Data-Dependent Stability of Stochastic Gradient Descent

Ilja Kuzborskij\textsuperscript{a,b,c} and Christoph Lampert\textsuperscript{d}

\textsuperscript{a}Idiap Research Institute, Switzerland
\textsuperscript{b}EPFL, Switzerland
\textsuperscript{c}University of Rome La Sapienza, Italy
\textsuperscript{d}IST Austria

March 7, 2017

Abstract
We establish a data-dependent notion of algorithmic stability for Stochastic Gradient Descent (SGD) and employ it to develop novel generalization bounds. This is in contrast to previous distribution-free algorithmic stability results for SGD which depend on the worst-case constants. By virtue of the data-dependent argument, our bounds provide new insights into learning with SGD on convex and non-convex problems.

In the convex case, we show that the bound on the generalization error is multiplicative in the risk at the initialization point. In the non-convex case, we prove that the expected curvature of the objective function around the initialization point has crucial influence on the generalization error. In both cases, our results suggest a simple data-driven strategy to stabilize SGD by pre-screening its initialization.

1 Introduction
Stochastic gradient descent (SGD) has become one of the workhorses of modern machine learning. In particular, it is the optimization method of choice for training highly complex and non-convex models, such as neural networks. When it was observed that these models generalize better (suffer less from overfitting) than classical machine learning theory suggests, a large theoretical interest emerged to explain this phenomenon. Given that SGD at best finds a local minimum of the non-convex objective function, it has been argued that all such minima might be equally good. However, at the same time, a large body of empirical work and tricks of trade, such as early stopping, suggests that in practice one might not even reach a minimum, yet nevertheless observes excellent performance.

In this work we follow an alternative route that aims to directly analyze the generalization ability of SGD by studying how sensitive it is to small perturbations in the training set. This is known as algorithmic stability approach (Bousquet and Elisseeff, 2002) and recently Hardt et al. (2016) used it to establish generalization bounds for both convex and non-convex learning settings. To do so they employed a rather restrictive notion of stability that does not depend on the data, but captures only intrinsic characteristics of the learning algorithm and global properties of the objective function. Consequently, their analysis results in worst-case guarantees that in some cases

\textsuperscript{*}ilja.kuzborskij@idiap.ch, work performed at IST Austria.
\textsuperscript{†}chl@ist.ac.at
tend to be too pessimistic. As recently pointed out by Zhang et al. (2017), deep learning might indeed be such a case, as this notion of stability is insufficient to give deeper theoretical insights, and a less restrictive one is desirable.

**Our main contribution** in this work is two-fold: we introduce a new data-dependent notion of algorithmic stability and prove that this stability property holds for SGD as a learning algorithm for convex as well as non-convex problems. As a consequence we obtain new generalization bounds that depend on the data-generating distribution and the initialization point of an algorithm. For convex loss functions, the bound on the generalization error is multiplicative in the risk at the initialization point. For the non-convex loss functions, besides the risk, it is also critically controlled by the expected second-order information about the objective function at the initialization point.

In particular, our findings justify the intuition that SGD is more stable in flat areas of the objective function and link it to the generalization ability. This also backs up numerous empirical findings in the deep learning literature that solutions with low generalization error occur in flat regions. At the same time, in pessimistic scenarios, our bounds are no worse than those of Hardt et al. (2016).

Finally, we exemplify an application of our bounds, and propose a simple yet principled transfer learning scheme for the convex and non-convex case, which is guaranteed to transfer from the best source of information. In addition, this approach can also be used to select a good initialization given a number of random starting positions. This is a theoretically sound alternative to the purely random start popular in non-convex learning.

The rest of the paper is organized as follows. We revisit the connection between stability and generalization of SGD in Section 3 and introduce a data-dependent notion of stability in Section 4. Next, we state the main results in Section 5, in particular, Theorem 3 for the convex case, and Theorem 4 for the non-convex one. We demonstrate applications of these bounds by showcasing principled transfer learning approaches in Section 5.3. Finally, in Section 6 we present proofs, and conclude in Section 7.

## 2 Related Work

Algorithmic stability has been a topic of interest in learning theory for a long time, however, the modern approach on the relationship between stability and generalization goes back to the milestone work of Bousquet and Elisseeff (2002). They analyzed several notions of stability, which fall into two categories: distribution-free and distribution-dependent ones. The first category is usually called uniform stability and focuses on the intrinsic stability properties of an algorithm without regard to the data-generating distribution. Uniform stability was used to analyze many algorithms, including regularized Empirical Risk Minimization (ERM) (Bousquet and Elisseeff, 2002), randomized aggregation schemes (Elisseeff et al., 2005), and recently SGD by Hardt et al. (2016); London (2016), and Poggio et al. (2011). Despite the fact that uniform stability has been shown to be sufficient to guarantee learnability, it can be too pessimistic, resulting in the worst-case rates.

In this work we are interested in the data-dependent behavior of SGD, thus the emphasis will fall on the distribution-dependent notion of stability, known as the hypothesis stability and also as the average stability (Shalev-Shwartz et al., 2010). The attractive quality of this less restrictive stability type is that the resulting bounds are controlled by how stable the algorithm is under the data-generating distribution. For instance, in works of Bousquet and Elisseeff (2002) and Devroye and Wagner (1979), the hypothesis stability is related to the variance of an estimator. Shalev-Shwartz and Ben-David (2014, Sec. 13) show risk bounds that depend on the expected empirical risk of a solution to the regularized ERM. In turn, one can exploit this fact to state improved risk bounds, for instance, ones that exhibit fast-rate regimes (Koren and Levy, 2015; Gonen and Shalev-Shwartz, 2017), or even to design enhanced algorithms that minimize these bounds in a
data-driven way, e.g. by exploiting side information as in transfer (Kuzborskij and Orabona, 2013; Ben-David and Urner, 2013) and metric learning (Perrot and Habrard, 2015). Here, we focus on the later direction in the context of SGD: how stable is SGD under the data-generating distribution given an initialization point of interest?

We will study the hypothesis stability of SGD for both convex and non-convex loss functions. In the convex setting, we will relate stability to the risk at the initialization point, while previous data-driven stability arguments usually consider minimizers of convex ERM rather than a stochastic approximation (Shalev-Shwartz and Ben-David, 2014; Koren and Levy, 2015). Beside convex problems, our work also touches generalization ability of SGD on non-convex problems. Here, we borrow techniques of Hardt et al. (2016) and extend them to the distribution-dependent setting. That said, while bounds of Hardt et al. (2016) are stated in terms of worst-case quantities, ours reveal new connections to the data-dependent second-order information. These new insights also partially justify empirical observations in deep learning about the link between the curvature and the generalization error (Hochreiter and Schmidhuber, 1997; Keskar et al., 2017; Chaudhari et al., 2017). At the same time, our work is an alternative to the theoretical studies of neural network objective functions (Choromanska et al., 2015; Kawaguchi, 2016), as we focus on the direct connection between the generalization and the curvature.

In this light, our work is also related to non-convex optimization by SGD. Literature on this subject typically studies rates of convergence to the stationary points (Ghadimi and Lan, 2013; Allen-Zhu and Hazan, 2016; Reddi et al., 2016), and ways to avoid saddles (Ge et al., 2015; Lee et al., 2016). However, unlike these works, and similarly to Hardt et al. (2016), we are interested in the generalization ability of SGD, and thanks to the stability approach, involvement of stationary points in our analysis is not necessary.

Finally, we propose an example application of our findings in Transfer Learning (TL). For instance, by controlling the stability bound in a data-driven way, one can choose an initialization that leads to improved generalization. This is related to TL where one transfers from pre-trained models (Kuzborskij and Orabona, 2016; Tommasi et al., 2014; Pentina and Lampert, 2014; Ben-David and Urner, 2013), especially popular in deep learning due to its data-demanding nature (Galanti et al., 2016). Theoretical literature on this topic is mostly focused on the ERM setting and PAC-bounds, while our analysis of SGD yields such guarantees as a corollary.

3 Stability of Stochastic Gradient Descent

First we introduce definitions used in the rest of the paper.

3.1 Definitions

We will denote with small and capital bold letters respectively column vectors and matrices, e.g., $a = [a_1, a_2, \ldots, a_d]^T \in \mathbb{R}^d$ and $A \in \mathbb{R}^{d_1 \times d_2}$, $\|a\|$ is understood as a Euclidean norm and $\|A\|_2$ as a spectral norm. We denote enumeration by $[n] = \{1, \ldots, n\}$ for $n \in \mathbb{N}$.

