HOW DOES SHARPNESS-AWARE MINIMIZATION MINIMIZE SHARPNESS?

Anonymous authors
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ABSTRACT

Sharpness-Aware Minimization (SAM) is a highly effective regularization technique for improving the generalization of deep neural networks for various settings. However, the underlying working of SAM remains elusive because of various intriguing approximations in the theoretical characterizations. SAM intends to penalize a notion of sharpness of the model but implements a computationally efficient variant; moreover, a third notion of sharpness was used for proving generalization guarantees. The subtle differences in these notions of sharpness can indeed lead to significantly different empirical results. This paper rigorously nails down the exact sharpness notion that SAM regularizes and clarifies the underlying mechanism. We also show that the two steps of approximations in the original motivation of SAM individually lead to inaccurate local conclusions, but their combination accidentally reveals the correct effect, when full-batch gradients are applied. Furthermore, we also prove that the stochastic version of SAM in fact regularizes the third notion of sharpness mentioned above, which is most likely to be the preferred notion for practical performance. The key mechanism behind this intriguing phenomenon is the alignment between the gradient and the top eigenvector of Hessian when SAM is applied.

1 INTRODUCTION

Modern deep nets are often overparametrized and have the capacity to fit even randomly labeled data (Zhang et al., 2016). Thus, a small training loss does not necessarily imply good generalization. Yet, standard gradient-based training algorithms such as SGD are able to find generalizable models. Recent empirical and theoretical studies suggest that generalization is well-correlated with the sharpness of the loss landscape at the learned parameter (Keskar et al., 2016; Dinh et al., 2017; Dziugaite & Roy, 2017; Neyshabur et al., 2017; Jiang et al., 2019). Partly motivated by these studies, Foret et al. (2021); Wu et al. (2020); Zheng et al. (2021) propose to penalize the sharpness of the landscape to improve the generalization. We refer this method to *Sharpness-Aware Minimization* (SAM) and focus on the version of Foret et al. (2021) in this paper.

Despite its empirical success, the underlying working of SAM remains elusive because of the various intriguing approximations made in its derivation and analysis. There are three different notions of sharpness involved – SAM intends to optimize the first notion, the sharpness along the worst direction but actually implements a computationally efficient notion, the sharpness along the direction of the gradient. But in the analysis, a third notion of sharpness is actually used to prove generalization guarantees, which admits the first notion as an upper bound. The subtle difference between the three notions can lead to very different explicit biases. (see Figure 1 for demonstraion)

More concretely, let L be the training loss, x be the parameter and ρ be the *perturbation radius*, a hyperparameter requiring tuning. The first notion corresponds to the following optimization problem (1), where we call $R_\rho^{\max}(x) = L_\rho^{\max}(x) - L(x)$ the *worst-direction sharpness* at x and thus SAM is intended to minimize the original training loss plus the worst-direction sharpness at x.

$$\min_x L_\rho^{\max}(x), \quad \text{where} \quad L_\rho^{\max}(x) = \max_{\|v\|_2 \le 1} L(x + \rho v), \tag{1}$$

However, even evaluation of $L_\rho^{\max}(x)$ is computationally expensive, not to mention optimization. Thus Foret et al. (2021); Zheng et al. (2021) propose to approximate the worst perturbation direction by the direction of the gradient and implement the second notion of sharpness, which corresponds

Type of Sharpness	Symbol	Definition	Explicit Bias Among Minimizers
Worst-direction	$L_\rho^{\max}$	$\max_{\|v\|_2 \le 1} L(x+\rho v)$	$\min_x \lambda_1(\nabla^2 L(x))$
Ascent-direction	L_ρ^{asc}	$L\left(x+\rho\frac{\nabla L(x)}{\|\nabla L(x)\|_2}\right)$	$\min_x \lambda_{\min}(\nabla^2 L(x))$
Average-direction	L_ρ^{avg}	$\mathbb{E}_{v\sim N(0,I)} L(x+\rho\frac{v}{\|v\|_2})$	$\min_x \operatorname{Tr}(\nabla^2 L(x))$

Table 1: Definitions and explicit biases of different notions of sharpness. Here $\lambda_{\min}$ denotes to the smallest *non-zero* eigenvalue.

to (2). We call $R_\rho^{\text{asc}}(x) = L_\rho^{\text{asc}}(x) - L(x)$ the *ascent-direction sharpness* at x.

$$\min_x L_\rho^{\text{asc}}(x), \quad \text{where} \quad L_\rho^{\text{asc}}(x) = L\left(x+\rho\frac{\nabla L(x)}{\|\nabla L(x)\|_2}\right). \tag{2}$$

Intriguingly, in the generalization analysis of SAM by Foret et al. (2021); Wu et al. (2020), the first notion of sharpness, *i.e.*, the worst-direction sharpness, is only used for upper bounding the third notion of sharpness via the PAC Bayesian theory (McAllester, 2003). We call the third notion $R_\rho^{\text{avg}}(x) = L_\rho^{\text{avg}}(x) - L(x)$ the *average-direction sharpness* at x, where $L_\rho^{\text{avg}}(x) = \mathbb{E}_{g\sim N(0,I)} L\left(x+\rho g/\|g\|\right)$.

