theta_{A,\alpha})} d\xi = \int_{\xi} \frac{\langle \theta_{B,\alpha} - \theta'_{B,\alpha}, \xi - \nabla \theta_{B,\alpha} \psi(\xi; \tilde{\theta}_{B,\alpha}) \rangle^2}{p_\psi(\xi; \theta_{A,\alpha})} p_\psi(\xi; \tilde{\theta}_{B,\alpha}) d\xi,$$

(14)

where since $p_\psi(\xi; \tilde{\theta}_{B,\alpha}) = \exp(\langle \xi, \tilde{\theta}_{B,\alpha} \rangle - \psi(\tilde{\theta}_{B,\alpha})) \pi_0(\xi)$ we have

$$\nabla \theta_{B,\alpha} p_\psi(\xi; \tilde{\theta}_{B,\alpha}) = (\xi - \nabla \theta_{B,\alpha} \psi(\xi; \tilde{\theta}_{B,\alpha})) p_\psi(\xi; \tilde{\theta}_{B,\alpha}).$$

**Handling Distributional Dependence of $\tilde{\theta}_{B,\alpha}$.** Note that it is difficult to proceed with the analysis with the density term depending on parameter $\tilde{\theta}_{B,\alpha}$ since $\tilde{\theta}_{B,\alpha}$ depends on $\xi$ and there is an outside integral over $\xi$ in (14). So, we first bound the density term depending on $\theta_{B,\alpha}$ in terms of exponential family densities with parameters $\theta_{B,\alpha}$ and $\theta'_{B,\alpha}$ essentially using $c_2$-smoothness of $\psi$.

**Lemma 2.** With $\tilde{\theta}_{B,\alpha} = \gamma_\xi \theta_{B,\alpha} + (1 - \gamma_\xi) \theta'_{B,\alpha}$ for some $\gamma_\xi \in [0,1]$, we have

$$\exp \left[ \frac{\langle \xi, \tilde{\theta}_{B,\alpha} \rangle - \psi(\tilde{\theta}_{B,\alpha})}{\max \left( \exp \left[ \langle \xi, \theta_{B,\alpha} \rangle - \psi(\theta_{B,\alpha}) \right], \exp \left[ \langle \xi, \theta'_{B,\alpha} \rangle - \psi(\theta'_{B,\alpha}) \right] \right)} \right] \leq \exp \left[ c_2 \| \theta_{B,\alpha} - \theta'_{B,\alpha} \|_2^2 \right].$$

In other words, for any $\xi$ we have

$$p_\psi(\xi; \tilde{\theta}_{B,\alpha}) \leq \exp \left[ c_2 \| \theta_{B,\alpha} - \theta'_{B,\alpha} \|_2^2 \right] \max \left( p_\psi(\xi; \theta_{B,\alpha}), p_\psi(\xi; \theta'_{B,\alpha}) \right).$$

Since the parameters $\theta_{B,\alpha}, \theta'_{B,\alpha}$ in the right-hand-side depend on $\xi$, the outside integral over $\xi$ in (14) will not pose any unusual challenges.

**Bounding the Density Ratio.** Next we focus on the density ratio $p_\psi^2(\xi; \tilde{\theta}_{B,\alpha})/p_\psi(\xi; \theta_{A,\alpha})$ in (14). By Lemma 2 it suffices to focus on $p_\psi^2(\xi; \theta_{B,\alpha})/p_\psi(\xi; \theta_{A,\alpha})$ or the equivalent term for $\theta'_{B,\alpha}$. We show that the density ratio can be bounded by another distribution in the same exponential family $p_\psi$ with parameters $(\theta_{B,\alpha} - \theta_{A,\alpha})$.

**Lemma 3.** For any $\xi$, we have

$$\frac{\exp \left[ \langle \xi, 2\theta_{B,\alpha} \rangle - 2 \psi(\theta_{B,\alpha}) \right]}{\exp \left[ \langle \xi, \theta_{A,\alpha} \rangle - \psi(\theta_{A,\alpha}) \right]} \leq \exp \left[ 2c_2 \| \theta_{B,\alpha} - \theta_{A,\alpha} \|_2^2 \right] \exp \left[ \langle \xi, (2\theta_{B,\alpha} - \theta_{A,\alpha}) - \psi(2\theta_{B,\alpha} - \theta_{A,\alpha}) \right].$$

In other words, for any $\xi$ we have

$$\frac{p_\psi^2(\xi; \theta_{B,\alpha})}{p_\psi(\xi; \theta_{A,\alpha})} \leq \exp \left[ 2c_2 \| \theta_{B,\alpha} - \theta_{A,\alpha} \|_2^2 \right] p_\psi(\xi; 2\theta_{B,\alpha} - \theta_{A,\alpha}).$$

The analysis for the term $p_\psi^2(\xi; \theta'_{B,\alpha})/p_\psi(\xi; \theta_{A,\alpha})$ is exactly the same.

**Bounding the Integral.** Ignoring multiplicative terms which do not depend on $\xi$ for the moment, the analysis needs to bound an integral term of the form

$$\int_{\xi} \langle \theta_{B,\alpha} - \theta'_{B,\alpha}, \xi - \nabla \psi(\xi; \tilde{\theta}_{B,\alpha}) \rangle^2 p_\psi(\xi; 2\theta_{B,\alpha} - \theta_{A,\alpha}) d\xi,$$
We now establish optimization guarantees for two examples of EFLD, i.e., Noisy Sign-SGD with Bernoulli Assumption 2.

The loss function \( \theta \) where the expectation yields the covariance matrix of an exponential family is the Hessian of the log-partition function (Wainwright and Jordan 2008; Banerjee et al. 2005). The integral, however, is with respect to \( p_\psi(\xi; 2\theta_{B,\alpha} - \theta_{A,\alpha}) \), not \( p_\psi(\xi; \theta_{B,\alpha}) \). We handle this discrepancy by using

\[
\langle \theta_{B,\alpha} - \theta'_{B,\alpha}, \xi - \nabla_\psi(\xi; \tilde{\theta}_{B,\alpha}) \rangle^2 = \langle \theta_{B,\alpha} - \theta'_{B,\alpha}, (\xi - \mathbb{E}[\xi]) + (\mathbb{E}[\xi] - \nabla_\psi(\xi; \tilde{\theta}_{B,\alpha})) \rangle^2 \\
\leq 2 \langle \theta_{B,\alpha} - \theta'_{B,\alpha}, \xi - \mathbb{E}[\xi] \rangle^2 + 2 \langle \theta_{B,\alpha} - \theta'_{B,\alpha}, \mathbb{E}[\xi] - \nabla_\psi(\xi; \tilde{\theta}_{B,\alpha}) \rangle^2,
\]

where the expectation \( \mathbb{E}[\xi] \) is with respect to \( p_\psi(\xi; 2\theta_{B,\alpha} - \theta_{A,\alpha}) \). Quadratic form for the first term yields the covariance \( \mathbb{E}[(\xi - \mathbb{E}[\xi])(\xi - \mathbb{E}[\xi])^T] = \nabla^2 \psi(2\theta_{B,\alpha} - \theta_{A,\alpha}) \leq c_2 \mathbb{I} \), by smoothness and since the covariance matrix of an exponential family is the Hessian of the log-partition function (Wainwright and Jordan 2008). Since \( \mathbb{E}[\xi] = \nabla_\psi(2\theta_{B,\alpha} - \theta_{A,\alpha}) \), the second term depends on the difference of gradients \( \nabla_\psi(2\theta_{B,\alpha} - \theta_{A,\alpha}) - \nabla_\psi(\tilde{\theta}_{B,\alpha}) \) which, using smoothness and additional analysis, can be bounded by the norm of \( \theta_{B,\alpha} - \theta_{A,\alpha} \). All the pieces can be put together to get the bound in Theorem 1 which when used in Lemma 1 yields Theorem 2.

### 4.4 Optimization Guarantees for EFLD

We now establish optimization guarantees for two examples of EFLD, i.e., Noisy Sign-SGD with Bernoulli noise over \( \{ -1, +1 \} \) and SGLD with Gaussian noise.

**Noisy Sign-SGD.** From Example 4.2 in Section 4.1 for noisy sign-SGD, for mini-batch \( B_t \) and scaling \( \alpha_t \), mini-batch Noisy Sign-SGD updates the parameters as \( w_t = w_{t-1} - \eta_t \xi_t \), where each component \( j \in [p] \)

\[
\xi_{t,j} \sim p_{\theta_{B_t,\alpha_t}}(\xi_j) = \frac{\exp(\xi_j \theta_{B_t,\alpha_t})}{\exp(-\theta_{B_t,\alpha_t}) + \exp(\theta_{B_t,\alpha_t})}, \quad \xi_j \in \{ -1, +1 \}
\]

where \( \theta_{B_t,\alpha_t} = \nabla \ell(w_{t-1}, S_{B_t})/\alpha_t \) is the scaled mini-batch gradient. The full-batch version uses parameters \( \mathbb{E}_{B_t}[\theta_{B_t,\alpha_t}] = \nabla L_S(w_{t-1}) \). For the optimization analysis for full batch gradient descent, we assume that the loss is smooth.

**Assumption 1.** The loss function \( L_S(w) = \frac{1}{n} \sum_{i=1}^n \ell(w, z_i) \) satisfies: \( \forall w, w' \), for some non-negative constants \( K := [K_1, \ldots, K_p] \), we have \( L_S(w) \leq L_S(w') + \nabla L_S(w')^T (w - w') + \frac{1}{2} \sum_i K_i (w_i - w'_i)^2 \).

For the mini-batch analysis, we additionally assume that the mini-batch gradients are unbiased, symmetric, and sub-Gaussian.

**Assumption 2.** Given \( w_{t-1} \), the mini-batch gradient \( \nabla \ell(w_{t-1}, S_{B_t}) \) is

(a) unbiased, i.e., \( \mathbb{E}_{B_t|w_{t-1}} \nabla \ell(w_{t-1}, S_{B_t}) = \nabla L_S(w_{t-1}) \);

(b) symmetric, i.e., the density \( p_{B_t|w_{t-1}}(\xi) \) of \( \xi \equiv \nabla \ell(w_{t-1}, S_{B_t}) \) is symmetric around its expectation \( L_S(w_{t-1}) \): \( p_{B_t|w_{t-1}}(\xi) = p_{B_t|w_{t-1}}(2\nabla L_S(w_{t-1}) - \xi) \); and

(c) sub-Gaussian, i.e., for any \( \lambda > 0 \), any \( v \) s.t. \( \|v\|_2 = 1 \),

\[
\mathbb{E}_{B_t|w_{t-1}}[\exp \lambda \langle v, \nabla \ell(w_{t-1}, S_{B_t}) - \nabla L_S(w_{t-1}) \rangle] \leq \exp(\lambda^2 \kappa_t^2/2),
\]

for some constant \( \kappa_t > 0 \).
The smoothness assumption in Assumption 1 is standard in non-convex optimization especially for sign-SGD literature (Bernstein et al. 2018a,b). Assumption 2 for the mini-batch setting helps the theoretical analysis, where (a) is satisfied when the batches $S_{B_i}$ are taken uniformly from samples $S$ as the standard training does; (b) assumes symmetry of the mini-batch gradients; and (c) is similar and stronger assumption compared to Assumption 3 in Bernstein et al. (2018a), where they assume bounded variance for stochastic gradient and our assumption implies suitably bounded higher moments of $\nabla \ell(w_{t-1}, S_{B_i}) - \nabla L_S(w_{t-1})$, which is referred as the minibatch noise in recent noisy SGD literature e.g. Damian et al. (2021). Similar to such literature, if we consider mini-batch stochastic gradient be modeled as the average of $|B_i|$ calls to the full-batch gradient, from the Hoeffding’s inequality for bounded variables, $\kappa_t$ is scaled by $1/\sqrt{|B_t|}$.

Based on the assumptions, we have the following optimization guarantee for full-batch and mini-batch noisy Sign-SGD.

**Theorem 3.** If the loss satisfies Assumption 1 for full-batch noisy Sign-SGD with step size $\rho_t = 1/\sqrt{T}$ and $\alpha_t$ satisfying $c \geq \alpha_t \geq \|L_S(w_t)\|_\infty$, we have

$$E \left[ \frac{1}{T} \sum_{t=1}^{T} \|\nabla L_S(w_t)\|_2^2 \right] \leq \frac{5c}{3\sqrt{T}} \left( L_S(w_0) - L_S(w^*) + \frac{1}{2}\|\bar{K}\|_1 \right).$$

Further, if Assumption 2 holds, for mini-batch noisy Sign-SGD with step size $\eta_t = 1/\sqrt{T}$, and $\alpha_t$ satisfying $c \geq \alpha_t \geq \max[\sqrt{2}\kappa_t, 4\|L_S(w_t)\|_\infty]$, we have

$$E \left[ \frac{1}{T} \sum_{t=1}^{T} \|\nabla L_S(w_t)\|_2^2 \right] \leq \frac{4c}{\sqrt{T}} \left( L_S(w_0) - L_S(w^*) + \frac{1}{2}\|\bar{K}\|_1 \right),$$

where equation (16;17) holds for any $S$, any initialization $w_0$, and the expectation is taken over the randomness of algorithm.

**Stochastic Gradient Langevin Dynamics (SGLD).** We acknowledge that the following optimization result for SGLD exists in various forms, as noisy gradient descent algorithms with Gaussian noise have been studied in literature such as differential privacy, where SGLD can be viewed as DP-SGD (Bassily et al. 2014; Wang and Xu 2019) and the proof technique boils down to bounding the stochastic variance of the noisy gradient (Shamir and Zhang 2013).

**Theorem 4.** Under Assumptions 1 and 2 with $K_i = K, \forall i \in [p]$, for any training set $S$, SGLD, i.e., EFLD with Gaussian noise, $\rho_t = \eta_t$, $\alpha_t = \sigma_t/\eta_t$, batch size $|B_t| = b$, and step size $\eta_t = 1/\sqrt{T}$ satisfies

$$\frac{1}{T} \sum_{t=1}^{T} E\|\nabla L_S(w_t)\|^2 \leq \frac{L_S(w_1) - L_S(w^*)}{\sqrt{T}} + \frac{K^2}{2T} \sum_{t=1}^{T} (p\alpha_t^2 + c_3\kappa_t^2),$$

where $w_1$ are the initial parameters, $w^*$ is a minima of $L_S(w)$, $c_3$ is an absolute constant, and the expectation is over the randomness of the algorithm.

The error rate of SGLD depends on the noise level $\alpha_t$ and the sub-Gaussian parameter $\kappa_t$. The bound has a $O(1/\sqrt{T})$ rate as long as the average noise level and sub-Gaussian parameter are bounded by a constant. We note that similar to the optimization guarantees of differentially private SGD, the convergence rate depends on the dimension of the gradient $p$ due to the isotropic Gaussian noise. Special noise structures such as anisotropic noise that align with the gradient structure can improve the dependence on dimension (Kairouz et al. 2020; Zhang et al. 2021; Asi et al. 2021; Zhou et al. 2020).
Figure 1: Results for training CNN using SGLD on MNIST, Fashion-MNIST and CIFAR-10. X-axis shows the number of training epochs. (a)-(d) shows our bound is non-vacuous and can be used to bound the empirical test error. (e)-(h) compare our bound with the existing bounds and show the effect on $\alpha^2_t$. Our bounds are numerically sharper than existing bounds, and larger $\alpha^2_t$ leads to tighter generalization bounds which is consistent with the theoretical analysis. (i)-(l) show the key factors in each bound, i.e., the squared gradient norm in Li et al. (2020), the gradient incoherence in Negrea et al. (2019), the two-sample incoherence in Rodríguez-Gálvez et al. (2021), and the gradient discrepancy in our bound. Incoherence or discrepancy based quantities are orders of magnitude smaller than the gradient norm.