We indicate an example space by $\mathcal{Z}$ and its member by $z \in \mathcal{Z}$. For instance, in a supervised setting $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$, such that $\mathcal{X}$ is the input and $\mathcal{Y}$ is the output space of a learning problem. We assume that training and testing examples are drawn from probability distribution $\mathcal{D}$ over $\mathcal{Z}$. In particular, we will denote the training set as $S = \{z_i\}_{i=1}^m \sim \mathcal{D}^m$.

For a parameter space $\mathcal{H}$, we define a learning algorithm as a map

$$A : \mathcal{Z}^m \mapsto \mathcal{H},$$

and for brevity we will use notation $A_S = A(S)$. In the following we assume that $\mathcal{H} \subseteq \mathbb{R}^d$. To measure the accuracy of a learning algorithm $A$, we have a loss function $f(w, z)$, which measures
the cost incurred of predicting with parameters $w \in \mathcal{H}$ on an example $z$. The risk of $w$, with respect to the distribution $\mathcal{D}$, is defined as

$$R(w) := \mathbb{E}_{z \sim \mathcal{D}}[f(w, z)] ,$$

while the empirical risk given a training set $S$ is

$$\hat{R}_S(w) := \frac{1}{m} \sum_{i=1}^{m} f(w, z_i) .$$

### 3.2 Uniform Stability and Generalization

On an intuitive level, a learning algorithm is said to be stable whenever a small perturbation in the training set does not affect its outcome too much. Of course, there is a number of ways to formalize the perturbation and the extent of the change in the outcome, and we will discuss some of them below. The most important consequence of a stable algorithm is that it generalizes from the training set to the unseen data sampled from the same distribution. In other words, the difference between the risk $R(A_S)$ and the empirical risk $\hat{R}_S(A_S)$ of the algorithm’s output is controlled by the quantity that captures how stable the algorithm is. So, to observe good performance, or a decreasing true risk, we must have a stable algorithm and decreasing empirical risk (training error), which usually comes by design of the algorithm. In this work we focus on the stability of the Stochastic Gradient Descent (SGD) algorithm, and thus, as a consequence, we study its generalization ability.

Recently, Hardt et al. (2016) used a stability argument to prove generalization bounds for learning with SGD. Specifically, they have extended the notion of the uniform stability originally proposed by Bousquet and Elisseeff (2002), to accommodate randomized algorithms.

**Definition 1 (Uniform stability).** A randomized algorithm $A$ is $\epsilon$-uniformly stable if for all datasets $S, S^{(i)} \in \mathcal{Z}^m$ such that $S$ and $S^{(i)}$ differ in the $i$-th example, we have

$$\sup_{z \in \mathcal{Z}, i \in [m]} \mathbb{E}_{A}[f(A_S, z) - f(A_{S^{(i)}}, z)] \leq \epsilon .$$

Since SGD is a randomized algorithm, we have to cope with two sources of randomness: the data-generating process and the randomization of the algorithm $A$ itself, hence we have statements in expectation. The following theorem of Hardt et al. (2016) shows that the uniform stability implies generalization in expectation.

**Theorem 1.** Let $A$ be $\epsilon$-uniformly stable. Then,

$$\left| \mathbb{E}_{S,A} \left[ \hat{R}_S(A_S) - R(A_S) \right] \right| \leq \epsilon .$$

Thus it suffices to characterize the uniform stability of an algorithm to state a generalization bound. In particular, Hardt et al. (2016) showed generalization bounds for SGD under different assumptions on the loss function $f$. Despite that these results hold in expectation, other forms of generalization bounds, such as high-probability ones, can be derived from the above (Shalev-Shwartz et al., 2010).

Apart from SGD, uniform stability has been used before to prove generalization bounds for many learning algorithms (Bousquet and Elisseeff, 2002). However, these bounds typically suggest the worst-case generalization rates, and rather reflect intrinsic stability properties of an algorithm. In other words, uniform stability is oblivious to the data-generating process and any other side information, which might reveal scenarios where generalization occurs at a faster rate. In turn,
these insights could motivate the design of improved learning algorithms. In the following we address some limitations of analysis through uniform stability by using a less restrictive notion of stability. We extend the setting of Hardt et al. (2016) by proving data-dependent stability bounds for convex and non-convex loss functions. In addition, we also take into account the initialization point of an algorithm as a form of supplementary information, and we dedicate special attention to its interplay with the data-generating distribution. Finally, we discuss situations where one can explicitly control the stability of SGD in a data-dependent way.

4 Data-dependent Stability Bounds for SGD

In this section we present a notion of data-dependent algorithmic stability, that allows us to state generalization bounds which depend not only on the properties of the learning algorithm, but also on the additional parameters of the algorithm. We indicate such additional parameters by $\theta$, and therefore we denote stability as a function $\epsilon(\theta)$. In particular, in the following we will be interested in scenarios where $\theta$ describes the data-generating distribution and the initialization point of SGD.

Definition 2 (Hypothesis stability). A randomized algorithm $A$ is $\epsilon(\theta)$-hypothesis stable if it is true that

$$\sup_{i \in [m]} \left\{ \mathbb{E}_{A,S,z} [f(A_S, z) - f(A_{S(i)}, z)] \right\} \leq \epsilon(\theta),$$

where $S \overset{iid}{\sim} D^m$ and $S^{(i)}$ is its copy with $i$-th example replaced by $z \overset{iid}{\sim} D$.

Our definition of hypothesis stability resembles the notion introduced by Bousquet and Elisseeff (2002). The difference lies in the fact that an example in the training set is replaced rather than deleted, and, in addition, that the randomness of the algorithm is taken into account. A similar notion was also used by Elisseeff et al. (2005) for analysis of a randomized aggregation schemes, however their definition involves absolute difference of losses. The dependence on $\theta$ also bears similarity to recent work of London (2016), however, there, it is used in the context of uniform stability. The following theorem shows that hypothesis-stable random algorithm is guaranteed to generalize in expectation.

Theorem 2. Let an algorithm $A$ be $\epsilon(\theta)$-hypothesis stable. Then,

$$\mathbb{E}_{S} \left[ R(A_S) - \hat{R}_S(A_S) \right] \leq \epsilon(\theta).$$

Proof. Indicate by $S = \{z_i\}_{i=1}^m$ and $S' = \{z'_i\}_{i=1}^m$ independent training sets sampled i.i.d. from $D$, and let $S^{(i)} = \{z_1, \ldots, z_{i-1}, z'_i, z_{i+1}, \ldots, z_m\}$, such that $z'_i \overset{iid}{\sim} D$. We relate expected empirical risk and expected risk by

$$\mathbb{E}_{S} \left[ \hat{R}_S(A_S) \right] = \mathbb{E}_{SA} \left[ \frac{1}{m} \sum_{i=1}^m f(A_S, z_i) \right]$$

$$= \mathbb{E}_{SS'} \left[ \frac{1}{m} \sum_{i=1}^m f(A_{S(i)}, z'_i) \right]$$

$$= \mathbb{E}_{SS'} \left[ \frac{1}{m} \sum_{i=1}^m f(A_S, z'_i) \right] - \delta$$

$$= \mathbb{E}_{S} \left[ R(A_S) \right] - \delta,$$
where
\[
\delta = \mathbb{E}_{S,S'} \mathbb{E}_{A} \left[ \frac{1}{m} \sum_{i=1}^{m} (f(A_S, z'_i) - f(A_{S(i)}, z'_i)) \right] = \frac{1}{m} \sum_{i=1}^{m} \mathbb{E}_{S,z'_i} \mathbb{E}_{A} \left[ f(A_S, z'_i) - f(A_{S(i)}, z'_i) \right].
\]
Renaming \(z'_i\) as \(z\) and taking sup over \(i\) we get that
\[
\delta \leq \sup_{i \in [m]} \left\{ \mathbb{E}_{S,z} \mathbb{E}_{A} \left[ f(A_S, z) - f(A_{S(i)}, z) \right] \right\}.
\]
This completes the proof.

5 Main Results

Before presenting our main results in this section, we discuss algorithmic details and assumptions.