For further acceleration, Foret et al. (2021); Zheng et al. (2021) omit the gradient through other occurrence of x and approximate the gradient of ascent-direction sharpness by gradient taken after one-step ascent, *i.e.*, $\nabla L_\rho^{\text{asc}}(x) \approx \nabla L\left(x+\rho\frac{\nabla L(x)}{\|\nabla L(x)\|_2}\right)$ and derive the update rule of SAM, where η is the learning rate.

$$\text{Sharpness-Aware Minimization (SAM):} \quad x(t+1) = x(t) - \eta\nabla L\left(x+\rho\frac{\nabla L(x)}{\|\nabla L(x)\|_2}\right) \tag{3}$$

In this paper, we analyze the explicit bias of various notions of sharpness and the optimization trajectory of SAM. Our analysis is performed for small perturbation radius ρ and learning rate η under the setting where the minimizers of loss form a manifold following Fehrman et al. (2020); Li et al. (2021) In particular, we make the following theoretical contributions.

1. We prove that full-batch SAM does minimize worst-direction sharpness. (Theorem 4.9)
2. Surprisingly, when batch size is 1, SAM minimizes average-direction sharpness. (Theorem 4.9)
3. We characterize the explicit biases of three notions of sharpness among minimizers when perturbation radius ρ goes to zero. (Theorems 4.5 to 4.7, also see Table 1) Surprisingly, both heuristic approximations made for the update rule of SAM lead to inaccurate solutions, that is, (1) minimizing worst-direction sharpness and ascent-direction sharpness induce different biases among minimizers, and (2) SAM doesn't minimize ascent-direction sharpness.

The key mechanism behind this implicit bias of SAM is the implicit alignment between the gradient and the top eigenvector of Hessian when running SAM.

2 Related Works

Sharpness and Generalization. The study on the connection between sharpness and generalization can be traced back to Hochreiter & Schmidhuber (1997). Keskar et al. (2016) observed a positive correlation between the batch size, the generalization error, and the sharpness of the loss landscape when changing the batch size. Jastrzebski et al. (2017) extends this by finding a correlation of the sharpness and the ratio between learning rate to batch size. Dinh et al. (2017) show that one can easily construct networks with good generalization but with arbitrary large sharpness by reparametrization. Dziugaite & Roy (2017); Neyshabur et al. (2017); Wei & Ma (2019) give theoretical guarantees on the generalization error using sharpness-related measures. Jiang et al. (2019) perform a large-scale empirical study on various generalization measures and showed that sharpness-based measures have the highest correlation with generalization.

Background on Sharpness Aware-Minimization. Foret et al. (2021); Zheng et al. (2021) concurrently proposed to minimize the loss at the perturbed from current parameter towards the worst direction to improve generalization. Wu et al. (2020) propose the almost identical method for a different purpose, robust generalization of adversarial training. Kwon et al. (2021) proposed a different metric for SAM to fix the rescaling problem pointed out by Dinh et al. (2017). Liu et al. (2022) propose an more computationally efficient version of SAM. Zhao et al. (2022) proposed to improve generalization by penalizing gradient norm. Their proposed algorithm can be viewed as a