5 Experiments

In this section, we conduct a series of experiments to evaluate our generalization error bounds. For SGLD, we aim to compare the proposed bound in Theorem 2 with existing bounds in Li et al. (2020), Negrea et al. (2019), and Rodríguez-Gálvez et al. (2021) for various datasets. Note that the bound presented in Rodríguez-Gálvez et al. (2021) is an extension of that in Haghifam et al. (2020) from full-batch setting to mini-batch setting. We also evaluate the optimization performance of proposed Noisy Sign-SGD by comparing it with the original sign-SGD (Bernstein et al., 2018a) and present the corresponding generalization bound in Theorem 2.

The details of our model architectures, learning rate scheduling, hyper-parameter selections and additional experimental results can be found in Appendix D. We emphasize that the goal for the experiments was to do a comparative study relative to existing approaches and bounds. We note that the empirical performance of the methods can potentially be improved with better architectures and training strategies, e.g., deeper/wider
Figure 2: Results for training CNN using SGLD on a subset of MNIST \((n = 10000)\) with different randomness on labels. (a) Test error and bound: As the label randomness increases, the empirical test error (dashed lines) increases and so does the test error bound (solid lines); overall, the bounds stays valid. (b) Generalization bound: As the label randomness increases, so does the generalization bound in Theorem 2. (c) Gradient discrepancy: As the label randomness increases, so does the gradient discrepancy \(\| \nabla \ell (w_t, z_n) - \nabla \ell (w_t, z'_n) \|^2 \), which in turn leads to the increase in the generalization bound. (d) Training error: While training takes more epochs with random labels, training error does go to zero.

Figure 3: (a)-(d) show the training dynamics of CNN on MNIST and Fashion-MNIST, and ResNet-18 on CIFAR-10 and CIFAR-100 using noisy sign-SGD with different scaling \(\alpha_t\). Legends indicate the choice of \(\alpha_t\) and the numbers in brackets are test errors at convergence. As \(\alpha_t \to 0\), Noisy sign-SGD matches both the optimization trajectory as well as the final test accuracy of the original sign-SGD (Bernstein et al., 2018a). (e)-(f) show that empirical test error can be bounded based on our generalization bound and the corresponding training error. The larger \(\alpha_t\) (noise) is the sharper our bound is.

5.1 Stochastic Gradient Langevin Dynamics

Comparison with existing work. We have derived generalization error bounds that depend on the data-dependent quantity gradient discrepancy, i.e., \(\| \nabla \ell (w_t, z_n) - \nabla \ell (w_t, z'_n) \|^2 \). Existing bounds in Li et al.
(2020) and Negrea et al. (2019) have also improved the Lipschitz constant in Mou et al. (2018) to a data-dependent quantity. As shown in Figure 1(a)-(d), by combining with the empirical training error, all four generalization error bounds can be used to bound the empirical test error, but our bound is able to generate a much tighter upper bound. Such difference is mainly due to the fact that we replace the squared gradient norm in Li et al. (2020), the squared norm of gradient incoherence in Negrea et al. (2019), and that of two-sample incoherence in Rodriguez-Gálvez et al. (2021) with the gradient discrepancy while maintaining a $1/n$ sample dependence. Results in Figure 1(e)-(h) show that our bounds are much sharper than those of Li et al. (2020) because our gradient discrepancy (Figure 1(i)-(l)) is usually 2-4 order of magnitude smaller than the squared gradient norms appeared in Li et al. (2020). Our bounds are also sharper than those of Negrea et al. (2019) and Rodriguez-Gálvez et al. (2021) due to an improved dependence on $n$ from an order of $1/\sqrt{n}$ to $1/n$. Note that, even though the gradient incoherence in Negrea et al. (2019) is about 1 to 2 order of magnitude smaller than the gradient discrepancy for simple problems such as MNIST and Fashion-MNIST, the difference between the gradient incoherence and our gradient discrepancy reduces as the problem becomes harder (see results for CIFAR-10 in Figure 1(j)).

Effect of Random Labels. Motivated by Zhang et al. (2017), we train CNN with SGLD on a smaller subset of MNIST dataset ($n = 10000$) with randomly corrupted labels. The corruption fraction varies from 0% (without label corruption) to 60%. As shown in Figure 2(d), for long enough training time, all experiments with different level of label randomness can achieve almost zero training error. However, the one with higher level of randomness has higher generalization/test error (Figure 2(a) dashed lines). Our generalization bound also becomes larger as the randomness increases since the corresponding gradient discrepancy increases.

5.2 Noisy Sign-SGD

In this section, we present numerical results for Noisy Sign-SGD proposed in Example 4.2. Since none of the existing bounds can give a valid generalization bound for Noisy Sign-SGD, we only present our bound here.

Optimization. Figures 3(a)-(d) show the training dynamics of Noisy Sign-SGD under various choices of $\alpha_t$. As $\alpha_t \rightarrow 0$, Noisy Sign-SGD matches both the optimization trajectory as well as the final test accuracy of the original Sign-SGD (Bernstein et al., 2018a). However, as $\alpha_t$ increases, the distribution over $\{-1, +1\}$ approaches the uniform distribution, and with such high noise, the corresponding Noisy Sign-SGD seems to converge but to a rather sub-optimal value.

Generalization Bound. Figure 3(e)-(f) show that our bound successfully bounds the empirical test error. Larger $\alpha_t$ leads to sharper generalization bounds. However, larger $\alpha_t$ adversely affects the optimization, e.g., Figure 3(a)-(d) blue and orange lines. The results illustrate the trade-off between the empirical optimization and the generalization bound. In practice, one needs to balance the optimization error and generalization by choosing a suitable scaling $\alpha_t$.

6 Conclusions

Inspired by recent advances in stability based and information theoretic approaches to generalization bounds (Mou et al., 2018; Pensia et al., 2018; Negrea et al., 2019; Li et al., 2020; Haghifam et al., 2020), we have presented a framework for developing such bounds based on expected stability for noisy stochastic iterative learning algorithms. We have also introduced Exponential Family Langevin Dynamics (EFLD), a large family of noisy gradient descent algorithms based on exponential family noise, which includes SGLD and Noisy Sign-SGD as two special cases. We have developed an expected stability based generalization
bound applicable to any EFLD algorithm with a $O(1/n)$ sample dependence and a dependence on gradient incoherence, rather than gradient norms. Further, we have provided optimization guarantees for special cases of EFLD, viz. Noisy Sign-SGD and SGLD. Our experiments on various benchmarks illustrate that our bounds are non-vacuous and quantitatively much sharper than existing bounds [Li et al., 2020; Negrea et al., 2019].

**Acknowledgements.** The research was supported by NSF grants IIS-1908104, OAC-1934634, IIS-1563950, and a C3.ai research award. We would like to thank the Minnesota Super-computing Institute (MSI) for providing computational resources and support.

**References**

Alistarh, D., Grubic, D., Li, J., Tomioka, R., and Vojnovic, M. (2017). Qsgd: Communication-efficient sgd via gradient quantization and encoding. In Guyon, I., Luxburg, U. V., Bengio, S., Wallach, H., Fergus, R., Vishwanathan, S., and Garnett, R., editors, *Advances in Neural Information Processing Systems 30*, pages 1709–1720. Curran Associates, Inc.

Asi, H., Duchi, J., Fallah, A., Javidbakht, O., and Talwar, K. (2021). Private adaptive gradient methods for convex optimization. In *International Conference on Machine Learning*, pages 383–392. PMLR.

Banerjee, A., Merugu, S., Dhillon, I. S., and Ghosh, J. (2005). Clustering with bregman divergences. *Journal of machine learning research*, 6(10).

Barndorff-Nielsen, O. (2014). *Information and exponential families: in statistical theory*. John Wiley & Sons.

Bassily, R., Feldman, V., Guzmán, C., and Talwar, K. (2020). Stability of stochastic gradient descent on nonsmooth convex losses. *Advances in Neural Information Processing Systems*, 33.

Bassily, R., Feldman, V., Talwar, K., and Guha Thakurta, A. (2019). Private stochastic convex optimization with optimal rates. *Advances in neural information processing systems*.

Bassily, R., Smith, A., and Thakurta, A. (2014). Private empirical risk minimization: Efficient algorithms and tight error bounds. In *2014 IEEE 55th Annual Symposium on Foundations of Computer Science*, pages 464–473. IEEE.

Bernstein, J., Wang, Y.-X., Azizzadenesheli, K., and Anandkumar, A. (2018a). signsgd: Compressed optimisation for non-convex problems. In *International Conference on Machine Learning*, pages 560–569. PMLR.

Bernstein, J., Zhao, J., Azizzadenesheli, K., and Anandkumar, A. (2018b). signsgd with majority vote is communication efficient and fault tolerant. In *International Conference on Learning Representations*.

Boucheron, S., Lugosi, G., and Massart, P. (2013). *Concentration inequalities: A nonasymptotic theory of independence*. Oxford university press.

Bousquet, O. and Elisseeff, A. (2002). Stability and generalization. *Journal of Machine Learning Research*, 2:499–526.

Bousquet, O., Klochkov, Y., and Zhivotovskiy, N. (2020). Sharper bounds for uniformly stable algorithms. In *Conference on Learning Theory*, pages 610–626. PMLR.
Brown, L. D. (1986). Fundamentals of statistical exponential families: with applications in statistical decision theory. Ims.

Bu, Y., Zou, S., and Veeravalli, V. V. (2019). Tightening mutual information based bounds on generalization error. In 2019 IEEE International Symposium on Information Theory (ISIT), pages 587–591. IEEE.

Bun, M., Dwork, C., Rothblum, G. N., and Steinke, T. (2018). Composable and versatile privacy via truncated cdp. In Proceedings of the 50th Annual ACM SIGACT Symposium on Theory of Computing, pages 74–86.

Canonne, C. L., Kamath, G., and Steinke, T. (2020). The discrete gaussian for differential privacy. In NeurIPS.

Chen, X., Chen, T., Sun, H., Wu, Z. S., and Hong, M. (2019). Distributed training with heterogeneous data: Bridging median-and mean-based algorithms. arXiv preprint arXiv:1906.01736.

Damian, A., Ma, T., and Lee, J. (2021). Label noise sgd provably prefers flat global minimizers. arXiv preprint arXiv:2106.06530.

Devroye, L. and Wagner, T. (1979). Distribution-free inequalities for the deleted and holdout error estimates. IEEE Transactions on Information Theory, 25(2):202–207.

Elisseeff, A., Evgeniou, T., Pontil, M., and Kaelbing, L. P. (2005). Stability of randomized learning algorithms. Journal of Machine Learning Research, 6(1).

Feldman, V. and Vondrak, J. (2018). Generalization bounds for uniformly stable algorithms. In Proceedings of the 32nd International Conference on Neural Information Processing Systems, pages 9770–9780.

Feldman, V. and Vondrak, J. (2019). High probability generalization bounds for uniformly stable algorithms with nearly optimal rate. In Conference on Learning Theory, pages 1270–1279. PMLR.

Grünwald, P., Steinke, T., and Zakynthinou, L. (2021). Pac-bayes, mac-bayes and conditional mutual information: Fast rate bounds that handle general vc classes. arXiv preprint arXiv:2106.09683.

Haghifam, M., Negrea, J., Khisti, A., Roy, D. M., and Dziugaite, G. K. (2020). Sharpened generalization bounds based on conditional mutual information and an application to noisy, iterative algorithms. Advances in Neural Information Processing Systems.

Hardt, M., Recht, B., and Singer, Y. (2016). Train faster, generalize better: Stability of stochastic gradient descent. In International Conference on Machine Learning, pages 1225–1234.

Hellström, F. and Durisi, G. (2020). Generalization bounds via information density and conditional information density. IEEE Journal on Selected Areas in Information Theory, 1(3):824–839.

Hellström, F. and Durisi, G. (2021). Fast-rate loss bounds via conditional information measures with applications to neural networks. In 2021 IEEE International Symposium on Information Theory (ISIT), pages 952–957. IEEE.

Jiang, P. and Agrawal, G. (2018). A linear speedup analysis of distributed deep learning with sparse and quantized communication. In Bengio, S., Wallach, H., Larochelle, H., Grauman, K., Cesa-Bianchi, N., and Garnett, R., editors, Advances in Neural Information Processing Systems 31, pages 2525–2536. Curran Associates, Inc.
Jin, C., Ge, R., Netrapalli, P., Kakade, S. M., and Jordan, M. I. (2017). How to escape saddle points efficiently. In *International Conference on Machine Learning*, pages 1724–1732.

Jin, C., Netrapalli, P., Ge, R., Kakade, S. M., and Jordan, M. I. (2019). On nonconvex optimization for machine learning: Gradients, stochasticity, and saddle points. *arXiv preprint arXiv:1902.04811*.

Jin, R., Huang, Y., He, X., Wu, T., and Dai, H. (2020). Stochastic-sign sgd for federated learning with theoretical guarantees. *arXiv preprint arXiv:2002.10940*.

Kairouz, P., Ribero, M., Rush, K., and Thakurta, A. (2020). Dimension independence in unconstrained private erm via adaptive preconditioning. *arXiv preprint arXiv:2008.06570*.

Krizhevsky, A. (2009). Learning Multiple Layers of Features from Tiny Images. Technical Report Vol. 1. No. 4., University of Toronto.

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

Li, B., Chen, C., Liu, H., and Carin, L. (2019). On connecting stochastic gradient mcmc and differential privacy. In *The 22nd International Conference on Artificial Intelligence and Statistics*, pages 557–566. PMLR.

Li, J., Luo, X., and Qiao, M. (2020). On generalization error bounds of noisy gradient methods for non-convex learning. In *International Conference on Learning Representations*.

Mou, W., Wang, L., Zhai, X., and Zheng, K. (2018). Generalization bounds of sgld for non-convex learning: Two theoretical viewpoints. In *Conference on Learning Theory*, pages 605–638. PMLR.

Negrea, J., Haghifam, M., Dziugaite, G. K., Khisti, A., and Roy, D. M. (2019). Information-theoretic generalization bounds for sgld via data-dependent estimates. In *Advances in Neural Information Processing Systems*.

Neu, G., Dziugaite, G. K., Haghifam, M., and Roy, D. M. (2021). Information-theoretic generalization bounds for stochastic gradient descent. In *COLT*.

Pensia, A., Jog, V., and Loh, P.-L. (2018). Generalization error bounds for noisy, iterative algorithms. In *2018 IEEE International Symposium on Information Theory (ISIT)*, pages 546–550. IEEE.

Pollard, D. (2002). *A user’s guide to measure theoretic probability*. Number 8. Cambridge University Press.