We will study the following variant of SGD: given a training set \(S = \{z_i\}_{i=1}^{m} \overset{iid}{\sim} \mathcal{D}^m\), step sizes \(\{\alpha_t\}_{t=1}^{T}\), random indices \(I = \{j_t\}_{t=1}^{T}\), and an initialization point \(w_1\), perform updates
\[
w_{t+1} = w_t - \alpha_t \nabla f(w_t, z_{j_t})
\]
for \(T \leq m\) steps. We assume that the indices in \(I\) are sampled from the uniform distribution over \([m]\) without replacement, and that this is the only source of randomness for SGD. In practice this corresponds to permuting the training set before making a pass through it, as it is commonly done in practical applications. Next, we introduce statements about the loss functions \(f\) used in the following.

**Definition 3 (Lipschitz \(f\)).** A loss function \(f\) is \(L\)-Lipschitz if \(\|\nabla f(w, z)\| \leq L, \forall w \in \mathcal{H} \text{ and } \forall z \in \mathcal{Z}\). Note that this also implies that
\[
|f(w, z) - f(v, z)| \leq L\|w - v\|.
\]

**Definition 4 (Smooth \(f\)).** A loss function is \(\beta\)-smooth if \(\forall w, v \in \mathcal{H} \text{ and } \forall z \in \mathcal{Z},\)
\[
\|\nabla f(w, z) - \nabla f(v, z)\| \leq \beta\|w - v\|.
\]
\(\beta\)-smoothness also implies that
\[
f(w, z) - f(v, z) \leq \nabla f(v, z)^T (w - v) + \frac{\beta}{2}\|w - v\|^2.
\]

**Definition 5 (Lipschitz Hessians).** A loss function \(f\) has a \(\rho\)-Lipschitz Hessian if \(\forall w, v \in \mathcal{H} \text{ and } \forall z \in \mathcal{Z},\)
\[
\|\nabla^2 f(w, z) - \nabla^2 f(v, z)\|_2 \leq \rho\|w - v\|.
\]

The last condition is occasionally used in analysis of SGD (Ge et al., 2015) and holds whenever \(f\) has a bounded third derivative. All presented theorems assume that the loss function used by SGD is non-negative, Lipschitz, and \(\beta\)-smooth. Examples of such commonly used loss functions are the logistic/softmax losses and neural networks with sigmoid activations. Convexity of loss functions or Lipschitzness of Hessians will only be required for some results, and we will denote it explicitly when necessary.
5.1 Convex Losses

First, we present a new and data-dependent stability result for convex losses.

**Theorem 3.** Assume that $f$ is convex, and that SGD’s step sizes satisfy $\alpha_t \leq \frac{2}{\beta}$, $\forall t \in [T]$. Then SGD is $\epsilon(D, w_1)$-hypothesis stable with

$$\epsilon(D, w_1) \leq \frac{2L\sqrt{2\beta R(w_1)}}{m} \sum_{t=1}^{T} \alpha_t.$$  

The proof is given in Section 6.2. Under the same assumptions, Hardt et al. (2016) showed a uniform stability bound $\epsilon \leq \frac{2L_2}{m} \sum_{t=1}^{T} \alpha_t$. Our bound differs since it involves a multiplicative risk at the initialization point, that is $\sqrt{R(w_1)}$, in place of a Lipschitz constant. Thus, our bound corroborates the intuition that whenever we start at a good location of the objective function, the algorithm is more stable and thus generalizes better. We note that this result cannot be obtained through a more restrictive uniform stability, precisely because bounds on the stability must hold for a worst-case choice of data. In contrast, the notion of stability we employ depends on the data-generating distribution, which allowed us to introduce dependency on the risk.

Furthermore, consider that we start at arbitrary location $w_1$: assuming that the loss function is bounded for a concrete $H$ and $Z$, the rate of our bound up to a constant is no worse than that of Hardt et al. (2016). Finally, one can always tighten this result by taking the minimum of two stability bounds.

5.2 Non-convex Losses

Now we state a new stability result for non-convex losses.

**Theorem 4.** Assume that $f(\cdot, z) \in [0, 1]$ and has a $\rho$-Lipschitz Hessian, and that step sizes of a form $\alpha_t = \frac{c_t}{T}$, satisfy $c \leq \min\left\{\frac{1}{\beta}, \frac{1}{4(2\beta \ln(T))^2}\right\}$. Then SGD is $\epsilon(D, w_1)$-hypothesis stable with

$$\epsilon(D, w_1) \leq 1 + \frac{1}{m} \left\{2\rho \frac{L}{\beta} \right\}^{\frac{1}{1 + \gamma}} T^{\frac{\gamma}{1 + \gamma}},$$

where

$$\gamma := \min\left\{\beta, \frac{1}{\rho} \mathbb{E}_z \left[\|\nabla^2 f(w_1, z)\|_2\right] + c \rho (1 + \ln(T)) \sqrt{2\beta R(w_1)}\right\}.$$  

In particular, $\gamma$ characterizes how the curvature at the initialization point affects stability, and hence the generalization error of SGD. Since $\gamma$ heavily affects the rate of convergence in (1), and in most situations smaller $\gamma$ yields higher stability, we now look at few cases of its behavior.

Consider a regime such that $\gamma$ is of the order $\tilde{\Theta} \left(\mathbb{E}[\|\nabla^2 f(w_1, z)\|_2] + \sqrt{R(w_1)}\right)$, or in other words, that stability is controlled by the curvature and the risk of the initialization point $w_1$. This suggests that starting from a point in a flat region with low risk should yield higher stability, and therefore as predicted by our theory, allow for faster generalization. In addition, we observe that considered stability regime offers a principled way to pre-screen a good initialization point in practice, by choosing the one that minimizes spectral norm of the Hessian and the risk.

Next, we focus on a more specific case. Suppose that we choose a step size $\alpha_t = \frac{c_t}{T}$ such that $\gamma \leq \tilde{\Theta} \left(\mathbb{E}[\|\nabla^2 f(w_1, z)\|_2]\right)$, yet not too small, so that the empirical risk can still be decreased. Then, stability is dominated by the curvature around $w_1$. Indeed, lower generalization error on non-convex problems, such as training deep neural networks, has been observed empirically when SGD is actively guided (Hochreiter and Schmidhuber, 1997; Goodfellow et al., 2016; Chaudhari
et al., 2017) or converges to solutions with low curvature (Keskar et al., 2017). However, to the best of our knowledge, Theorem 4 is the first to establish a theoretical link between the curvature of the loss function and the generalization ability of SGD in a data-dependent sense.

Finally, we note that Hardt et al. (2016, Theorem 3.8) showed a bound similar to (1), however, in place of $\gamma$ their bound has a Lipschitz constant of the gradient. The crucial difference lies in term $\gamma$ which is now not merely a Lipschitz constant, but rather depends on the data-generating distribution and initialization point of SGD. We compare to their bound by considering the worst case scenario, namely, that SGD is initialized in a point with high curvature, or altogether, that the objective function is highly curved everywhere. Then, at least our bound is no worse than the one of Hardt et al. (2016), since $\gamma \leq \beta$.

5.3 Application to Transfer Learning

One example application of data-dependent bounds presented before lies in Transfer Learning (TL), where we are interested in achieving faster generalization on a target task by exploiting side information that originates from different but related source tasks. The literature on TL explored many ways to do so, and here we will focus on the one that is most compatible with our bounds.

More formally, suppose that the target task at hand is characterized by a joint probability distribution $D$, and as before we have a training set $S \stackrel{iid}{\sim} D^m$. Some TL approaches also assume access to the data sampled from the distributions associated with the source tasks. Here we follow a conservative approach – instead of the source data, we receive a set of source hypotheses $\{w_{src}^k\}_{k=1}^K \subset \mathcal{H}$, trained on the source tasks. At the same time we assume no access to the source data directly. The goal of a learner is to come up with a target hypothesis $w_{trg}$, which in the optimistic scenario generalizes better by relying on source hypotheses. In the TL literature this is known as Hypothesis Transfer Learning (HTL) (Kuzborskij and Orabona, 2016), that is, we transfer from the source hypotheses which act as a proxy to the source tasks and the risk $R(w_{src}^k)$ quantifies how much source and target tasks are related.

In the following we will consider SGD for HTL, where the source hypotheses act as initialization points. First, consider learning with convex losses: Theorem 3 depends on $R(w_1)$, thus it immediately quantifies the relatedness of source and target tasks. This suggests that it is enough to pick the point that minimizes the stability bound to transfer from the most related source task. Then, bounding $R(w_{src}^k)$ by its empirical counterpart through Hoeffding inequality, the most related source is $w_{src}^k \star$ such that

$$k \star = \arg \min_{k \in [K]} \hat{R}_S(w_{src}^k) .$$

Similar conclusions where drawn in HTL literature, albeit in the context of ERM.