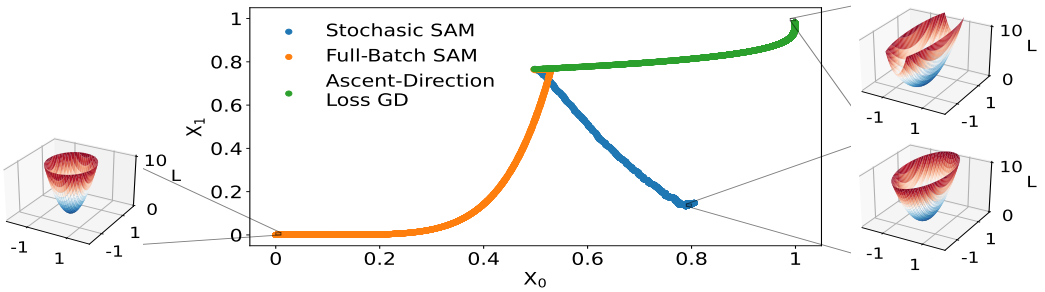

Figure 1: Visualization of the different biases of different sharpness notions on a 4D-toy example. For $x, y \in \mathbb{R}^2$, consider loss $L(x, y) = F_0(x)y_0^2 + F_1(x)y_1^2$ with $F_0(x) = x_0^2 + 6x_1^2 + 8$ and $F_1(x) = 4(1 - x_0)^2 + (1 - x_1)^2 + 1$. L has a zero loss manifold $\{y = 0\}$ and the eigenvalues of its Hessian on manifold are $F_0(x)$ and $F_1(x)$ with $F_0(x) \geq 8 > 6 \geq F_1(x)$ on $[0, 1]^2$. As our theory predicts, (1). full-batch SAM (3) finds the minimizer with the smallest top eigenvalue, $F_0(x)$; (2). GD on Ascent-direction Loss L_ρ^{asc} (2) finds the minimizer with the smallest bottom eigenvalue, $F_0(x)$. (3). Stochastic SAM (16) (with $L_0(x, y) = F_0(x)x_0^2, L_1(x, y) = F_1(x)y_1^2$) finds the minimizer with smallest trace of Hessian. Loss landscape $L(x, \cdot)$ are visualized as 3D plots at converged x to illustrate the different biases. (*cf.*Table 1)

generalization of SAM. Andriushchenko & Flammarion (2022) studied a variant of SAM where the step size of ascent step is ρ instead of $\frac{\rho}{\|\nabla L(x)\|_2}$. They showed that for a simple model this variant of SAM has a stronger regularization effect when batch size is 1 compared to the full-batch case and argued that this might be the explanation that SAM generalizes better with small batch sizes.

3 Notations and Assumptions

For any integer k, we define $\mathcal{C}^k$ as the set of k times continuously differentiable functions. For any mapping F, we define $\partial F(x)[u]$ and $\partial^2 F(x)[u, v]$ as the first and second order directional derivative of $F(x)$ along the direction u (and v). Given a differential submanifold Γ of $\mathbb{R}^D$ and a point $x \in \Gamma$, define $P_{x,\Gamma}$ as the projection operator onto the manifold of the normal space of Γ at x and $P_{x,\Gamma}^\top = I_D - P_{x,\Gamma}$. We fix our initialization as x_{init} and our loss function as $L : \mathbb{R}^D \to \mathbb{R}$. Given the loss function, the gradient flow can be defined as mapping $\phi : \mathbb{R}^D \times [0, \infty) \to \mathbb{R}^D$ satisfying $\phi(x, \tau) = x - \int_0^\tau \nabla L(\phi(x, t))dt$. We further define the limiting map $\Phi : \mathbb{R}^D \to \mathbb{R}^D$ as $\Phi(x) = \lim_{\tau\to\infty} \phi(x, \tau)$. For any positive definite symmetry matrix $A \in \mathbb{R}^{D\times D}$, define $\{\lambda_i(A), v_i(A)\}_{i\in[D]}$ as all its eigenvalues and eigenvectors satisfying $\lambda_1(A) \geq \lambda_2(A) ... \geq \lambda_3(A)$ and $\|v_i(A)\|_2 = 1$. Our analysis assumes sufficiently small η and ρ and uses $O(\cdot)$ to hide constant.

Following Fehrman et al. (2020); Li et al. (2021); Arora et al. (2022), we make the below assumption.

Assumption 3.1. *Assume loss $L : \mathbb{R}^D \to \mathbb{R}$ belongs to $\mathcal{C}^4$, and there exists a manifold Γ that is $D - M$ dimensional $\mathcal{C}^2-$submanifold of $\mathbb{R}^D$ for some integer $1 \leq M \leq D$, where for all $x \in \Gamma$, x is a global minimizer of L, $L(x) = 0$ and rank$(\nabla^2 L(x)) = M$.*

The smoothness assumption is meet with networks with smooth activation functions and the existence of the manifold is due to the vast overparameterization of the modern neural network. The full rank assumption is necessary for the analysis to guarantee the differentiability of Φ.

Definition 3.2 (Attraction Set)**.** *Let U be the attraction set of Γ under gradient flow, that is, a neighborhood of Γ containing all points starting from which gradient flow w.r.t. loss L converges to some point in Γ, or mathematically, $U \triangleq \{x \in \mathbb{R}^D | \Phi(x)$ exists and $\Phi(x) \in \Gamma\}$.*

Assumption 3.1 implies that U is open and Φ is in $\mathcal{C}^3$ on U (from Lemma B.15 Arora et al. (2022)).