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

Rodriguez-Gálvez, B., Bassi, G., Thobaben, R., and Skoglund, M. (2021). On random subset generalization error bounds and the stochastic gradient langevin dynamics algorithm. In *2020 IEEE Information Theory Workshop (ITW)*, pages 1–5. IEEE.

Rogers, W. H. and Wagner, T. J. (1978). A finite sample distribution-free performance bound for local discrimination rules. *The Annals of Statistics*, pages 506–514.

Russo, D. and Zou, J. (2016). Controlling bias in adaptive data analysis using information theory. In *Artificial Intelligence and Statistics*, pages 1232–1240. PMLR.
Sason, I. and Verdu, S. (2016). *f*-divergence inequalities. *IEEE Transactions on Information Theory*, 62.

Shalev-Shwartz, S., Shamir, O., Srebro, N., and Sridharan, K. (2009). Stochastic convex optimization. In *COLT*.

Shamir, O. and Zhang, T. (2013). Stochastic gradient descent for non-smooth optimization: Convergence results and optimal averaging schemes. In *International conference on machine learning*, pages 71–79. PMLR.

Steinke, T. and Zakynthinou, L. (2020). Reasoning about generalization via conditional mutual information. In *Conference on Learning Theory*, pages 3437–3452. PMLR.

Tsybakov, A. B. (2008). *Introduction to nonparametric estimation*. Springer Science & Business Media.

Wainwright, M. J. and Jordan, M. I. (2008). *Graphical models, exponential families, and variational inference*. Now Publishers Inc.

Wang, D. and Xu, J. (2019). Differentially private empirical risk minimization with smooth non-convex loss functions: A non-stationary view. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 33, pages 1182–1189.

Wang, Y.-X., Fienberg, S., and Smola, A. (2015). Privacy for free: Posterior sampling and stochastic gradient monte carlo. In *International Conference on Machine Learning*, pages 2493–2502. PMLR.

Welling, M. and Teh, Y. W. (2011). Bayesian learning via stochastic gradient langevin dynamics. In *International Conference on Machine Learning*, ICML ’11, pages 681–688.

Xiao, H., Rasul, K., and Vollgraf, R. (2017). Fashion-mnist: a novel image dataset for benchmarking machine learning algorithms.

Xu, A. and Raginsky, M. (2017). Information-theoretic analysis of generalization capability of learning algorithms. *Advances in Neural Information Processing Systems*, 2017:2525–2534.

Yang, G., Zhang, T., Kirichenko, P., Bai, J., Wilson, A. G., and De Sa, C. (2019). Swalp: Stochastic weight averaging in low-precision training. *36th International Conference on Machine Learning (ICML)*.

Zhang, C., Bengio, S., Hardt, M., Recht, B., and Vinyals, O. (2017). 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.

Zhang, H., Mironov, I., and Hejazinia, M. (2021). Wide network learning with differential privacy. *arXiv preprint arXiv:2103.01294*.

Zhou, R., Tian, C., and Liu, T. (2021). Individually conditional individual mutual information bound on generalization error. In *2021 IEEE International Symposium on Information Theory (ISIT)*, pages 670–675. IEEE.

Zhou, Y., Wu, S., and Banerjee, A. (2020). Bypassing the ambient dimension: Private sgd with gradient subspace identification. In *International Conference on Learning Representations*. 
A  Analysis and Proofs for Expected Stability (Section 3)

Proposition 1. Let $S_n \sim D^n$ and let $S_n'$ be a dataset obtained by replacing $z_n \in S_n$ with $z_n' \sim D$. Let $A(S_n), A(S_n')$ respectively denote the distributions over the hypothesis space $W$ obtained by running randomized algorithm $A$ on $S_n, S_n'$. Assume that for all $S_n \in Z^n, z \in Z, E_{W \sim A(S_n)}[\ell^2(W, z)] \leq c_0^2/4$ for some constant $c_0 > 0$. With $H(\cdot, \cdot)$ denoting the Hellinger divergence, we have

$$|E_{S_n \sim D^n}[L_D(A(S_n)) - L_S(A(S_n))]| \leq c_0 E_{S_n \sim D^n} E_{z_n' \sim D} \sqrt{2H^2(A(S_n), A(S_n'))}.$$  (3)

Proof. Let $S_n = (z_1, \ldots, z_n)$ and $	ilde{S}_n' = (z_1', \ldots, z_n')$ two independent random samples and let $S_n^{(i)} = (z_1, \ldots, z_{i-1}, z_i', z_{i+1}, \ldots, z_n)$ be the sample that is identical to $S$ except in the $i$-th example where we replace $z_i$ with $z_i'$. Note that $S_n^{(n)} = S_n'$, where $S_n'$ is the dataset obtained by replacing $z_n \in S_n$ with $z_n'$ as in the Proposition statement. Now, by definition we have

$$|E_{S_n \sim D^n}[L_D(A(S_n)) - L_S(A(S_n))]| = |E_{S_n} E_{S_n'} E_{A} \left[ \frac{1}{n} \sum_{i=1}^{n} \left( \ell(A(S_n^{(i)}), z_i') - \ell(A(S_n), z_i') \right) \right] |
\leq E_{S_n} E_{S_n'} E_{A} \left[ \frac{1}{n} \sum_{i=1}^{n} \left| \int_{\mathbb{R}^d} \ell(w; z_i') p_i(w) dw - \int_{\mathbb{R}^d} \ell(w; z_i') p(w) dw \right| \right]
\leq E_{S_n} E_{S_n'} E_{A} \left[ \frac{1}{n} \sum_{i=1}^{n} \int_{\mathbb{R}^d} \ell(w; z_i') \left( \sqrt{p_i(w)} + p(w) \right) \left( \sqrt{p_i(w)} - \sqrt{p(w)} \right) dw \right]
\leq E_{S_n} E_{S_n'} E_{A} \left[ \frac{1}{n} \sum_{i=1}^{n} \left( \int_{\mathbb{R}^d} \ell^2(w; z_i') \left( \sqrt{p_i(w)} + \sqrt{p(w)} \right)^2 dw \right)^{1/2} \left( \int_{\mathbb{R}^d} \left( \sqrt{p_i(w)} - \sqrt{p(w)} \right)^2 dw \right)^{1/2} \right].

where in (a) $p_i(w), p(w)$ are respectively the distributions obtained by $A(S_n^{(i)}), A(S_n)$, and (b) follows by Cauchy-Schwarz inequality. Focusing on the first integral, we have:

$$\left( \int_{\mathbb{R}^d} \ell^2(w; z_i') \left( \sqrt{p_i(w)} + \sqrt{p(w)} \right)^2 dw \right)^{1/2} \leq \left( 2 \int_{\mathbb{R}^d} \ell^2(w; z_i') p_i(w) dw + 2 \int_{\mathbb{R}^d} \ell^2(w; z_i') p(w) dw \right)^{1/2} \leq \left( c_0^2/2 + c_0^2/2 \right)^{1/2} = c_0.

Hence, by definition of the Hellinger divergence, we have

$$E_{S_n \sim D^n}[L_D(A(S_n)) - L_S(A(S_n))] \leq E_{S_n} E_{S_n'} \frac{1}{n} \sum_{i=1}^{n} c_0 \sqrt{2H^2(A(S_n), A(S_n^{(i)})},

20
\[
\begin{align*}
&= (a) \mathbb{E}_{S_n} \mathbb{E}_{\tilde{S}_n} \frac{1}{n} \sum_{i=1}^{n} c_0 \sqrt{2H^2(A(S_n), A(S'_n))} \\
&= c_0 \mathbb{E}_{S_n \sim D_n} \mathbb{E}_{\tilde{S}_n \sim D} \sqrt{2H^2(A(S_n), A(S'_n))} ,
\end{align*}
\]
where (a) follows since the samples are drawn i.i.d. and the randomized algorithm \(A(\cdot)\) is permutation invariant. That completes the proof.

\[\Box\]

**Proposition 2.** For any distributions \(P\) and \(P'\), \(2H^2(P, P') \leq \min \{ KL(P, P'), \sqrt{\frac{1}{2} KL(P, P')} \} \).

**Proof.** For the first part, note that:

\[
KL(P, P') = \int \left( \log \frac{p(w)}{p'(w)} \right) p(w) \, dw \\
= 2 \int \left( -\log \sqrt{\frac{p'(w)}{p(w)}} \right) p(w) \, dw \\
\geq (a) 2 \int \left( 1 - \sqrt{\frac{p'(w)}{p(w)}} \right) p(w) \, dw \\
= 2 \int \left( p(w) - \sqrt{p(w)p'(w)} \right) \, dw \\
= \int \left( p(w) + p'(w) - 2\sqrt{p(w)p'(w)} \right) \, dw \\
= \int \left( \sqrt{p(w)} - \sqrt{p'(w)} \right)^2 \, dw \\
= 2H^2(P, P') ,
\]

where (a) follows since for \(z > -1\), \(\log(1+z) \leq z\), using \(x = 1+z\) and changing signs gives \(-\log x \geq 1-x\).

For the second part, note that:

\[
2H^2(P, P') = \int_w (\sqrt{p(w)} - \sqrt{p'(w)})^2 \, dw \\
= \int_w |\sqrt{p(w)} - \sqrt{p'(w)}| \times |\sqrt{p(w)} - \sqrt{p'(w)}| \, dw \\
\leq \int_w |\sqrt{p(w)} - \sqrt{p'(w)}| \times |\sqrt{p(w)} + \sqrt{p'(w)}| \, dw \\
= \int_w |p(w) - p'(w)| \, dw \\
= TV(P, P') ,
\]

where \(TV(P, P')\) denotes the total variation distance \([\text{Pollard} 2002]\). Further, from Pinsker’s inequality \([\text{Tsybakov} 2008]\), we have

\[
TV(P, P') \leq \sqrt{\frac{1}{2} KL(P, P')} .
\]

Combining the two results completes the proof. \(\Box\)
A.1 Proofs for Section 3.2

Our first result establishes a bound on the KL-divergence between two component mixture models in terms of the mixing weight of the unique components. Similar results have appeared in (Li et al., 2020; Bun et al., 2018) in related contexts. Our proof is different, simple, and self-contained.

**Lemma 4.** Let $Q, Q', R$ be any three distributions such that $Q, Q'$ are both absolutely continuous w.r.t. $R$. Then, for any $s \in (0, 1)$

\[
KL\left( sQ + (1-s)R \middle|\middle| sQ' + (1-s)R \right) \leq \frac{s^2}{1-s} \int_w \frac{(Q(w) - Q'(w))^2}{R(w)} dw .
\]

**Proof.** Let $U = sQ' + (1-s)R$. Then, with $F(x) = Q(x) - Q'(x)$, we have

\[
KL(sQ + (1-s)R || sQ' + (1-s)R) = KL(U + s(Q - Q') || U)
\]

\[
= \int (U(x) + sF(x)) \log \left( \frac{U(x) + sF(x)}{U(x)} \right) dx
\]

\[
= \int (U(x) + sF(x)) \log \left( 1 + \frac{sF(x)}{U(x)} \right) dx
\]

\[
= \int sF(x) + \frac{s^2F^2(x)}{2U(x)} - \frac{s^3F^3(x)}{6U^2(x)} + \frac{s^4F^4(x)}{12U^3(x)} - \cdots dx
\]

\[
= s^2 \int \frac{F^2(x)}{U(x)} \left( \frac{1}{2} - \frac{sF(x)}{6U(x)} + \frac{s^2F^2(x)}{12U^2(x)} - \cdots \right) dx ,
\]

where the first term vanishes since $\int F(x) dx = \int (Q(x) - Q'(x)) dx = 0$. This is the reason the dependency is on $s^2$, not $s$. With $W(x) = sF(x)/U(x)$, noting that $W(x) > -1$, and

\[
\left( \frac{1}{2} - \frac{W(x)}{6} + \frac{W^2(x)}{12} - \cdots \right) = \frac{(1 + W(x)) \log(1 + W(x)) - W(x)}{W^2(x)} \leq 1 ,
\]

we have

\[
KL(sP + (1-s)R || sQ + (1-s)R) = s^2 \int \frac{F^2(x)}{U(x)} \left( \frac{(1 + W(x)) \log(1 + W(x)) - W(x)}{W^2(x)} \right) dx
\]

\[
\leq s^2 \int \frac{F^2(x)}{U(x)} dx
\]

\[
\leq \frac{s^2}{(1-s)} \int \frac{(Q(x) - Q'(x))^2}{R(x)} dx .
\]

That completes the proof.

\[\square\]

**Proposition 3.** Consider the mixture models $Q_t = \frac{1}{|G_1|} \sum_{B_t \in G_1} P_{B_t,t}$, $Q'_t = \frac{1}{|G_1|} \sum_{B_t \in G_1} P'_{B_t,t}$, $R_t = \frac{1}{|G_0|} \sum_{A_t \in G_0} P_{A_t,t}$. Then, with $s = \frac{|G_1|}{|G|} = \frac{(k-1)}{(b)} = \frac{b}{n}$, we have

\[
P_t = sQ_t + (1-s)R_t , \quad \text{and} \quad P'_t = sQ'_t + (1-s)R_t .
\]

**Proof.** The proof follows the argument in the proof of Lemma 21 in (Li et al., 2020). \[\square\]
Lemma 5. Consider a general noisy stochastic iterative algorithm with updates of the form (4) with mini-batch size $B_t = b$. Then, conditioned on any trajectory $w_{0:t-1}$, we have

$$KL \left( P_t \| P'_t \right) \leq \frac{b^2}{n^2} \frac{n}{n-b} \mathbb{E}_{B_t \in G_1} \mathbb{E}_{A_t \in G_0} \left[ \int_{\xi_t} \left( \frac{dP_{B_t, \xi_t} - dP'_{B_t, \xi_t}}{dP_{A_t, \xi_t}} \right)^2 d\xi_t \right]. \quad (21)$$

Proof. By definition, Proposition 3 and Lemma 4 with $s = b/n$, we have

$$KL \left( P_t \| P'_t \right) \overset{(a)}{\leq} \frac{b^2}{n^2} \left( 1 + \frac{b}{n-b} \right) \int_{w} \left( \frac{1}{|G_1|} \sum_{B \in G_1} dP_B(w) - \sum_{A \in G_0} dP_A(w) \right)^2 d\xi,$$

$$\overset{(b)}{=} \frac{b^2}{n^2} \left( 1 + \frac{b}{n-b} \right) \int_{w} \frac{1}{|G_1|} \sum_{B \in G_1} \left( \frac{dP_B(w) - dP'_B(w)}{dP_A(w)} \right)^2 d\xi,$$

$$\overset{(c)}{=} \frac{b^2}{n^2} \left( 1 + \frac{b}{n-b} \right) \int_{w} \frac{1}{|G_1|} \sum_{B \in G_1} \left( \frac{dP_B(w) - dP'_B(w)}{dP_A(w)} \right)^2 d\xi,$$

where (a) is from Lemma 4, (b) is from Jensen’s inequality since function $f(x) = x^2$ is convex and $f(x) = \frac{1}{2} x$ is convex on $(0, \infty)$. That completes the proof.