Matters are slightly more complicated in the non-convex case. We take a similar approach, however, now we minimize stability bound (1), and for the sake of simplicity assume that we make a full pass over the data, so $T = m$. Then the best source is $w_{src}^k$ such that

$$k \star = \arg \min_{k \in [K]} \left\{ 1 + \frac{1}{c|k|} \left( \frac{cL^2}{m} \right)^{\frac{1}{1+\gamma_k}} \right\} ,$$

where

$$\hat{\gamma}_k := \frac{1}{m} \sum_{i=1}^m \|\nabla^2 f(w_{src}^k, z_i)\|_2 + \lambda \sqrt{\hat{R}_S(w_{src}^k)} + \frac{1}{\sqrt{m}} ,$$

and $\lambda := c\rho(1 + \ln(T))$. Note that we again have replaced expectation terms with empirical estimates by applying Hoeffding inequality. Thus, once again, we get a simple and principled
way to speed up generalization by transferring from the most related source task on non-convex problems. We also note that there is no restriction on the origin of the source hypotheses \( w_k^{src} \). In general, these can even be random guesses, in which case we would be pre-screening a good starting position. Finally, it is worth mentioning that \( \hat{\gamma}_k \) involves estimating the spectral norm of the Hessian, which is computationally cheaper to evaluate compared to the complete Hessian matrix (Pearlmutter, 1994). This is particularly relevant for deep learning, where computation of the Hessian matrix can be prohibitively expensive.

6 Proofs

In this section we present proofs of all the statements.

6.1 Preliminaries

We say that the SGD gradient update rule is an operator \( G_t : \mathcal{H} \rightarrow \mathcal{H} \), such that

\[
G_t(w) := w - \alpha_t \nabla f(w, z_i),
\]

and it is also a function of the training set \( S \) and a random index set \( I \). Then, \( w_{t+1} = G_t(w_t) \), throughout \( t = 1, \ldots, T \). Moreover we will use the notation \( w_{S,t} \) to indicate the output of SGD ran on a training set \( S \), at step \( t \), and define

\[
\delta_t(S, z) := \| w_{S,t} - w_{S(\cdot), t} \|.
\]

Next, we summarize a few instrumental facts about \( G_t \) and few statements about the loss functions used in our proofs.

**Definition 6 (Expansiveness).** A gradient update rule is \( \eta \)-expansive if for all \( w, v \),

\[
\| G_t(w) - G_t(v) \| \leq \eta \| w - v \|.
\]

The following lemma characterizes expansiveness for the gradient update rule under different assumptions on \( f \).

**Lemma 1** (Lemma 3.6 in (Hardt et al., 2016)). Assume that \( f \) is \( \beta \)-smooth. Then, we have that:

1) \( G_t \) is \((1 + \alpha_t \beta)\)-expansive,

2) If \( f \) in addition is convex, then, for any \( \alpha_t \leq \frac{2}{\beta} \), the gradient update rule \( G_t \) is 1-expansive.

An important consequence of \( \beta \)-smoothness of \( f \) is self-boundedness (Shalev-Shwartz and Ben-David, 2014), which we will use on many occasions.

**Lemma 2** (Self-boundedness). For \( \beta \)-smooth non-negative function \( f \) we have that \( \| \nabla f(w, z) \| \leq \sqrt{2\beta f(w, z)} \).

Self-boundedness in turn implies the following boundedness of a gradient update rule.

**Corollary 1.** Assume that \( f \) is \( \beta \)-smooth and non-negative. Then,

\[
\| w - G_t(w) \| \leq \alpha_t \min \left\{ \sqrt{2\beta f(w, z_i)}, L \right\}.
\]
Proof. By Lemma 2

\[ \|w - G_t(w)\| = \|\alpha_t \nabla f(w, z_{j_t})\| \leq \sqrt{2\alpha_t^2 \beta f(w, z_{j_t})}, \]

and also by Lipschitzness of \( f \), \( \|\alpha_t \nabla f(w, z_{j_t})\| \leq \alpha_t L. \)

Next we introduce a bound that relates the risk of the output at step \( t \) to the risk of the initialization point \( w_1 \) through the variance of the gradient. Given an appropriate choice of step size, this bound will be crucial at stating stability bounds that depend on the risk at \( w_1 \). The proof idea is similar to the one of (Ghadimi and Lan, 2013). In particular, it does not require convexity of the loss function.

**Lemma 3.** Assume that the loss function \( f \) is \( \beta \)-smooth. Then, for \( w_{S,t} \) we have that

\[ E_{S} [f(w_{S,t}, z_{j_t}) - f(w_1, z_{j_t})] \leq \sum_{k=1}^{t-1} \alpha_k \left( \frac{\alpha_k \beta}{2} - 1 \right) E_{S} [\|\nabla f(w_{S,k}, z_{j_k})\|^2]. \]

Proof. For brevity let \( w_k = w_{S,k} \). The \( \beta \)-smoothness of \( f \) for any \( z_{j_t} \) we have

\[ f(w_{k+1}, z_{j_t}) - f(w_k, z_{j_t}) \leq \nabla f(w_k, z_{j_t})^T(w_{k+1} - w_k) + \frac{\beta}{2}\|w_{k+1} - w_k\|^2. \]

Considering SGD update \( w_{k+1} = w_k - \alpha_k \nabla f(w_k, z_{j_k}) \), where \( z_{j_k} \sim D \), and summing both sides from \( 1 \) to \( t-1 \) we get

\[ f(w_{t}, z_{j_t}) - f(w_1, z_{j_t}) \leq -\sum_{k=1}^{t-1} \alpha_k \nabla f(w_k, z_{j_k})^T \nabla f(w_k, z_{j_k}) + \frac{\beta}{2} \sum_{k=1}^{t-1} \alpha_k^2 \|\nabla f(w_k, z_{j_k})\|^2. \]

Taking expectation w.r.t. \( S \) and \( z \) on both sides, using the fact that \( w_{S,k} \) does not depend on \( z_{j_k} \) nor on \( z_{j_t} \), and that \( z_{j_k}, z_{j_t} \sim D \), we have that

\[
E_{S,z} [f(w_{S,t}, z_{j_t}) - f(w_1, z_{j_t})] \\
\leq -\sum_{k=1}^{t-1} \alpha_k \ E_{S,z} [\nabla f(w_{S,k}, z_{j_k})^T \nabla f(w_{S,k}, z_{j_k})] + \frac{\beta}{2} \sum_{k=1}^{t-1} \alpha_k^2 \ E_{S,z} [\|\nabla f(w_{S,k}, z_{j_k})\|^2] \\
= \alpha_k \left( \frac{\alpha_k \beta}{2} - 1 \right) \sum_{k=1}^{t-1} \alpha_k^2 \ E_{S,z} [\|\nabla f(w_{S,k}, z_{j_k})\|^2].
\]

\[ \square \]

Next, we show that, in expectation, deviations between SGD updates are controlled by the risk at the initialization point for an appropriate choice of a step size.

**Lemma 4.** Assume that the loss function \( f \) is \( \beta \)-smooth and non-negative, and that step sizes obey \( \alpha_t \leq \frac{2}{\beta} \). Then, for the gradient update rule \( G_t \) we have

\[ E_{S,z} [\|G_t(w_{S,t}) - G_t(w_{S(t-1),1})\|] \leq E_{S,z} [\delta_t(S,z)] + 2\alpha_t \sqrt{2\beta R(w_1)}. \]
Proof. By triangle inequality and Corollary 1 claiming that updates are \( \alpha_t \sqrt{2\beta f(S,t,z_j)} \)-bounded, we have that
\[
\|G_t(w_{S,t}) - G_t(w_{S^{(i)},t})\|
= \|G_t(w_{S,t}) - w_{S,t} + w_{S,t} - w_{S^{(i)},t} + w_{S^{(i)},t} - G_t(w_{S^{(i)},t})\|
\leq \|w_{S,t} - w_{S^{(i)},t}\| + \alpha_t \sqrt{2\beta} \left( \sqrt{f(w_{S,t}, z_j)} + \sqrt{f(w_{S^{(i)},t}, z'_j)} \right).
\]
Taking expectation w.r.t. the training set and applying Jensen’s inequality we further have
\[
\mathbb{E}_{S,z} \left[ \|G_t(w_{S,t}) - G_t(w_{S^{(i)},t})\| \right]
\leq \mathbb{E}_{S,z} \left[ \|w_{S,t} - w_{S^{(i)},t}\| \right] + \alpha_t \sqrt{2\beta} \left( \mathbb{E}_{S} \left[ f(w_{S,t}, z_j) \right] + \mathbb{E}_{S} \left[ f(w_{S^{(i)},t}, z'_j) \right] \right),
\]
where the last identity comes by renaming \( z'_j \) into \( z_j \), because \( w_{S^{(i)},t} \) does not depend on \( z'_j \) and the fact that \( z'_j, z_j \) i.i.d. \( \mathcal{D} \). Finally we invoke Lemma 3 assuming that the step size is set such that \( \alpha_t \leq \frac{2}{\beta} \) to get
\[
\mathbb{E}_{S} \left[ f(w_{S,t}, z_j) \right] \leq \mathbb{E}_{S} \left[ f(w_1, z_j) \right] = R(w_1).
\]
Plugging this into (3) proves the statement.

6.2 Convex Losses

In this section we prove hypothesis stability for loss functions that are non-negative, \( \beta \)-smooth, and convex.

Proof of Theorem 3. The proof follows the outline of the proof of Theorem 3.7 in (Hardt et al., 2016). By Lipschitzness of \( f \) we get that
\[
\mathbb{E}_{S,z} \mathbb{E}_{A} \left[ f(w_{S,T}, z) - f(w_{S^{(i)},T}, z) \right] \leq L \mathbb{E}_{S,z} \mathbb{E}_{A} \left[ \|w_{S,T} - w_{S^{(i)},T}\| \right] = L \mathbb{E}_{S,z} \mathbb{E}_{A} \left[ \delta_T(S,z) \right].
\]
The strategy of our proof will be to establish the bound on \( \mathbb{E}_{S,z} \mathbb{E}_{A} \left[ \delta_T(S,z) \right] \) by using a recursive argument. In fact we will state the bound on \( \mathbb{E}_{A} \mathbb{E}_{S,z} \left[ \delta_{t+1}(S,z) \right] \) in terms of \( \mathbb{E}_{A} \mathbb{E}_{S,z} \left[ \delta_t(S,z) \right] \) and then unravel the recursion.

To do so, we distinguish two cases: 1) SGD encounters a perturbed point at step \( t \), that is \( t = i \), and 2) the current point is the same in \( S \) and \( S^{(i)} \), so \( t \neq i \). To handle the first case, we will use the data-dependent boundedness of the gradient update rule, and by Lemma 4 we have that
\[
\mathbb{E}_{S,z} \left[ \delta_{i+1}(S,z) \right] \leq \mathbb{E}_{S,z} \left[ \delta_t(S,z) \right] + 2\alpha_t \sqrt{2\beta R(w_1)}.
\]
To handle the second case, we will use the expansiveness of the gradient update rule, Lemma 1, which states that for convex loss functions, the gradient update rule is 1-expansive, so \( \delta_{i+1}(S,z) \leq \delta_t(S,z) \). Considering both cases of example selection, and noting that SGD encounters the perturbation w.p. \( \frac{1}{m} \), we write \( \mathbb{E}_{A} \) for a step \( t \) as
\[
\mathbb{E}_{A} \mathbb{E}_{S,z} \left[ \delta_{i+1}(S,z) \right] \leq \left( 1 - \frac{1}{m} \right) \mathbb{E}_{A} \mathbb{E}_{S,z} \left[ \delta_t(S) \right] + \frac{1}{m} \left( \mathbb{E}_{A} \mathbb{E}_{S,z} \left[ \delta_t(S,z) \right] + 2\alpha_t \sqrt{2\beta R(w_1)} \right)
= \mathbb{E}_{A} \mathbb{E}_{S,z} \left[ \delta_t(S,z) \right] + \frac{2\alpha_t \sqrt{2\beta R(w_1)}}{m}.
\]

Unraveling the recursion from \( T \) to 1 yields

\[
E \mathbb{E}_{S,z} [\delta_T(S, z)] \leq 2\sqrt{2\beta R(w_1)} \frac{T}{m} \sum_{t=1}^T \alpha_t.
\]

Plugging this into (4) we get the statement of Theorem 3.

\[
\square
\]

6.3 Non-convex Losses

Our proof of a stability bound for non-convex loss functions, Theorem 4, follows a general outline of Hardt et al. (2016, Theorem 3.8). Namely, the outputs of SGD run on a training set \( S \) and its perturbed version \( S^{(i)} \) will not differ too much, because by the time a perturbation is encountered, the step size has already decayed enough. So, on the one hand, stabilization is enforced by the diminishing the step size, and on the other hand, by how much updates expand the distance between the gradients after the perturbation. Since Hardt et al. (2016) work with uniform stability, they capture the expansiveness of post-perturbation update by the Lipschitzness of the gradient. In combination with a recursive argument, their bound has exponential dependency on the Lipschitz constant of the gradient. We argue that the Lipschitz continuity of the gradient can be too pessimistic in general. Instead, we rely on a local data-driven argument: considering that we initialize SGD at point \( w_1 \), how much do updates expand the gradient under the distribution of interest? The following crucial lemma characterizes such behavior in terms of the curvature at \( w_1 \).

**Lemma 5.** Assume that the loss function \( f(\cdot, z) \) is \( \beta \)-smooth and that its Hessian is \( \rho \)-Lipschitz. Then,

\[
\|G_t(w_{S,t}) - G_t(w_{S^{(i)},t})\| \leq (1 + \alpha_t \xi_t(S, z)) \delta_t(S, z)
\]

where

\[
\xi_t(S, z) := \|\nabla^2 f(w_1, z_t)\|_2 + \rho \sqrt{\frac{\beta}{2}} \sum_{k=1}^T \alpha_k \left( \sqrt{f(w_{S,k}, z_{j_k})} + \sqrt{f(w_{S^{(i)},k}, z_{j_k}')} \right).
\]

Furthermore, for any \( t \in [T] \),

\[
E_{S,t} [\xi_t(S, z)] \leq E_z [\|\nabla^2 f(w_1, z)\|_2] + c\rho (1 + \ln(T)) \sqrt{2\beta R(w_1)}.
\]

**Proof.** Recall that the randomness of the algorithm is realized through sampling without replacement from the uniform distribution over \([m]\). Apart from that we will not be concerned with the randomness of the algorithm, and given the set of random variables \( \{j_i\}_{i=1}^m \), for brevity we will use indexing notation \( z_1, z_2, \ldots, z_m \) to indicate \( z_{j_1}, z_{j_2}, \ldots, z_{j_m} \). Next, let \( S^{(i)} = \{z_i'\}_{i=1}^m \), and introduce a shorthand notation \( f_k(w) = f(w, z_k) \) and \( f_k'(w) = f(w, z_k') \). We start by applying triangle inequality to get

\[
\|G_t(w_{S,t}) - G_t(w_{S^{(i)},t})\| \leq \|w_{S,t} - w_{S^{(i)},t}\| + \alpha_t \|\nabla f_t(w_{S,t}) - \nabla f_t(w_{S^{(i)},t})\|.
\]

In the following we will focus on the second term of r.h.s. above. Given SGD outputs \( w_{S,t} \) and \( w_{S^{(i)},t} \) with \( t > i \), our goal here is to establish how much do gradients grow apart with every new update. This behavior can be characterized assuming that gradient is Lipschitz continuous, however, we conduct a local analysis. Specifically, we observe how much do updates expand gradients, given that we start at some point \( w_1 \) under the data-generating distribution. So, instead of the Lipschitz constant, expansiveness rather depends on the curvature around \( w_1 \). On the other hand, we are dealing with outputs at an arbitrary time step \( t \), and therefore we first have to relate
1) Decomposition. Introduce \( \delta_t \coloneqq w_{S^{(i)},t} - w_{S,t} \). By Taylor theorem we get that

\[
\nabla f_t(w_{S,t}) - \nabla f_t(w_{S^{(i)},t}) = \int_0^1 \left( \nabla^2 f_t(w_{S,t} + \tau \delta_t) - \nabla^2 f_t(w_1) \right) d\tau \delta_t + \nabla^2 f_t(w_1) \delta_t.
\]