Now we have all the pieces to prove the following result:

Lemma 1. Consider a noisy stochastic iterative algorithms of the form (4) with mini-batch size $b \leq n/2$. Then, with $c_1 = \sqrt{2} c_0$ (with $c_0$ as in Proposition 7), we have

$$\mathbb{E}_{S_n}[L_D(A(S_n)) - L_S(A(S_n))] \leq c_1 \mathbb{E}_{S_n} \mathbb{E}_{z_n} \mathbb{E}_{z'_n} \left[ \sum_{t=1}^{T} \mathbb{E}_{W_{0:(t-1)}} \mathbb{E}_{B_t \in G_1} \mathbb{E}_{A_t \in G_0} \left[ \int_{\xi_t} \left( \frac{dP_{B_t, \xi_t} - dP'_{B_t, \xi_t}}{dP_{A_t, \xi_t}} \right)^2 d\xi_t \right] \right]. \quad (7)$$

Proof. Based on Propositions 1 and 2 and 5, we have

$$\mathbb{E}_{S \sim D^n}[L_D(A(S)) - L_S(A(S))] \leq \sqrt{KL \left( P_T \| P'_T \right)} \leq \sqrt{\sum_{t=1}^{T} \mathbb{E}_{P_{0:(t-1)}} \left[ KL \left( P_t \| P'_t \right) \right]}.$$

Applying Lemma 5 to bound $KL \left( P_t \| P'_t \right)$ and noting that $b/(n-b) \leq 1$ for $b \leq n/2$ completes the proof.
\[ Y(S) = \sum_{i=1}^{n} \mathbb{E}_A[\mathbb{E}_{Z \sim D}[\ell(A(S), Z)] - \ell(A(S), Z_i)] = n(\text{LD}(A(S)) - \text{LS}(A(S))). \] (22)

Theorem 1 establishes a bound on \(|\frac{1}{n} \mathbb{E}_S[Y(S)]|\). We now focus on establishing a high probability bound on \(\frac{1}{n}(Y(S) - \mathbb{E}_S[Y(S)])\). Let \(S' = (Z'_1, \ldots, Z'_n)\) be such that \(Z'_i\) is an independent copy of \(Z_i\). Further, let \(S'_i = (Z_1, \ldots, Z_{i-1}, Z'_i, Z_{i+1}, \ldots, Z_n)\). Then, the change in SGE

\[ Y(S) - Y(S'_i) = n \left[ (\text{LD}(A(S)) - \text{LD}(A(S'_i))) - (\text{LS}(A(S)) - \text{LS}(A(S'_i))) \right] \] (23)

is a symmetric random variable, and is identically distributed for \(i = 1, \ldots, n\). Our analysis is based on the following assumption:

**Assumption 3.** The random variable \((Y(S) - Y(S'_i))^2\) is sub-Gaussian with \(\psi_2\)-norm \(\kappa^2_A\), i.e., \(\|Y - Y'_i\|_{\psi_2} = \sup_{q \geq 1} (\mathbb{E}_{S,S'}|Y(S) - Y(S'_i)|^{2q})^{1/2} \leq \kappa^2_A\).

Assumption 3 implies that \(\|Y - Y'_i\|_{\psi_2} \leq \kappa_A\). Note that since \(Y(S) - Y(S'_i)\) is identically distributed for all \(i\), \(\kappa_A\) is the same for all \(i\). Further, \(\kappa_A\) is a property of the algorithm \(A\), and can be viewed as a measure of stability. If \(\kappa_A = O(1)\), i.e., swapping one point effectively leads to \(O(\frac{1}{n})\) change in the generalization error, then \(A\) can be considered stable; on the other hand, if \(\kappa_A = O(\sqrt{n})\), then \(A\) is not stable since the effective change in generalization error \(\frac{1}{n}(Y(S) - Y(S'_i))\) is \(O(1/\sqrt{n})\), the same order as typical generalization error \(\frac{1}{n}Y(S)\) itself. The sharpness of the high-probability bound we present meaningfully depends on \(\kappa_A\), with smaller values implying sharper bounds.

**Theorem 5.** Under Assumption 3 with probability at least \((1 - \delta)\) over the draw \(S \sim D^n\), we have

\[ L_D(A(S)) \leq L_S(A(S)) + \mathbb{E}_S \left[ L_D(A(S) - L_S(A(S)) \right] + \max \left( \frac{1}{n}, \frac{c_1 \kappa_A}{\sqrt{n}} \right) \log \left( \frac{16}{\delta} \right). \] (24)

If \(\kappa_A = O(1)\), i.e., swapping one point effectively leads to \(O(\frac{1}{n})\) change in the generalization error, then \(A\) can be considered very stable; if \(\kappa_A = O(\sqrt{n})\), then \(A\) can be considered somewhat stable; and if \(\kappa_A^2 = O(\sqrt{n})\), then \(A\) is not stable since the effective change in generalization error \(\frac{1}{n}(Y(S) - Y(S'_i))\) is \(O(1/\sqrt{n})\), the same order as the generalization error \(\frac{1}{n}Y(S)\) itself.

**Proof.** Let \(S = (Z_1, \ldots, Z_n)\) and let \(S' = (Z'_1, \ldots, Z'_n)\) be such that \(Z'_i\) is an independent copy of \(Z_i\). With \((x)_+ = \max(x, 0)\), let

\[ V^+ = V^+(S) = \sum_{i=1}^{n} \mathbb{E}_{S'_i}[(Y - Y'_i)_+] \] (25)

Our proof uses the following exponential version of the Efron-Stein inequality [Theorem 6.16 in Boucheron et al. (2013)], whose proof is based on a combination of the symmetric modified log-Sobolev inequality [Theorem 6.15 in Boucheron et al. (2013)] with the change of measure:
Theorem 6. Let $Y = f(Z_1, \ldots, Z_n)$, where $Z_i, i = 1, \ldots, n$ are independent. Let $\theta, \lambda > 0$ be such that $\theta \lambda < 1$ and $E[\exp(\lambda V^+/\theta)] < \infty$. Then,

$$\log E \left[ e^{\lambda(Y - EY)} \right] \leq \frac{\lambda \theta}{1 - \lambda \theta} \log E \left[ e^{\lambda V^+/\theta} \right].$$

(26)

For the proof of Theorem 5, note that $V^+$ is sub-Gaussian with $\|V^+\|_{\psi^2} \leq n \kappa_A^2$. Let $\mu_+ = E[V^+]$ and $\kappa_+ = \|V^+\|_{\psi^2}$. Then from Theorem 6, we have

$$\psi(\lambda) \triangleq \log E \left[ e^{\lambda(Y - EY)} \right] \leq \frac{\lambda \mu_+}{1 - \lambda \theta} \left[ \frac{\lambda \mu_+}{\theta} + c \frac{\lambda^2 \kappa_+^2}{\theta^2} \right].$$

Then, by Markov’s inequality we have

$$\log P(Y - EY > t) \leq \psi(\lambda) - \lambda t$$

$$\leq \frac{1}{1 - \lambda \theta} \left[ \lambda^2 \mu_+ + c \lambda^3 \kappa_+^2 / \theta - (1 - \lambda \theta) \lambda t \right].$$

Choosing $\theta = 1/(2\lambda)$, we have

$$\log P(Y - EY > t) \leq 2\lambda^2 \mu_+ + 4c \lambda^4 \kappa_+^2 - \lambda t.$$

Consider choosing $\lambda = \min \left\{ 1, \frac{1}{c_0 \sqrt{2\kappa_+}} \right\}$, where $c_0 = \max(1, \sqrt{c})$. Since $\mu_+ \leq \kappa_+$, we have

$$\log P(Y - EY > t) \leq 2 - \min \left\{ 1, \frac{1}{c_0 \sqrt{2\kappa_+}} \right\} t$$

$$\Rightarrow P(Y - EY > t) \leq 8 \exp \left( -\min \left\{ 1, \frac{1}{c_0 \sqrt{2\kappa_+}} \right\} t \right).$$

With $t = n\epsilon$, and noting that $\kappa_+ \leq n \kappa_A^2$, with $c_1 = c_0 \sqrt{2}$, we have

$$P(Y - EY > n\epsilon) \leq 8 \exp \left( -\min \left\{ n, \frac{\sqrt{n}}{c_1 \kappa_A} \right\} \epsilon \right).$$

Now, we choose $\delta$ such that

$$8 \exp \left( -\min \left\{ n, \frac{\sqrt{n}}{c_1 \kappa_A} \right\} \epsilon \right) \leq 8 \exp (-n\epsilon) + 8 \exp \left( -\frac{\sqrt{n}}{c_1 \kappa_A} \epsilon \right) \leq \delta.$$

It suffices to choose $\epsilon$ such that

$$8 \exp (-n\epsilon) \leq \delta/2 \quad \Rightarrow \quad \epsilon \geq \frac{1}{n} \log \left( \frac{16}{\delta} \right)$$

$$8 \exp \left( -\frac{\sqrt{n}}{c_1 \kappa_A} \epsilon \right) \leq \delta/2 \quad \Rightarrow \quad \epsilon \geq \frac{c_1 \kappa_A}{\sqrt{n}} \log \left( \frac{16}{\delta} \right).$$

As a result,

$$P \left( \frac{1}{n}(Y - EY) > \max \left\{ \frac{1}{n}, \frac{c_1 \kappa_A}{\sqrt{n}} \right\} \log \left( \frac{16}{\delta} \right) \right) \leq \delta.$$

That completes the proof. □
B Analysis and Proofs for EFLD (Section 4)

In this section, we provide the proofs for Section 4. We first review and show details of a few examples of exponential family.

B.1 Examples of Exponential Family

Example B.1 (Gaussian). For univariate Gaussians with fixed variance $\sigma^2$, the scaling $\alpha = \sigma$, the sufficient statistic $\xi = x/\sigma$, the log-partition function $\psi(\theta) = \theta^2/2$, and the base measure $\pi_0(\xi) = \frac{1}{\sqrt{2\pi}\sigma} \exp(-\xi^2/2\sigma^2)$ or equivalently $\pi_0(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp(-x^2/2\sigma^2)$ using $\xi = x/\sigma$ and $d\xi = dx/\sigma$. The scaled parameter $\theta_\alpha = \theta/\sigma$. Then, the distribution from the natural parameter form is:

$$p_{\theta/\sigma}(x) = \exp(x\theta/\sigma^2 - \theta^2/(2\sigma^2)) \times \frac{1}{\sqrt{2\pi}\sigma} \exp(-x^2/2\sigma^2) = \frac{1}{\sqrt{2\pi}\sigma} \exp(-(x - \mu)^2/2\sigma^2).$$

(27)

The expectation parameter $\mu = \nabla \psi(\theta) = \theta$. The scaled expectation parameter $\mu_\alpha = \nabla \psi(\theta_\alpha) = \theta_\alpha = \theta/\sigma = \mu/\sigma$. Since $\xi = x/\sigma$ and the Bregman divergence is given by:

$$d_\phi(\xi,\mu) = \frac{1}{2}(\xi - \mu)^2,$$

the expectation parameter form

$$p_{\mu_\alpha}(\xi) = \exp(-(x/\sigma - \mu/\sigma)^2/2) \frac{1}{\sqrt{2\pi}\sigma} = \frac{1}{\sqrt{2\pi}\sigma} \exp(-(x - \mu)^2/2\sigma^2).$$

(28)

Example B.2 (Bernoulli over $\{0, 1\}$). For Bernoulli over $\{0, 1\}$, the sufficient statistic $\xi = x \in \{0, 1\}$, base measure is 1 on $\{0, 1\}$, and the log-partition function $\psi(\theta) = \log(1 + \exp(\theta))$ for natural parameter $\theta \in \mathbb{R}$. The expectation parameter $\mu = \nabla \psi(\theta) = \frac{\exp(\theta)}{1 + \exp(\theta)}$, the sigmoid function of $\theta$. The Bregman divergence is the Bernoulli KL-divergence given by: $d_\phi(\xi,\mu) = x \log \frac{x}{\mu} + (1 - x) \log \frac{1 - x}{1 - \mu}$. For scaled parameters $\theta_\alpha = \theta/\alpha$, the corresponding expectation parameter $\mu_\alpha = \frac{\exp(\theta)}{1 + \exp(\theta)}$. The mean parameter form distribution is given by

$$p_{\mu_\alpha}(\xi) = \exp(-d_\phi(\xi,\mu_\alpha)) = \mu_\alpha^{\xi} (1 - \mu_\alpha)^{1-\xi}.$$  

(29)

Example B.3 (Bernoulli over $\{-1, 1\}$). For Bernoulli over $\{-1, 1\}$, the sufficient statistic $\xi = x \in \{-1, 1\}$, base measure is 1 on $\{-1, 1\}$, and the log-partition function $\psi(\theta) = \log(\exp(-\theta) + \exp(\theta))$ for natural parameter $\theta \in \mathbb{R}$. The expectation parameter $\mu = \nabla \psi(\theta) = \frac{\exp(\theta)}{\exp(-\theta) + \exp(\theta)} = \frac{\exp(2\theta) - 1}{\exp(2\theta) + 1}$, then its inverse function $\theta = \nabla \phi(\mu) = \frac{1}{2} \log \left( \frac{1 + \mu}{1 - \mu} \right)$, by integration we have $\phi(\mu) = \frac{1 + \mu}{2} \log \frac{1 + \mu}{1 - \mu} + \frac{1 - \mu}{2} \log \frac{1 - \mu}{1 + \mu}$. The Bregman divergence is given by: $d_\phi(\xi,\mu) = \frac{1 + \xi}{2} \log \frac{1 + \xi}{1 + \mu} + \frac{1 - \xi}{2} \log \frac{1 - \xi}{1 - \mu}$. For scaled parameters $\theta_\alpha = \theta/\alpha$, the corresponding expectation parameter $\mu_\alpha = \frac{\exp(2\theta_\alpha) - 1}{\exp(2\theta_\alpha) + 1}$. Noting that $\frac{1 + \xi}{2} \log \frac{1 + \xi}{2} - \frac{1 - \xi}{2} \log \frac{1 - \xi}{2} = 0$ for the base measure, the distribution is given by

$$p_{\mu_\alpha}(\xi) = \exp(-d_\phi(\xi,\mu_\alpha)) = \left( \frac{1 + \mu_\alpha}{2} \right)^{\frac{1 + \xi}{2}} \left( \frac{1 - \mu_\alpha}{2} \right)^{\frac{1 - \xi}{2}},$$

(30)

which is $\xi = 1$ with probability $\frac{1 + \mu_\alpha}{2}$ and $\xi = -1$ with probability $\frac{1 - \mu_\alpha}{2}$.

B.2 Proof of Theorem 1

Theorem 1. For a given set $S_{n+1} \sim D_{n+1}$ and $w_{t-1}$ at iteration $(t-1)$, let $\Delta_t(w_{t-1}) = \max_{z,z' \in S_{n+1}} \|\nabla \ell(w_{t-1}, z) - \nabla \ell(w_{t-1}, z')\|_2$. Further, for a $c_2$-smooth log-partition function $\psi$, let the scaling $\alpha_t(w_{t-1})$ be data-dependent.
such that \( \alpha_{t|w_{t-1}}^2 \geq 8 c_2 \Delta_{t|w_{t-1}}^2 (\bar{S}_{n+1}) \). Then, we have

\[
I_{A_t,B_t} \leq 5c_2 \| \theta_{B_t;\alpha_t} - \theta_{B'_t;\alpha_t} \|^2 = \frac{5c_2}{2\alpha_{t|w_{t-1}}^2} \left\| \nabla \ell (w_{t-1}, S_{B_t}) - \nabla \ell (w_{t-1}, S_{B'_t}) \right\|^2 . \tag{11}
\]

To avoid clutter, we drop the subscript \( t \) for the analysis and note that the analysis holds for any step \( t \).