Taking norm on both sides, applying triangle inequality, Cauchy-Schwartz inequality, and assuming that Hessians are \( \rho \)-Lipschitz we obtain

\[
\|\nabla f_t(w_{S,t}) - \nabla f_t(w_{S^{(i)},t})\| \\
\leq \int_0^1 \|\nabla^2 f_t(w_{S,t} + \tau \delta_t) - \nabla^2 f_t(w_1)\| d\tau \|\delta_t\| + \|\nabla^2 f_t(w_1)\| \|\delta_t\| \\
\leq \rho \int_0^1 \|w_{S,t} - w_1 + \tau \delta_t\| d\tau \|\delta_t\| + \|\nabla^2 f_t(w_1)\| \|\delta_t\|.
\]

2) Bounding gradients. Using telescoping sums and SGD update rule we get that

\[
w_{S,t} - w_1 + \tau \delta_t \\
= w_{S,t} - w_1 + \tau \left( w_{S^{(i)},t} - w_1 + w_1 - w_{S,t} \right) \\
= \sum_{k=1}^{t-1} (w_{S,k+1} - w_{S,t}) + \tau \sum_{k=1}^{t-1} (w_{S^{(i)},k+1} - w_{S^{(i)},k}) - \tau \sum_{k=1}^{t-1} (w_{S,k+1} - w_{S,k}) \\
= (\tau - 1) \sum_{k=1}^{t-1} \alpha_k \nabla f_k(w_{S,k}) - \tau \sum_{k=1}^{t-1} \alpha_k \nabla f_k(w_{S^{(i)},k}).
\]

Plugging above into the integral of (6) we have

\[
\int_0^1 \left\| \sum_{k=1}^{t-1} \alpha_k \left( (\tau - 1) \nabla f_k(w_{S,k}) - \tau \nabla f_k(w_{S^{(i)},k}) \right) \right\| d\tau \\
\leq \frac{1}{2} \left\| \sum_{k=1}^{t-1} \alpha_k \nabla f_k(w_{S,k}) \right\| + \frac{1}{2} \left\| \sum_{k=1}^{t-1} \alpha_k \nabla f_k(w_{S^{(i)},k}) \right\| \\
\leq \sqrt{\frac{\beta}{2}} \sum_{k=1}^{t-1} \alpha_k \left( \sqrt{f_k(w_{S,k})} + \sqrt{f_k(w_{S^{(i)},k})} \right),
\]

where the last inequality comes from the self-bounding property of \( \beta \)-smooth functions, Lemma 2. Plugging this result back into (6) completes the proof of the first statement.

Bounding \( \mathbb{E}_{S,z} [\xi_t(S, z)] \). Now we briefly focus on the expectation of \( \xi_t(S, z) \), and relate it to the risk of \( w_1 \) and expectation Hessian. By definition of \( \xi_t(S, z) \)

\[
\mathbb{E}_{S,z} [f_t(S, z)] \leq \rho \sqrt{\frac{\beta}{2}} \sum_{k=1}^T \alpha_k \left( \mathbb{E}_{S,z} \left[ \sqrt{f(w_{S,k}, z_k)} \right] + \mathbb{E}_{S,z} \left[ \sqrt{f(w_{S^{(i)},k}, z'_k)} \right] + \mathbb{E}_{S,z} \left[ \|\nabla^2 f(w_1, z_t)\|_2 \right] \right).
\]
By Jensen’s inequality and applying Lemma 3 assuming that \( \alpha_t \leq \frac{2}{3} \) we have,

\[
\mathbb{E} \left[ \sqrt{f(w_{S,k}, z_{j_k})} \right] \leq \sqrt{\mathbb{E} [f(w_{S,k}, z_{j_k})]} \leq \sqrt{R(w_1)}.
\]

We arrive at the same bound for the perturbed term by renaming \( z'_{j_k} \) into \( z_{j_k} \), using the fact that \( w_{S(t),k} \) does not depend on \( z'_{j_k} \) under the randomization of SGD. Finally putting things together,

\[
\mathbb{E}_{S,z} [\zeta_t(S, z)] \leq \rho \sqrt{2R(w_1)} \sum_{k=1}^T \alpha_k + \mathbb{E}_{z} [||\nabla^2 f(w_1, z)||],
\]

and upper bounding \( \sum_{k=1}^T \alpha_k \leq c (1 + \ln(T)) \) proves the second statement.

The following lemma is similar to Lemma 3.11 of (Hardt et al., 2016), and is instrumental in bounding the stability of SGD for non-convex objectives. However, we make an adjustment and state it in expectation over the data.

**Lemma 6.** Assume that the loss function \( f(\cdot, z) \in [0, 1] \) is \( L \)-Lipschitz for all \( z \). Then, for every \( t_0 \in \{0, 1, 2, \ldots, m\} \) we have that,

\[
\mathbb{E}_{S,z,A} [f(w_{S,T}, z) - f(w_{S(t),T}, z)] \leq L \mathbb{E}_{S,z,A} [\mathbb{E}_A [\delta_T(S, z) \mid \delta_{t_0}(S, z) = 0]] + \frac{t_0}{m}.
\]

**Proof.** Denote event \( \mathcal{E} = I \{\delta_{t_0}(S, z) = 0\} \). Then we have

\[
\mathbb{E}_{S,z,A} [f(w_{S,T}, z) - f(w_{S(t),T}, z)] = \mathbb{E}_{S,z,A} \left[ \mathbb{P} \{\mathcal{E} \} \mathbb{E}_A [f(w_{S,T}, z) - f(w_{S(t),T}, z) \mid \mathcal{E}] + \mathbb{P} \{-\mathcal{E}\} \mathbb{E}_A [f(w_{S,T}, z) - f(w_{S(t),T}, z) \mid -\mathcal{E}] \right]\]

\[
\leq \mathbb{E}_{S,z,A} [f(w_{S,T}, z) - f(w_{S(t),T}, z) \mid \mathcal{E}] + \mathbb{P} \{-\mathcal{E}\} \mathbb{E}_A [f(w_{S,T}, z) \mid -\mathcal{E}] \]

\[
\leq \mathbb{E}_{S,z,A} [L \mathbb{E}_A [\delta_T(S, z) \mid \mathcal{E}] + \mathbb{P} \{-\mathcal{E}\} \mathbb{E}_A [f(w_{S,T}, z) \mid -\mathcal{E}]] + \frac{t_0}{m}.
\]

The rest of the proof concerns bounding the second summand above, and is similar to the one of Lemma 3.11 of Hardt et al. (2016). Recall that \( i \in [m] \) is the index where \( S \) and \( S^{(i)} \) differ, and introduce a random variable \( \tau \) taking on the index of the first time step where SGD uses the example \( z_i \) or a replacement \( z \). Note also that \( \tau \) does not depend on the data. When \( \tau > t_0 \), then it must be that \( \delta_{t_0}(S, z) = 0 \), because updates on both \( S \) and \( S^{(i)} \) are identical until \( t_0 \). Thus we have that

\[
\mathbb{P} \{-\mathcal{E}\} = \mathbb{P} \{\delta_{t_0}(S, z) \neq 0\} \leq \mathbb{P} \{\tau \leq t_0\}.
\]

Now assuming that \( \tau \) is a uniformly distributed over \([m] \) we have that

\[
\mathbb{P} \{\tau \leq t_0\} = \frac{t_0}{m}.
\]

Then (9) is bounded by

\[
L \mathbb{E}_{S,z} [\mathbb{E}_A [\delta_T(S, z) \mid \mathcal{E}]] + \mathbb{E}_{S,z} [\mathbb{E}_A [f(w_{S,T}, z) \mid -\mathcal{E}]] \frac{t_0}{m}
\]

\[
\leq L \mathbb{E}_{S,z} [\mathbb{E}_A [\delta_T(S, z) \mid \mathcal{E}]] + \frac{t_0}{m}
\]

\[
= L \mathbb{E}_{S,z} [\mathbb{E}_A [\delta_T(S, z) \mid \delta(S, z) = 0]] + \frac{t_0}{m},
\]

which completes the proof. \( \square \)
We spend a moment to highlight the role of conditional expectation in (8). Observe that we could naively bound (7) by the Lipschitzness of \( f \), but Lemma 6 follows a more careful argument. First note that \( t_0 \) is a free parameter. The expected distance in (8) between SGD outputs \( w_{S,t} \) and \( w_{S(0),t} \) is conditioned on the fact that at step \( t_0 \) outputs of SGD are still the same. This means that the perturbed point is encountered after \( t_0 \). Then, the conditional expectation should be a decreasing function of \( t_0 \): the later the perturbation occurs, the smaller deviation between \( w_{S,t} \) and \( w_{S(0),t} \) we should expect. Later we use this fact to minimize the bound (8) over \( t_0 \). Next, we need the following statement to prove our stability bound.

**Proposition 1** (Bernstein-type inequality). Let \( Z \) be a zero-mean real-valued r.v., such that \( |Z| \leq b \) and \( E[Z^2] \leq \sigma^2 \). Then for all \( |c| \leq \frac{1}{2\sigma} \), we have that \( E[e^{cZ}] \leq e^{c^2\sigma^2} \).

**Proof.** Stated inequality is a consequence of a Bernstein-type inequality for moment generating functions, Theorem 2.10 in (Boucheron et al., 2013). Observe that zero-centered r.v. \( Z \) bounded by \( b \) satisfies Bernstein’s condition, that is

\[
|E[(Z - E[Z])^q]| \leq \frac{q!}{2} \sigma^2 b^{k-2} \quad \text{for all integers } q \geq 3.
\]

This in turn satisfies condition for Bernstein-type inequality stating that

\[
E[\exp(c(Z - E[Z]))] \leq \exp\left(\frac{c^2\sigma^2/2}{1 - bc}\right).
\]

Choosing \( |c| \leq \frac{1}{2\sigma} \) verifies the statement. \( \square \)

Now we are ready to prove Theorem 4, which bounds the \( \epsilon(D, w_1) \)-hypothesis stability of SGD.

**Proof of Theorem 4.** By Lemma 6, for all \( t_0 \in [m] \),

\[
E_{S,z} E_A[f(w_{S,T}, z) - f(w_{S(0),T}, z)] \\
\leq L E_{S,z} E_A[f_T(S, z) \mid \delta_{t_0}(S, z) = 0] + \frac{t_0}{m}. \tag{10}
\]

Most of the proof is dedicated to bounding the first term in (10). We deal with this similarly as in (Hardt et al., 2016). Introduce \( \Delta_t(S, z) := E_A[\delta_{t}(S, z) \mid \delta_{t_0}(S, z) = 0] \). Specifically, we state the bound on \( \Delta_T(S, z) \) by using a recursion. In our case, however, we also have an expectation w.r.t. the data, and to avoid complications with dependencies, we first unravel the recursion for the random quantities, and only then take the expectation. At this point the proof crucially relies on the product of exponentials arising from the recursion, and all relevant random quantities end up inside of them. We alleviate this by Proposition 1. Finally, we conclude by minimizing (10) w.r.t. \( t_0 \). Thus we have three steps: 1) recursion, 2) bounding \( E[\exp(\cdot)] \), and 3) tuning of \( t_0 \).

1) **Recursion.** We begin by stating the bound on \( \Delta_T(S, z) \) by recursion. Thus we will first state the bound on \( \Delta_{t+1}(S, z) \) in terms of \( \Delta_t(S, z) \), and other relevant quantities and then unravel the recursion. As in the convex case, we distinguish two cases: 1) SGD encounters the perturbed point at step \( t \), that is \( t = i \), and 2) the current point is the same in \( S \) and \( S(i) \), so \( t \neq i \). For the first case, we will use worst-case boundedness of \( G_t \), Corollary 1, that is, \( \|G_t(w_{S,t}) - G_t(w_{S(0),t})\| \leq \delta_t(S, z) + 2\alpha_t L \). To handle the second case we will use Lemma 5, namely,

\[
\|G_t(w_{S,t}) - G_t(w_{S(0),t})\| \leq (1 + \alpha_t \beta_t(S, z)) \delta_t(S, z).
\]

In addition, as a safety measure we will also take into account that the gradient update rule is at most \((1 + \alpha_t \beta)\)-expansive by Lemma 1. So we will work with the function \( \psi_t(S, z) := \]
\( \min \{ \xi_t(S, z), \beta \} \) instead of \( \xi_t(S, z) \) and decompose the expectation w.r.t. \( A \) for a step \( t \). Noting that SGD encounters the perturbed example with probability \( \frac{1}{m} \),

\[
\Delta_{t+1}(S, z) \leq \left( 1 - \frac{1}{m} \right) (1 + \alpha_t \psi_t(S, z)) \Delta_t(S, z) + \frac{1}{m} (2\alpha_t L + \Delta_t(S, z))
\]

\[
= \left( 1 + \left( 1 - \frac{1}{m} \right) \alpha_t \psi_t(S, z) \right) \Delta_t(S, z) + \frac{2\alpha_t L}{m}
\]

\[
\leq \exp (\alpha_t \psi_t(S, z)) \Delta_t(S, z) + \frac{2\alpha_t L}{m},
\]

(11)

where the last inequality follows from \( 1 + x \leq \exp(x) \). This inequality is not overly loose for \( x \in [0, 1] \), and, in our case it becomes instrumental in handling the recursion.

Now, observe that relation \( x_{t+1} \leq a_t x_t + b_t \) with \( x_{t_0} = 0 \) unwinds from \( T \) to \( t_0 \) as \( x_T \leq \sum_{t=t_0+1}^{T} b_t \prod_{k=t+1}^{T} a_k \). Consequently, having \( \Delta_{t_0}(S, z) = 0 \), we unwind (11) to get

\[
\Delta_T(S, z) \leq \sum_{t=t_0+1}^{T} \left( \prod_{k=t+1}^{T} \exp \left( \frac{c \psi_k(S, z)}{k} \right) \right) \frac{2cL}{mt}
\]

\[
= \sum_{t=t_0+1}^{T} \exp \left( c \sum_{k=t+1}^{T} \frac{\psi_k(S, z)}{k} \right) \frac{2cL}{mt}.
\]

(12)

2) **Bounding** \( \mathbb{E}[\exp(\cdots)] \). We take expectation w.r.t. \( S \) and \( z \) on both sides and focus on the expectation of the exponential in (12). First, introduce \( \mu_k := \mathbb{E}_{S, z}[\psi_k(S, z)] \), and proceed as

\[
\mathbb{E}_{S, z} \left[ \exp \left( c \sum_{k=t+1}^{T} \frac{\psi_k(S, z)}{k} \right) \right] = \mathbb{E}_{S, z} \left[ \exp \left( c \sum_{k=t+1}^{T} \frac{\psi_k(S, z) - \mu_k}{k} \right) \right] \exp \left( c \sum_{k=t+1}^{T} \frac{\mu_k}{k} \right).
\]

(13)

Observe that zero-mean version of \( \psi_k(S, z) \) is bounded as

\[
\sum_{k=t+1}^{T} \left| \frac{\psi_k(S, z) - \mu_k}{k} \right| \leq 2\beta \ln(T),
\]
and assume the setting of $c$ as $c \leq \frac{1}{1 + 2\ln(T)/T}$. By Proposition 1, we have

$$
\mathbb{E} \left[ \exp \left( c \frac{\sum_{k=t+1}^{T} \psi_k(S,z) - \mu_k}{k} \right) \right] 
\leq \exp \left( c^2 \mathbb{E} \left[ \left( \frac{\sum_{k=t+1}^{T} \psi_k(S,z) - \mu_k}{k} \right)^2 \right] \right) 
= \exp \left( \frac{c}{2} \mathbb{E} \left[ \left( \frac{1}{2\beta \ln(T)} \sum_{k=t+1}^{T} \psi_k(S,z) - \mu_k \right)^2 \right] \right) 
\leq \exp \left( \frac{c}{2} \mathbb{E} \left[ \left( \sum_{k=t+1}^{T} \psi_k(S,z) - \mu_k \right)^2 \right] \right) 
\leq \exp \left( \frac{c}{2} \sum_{k=t+1}^{T} \mathbb{E} \left[ |\psi_k(S,z) - \mu_k| \right] \right) 
\leq \exp \left( \frac{c}{2} \sum_{k=t+1}^{T} \mu_k \right).
$$

Getting back to (13) we conclude that

$$
\mathbb{E}_{S,z} \left[ \exp \left( c \frac{\sum_{k=t+1}^{T} \psi_k(S,z)}{k} \right) \right] \leq \exp \left( c \sum_{k=t+1}^{T} \frac{2\mu_k}{k} \right). \tag{14}
$$

Next, we give an upper-bound on $\mu_k$, that is $\mu_k \leq \min \{\beta, \mathbb{E}_{S,z} [\xi_k(S,z)]\}$. Finally, we bound $\mathbb{E}_{S,z} [\xi_k(S,z)]$ using the second result of Lemma 5, which holds for any $k \in [T]$, to get that $\mu_k \leq \gamma$, with $\gamma$ defined in (2).