When the density \( dP_{B,A} = p_\psi (\xi; \theta_{B,\alpha}) \), by mean-value theorem, for each \( \xi \), we have

\[
p_\psi (\xi; \theta_{B,\alpha}) - p_\psi (\xi; \theta'_{B,\alpha}) = \langle \theta_{B,\alpha} - \theta'_{B,\alpha}, \nabla \theta_{B,\alpha} p_\psi (\xi; \tilde{\theta}_{B,\alpha}) \rangle , \tag{31}
\]

for some \( \tilde{\theta}_{B,\alpha} = \gamma \xi \theta_{B,\alpha} + (1 - \gamma \xi) \theta'_{B,\alpha} \) where \( \gamma \in [0,1] \). Then,

\[
I_{A,B} = \int_\xi \frac{(p_\psi (\xi; \theta_{B,\alpha}) - p_\psi (\xi; \theta'_{B,\alpha}))^2}{p_\psi (\xi; \theta_{A,\alpha})} \, d\xi = \int_\xi \frac{(\theta_{B,\alpha} - \theta'_{B,\alpha}, \nabla \theta_{B,\alpha} p_\psi (\xi; \tilde{\theta}_{B,\alpha}))^2}{p_\psi (\xi; \theta_{A,\alpha})} \, d\xi
\]

\[
= \int_\xi \frac{(\theta_{B,\alpha} - \theta'_{B,\alpha}, \xi - \nabla \theta'_{B,\alpha} \psi (\xi; \tilde{\theta}_{B,\alpha}))^2}{p_\psi (\xi; \theta_{A,\alpha})} \, d\xi , \tag{32}
\]

since \( p_\psi (\xi; \tilde{\theta}_{B,\alpha}) = \exp (\langle \xi, \tilde{\theta}_{B,\alpha} \rangle - \psi (\tilde{\theta}_{B,\alpha}) ) \pi_0 (\xi) \).

### B.2.1 Handling Distributional Dependency of \( \tilde{\theta}_{B} \)

Note that we cannot proceed with the analysis with the density term depending on \( \tilde{\theta}_B \) since \( \tilde{\theta}_B \) depends on \( \xi \).

In this step we focus on bounding the density term depending on \( \tilde{\theta}_B \) in terms of exponential family densities with parameters \( \theta_B \) and \( \theta'_B \).

**Lemma 2.** With \( \tilde{\theta}_{B,\alpha} = \gamma \xi \theta_{B,\alpha} + (1 - \gamma \xi) \theta'_{B,\alpha} \) for some \( \gamma \xi \in [0,1] \), we have

\[
\exp \left[ \langle \xi, \tilde{\theta}_{B,\alpha} \rangle - \psi (\tilde{\theta}_{B,\alpha}) \right] \leq \exp \left[ \langle \xi, \theta_{B,\alpha} \rangle - \psi (\theta_{B,\alpha}) \right] \leq \exp \left[ \langle \xi, \theta'_{B,\alpha} \rangle - \psi (\theta'_{B,\alpha}) \right] = \exp \left[ c_2 \| \theta_{B,\alpha} - \theta'_{B,\alpha} \|^2 \right] .
\]

**Proof.** Denoting \( \gamma \xi \) as \( \gamma \) for convenience (the dependence on \( \xi \) does not play a role in the analysis), we have

\[
\langle \xi, \tilde{\theta}_{B,\alpha} \rangle - \psi (\tilde{\theta}_{B,\alpha}) = \langle \xi, \gamma \theta_{B,\alpha} + (1 - \gamma) \theta'_{B,\alpha} \rangle - \psi (\gamma \theta_{B,\alpha} + (1 - \gamma) \theta'_{B,\alpha})
\]

\[
= \gamma \left[ \langle \xi, \theta_{B,\alpha} \rangle - \psi (\theta_{B,\alpha}) \right] + (1 - \gamma) \left[ \langle \xi, \theta'_{B,\alpha} \rangle - \psi (\theta'_{B,\alpha}) \right]
\]

\[
+ \gamma \psi (\theta_{B,\alpha}) + (1 - \gamma) \psi (\theta'_{B,\alpha}) - \psi (\gamma \theta_{B,\alpha} + (1 - \gamma) \theta'_{B,\alpha})
\]

\[
\leq \max \left( \langle \xi, \theta_{B,\alpha} \rangle - \psi (\theta_{B,\alpha}), \langle \xi, \theta'_{B,\alpha} \rangle - \psi (\theta'_{B,\alpha}) \right)
\]

\[
+ \gamma d_\psi (\theta_{B,\alpha}, \tilde{\theta}_{B,\alpha}) + (1 - \gamma) d_\psi (\theta'_{B,\alpha}, \tilde{\theta}_{B,\alpha}) ,
\]

where the second term in (a) follows since difference between two sides of Jensen’s inequality is given by the Bregman information, i.e., expected Bregman divergence to the expectation (See section 3.1.1 in Banerjee et al. (2005));

\[
\gamma \psi (\theta_{B,\alpha}) + (1 - \gamma) \psi (\theta'_{B,\alpha}) - \psi (\gamma \theta_{B,\alpha} + (1 - \gamma) \theta'_{B,\alpha}) = \gamma d_\psi (\theta_{B,\alpha}, \tilde{\theta}_{B,\alpha}) + (1 - \gamma) d_\psi (\theta'_{B,\alpha}, \tilde{\theta}_{B,\alpha}) .
\]
Now, note that
\[
\gamma d_\psi(\theta_{B,a}, \tilde{\theta}_{B,a}) + (1 - \gamma) d_\psi(\theta'_{B,a}, \tilde{\theta}_{B,a}) \leq \gamma d_\psi(\theta_{B,a}, \theta'_{B,a}) + (1 - \gamma) d_\psi(\theta'_{B,a}, \theta_{B,a}) \\
\leq \gamma c_2 \|\theta'_{B,a} - \theta_{B,a}\|^2 + (1 - \gamma) c_2 \|\theta_{B,a} - \theta'_{B,a}\|^2 \\
\leq c_2 \|\theta_{B,a} - \theta'_{B,a}\|^2.
\]
As a result,
\[
\exp \left[ (\xi, \tilde{\theta}_{B,a}) - \psi(\tilde{\theta}_{B,a}) \right] \\
\leq \exp \left[ c_2 \|\theta_{B,a} - \theta'_{B,a}\|^2 \right] \exp \left[ \max \left( (\xi, \theta_{B,a}) - \psi(\theta_{B,a}), (\xi, \theta'_{B,a}) - \psi(\theta'_{B,a}) \right) \right] \\
\leq \exp \left[ c_2 \|\theta_{B,a} - \theta'_{B,a}\|^2 \right] \\
= \exp \left[ c_2 \|\theta_{B,a} - \theta'_{B,a}\|^2 \right].
\]
That completes the proof. \(\square\)

### B.2.2 Bounding the Density Ratio

Focusing on density ratio, we have

**Lemma 3.** For any \(\xi\), we have
\[
\frac{\exp [(\xi, 2\theta_{B,a}) - 2\psi(\theta_{B,a})]}{\exp [(\xi, \theta_{A,a}) - \psi(\theta_{A,a})]} \leq \exp \left[ c_2 \|\theta_{B,a} - \theta_{A,a}\|^2 \right] \exp \left[ (\xi, (2\theta_{B,a} - \theta_{A,a}) - \psi(2\theta_{B,a} - \theta_{A,a})) \right].
\]

**Proof.** Note that
\[
\frac{\exp [(\xi, 2\theta_{B,a}) - 2\psi(\theta_{B,a})]}{\exp [(\xi, \theta_{A,a}) - \psi(\theta_{A,a})]} = \exp \left[ (\xi, (2\theta_{B,a} - \theta_{A,a}) - (2\psi(\theta_{B,a}) - \psi(\theta_{A,a})) \right] \\
= \beta_{B,A,a} \exp [(\xi, (2\theta_{B,a} - \theta_{A,a}) - \psi(2\theta_{B,a} - \theta_{A,a}))],
\]
where
\[
\beta_{B,A,a} = \exp \left[ \psi((2\theta_{B,a} - \theta_{A,a}) - (2\psi(\theta_{B,a}) - \psi(\theta_{A,a})) \right).
\]

Note that
\[
\log \beta_{B,A,a} = \psi((2\theta_{B,a} - \theta_{A,a}) - (2\psi(\theta_{B,a}) - \psi(\theta_{A,a})) \\
= -\left( \psi(\theta_{B,a}) - \psi((2\theta_{B,a} - \theta_{A,a}) \right) - \left( \psi(\theta_{B,a}) - \psi(\theta_{A,a}) \right) \\
\leq \left\langle \theta_{B,a} - \theta_{A,a}, \nabla \psi((2\theta_{B,a} - \theta_{A,a}) \right) + \left\langle \theta_{A,a} - \theta_{B,a}, \nabla \psi(\theta_{A,a}) \right) \\
\leq \|\theta_{B,a} - \theta_{A,a}\|_2 \|\nabla \psi((2\theta_{B,a} - \theta_{A,a}) - \nabla \psi(\theta_{A,a}))\|_2
\]
where (a) follows from the convexity of $\psi$, (b) follows from Cauchy-Schwartz, and (c) follows by smoothness of $\psi$.

As a result, we have

$$
\exp \left[ \langle \xi, 2\theta_{B,\alpha} \rangle - 2\psi(\theta_{B,\alpha}) \right] \leq \exp \left[ 2c_2 \| \theta_{B,\alpha} - \theta_{A,\alpha} \|_2^2 \right] \exp \left[ \langle \xi, (2\theta_B - \theta_A) / \alpha \rangle - \psi((2\theta_B - \theta_A) / \alpha) \right].
$$

That completes the proof. \[\square\]

The analysis for the term involving $\theta'_B$ is exactly the same.

Combining Lemma 2 and 3 we have the following result:

**Lemma 6.** We have

$$
\frac{p^2_{\psi}(\xi; \tilde{\theta}_{B,\alpha})}{p_{\psi}(\xi; \theta_{A,\alpha})} \leq \exp \left[ 2c_2 \| \theta_{B,\alpha} - \theta_{B',\alpha} \|_2^2 \right] \cdot \max \left( \exp \left[ 2c_2 \| \theta_{B,\alpha} - \theta_{A,\alpha} \|_2^2 \right] p_{\psi}(\xi; 2\theta_{B,\alpha} - \theta_{A,\alpha}), \right.
\exp \left[ 2c_2 \| \theta_{B',\alpha} - \theta_{A,\alpha} \|_2^2 \right] p_{\psi}(\xi; 2\theta_{B',\alpha} - \theta_{A,\alpha}) \right).
$$

**Proof.** From Lemma 2 we have

$$
p^2_{\psi}(\xi; \tilde{\theta}_{B,\alpha}) = \exp \left[ 2 \langle \xi, \tilde{\theta}_{B,\alpha} \rangle - 2\psi(\tilde{\theta}_{B,\alpha}) \right] \leq \exp \left[ c_2 \| \theta_{B,\alpha} - \theta_{B',\alpha} \|_2^2 \right] \cdot \max \left( \exp \left[ \langle \xi, \theta_{B,\alpha} \rangle - \psi(\theta_{B,\alpha}) \right], \exp \left[ \langle \xi, \theta_{B',\alpha} \rangle - \psi(\theta_{B',\alpha}) \right] \right)
$$

Thus,

$$
\frac{p^2_{\psi}(\xi; \tilde{\theta}_{B,\alpha})}{p_{\psi}(\xi; \theta_{A,\alpha})} \leq \exp \left[ 2c_2 \| \theta_{B,\alpha} - \theta_{B',\alpha} \|_2^2 \right] \cdot \max \left( \exp \left[ 2 \langle \xi, \theta_{B,\alpha} \rangle - 2\psi(\theta_{B,\alpha}) \right], \exp \left[ 2 \langle \xi, \theta_{B',\alpha} \rangle - 2\psi(\theta_{B',\alpha}) \right] \right) \frac{\exp \left[ \langle \xi, (2\theta_B - \theta_A) / \alpha \rangle - \psi((2\theta_B - \theta_A) / \alpha) \right]}{\exp \left[ \langle \xi, \theta_{A,\alpha} \rangle - \psi(\theta_{A,\alpha}) \right]}
$$

Based on Lemma 3 we have

$$
\frac{\exp \left[ \langle \xi, 2\theta_{B,\alpha} \rangle - 2\psi(\theta_{B,\alpha}) \right]}{\exp \left[ \langle \xi, \theta_{A,\alpha} \rangle - \psi(\theta_{A,\alpha}) \right]} \leq \exp \left[ 2c_2 \| \theta_{B,\alpha} - \theta_{A,\alpha} \|_2^2 \right] \exp \left[ \langle \xi, (2\theta_B - \theta_A) / \alpha \rangle - \psi((2\theta_B - \theta_A) / \alpha) \right]
$$

Combining above inequalities we have

$$
\frac{p^2_{\psi}(\xi; \tilde{\theta}_{B,\alpha})}{p_{\psi}(\xi; \theta_{A,\alpha})} \leq \exp \left[ 2c_2 \| \theta_{B,\alpha} - \theta_{B',\alpha} \|_2^2 \right]
\times \max \left( \exp \left[ 2c_2 \| \theta_{B,\alpha} - \theta_{A,\alpha} \|_2^2 \right] p_{\psi}(\xi; 2\theta_{B,\alpha} - \theta_{A,\alpha}), \right.
\exp \left[ 2c_2 \| \theta_{B',\alpha} - \theta_{A,\alpha} \|_2^2 \right] p_{\psi}(\xi; 2\theta_{B',\alpha} - \theta_{A,\alpha}) \right).
$$

That completes the proof. \[\square\]
B.2.3 Bounding the Integral

Ignoring multiplicative terms which do not depend on \( \xi \) for the moment, the analysis needs to bound an integral term of the form

\[
\int_{\xi} \langle \theta_{B,\alpha} - \theta'_{B,\alpha}, \xi - \nabla \psi(\tilde{\theta}_{B,\alpha}) \rangle^2 p_\psi(\xi; 2\theta_{B,\alpha} - \theta_{A,\alpha}) d\xi,
\]

and a similar term with \( p_\psi^2(\xi; 2\theta_{B',\alpha} - \theta_{A,\alpha}) \). The proof of Theorem 1 can be done by suitably bounding the integral.

**Proof of Theorem 1** From Lemma \( \mathbb{1} \) we have

\[
I_{A,B} \leq \int_{\xi} \frac{\langle \theta_{B,\alpha} - \theta'_{B,\alpha}, \xi - \nabla \psi(\tilde{\theta}_{B,\alpha}) \rangle^2 p_\psi(\xi; \theta_{A,\alpha})}{p_\psi(\xi; 2\theta_{B,\alpha} - \theta_{A,\alpha})} d\xi
\]

\[
\leq \exp \left[ 2c_2 \| \theta_{B,\alpha} - \theta_{B',\alpha} \|_2^2 \right] \times \max \left( \exp \left[ 2c_2 \| \theta_{B,\alpha} - \theta_{A,\alpha} \|_2^2 \right] \int_{\xi} \langle \theta_{B,\alpha} - \theta_{B,\alpha}, \xi - \nabla \psi(\tilde{\theta}_{B,\alpha}) \rangle^2 p_\psi(\xi; 2\theta_{B,\alpha} - \theta_{A,\alpha}) d\xi,
\]

\[
\exp \left[ 2c_2 \| \theta_{B',\alpha} - \theta_{A,\alpha} \|_2^2 \right] \int_{\xi} \langle \theta_{B,\alpha} - \theta_{B',\alpha}, \xi - \nabla \psi(\tilde{\theta}_{B,\alpha}) \rangle^2 p_\psi(\xi; 2\theta_{B',\alpha} - \theta_{A,\alpha}) d\xi \right).
\]

Focusing on the integral in the first term (the analysis for the second term is essentially the same), we have

\[
\int_{\xi} \langle \theta_{B,\alpha} - \theta'_{B,\alpha}, \xi - \nabla \psi(\tilde{\theta}_{B,\alpha}) \rangle^2 p_\psi(\xi; 2\theta_{B,\alpha} - \theta_{A,\alpha}) d\xi
\]

\[
= \int_{\xi} \langle \theta_{B,\alpha} - \theta'_{B,\alpha}, (\xi - \mathbb{E}[\xi]) - (\nabla \psi(\tilde{\theta}_{B,\alpha}) - \mathbb{E}[\xi]) \rangle^2 p_\psi(\xi; 2\theta_{B,\alpha} - \theta_{A,\alpha}) d\xi
\]

\[
\leq 2 \int_{\xi} \langle \theta_{B,\alpha} - \theta'_{B,\alpha}, (\xi - \mathbb{E}[\xi])^2 p_\psi(\xi; 2\theta_{B,\alpha} - \theta_{A,\alpha}) d\xi
\]

\[
+ 2 \int_{\xi} \langle \theta_{B,\alpha} - \theta'_{B,\alpha}, \nabla \psi(\tilde{\theta}_{B,\alpha}) - \mathbb{E}[\xi] \rangle^2 p_\psi(\xi; 2\theta_{B,\alpha} - \theta_{A,\alpha}) d\xi.
\]

For \( T_1 \), note that

\[
T_1 = \mathbb{E}_{\xi \sim p_\psi(\xi; 2\theta_{B,\alpha} - \theta_{A,\alpha})} \left[ \langle \theta_{B,\alpha} - \theta'_{B,\alpha}, \xi - \mathbb{E}[\xi] \rangle^2 \right]
\]

\[
= (\theta_{B,\alpha} - \theta'_{B,\alpha})^T \mathbb{E}_{\xi \sim p_\psi(2\theta_{B,\alpha} - \theta_{A,\alpha})} \left[ (\xi - \mathbb{E}[\xi])(\xi - \mathbb{E}[\xi])^T \right] (\theta_{B,\alpha} - \theta'_{B,\alpha})
\]

\[
= (\theta_{B,\alpha} - \theta'_{B,\alpha})^T \nabla^2 \psi(2\theta_{B,\alpha} - \theta_{A,\alpha})(\theta_{B,\alpha} - \theta'_{B,\alpha}) \nabla^2 \psi(2\theta_{B,\alpha} - \theta_{A,\alpha})
\]

\[
\leq c_2 \| \theta_{B,\alpha} - \theta'_{B,\alpha} \|_2^2,
\]

since, by smoothness, the spectral norm of \( \nabla^2 \psi \) is bounded by \( c_2 \).
For $T_2$, first note that
\[
\mathbb{E}_{\xi \sim p_{\psi}}(\xi; 2\theta_{B,\alpha} - \theta_{A,\alpha})|\xi| = \nabla \psi(2\theta_{B,\alpha} - \theta_{A,\alpha}) .
\]
Hence, with $\tilde{\theta}_{B,\alpha} = \gamma\theta_{B,\alpha} + (1 - \gamma\xi)\theta_{B',\alpha}$ for some $\gamma \in [0, 1]$, we have
\[
T_2 = \mathbb{E}_{\xi \sim p_{\psi}}(\xi; 2\theta_{B,\alpha} - \theta_{A,\alpha}) \left[ \left( \theta_{B,\alpha} - \theta_{B',\alpha}, \nabla \psi(\tilde{\theta}_{B,\alpha}) - \mathbb{E}[\xi] \right)^2 \right] \\
= \mathbb{E}_{\xi \sim p_{\psi}}(\xi; 2\theta_{B,\alpha} - \theta_{A,\alpha}) \left[ \left( \theta_{B,\alpha} - \theta_{B',\alpha}, \nabla \psi(\tilde{\theta}_{B,\alpha}) - \nabla \psi(2\theta_{B,\alpha} - \theta_{A,\alpha}) \right)^2 \right] \\
\leq \left\| \theta_{B,\alpha} - \theta_{B',\alpha} \right\|^2 \mathbb{E}_{\xi \sim p_{\psi}}(\xi; 2\theta_{B,\alpha} - \theta_{A,\alpha}) \left[ \left\| \nabla \psi(\tilde{\theta}_{B,\alpha}) - \nabla \psi(2\theta_{B,\alpha} - \theta_{A,\alpha}) \right\|^2 \right] \\
= c_2^2 \left\| \theta_{B,\alpha} - \theta_{B',\alpha} \right\|^2 \mathbb{E}_{\xi \sim p_{\psi}}(\xi; 2\theta_{B,\alpha} - \theta_{A,\alpha}) \left[ \left\| \theta_{B,\alpha} - (2\theta_{B,\alpha} - \theta_{A,\alpha}) \right\|^2 \right] \\
= c_2^2 \left\| \theta_{B,\alpha} - \theta_{B',\alpha} \right\|^2 \mathbb{E}_{\xi \sim p_{\psi}}(\xi; 2\theta_{B,\alpha} - \theta_{A,\alpha}) \left[ \left\| \gamma\theta_{B,\alpha} + (1 - \gamma\xi)\theta_{B',\alpha} - \theta_{B,\alpha} - (2\theta_{B,\alpha} - \theta_{A,\alpha}) \right\|^2 \right] \\
= c_2^2 \left\| \theta_{B,\alpha} - \theta_{B',\alpha} \right\|^2 \mathbb{E}_{\xi \sim p_{\psi}}(\xi; 2\theta_{B,\alpha} - \theta_{A,\alpha}) \left[ \left\| (1 - \gamma\xi)(\theta_{B',\alpha} - \theta_{B,\alpha}) - (2\theta_{B,\alpha} - \theta_{A,\alpha}) \right\|^2 \right] \\
\leq c_2^2 \left\| \theta_{B,\alpha} - \theta_{B',\alpha} \right\|^2 \left( \left\| \theta_{B',\alpha} - \theta_{B,\alpha} \right\|^2 \mathbb{E}_{\xi \sim p_{\psi}}(\xi; 2\theta_{B,\alpha} - \theta_{A,\alpha}) \left[ (1 - \gamma\xi)^2 \right] + \mathbb{E}_{\xi \sim p_{\psi}}(\xi; 2\theta_{B,\alpha} - \theta_{A,\alpha}) \left[ \left\| \theta_{B,\alpha} - \theta_{A,\alpha} \right\|^2 \right] \right) \\
= c_2^2 \left\| \theta_{B,\alpha} - \theta_{B',\alpha} \right\|^2 \left( \left\| \theta_{B',\alpha} - \theta_{B,\alpha} \right\|^2 + \left\| \theta_{B,\alpha} - \theta_{A,\alpha} \right\|^2 \right) .
\]
Putting everything back together
\[
\int_{\xi} \left( \theta_{B,\alpha} - \theta_{B',\alpha}, \xi - \nabla \psi(\bar{\theta}_{B,\alpha}) \right)^2 p_{\psi}(\xi; 2\theta_{B,\alpha} - \theta_{A,\alpha}) d\xi = c_2\left\| \theta_{B,\alpha} - \theta_{B',\alpha} \right\|^2 \left( 1 + 2c_2\left\| \theta_{B,\alpha} - \theta_{B',\alpha} \right\|^2 + 2c_2\left\| \theta_{B,\alpha} - \theta_{A,\alpha} \right\|^2 \right) .
\]
Similarly
\[
\int_{\xi} \left( \theta_{B,\alpha} - \theta_{B',\alpha}, \xi - \nabla \psi(\bar{\theta}_{B,\alpha}) \right)^2 p_{\psi}(\xi; 2\theta_{B',\alpha} - \theta_{A,\alpha}) d\xi = c_2\left\| \theta_{B,\alpha} - \theta_{B',\alpha} \right\|^2 \left( 1 + 2c_2\left\| \theta_{B,\alpha} - \theta_{B',\alpha} \right\|^2 + 2c_2\left\| \theta_{B',\alpha} - \theta_{A,\alpha} \right\|^2 \right) .
\]
Then, plugging into bound on $I_{A,B}$, we have
\[
I_{A,B} \leq c_2\left\| \theta_{B,\alpha} - \theta_{B',\alpha} \right\|^2 \times \exp \left[ 2c_2\left\| \theta_{B,\alpha} - \theta_{B',\alpha} \right\|^2 \right] \times \max \left( \exp \left[ 2c_2\left\| \theta_{B,\alpha} - \theta_{A,\alpha} \right\|^2 \right] \times \left( 1 + 2c_2\left\| \theta_{B,\alpha} - \theta_{B',\alpha} \right\|^2 + 2c_2\left\| \theta_{B,\alpha} - \theta_{A,\alpha} \right\|^2 \right) \right) ,
\]
Since $\alpha^2 \geq 8c_2\Delta^2(S_{n+1})$ where $\Delta(S_{n+1}) = \max_{z,z' \in S_{n+1}} \| \nabla \ell(w, z) - \nabla \ell(w, z') \|_2$, recalling that $\theta_{B,\alpha} = \nabla \ell(w, B)/\alpha$, we have
\[
2c_2\left\| \theta_{B,\alpha} - \theta_{B',\alpha} \right\|^2 \leq \frac{1}{4}, \quad 2c_2\left\| \theta_{B,\alpha} - \theta_{A,\alpha} \right\|^2 \leq \frac{1}{4}, \quad 2c_2\left\| \theta_{B',\alpha} - \theta_{A,\alpha} \right\|^2 \leq \frac{1}{4} .
\]
As a result, we have

\[ I_{A,B} \leq c_2 \|\theta_{B,\alpha} - \theta_{B',\alpha}\|^2 \times \exp\left(\frac{1}{4}\right) \times \exp\left(\frac{1}{4}\right) \times \left(1 + \frac{1}{4} + \frac{1}{4}\right) \]

\[ \leq \frac{5c_2}{2\alpha^2} \|\nabla \ell(w, S_B) - \nabla \ell(w, S'_B)\|^2. \]

That completes the proof. \(\square\)

B.3 Expected Stability of EFLD

**Theorem 2.** Consider an exponential family Langevin dynamics (EFLD) algorithm of the form (8)-(9) with a \( c_2 \)-smooth log-partition function \( \psi \). Then, for mini-batch size \( b \leq n/2 \), with \( c = c_0\sqrt{5c_2} \) (with \( c_0 \) as in Proposition I) and \( \alpha^2 \geq 8c_2 \Delta^2_1(S_{n+1}) \) (as in Theorem I with the conditioning on \( w_{t-1} \) hidden to avoid clutter), we have

\[ |\mathbb{E}_S[L_D(A(S)) - L_S(A(S))]| \leq c_1 \frac{\mathbb{E}_{\xi_t}}{n} \sum_{t=1}^{T} \mathbb{E}_{W_0(t-1)} \mathbb{E}_{B_t \in G_t, A_t \in G_0} |I_{A_t, B_t}|. \]

**Proof.** Based on Lemma I we have

\[ |\mathbb{E}_S[L_D(A(S)) - L_S(A(S))]| \leq c_1 \frac{b}{n} \mathbb{E}_S \mathbb{E}_{\xi_t} \sum_{t=1}^{T} \mathbb{E}_{W_0(t-1)} \mathbb{E}_{B_t \in G_t, A_t \in G_0} |I_{A_t, B_t}|. \]

with \( I_{A_t, B_t} = \int_{\xi_t} \left(\frac{dP_{B_t, \xi_t} - dP_{B'_t, \xi_t}}{dP_{A_t, \xi_t}}\right)^2 d\xi_t \).

From Theorem I we have

\[ I_{A_t, B_t} \leq \frac{5c_2}{2\alpha^2|W_{t-1}|} \left[ \|\nabla \ell(w_{t-1}, S_{B_t}) - \nabla \ell(w_{t-1}, S'_{B_t})\|^2 \right] \]

\[ = \frac{5c_2}{2\alpha^2|W_{t-1}|} \left[ \left\| \frac{1}{b} \sum_{z \in S'_{B_t}} \nabla \ell(w_{t-1}, z) - \frac{1}{b} \sum_{z \in S_{B_t}} \nabla \ell(w_{t-1}, z) \right\|^2 \right] \]

\[ = \frac{5c_2}{2\alpha^2|W_{t-1}|} \left[ \left\| \nabla \ell(w_{t-1}, z_n) - \nabla \ell(w_{t-1}, z'_n) \right\|^2 \right], \]

where the last equation holds because \( S_{B_t} \) and \( S'_{B_t} \) only differ at \( z_n \) and \( z'_n \).

Combining the above two inequalities, we have

\[ |\mathbb{E}_S[L_D(A(S)) - L_S(A(S))]| \leq c_1 \frac{b^{\prime}}{n} \mathbb{E}_S \mathbb{E}_{\xi_t} \sum_{t=1}^{T} \mathbb{E}_{W_0(t-1)} \mathbb{E}_{B_t \in G_t, A_t \in G_0} |I_{A_t, B_t}|. \]

That completes the proof. \(\square\)
C  Optimization Guarantees for EFLD

C.1  Optimization Guarantees for Noisy Sign-SGD

The “density” for a mini-batch $B$ at scale $\alpha$ is:

$$p_\psi(\xi; \theta_{B,\alpha}) = \exp(\langle \xi, \theta_{B,\alpha} \rangle - \psi(\theta_{B,\alpha})) \pi_0(\xi), \quad \theta_{B,\alpha} \triangleq \frac{\nabla \ell(w_t, S_B)}{\alpha}.$$  \hspace{1cm} (37)

Note that the corresponding expectation parameter

$$\mu_{B,\alpha} = \nabla \theta_{B,\alpha} \psi(\theta_{B,\alpha}).$$  \hspace{1cm} (38)

The full-batch Noisy Sign-SGD updates the parameters as

$$w_{t+1} = w_t - \eta_t \xi_t; \quad \xi_{t,i} \sim \text{Rad} \left( \frac{1}{1 + \exp \left( -2 \nabla L_S(w_t)/\alpha_t \right)} \right), \quad \forall i \in [d],$$  \hspace{1cm} (39)

where $\text{Rad}(x)$ is the parametric Rademacher distribution with density $x$ at 1 and density $1-x$ at $-1$. For mini-batch $B_t$ and scaling $\alpha_t$, mini-batch Noisy Sign-SGD updates the parameters as

$$w_{t+1} = w_t - \eta_t \xi_t; \quad \xi_{t,i} \sim \text{Rad} \left( \frac{1}{1 + \exp \left( -2 \theta_{B_t,\alpha_t} \right)} \right), \quad \forall i \in [d].$$  \hspace{1cm} (40)

We make the following smoothness assumptions of the empirical loss function $L_S(w)$:

**Assumption 1.** The loss function $L_S(w) = \frac{1}{n} \sum_{i=1}^{n} \ell(w, z_i)$ satisfies: $\forall w, w'$, for some non-negative constants $K := [K_1, \ldots, K_p]$, we have $L_S(w) \leq L_S(w') + \nabla L_S(w')^T(w - w') + \frac{1}{2} \sum_i K_i (w_i - w_i')^2$.