3) Tuning of $t_0$. Now we turn our attention back to (12). Considering that we took an expectation w.r.t. the data, we use (14) and the fact that $\mu_k \leq \gamma$ to get that

$$
\mathbb{E}_{S,z} [\Delta_T(S,z)] \leq \sum_{t=t_0+1}^{T} \exp \left( 2\gamma \sum_{k=t+1}^{T} \frac{1}{k} \right) \frac{2cL}{mT} 
\leq \sum_{t=t_0+1}^{T} \exp \left( 2\gamma \ln \left( \frac{T}{t} \right) \right) \frac{2cL}{mT} 
= \frac{2cL}{m} \left( \frac{T}{t_0} \right)^{2\gamma} 
\leq \frac{1}{2\gamma} \frac{2cL}{m} \left( \frac{T}{t_0} \right)^{2\gamma}.
$$

Plug the above into (8) to get

$$
\mathbb{E}_{S,z} \mathbb{E}_{A} \left[ f(w_{S,T},z) - f(w_{S^{(i)},T},z) \right] \leq \frac{L^2}{\gamma m} \left( \frac{T}{t_0} \right)^{2\gamma} + \frac{t_0}{m}. \tag{15}
$$
Let $q = 2c\gamma$. Then, setting

$$t_0 = (2cL^2)^{\frac{1}{1+q}} T^{\frac{1}{1+q}}$$

minimizes (15). Plugging $t_0$ back we get that (15) equals to

$$\frac{1}{m} + \frac{1}{q} (2cL^2)^{\frac{1}{1+q}} T^{\frac{1}{1+q}}.$$

This completes the proof. □

7 Conclusions and Future Work

In this work we proved data-dependent stability bounds for SGD and revisited its generalization ability. We presented novel bounds for convex and non-convex smooth loss functions, controlled by data-dependent quantities, while previous stability bounds for SGD were derived through the worst-case analysis. In particular, for non-convex learning, we demonstrated theoretically that generalization of SGD is heavily affected by the expected curvature around the initialization point. Consequently, we exploited this fact, presenting a simple and data-driven transfer learning approach which directly minimizes the bound.

Since our bounds are data-dependent, it is likely that by following a similar analysis one could develop improved optimistic bounds (Srebro et al., 2010), that exhibit fast convergence rates subject to vanishing empirical risk of the output. Another direction lies in making our bounds adaptive. So far we have presented bounds that have data-dependent components, however the step size cannot be adjusted depending on the data, e.g. as in (Zhao and Zhang, 2015). This was partially addressed by London (2016), albeit in the context of uniform stability, and we plan to extend this idea to the context of data-dependent stability.

Acknowledgments

This work was in parts funded by the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation programme (grant agreement no 637076).

This work was in parts funded by the European Research Council under the European Union’s Seventh Framework Programme (FP7/2007-2013)/ERC grant agreement no 308036.

References

Z. Allen-Zhu and E. Hazan. Variance reduction for faster non-convex optimization. In International Conference on Machine Learning (ICML), pages 699–707, 2016.

S. Ben-David and R. Urner. Domain adaptation as learning with auxiliary information. NIPS workshop on New Directions in Transfer and Multi-Task, 2013.

S. Boucheron, G. Lugosi, and P. Massart. Concentration inequalities: A nonasymptotic theory of independence. Oxford University Press, 2013.

O. Bousquet and A. Elisseeff. Stability and Generalization. Journal of Machine Learning Research, 2:499–526, 2002.

P. Chaudhari, A. Choromanska, S. Soatto, Y. LeCun, C. Baldassi, C. Borgs, J. Chayes, L. Sagun, and R. Zecchina. Entropy-sgd: Biasing gradient descent into wide valleys. In International Conference on Learning Representations (ICLR), 2017.
A. Choromanska, M. Henaff, M. Mathieu, G. B. Arous, and Y. LeCun. The loss surfaces of multilayer networks. In Conference on Uncertainty in Artificial Intelligence (AISTATS), 2015.

L. Devroye and T. Wagner. Distribution-free performance bounds for potential function rules. IEEE Transactions on Information Theory, 25(5):601–604, 1979.

A. Elisseeff, T. Evgeniou, and M. Pontil. Stability of randomized learning algorithms. Journal of Machine Learning Research, 6(Jan):55–79, 2005.

T. Galanti, L. Wolf, and T. Hazan. A theoretical framework for deep transfer learning. Information and Inference, page iaw008, 2016.

R. Ge, F. Huang, C. Jin, and Y. Yuan. Escaping from saddle points-online stochastic gradient for tensor decomposition. In Workshop on Computational Learning Theory (COLT), pages 797–842, 2015.

S. Ghadimi and G. Lan. Stochastic first-and zeroth-order methods for nonconvex stochastic programming. SIAM Journal on Optimization, 23(4):2341–2368, 2013.

A. Gonen and S. Shalev-Shwartz. Fast rates for empirical risk minimization of strict saddle problems. arXiv preprint arXiv:1701.04271, 2017.

I. Goodfellow, Y. Bengio, and A. Courville. Deep learning. The MIT Press, 2016.

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

S. Hochreiter and J. Schmidhuber. Flat minima. Neural Computation, 9(1):1–42, 1997.

K. Kawaguchi. Deep learning without poor local minima. In Conference on Neural Information Processing Systems (NIPS), pages 586–594, 2016.

N. S. Keskar, D. Mudigere, J. Nocedal, M. Smelyanskiy, and P. T. P. Tang. On large-batch training for deep learning: Generalization gap and sharp minima. In International Conference on Learning Representations (ICLR), 2017.

T. Koren and K. Levy. Fast rates for exp-concave empirical risk minimization. In Conference on Neural Information Processing Systems (NIPS), pages 1477–1485, 2015.

I. Kuzborskij and F. Orabona. Stability and hypothesis transfer learning. In International Conference on Machine Learning (ICML), pages 942–950, 2013.

I. Kuzborskij and F. Orabona. Fast Rates by Transferring from Auxiliary Hypotheses. Machine Learning, pages 1–25, 2016.

J. D. Lee, M. Simchowitz, M. I. Jordan, and B. Recht. Gradient descent only converges to minimizers. In Workshop on Computational Learning Theory (COLT), pages 1246–1257, 2016.

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

B. A. Pearlmutter. Fast exact multiplication by the hessian. Neural Computation, 6(1):147–160, 1994.

A. Pentina and C. H. Lampert. A pac-bayesian bound for lifelong learning. In International Conference on Machine Learning (ICML), 2014.
M. Perrot and A. Habrard. A theoretical analysis of metric hypothesis transfer learning. In International Conference on Machine Learning (ICML), pages 1708–1717, 2015.

T. Poggio, S. Voinea, and L. Rosasco. Online learning, stability, and stochastic gradient descent. arXiv preprint arXiv:1105.4701, 2011.

S. J. Reddi, A. Hefny, S. Sra, B. Poczos, and A. Smola. Stochastic variance reduction for nonconvex optimization. In International Conference on Machine Learning (ICML), pages 314–323, 2016.

S. Shalev-Shwartz and S. Ben-David. Understanding Machine Learning: From Theory to Algorithms. Cambridge University Press, 2014.

S. Shalev-Shwartz, O. Shamir, N. Srebro, and K. Sridharan. Learnability, stability and uniform convergence. Journal of Machine Learning Research, 11(Oct):2635–2670, 2010.

N. Srebro, K. Sridharan, and A. Tewari. Smoothness, low noise and fast rates. In Conference on Neural Information Processing Systems (NIPS), pages 2199–2207, 2010.

T. Tommasi, F. Orabona, and B. Caputo. Learning categories from few examples with multi model knowledge transfer. IEEE Transactions on Pattern Analysis and Machine Intelligence, 36(5):928–941, 2014.

C. Zhang, S. Bengio, M. Hardt, B. Recht, and O. Vinyals. Understanding deep learning requires rethinking generalization. In International Conference on Learning Representations (ICLR), 2017.

P. Zhao and T. Zhang. Stochastic optimization with importance sampling for regularized loss minimization. In International Conference on Machine Learning (ICML), pages 1–9, 2015.