The assumption on on the empirical loss $L_S(w)$ is common in optimization analysis, besides that, we also assume some natural statistical properties of the batch gradient of the loss $\nabla \ell(w_t, S_{B_t})$, where the randomness comes from batches conditioned on $w_t$, satisfies the following assumptions:

**Assumption 2.** Given $w_{t-1}$, the mini-batch gradient $\nabla \ell(w_{t-1}, S_{B_t})$ is

(a) unbiased, i.e., $E_{B_t|w_{t-1}} \nabla \ell(w_{t-1}, S_{B_t}) = \nabla L_S(w_{t-1})$;

(b) symmetric, i.e., the density $p_{B_t|w_{t-1}}(\xi)$ of $\xi \equiv \nabla \ell(w_{t-1}, S_{B_t})$ is symmetric around its expectation $L_S(w_{t-1})$: $p_{B_t|w_{t-1}}(\xi) = p_{B_t|w_{t-1}}(2\nabla L_S(w_{t-1}) - \xi)$; and

(c) sub-Gaussian, i.e., for any $\lambda > 0$, any $v$ s.t. $\|v\|_2 = 1$,

$$E_{B_t|w_{t-1}}[\exp \lambda \langle v, \nabla \ell(w_{t-1}, S_{B_t}) - \nabla L_S(w_{t-1}) \rangle] \leq \exp(\lambda^2 \kappa_t^2/2),$$

for some constant $\kappa_t > 0$.

With Assumption [\ref{a1}] and Assumption [\ref{a2}], we have the following guarantee for convergence of noisy signSGD under full batch and mini batch settings. The following is a restate theorem from the main paper for the mini-batch Noisy Sign-SGD
Theorem 3. If the loss satisfies Assumption 1 for full-batch noisy Sign-SGD with step size $\rho_t = 1/\sqrt{T}$ and $\alpha_t$ satisfying $c \geq \alpha_t \geq \|\nabla S(w_t)\|\infty$, we have

$$E\left[\frac{1}{T} \sum_{t=1}^{T} \|\nabla L_S(w_t)\|^2 \right] \leq \frac{5c}{3\sqrt{T}} \left( L_S(w_0) - L_S(w^*) + \frac{1}{2} \|\tilde{K}\|_1 \right). \quad (16)$$

Further, if Assumption 2 holds, for mini-batch noisy Sign-SGD with step size $\eta_t = 1/\sqrt{T}$, and $\alpha_t$ satisfying $c \geq \alpha_t \geq \max[\sqrt{2}\kappa_t, 4\|\nabla L_S(w_t)\|\infty]$, we have

$$E\left[\frac{1}{T} \sum_{t=1}^{T} \|\nabla L_S(w_t)\|^2 \right] \leq \frac{4e}{\sqrt{T}} \left( L_S(w_0) - L_S(w^*) + \frac{1}{2} \|\tilde{K}\|_1 \right), \quad (17)$$

where equation (16) (17) holds for any $S$, any initialization $w_0$, and the expectation is taken over the randomness of algorithm.

Proof. First we prove Equation (16) for full-batched settings. Conditioned at $t$-th iteration, with Assumption 1 we have

$$L_S(w_{t+1}) - L_S(w_t) \leq \nabla L_S(w_t)^T (w_{t+1} - w_t) + \frac{1}{2} \sum_{i=1}^{d} K_i (w_{t+1,i} - w_{t,i})^2$$

$$= -\eta_t \nabla L_S(w_t)^T \xi_t + \eta_t^2 \sum_{i=1}^{d} K_i^2 / 2.$$ 

Then taking conditional expectation on both side for above equation we have

$$E[L_S(w_{t+1}) - L_S(w_t)] \leq -\eta_t \nabla L_S(w_t)^T E[\xi_t] + \eta_t^2 / 2 \|\tilde{K}\|_1$$

$$= -\eta_t \sum_i \nabla L_S(w_t)_i \left[ \frac{2}{1 + \exp(-2\nabla L_S(w_t)_i / \alpha_t)} - 1 \right] + \frac{\eta_t^2}{2} \|\tilde{K}\|_1$$

$$= -\eta_t \sum_i \nabla L_S(w_t)_i \left[ \frac{\exp(2\nabla L_S(w_t)_i / \alpha_t)}{\exp(2\nabla L_S(w_t)_i / \alpha_t) - 1} \right] + \frac{\eta_t^2}{2} \|\tilde{K}\|_1$$

$$= -\eta_t \sum_i \nabla L_S(w_t)_i \tanh(\nabla L_S(w_t)_i / \alpha_t) + \frac{\eta_t^2}{2} \|\tilde{K}\|_1$$

$$= -\eta_t \sum_i ||\nabla L_S(w_t)_i|| \tanh(\nabla L_S(w_t)_i / \alpha_t) + \frac{\eta_t^2}{2} \|\tilde{K}\|_1.$$ 

By taking $c \geq \alpha_t \geq ||\nabla L_S(w_t)||\infty$, and $\eta_t = 1/\sqrt{T}$, we have $\nabla L_S(w_t)_i / \alpha_t \leq 1$ so we can apply Lemma 7 to have

$$E[L_S(w_{t+1}) - L_S(w_t)] \leq -\frac{e^2 - 1}{(e^2 + 1)\alpha_t \sqrt{T}} \|\nabla L_S(w_t)\|_2^2 + \frac{1}{2T} \|\tilde{K}\|_1$$

$$\leq -\frac{3}{5c \sqrt{T}} \|\nabla L_S(w_t)\|_2^2 + \frac{1}{2T} \|\tilde{K}\|_1.$$ 

By telescope sum we have

$$E\left[\frac{1}{T} \sum_{t=1}^{T} \|\nabla L_S(w_t)\|^2 \right] \leq \frac{5c}{3\sqrt{T}} \left( L_S(w_0) - L_S(w^*) + \frac{1}{2} \|\tilde{K}\|_1 \right), \quad (41)$$
which completes the proof of full-batch updates.

Then we turn to prove Equation (17) for mini-batch settings. From smoothness condition Assumption 1, we have

\[
\mathbb{E}[L_S(w_{t+1}) - L_S(w_t)|w_t] \leq \mathbb{E}_{w_{t+1}|w_t} \nabla L_S(w_t)^T(w_{t+1} - w_t) + \frac{1}{2} \mathbb{E}_{w_{t+1}|w_t} \sum_{i=1}^{d} L_i(w_{t+1,i} - w_{t,i})^2
\]

\[
= \mathbb{E}_{\xi_i|w_t} \nabla L_S(w_t)^T(-\eta \xi_t) + \frac{1}{2} \mathbb{E}_{\xi_i|w_t} \sum_{i=1}^{d} L_i(-\eta \xi_t)^2
\]

\[
= -\eta \mathbb{E}_{\xi_i|w_t} \nabla L_S(w_t)^T(\mathbb{E}_{\xi_i|w_t} \xi_t) + \frac{1}{2} \mathbb{E}_{\xi_i|w_t} \sum_{i=1}^{d} L_i(-\eta \xi_t)^2
\]

\[
= -\eta \mathbb{E}_{\xi_i|w_t} \nabla L_S(w_t)^T(\mathbb{E}_{\xi_i|w_t} \xi_t) + \frac{\eta^2}{2} \|\vec{K}\|_1
\]

Focus on each individual term in the sum, we have

\[
\mathbb{E}_{\mathbb{B}_i|w_t}[\theta_{B,i}] \mathbb{E}_{\mathbb{B}_i|w_t} \left[ \frac{\exp(2\theta_{B,i}/\alpha_t) - 1}{\exp(2\theta_{B,i}/\alpha_t) + 1} \right] = \mathbb{E}_{\mathbb{B}_i|w_t}[\theta_{B,i}] \mathbb{E}_{\mathbb{B}_i|w_t} \left[ \frac{\exp(2\theta_{B,i}/\alpha_t - 2\mathbb{E}_{\mathbb{B}_i|w_t}[\theta_{B,i}/\alpha_t]) - \exp(-2\mathbb{E}_{\mathbb{B}_i|w_t}[\theta_{B,i}/\alpha_t])}{\exp(2\theta_{B,i}/\alpha_t - 2\mathbb{E}_{\mathbb{B}_i|w_t}[\theta_{B,i}/\alpha_t]) + \exp(-2\mathbb{E}_{\mathbb{B}_i|w_t}[\theta_{B,i}/\alpha_t])} \right]
\]

For ease of notation, denote \(2\theta_{B,i}/\alpha_t - \mathbb{E}_{\mathbb{B}_i|w_t}[2\theta_{B,i}/\alpha_t] = \theta, \mathbb{E}_{\mathbb{B}_i|w_t}[2\theta_{B,i}/\alpha_t] = \mu, \) and the pdf of \(\theta\) is \(p_\theta\) for the moment, then from Assumption 2, we have \(\theta\) is mean zero, symmetric around zero, and subgaussian with \(\psi_2\) norm \(2\kappa_t/\alpha_t\) by taking \(\lambda = 1, v = 1\), in the sub-Gaussian assumption: \(\mathbb{E}_{\theta}[\exp(\theta)] \leq \exp(2\kappa_t^2/\alpha_t^2)\).

Therefore, by changing notation we have

\[
\mathbb{E}_{\mathbb{B}_i|w_t}[\theta_{B,i}] \mathbb{E}_{\mathbb{B}_i|w_t} \left[ \frac{\exp(2\theta_{B,i}/\alpha_t) - 1}{\exp(2\theta_{B,i}/\alpha_t) + 1} \right] = \frac{\alpha_t \mu}{2} \mathbb{E}_{\theta} \left[ \frac{\exp(\theta) - \exp(-\mu)}{\exp(\theta) + \exp(-\mu)} \right].
\]

By symmetry of the distribution of \(\theta\), we have

\[
\frac{\alpha_t \mu}{2} \mathbb{E}_{\theta} \left[ \frac{\exp(\theta) - \exp(-\mu)}{\exp(\theta) + \exp(-\mu)} \right] = \frac{\alpha_t \mu}{2} \int_{-\infty}^{\infty} p_\theta(x) \left[ \frac{\exp(\theta) - \exp(-\mu)}{\exp(\theta) + \exp(-\mu)} \right] dx
\]

\[
= \frac{\alpha_t \mu}{2} \int_{-\infty}^{\infty} p_\theta(x) \left[ \frac{\exp(\theta) - \exp(-\mu)}{\exp(\theta) + \exp(-\mu)} + \frac{\exp(-x) - \exp(-\mu)}{\exp(-x) + \exp(-\mu)} \right] dx
\]

\[
= \frac{\alpha_t \mu}{2} \int_{0}^{\infty} \frac{p_\theta(x)(\exp(-x) - \exp(-\mu))(\exp(-x) + \exp(-\mu)) + (\exp(-x) - \exp(-\mu))(\exp(x) + \exp(-\mu))}{\exp(x) + \exp(-\mu)} dx
\]

\[
= \frac{\alpha_t}{2} \int_{0}^{\infty} \frac{2\mu(1 - \exp(-2\mu))}{\exp(x) + \exp(-\mu)} dx
\]

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By symmetry, we have \( p_\theta(x) = p_\theta(-x) \), and therefore
\[
\alpha_t / 2 \int_0^\infty p_\theta(x) \left( 2\mu(1 - \exp(-2\mu)) \right) \frac{dx}{(\exp x + \exp(-\mu))(\exp(-x) + \exp(-\mu))}
= \alpha_t / 2 \int_{-\infty}^\infty p_\theta(x) \left( \mu(1 - \exp(-2\mu)) \right) \frac{dx}{(\exp x + \exp(-\mu))(\exp(-x) + \exp(-\mu))}
= \frac{\alpha_t}{2} (\mu(1 - \exp(-2\mu))) \mathbb{E}_\theta \left( \frac{1}{\exp \theta + \exp(-\mu)} \right) \frac{1}{\exp \theta + \exp(-\mu) + \exp(-\mu)}
\]
Since \( \frac{\alpha_t}{2} (\mu(1 - \exp(-2\mu))) \geq 0 \), and \( \frac{1}{x} \) is convex on \( \mathbb{R}_+ \), we have
\[
\frac{\alpha_t}{2} (\mu(1 - \exp(-2\mu))) \mathbb{E}_\theta \left( \frac{1}{\exp \theta + \exp(-\mu)} \right) \frac{1}{\exp \theta - \exp(-\mu) + \exp(-\mu)}
\geq \frac{\alpha_t}{2} (\mu(1 - \exp(-2\mu))) \mathbb{E}_\theta \left( \frac{1}{\exp \theta + \exp(-\mu)} \right) \frac{1}{2 \exp(2\kappa_t^2/\alpha_t^2)}
\]
Using the sub-Gaussian property of \( \theta \): \( \mathbb{E}_\theta[\exp \theta] \leq \exp(2\kappa_t^2/\alpha_t^2) \), and symmetry so \( \mathbb{E}_\theta[\exp -\theta] \leq \exp(2\kappa_t^2/\alpha_t^2) \), we have
\[
\frac{\alpha_t}{2} (\mu(1 - \exp(-2\mu))) \mathbb{E}_\theta \left( \frac{1}{\exp \theta + \exp(-\mu)} \right) \frac{1}{2 \exp(2\kappa_t^2/\alpha_t^2)}
= \mathbb{E}_{B_i|\theta} B_i, \theta_{B_i}(1 - \exp(-4\mathbb{E}_{B_i|\theta} B_i, \theta_{B_i}/\alpha_t)) \frac{1}{2 \exp(2\kappa_t^2/\alpha_t^2)}
= \nabla L_S(w_\theta i)(1 - \exp(-4\nabla L_S(w_\theta i)/\alpha_t)) \frac{1}{2 \exp(2\kappa_t^2/\alpha_t^2)}
\]
Switching back to our previous notation:
\[
\frac{\alpha_t}{2} (\mu(1 - \exp(-2\mu))) \mathbb{E}_\theta \left( \frac{1}{\exp \theta + \exp(-\mu)} \right) \frac{1}{2 \exp(2\kappa_t^2/\alpha_t^2)}
= \mathbb{E}_{B_i|\theta} B_i, \theta_{B_i}(1 - \exp(-4\mathbb{E}_{B_i|\theta} B_i, \theta_{B_i}/\alpha_t)) \frac{1}{2 \exp(2\kappa_t^2/\alpha_t^2)}
\]
which implies we have
\[
\mathbb{E}[L_S(w_{t+1}) - L_S(w_t)|w_t] \leq -\frac{\eta_t}{2 \exp(2\kappa_t^2/\alpha_t^2)} \sum_i \nabla L_S(w_\theta i)(1 - \exp(-4\nabla L_S(w_\theta i)/\alpha_t)) + \frac{\eta_t^2}{2} \|K\|_1.
\]
Using Lemma\[8\] we have
\[
\mathbb{E}[L_S(w_{t+1}) - L_S(w_t)|w_t] \leq -\frac{\eta_t}{2(1 + \exp(2\kappa_t^2/\alpha_t^2))} \sum_i |\nabla L_S(w_\theta i)| \min \left[ 2\nabla L_S(w_\theta i)/\alpha_t, 0.5 \right] + \frac{\eta_t^2}{2} \|K\|_1.
\]
(42)
We choose \( \alpha_t \) such that \( \alpha_t \geq 4\|\nabla L_S(w_\theta)\|_\infty \), then we have
\[
\mathbb{E}[L_S(w_{t+1}) - L_S(w_t)|w_t] \leq -\frac{\eta_t}{\alpha_t(1 + \exp(2\kappa_t^2/\alpha_t^2))} \|\nabla L_S(w_\theta)\|^2 + \frac{\eta_t^2}{2} \|K\|_1.
\]
(43)
36
We choose \( \alpha_t \) such that \( c \geq \alpha_t \geq \max[\sqrt{2} \kappa_t, 4 \| \nabla L_S(w_t) \|_\infty] \), then we have

\[
\mathbb{E}[L_S(w_{t+1}) - L_S(w_t) | w_t] \leq -\frac{\eta_t}{c(1+e)} \| \nabla L_S(w_t) \|_2^2 + \frac{\eta_t^2}{2} \| \tilde{K} \|_1.
\] (44)

Therefore, if we choose \( \eta_t = 1/\sqrt{T} \), we have

\[
\mathbb{E}[L_S(w_{t+1}) - L_S(w_t) | w_t] \leq -\frac{1}{c(1+e)\sqrt{T}} \| \nabla L_S(w_t) \|_2^2 + \frac{1}{2T} \| \tilde{K} \|_1.
\] (45)

By telescope sum, we have

\[
\mathbb{E} \left[ \frac{1}{T} \sum_{t=1}^T \| \nabla L_S(w_t) \|_2^2 \right] \leq \frac{(1+e)c}{\sqrt{T}} \left( L_S(w_0) - L_S(w^*) + \frac{1}{2} \| \tilde{K} \|_1 \right).
\] (46)

and note that \( 1 + e < 4 \) which completes the proof.

**Lemma 7.** For any \(-1 \leq x \leq 1\), the following holds:

\[
| \tanh x | \geq \frac{e^2 - 1}{e^2 + 1} |x|
\] (47)

**Proof.** Without loss of generality, we focus on \( 0 < x \leq 1 \). We prove \( \tanh x/x \) is decreasing function on \( \mathbb{R}^+ \), which is equivalent to

\[
\left( \frac{\tanh x}{x} \right)' = \frac{x(1 - \tanh^2 x) - \tanh x}{x^2} \leq 0,
\]

and is equivalent to

\[
x \leq \frac{\tanh x}{1 - \tanh^2 x},
\]

where the right hand side is \( \sinh x \) and use the fact that \( x \leq \sinh x \) for \( x > 0 \) implies \( \tanh x/x \) is decreasing function, so

\[
\tanh x/x \geq \tanh 1 = \frac{e^2 - 1}{e^2 + 1},
\]

which completes the proof.

**Lemma 8.** For any \( x \),

\[
|1 - \exp(-2x)| \geq \min(|x|, \frac{1}{2}).
\]

**Proof.** Since \( \exp(-x) \geq 1 - x \), so we have for \( x < 0 \):

\[
1 - \exp(-2x) \leq 2x \leq x.
\]

For \( x > 0 \), since \( \exp x \geq 1 + x \), we have \( \exp -x \leq \frac{1}{1+x} \), so

\[
1 - \exp(-2x) \geq \frac{2x}{1+2x}.
\]
Then when $\frac{1}{2} > x > 0$,

$$\frac{2x}{1 + 2x} > x,$$

and when $x \geq \frac{1}{2}$,

$$\frac{2x}{1 + 2x} \geq \frac{1}{2},$$

which completes the proof.

**Theorem 4.** Under Assumptions 1 and 2 with $K_i = K, \forall i \in [p]$, for any training set $S$, SGLD, i.e., EFLD with Gaussian noise, $\rho_t = \eta_t, \alpha_t = \sigma_t / \eta_t$, batch size $|B_t| = b$, and step size $\eta_t = \frac{1}{\sqrt{T}}$ satisfies

$$\frac{1}{T} \sum_{t=1}^{T} \mathbb{E} \|\nabla L_S(w_t)\|^2 \leq \frac{L_S(w_1) - L_S(w^*)}{\sqrt{T}} + \frac{K \eta_T^2}{2 \sqrt{T}} \sum_{t=1}^{T} (p \alpha_t^2 + c_3 \kappa_t^2),$$

where $w_1$ are the initial parameters, $w^*$ is a minima of $L_S(w)$, $c_3$ is an absolute constant, and the expectation is over the randomness of the algorithm.

**Proof.** Recall that the update of SGLD is

$$w_{t+1} = w_t - \eta_t \nabla \ell (w_t, S_{B_t}) + \sigma_t N(0, I_d).$$

By smoothness of the loss, taking expectation w.r.t. the randomness of the mini-batch $B_t$ and the Gaussian draw $g_t \sim N(0, I_d)$ conditioned on $w_{1:t}$, we have

$$\mathbb{E}[L_S(w_{t+1})] \leq L_S(w_t) + \mathbb{E}[(\nabla L_S(w_t), w_{t+1} - w_t)] + \frac{K}{2} \mathbb{E} [\|w_{t+1} - w_t\|^2]$$

$$= L_S(w_t) + \mathbb{E}[\langle \nabla L_S(w_t), -\eta_t \nabla \ell (w_t, S_{B_t}) + \sigma_t g_t \rangle] + \frac{K}{2} \mathbb{E} [\| - \eta_t \nabla \ell (w_t, S_{B_t}) + \sigma_t g_t \|^2]$$

$$(a) \leq L_S(w_t) - \eta_t \|\nabla L_S(w_t)\|^2 + \frac{K \eta_t^2}{2} (c_3 \kappa_t^2 + p \alpha_t^2 / \eta_t^2),$$

where (a) follows since $\mathbb{E}[\nabla \ell (w_t, S_{B_t})] = 0$, $\mathbb{E}[g] = 0$, $\mathbb{E}[\|g\|^2] = p$, and $\mathbb{E}[\|\nabla \ell (w_t, S_{B_t})\|^2] \leq c_3 \kappa_t^2$ for some absolute constant $c_3$ since $\nabla \ell (w_t, S_{B_t})$ is sub-Gaussian with $\psi_2$-norm $\kappa_t$.

Rearranging the above inequality and using $\alpha_t = \sigma_t / \eta_t$ we have

$$\eta_t \|\nabla L_S(w_t)\|^2 \leq L_S(w_t) - \mathbb{E}[L_S(w_{t+1})] + \frac{K \eta_t^2}{2} (c_3 \kappa_t^2 + p \alpha_t^2).$$

Summing over $t = 1$ to $t = T$ and apply expectation over the trajectory at each step, we have

$$\sum_{t=1}^{T} \eta_t \mathbb{E} [\|\nabla L_S(w_t)\|^2] \leq L_S(w_1) - L_S(w^*) + \sum_{t=1}^{T} \frac{K \eta_t^2}{2} (p \alpha_t^2 + \kappa_t^2),$$

where $w^*$ is a minima of $L_S(w)$. With $\eta_t = \frac{1}{\sqrt{T}}$ for all $t \in [T]$, we have

$$\frac{1}{T} \sum_{t=1}^{T} \mathbb{E} [\|\nabla L_S(w_t)\|^2] \leq \frac{L_S(w_1) - L_S(w^*)}{\sqrt{T}} + \frac{K \eta_T^2}{2 \sqrt{T}} \sum_{t=1}^{T} (p \alpha_t^2 + c_3 \kappa_t^2).$$

That completes the proof.
D Experiment Details

Datasets. We use MNIST [LeCun et al. (1998)], Fashion-MNIST [Xiao et al. (2017)], CIFAR-10 [Krizhevsky (2009)] and CIFAR-100 [Krizhevsky (2009)] in our experiments.

MNIST dataset: 60,000 black and white training images, including handwritten digits 0 to 9. We use a subset of MNIST with \( n = 10,000 \) data points where 1,000 samples from each class are randomly selected. Each image of size \( 28 \times 28 \) is first re-scaled into \([0, 1]\) by dividing each pixel value by 255, then z-scored by subtracting the mean and dividing the standard deviation of the training set.

Fashion-MNIST dataset: 60,000 gray-scale training images and 10,000 test images, including 10 clothing categories such as shirts, dresses, sandals, etc. Each image of size \( 28 \times 28 \) is first re-scaled into \([0, 1]\) by dividing each pixel value by 255, then z-scored by subtracting the mean and dividing the standard deviation of the training set.

CIFAR-10/-100 dataset: 60,000 color images consisting of 10/100 categories, e.g., airplane, cat, dog etc. The training set includes 50,000 images while the test set contains the rest 10,000 images. Each image of size \( 32 \times 32 \) has 3 color channels. We first re-scale each image into \([0, 1]\) by dividing each pixel value by 255, then each image is normalized by subtracting the mean and dividing the standard deviation of the training set for each color channel. We also use RandomCrop and RandomHorizontalFlip for data augmentation.

Network Architectures. For experiments on both MNIST and Fashion-MNIST, we use a convolutional neural network with two convolutional layers followed by two fully connected layers with ReLU activations. For experiments use the CIFAR-10 dataset, we consider CNN architecture with two convolutional layers and three fully connected layers. The detail of each CNN architecture can be found in Table 1 and Table 2.

| Table 1: CNN architecture for MNIST and Fashion MNIST. | Parameters |
|---|---|
| Convolution | 32 filters of \( 5 \times 5 \) |
| Max-Pooling | \( 2 \times 2 \) |
| Convolution | 64 filters of \( 5 \times 5 \) |
| Max-Pooling | \( 2 \times 2 \) |
| Fully connected | 1024 units |
| Softmax | 10 units |

| Table 2: CNN architecture for CIFAR-10. | Parameters |
|---|---|
| Convolution | 64 filters of \( 5 \times 5 \) |
| Max-Pooling | \( 2 \times 2 \) |
| Convolution | 192 filters of \( 5 \times 5 \) |
| Max-Pooling | \( 2 \times 2 \) |
| Fully connected | 384 units |
| Fully connected | 192 units |
| Softmax | 10 units |

Experimental setup. We are interested in stochastic gradient Langevin dynamics, whose iterative updates are given by \( \mathbf{w}_t = \mathbf{w}_{t-1} - \eta_t \nabla \ell(\mathbf{w}_{t-1}, S_{B_t}) + N(0, \sigma_t^2 \mathbb{I}_d) \). We also denote \( \beta_t = 2\eta_t/\sigma_t^2 \) as the
inverse temperature at time $t$. For MNIST and Fashion-MNIST, the initial learning rate is $\eta_0 = 0.004$ and it decays by 0.96 after every 5 epochs. For CIFAR-10, the initial learning rate is $\eta_0 = 0.005$ and it decays by 0.995 after every 5 epochs. We use batch size $|B_t| = 100$ for MNIST and Fashion-MNIST, and $|B_t| = 200$ for CIFAR-10.

Motivated by Zhang et al. (2017), we train CNN with SGLD on a smaller subset of MNIST dataset ($n = 10000$) with randomly corrupted labels. The corruption fraction varies from 0% (without label corruption) to 60%. For different level of randomness, we use the same training setting with batch size $|B_t| = 100$, initial step size $\eta_0 = 0.005$, noise variance $\sigma_t = 0.2 \cdot \eta_t$, and we decay $\eta_t$ by 0.995 for every 30 epochs.

We are also interested in Noisy Sign-SGD whose iterative updates are given by $w_{t+1} = w_t - \eta \xi_t$, where $\xi_{t,j} \sim p_{\theta_{B_t},\alpha_t}(\xi_j) = \frac{\exp(\xi_j \theta_{B_t,\alpha_t})}{\exp(-\theta_{B_t,\alpha_t}) + \exp(\theta_{B_t,\alpha_t})}$. The initial learning rate is $\eta_0 = 10^{-4}$ and it decays by 0.1 after every 30 epochs. We use batch size $|B_t| = 100$ for all benchmarks.

All experiments minimize cross-entropy loss for a fixed number of epochs and have been run on NVIDIA Tesla K40m GPUs. For CNN, we repeat each experiment 30 times, and for ResNet-18, we repeat 5 times.

Table 3: Details of Experiments reported in Figure 1 and 4 for MNIST and Fashion-MNIST with CNN

| Parameter            | Values                                      |
|----------------------|---------------------------------------------|
| Dataset              | MNIST/ Fashion-MNIST                        |
| Architecture         | CNN with 2 conv. layers and 2 linear layers  |
| Batch Size           | 100                                         |
| Learning Rate        | $\eta_0 = 4 \times 10^{-3}$, decay epochs=5, decay rate=0.96 |
| Inverse Temperature  | $\beta \in [5000, 55000]$                  |
| Number of Epochs     | 50                                          |
| No. of training examples | 55000                                    |
| Number of Repeated Runs | 30                                          |

Table 4: Details of Experiments reported in Figure 1 and 5 for CIFAR-10 with CNN

| Parameter            | Values                                      |
|----------------------|---------------------------------------------|
| Dataset              | CIFAR-10                                    |
| Architecture         | CNN with 2 conv. layers and 3 linear layers  |
| Batch Size           | 200                                         |
| Learning Rate        | $\eta_0 = 5 \times 10^{-3}$, decay epochs=5, decay rate=0.995 |
| Inverse Temperature  | $\beta \in [5000, 55000]$                  |
| Number of Epochs     | 1000                                        |
| No. of training examples | 55000                                    |
| Number of Repeated Runs | 20                                          |
Table 5: Details of Experiments reported in Figure 2 for MNIST with CNN ($\sigma_t = 0.2 \cdot \eta_t$)

| Parameter                  | Values                                      |
|----------------------------|---------------------------------------------|
| Dataset                    | MNIST                                       |
| Architecture               | CNN with 2 conv. layers and 2 linear layers |
| Batch Size                 | 100                                         |
| Learning Rate              | $\eta_0 = 5 \times 10^{-3}$, decay epochs=30, decay rate=0.995 |
| Number of Epochs           | 1000                                        |
| No. of training examples   | 10000                                       |
| Number of Repeated Runs    | 30                                          |
Figure 4: Numerical results for CNN trained on MNIST using SGLD with a small noise variance $\sigma_t \approx 10^{-4}$. 
Figure 5: Numerical results for training CNN using SGLD on CIFAR-10.
Figure 6: Numerical results for CNN trained on MNIST using Noisy SGD. We follow the setting described in Li et al. (2020). The initial $\eta_t$ is $4 \times 10^{-3}$, and decays by 0.95 ($\alpha_t = 0.2$) or 0.995 ($\alpha_t = 0.002$) for every 5 epochs.
Figure 7: Numerical results for training CNN on MNIST and Fashion-MNIST using Noisy Sign-SGD. Increasing $\alpha_t$ leads to a tighter generalization bound even though it leads to a slightly larger gradient discrepancy.