4 Explicit and Implicit Bias in the Full-batch Setting

Section 4.1 provides a general theorem to properly analyze the explicit bias of various notions of sharpness among different minimizers. We then apply our machinery on *ascent-direction sharpness* and *worst-direction sharpness* and show that they have different explicit biases. In Section 4.2 we provide our main theorem in the full-batch setting, that SAM implicitly minimizes the worst-direction sharpness, via characterizing its limiting dynamics as learning rate ρ and η goes to 0 with

a Riemmanian gradient flow with respect to the top eigenvalue of the Hessian of the loss on the manifold of global minimizers. In Section 4.3 we sketch the proof of the implicit bias of SAM and identified a key property behind the implicit bias, which is the implicit alignment between the gradient and the top eigenvector of the Hessian throughout the training.

4.1 Worst- and Ascent-direction Sharpness have Different Explicit Bias

The intuition of approximating $R_\rho^{\max}$ by R_ρ^{asc} comes from the following Taylor expansions (Foret et al., 2021; Wu et al., 2020), which works for small ρ:

$$R_\rho^{\max}(x) = \sup_{\|v\|_2 \le 1} L(x+\rho v) - L(x) = \sup_{\|v\|_2 \le 1} \left(\rho v^\top \nabla L(x) + \frac{\rho^2}{2} v^\top \nabla^2 L(x) v + O(\rho^3) \right) \quad (4)$$

$$R_\rho^{\text{asc}}(x) = L\left(x + \rho \frac{\nabla L(x)}{\|\nabla L(x)\|_2} \right) - L(x) = \rho \|\nabla L(x)\|_2 + \frac{\rho^2}{2} \frac{\nabla L(x)^\top \nabla^2 L(x) \nabla L(x)}{\|\nabla L(x)\|_2^2} + O(\rho^3) \quad (5)$$

Here, the preference among the global minima is what we are mainly concerned with. Since $\sup_{\|v\|_2 \le 1} v^\top \nabla L(x) = \|\nabla L(x)\|_2$ when $\|\nabla L(x)\|_2 > 0$, the leading terms in Equations (4) and (5) are both the first order term, $\rho \|\nabla L(x)\|_2$, and are the same. However, it is erroneous to think that the first order term decides the explicit bias, as the first order term $\|\nabla L(x)\|_2$ vanishes at the global minimizers of the loss L and thus the second order term becomes the leading term. Any global minimizer x of the original loss L is an $O(\rho^2)$-approximate minimizer of the sharpness-aware loss because $\nabla L(x) = 0$. Therefore, the sharpness-aware loss needs to be of order ρ^2 so that we can guarantee the second-order terms in Equation (4) and/or Equation (5) to be non-trivially small.

In this section, we aim to understand under Assumption 3.1 what the explicit biases of various notions of sharpness among different minimizers are. Theorem 4.3 will be our main theoretic tool to analyze the explicit bias for small perturbation radius ρ. Below we first introduce some notations and assumption.

Notation for Regularizers. Let $R_\rho : \mathbb{R}^D \to \mathbb{R} \cup \{\infty\}$ be a family of regularizers parameterized by ρ. If R_ρ is not well-defined at some x, then we let $R_\rho(x) = \infty$. This convention will be useful when analyzing ascent-direction sharpness $R_\rho^{\text{asc}} = L_\rho^{\text{asc}} - L$ which is not defined when $\nabla L(x) = 0$. This convention will not change the minimizers of the regularized loss. Intuitively, a regularizer should always be non-negative, but however, when far away from manifold, regularizer $R_\rho(x)$ can actually be negative, *e.g.*, $R_\rho^{\text{avg}}(x) \approx \frac{\rho^2}{2D} \operatorname{Tr}[\nabla^2 L(x)]$. Therefore we make the following assumption to allow the regularizer to be mildly negative.

Assumption 4.1. *Suppose for any bounded closed set $B \subset U$, there exists $C > 0$, such that for sufficiently small ρ, $\forall x \in B, R_\rho(x) \ge -C\rho^2$.*

The following concept of limiting regularizer is of crucial role in our analysis.

Definition 4.2 (Limiting Regularizer)**.** *We define the* limiting regularizer *of $\{R_\rho\}$ as the function*

$$S : \Gamma \to \mathbb{R}, \quad S(x) = \lim_{\rho \to 0} \lim_{r \to 0} \inf_{\|x' - x\|_2 \le r} R_\rho(x')/\rho^2.$$

We say the limiting regularizer S of $\{R_\rho\}$ is a good *around some $x^* \in \Gamma$, if there is an open set V containing x^*, such that S is a non-negative continuous function in V and for any $\epsilon > 0$, there is some $\rho_{x^*} > 0$, it holds that $\forall x \in \Gamma \cap V, \rho \le \rho_{x^*}, \left| S(x) - \inf_{\|x'-x\|_2 \le \epsilon \cdot \rho} R_\rho(x')/\rho^2 \right| < \epsilon$. We say the limiting regularizer S is* good *on Γ, if S is good around every point $x \in \Gamma$.*

The high-level intuition behind the definition of limiting regularizer is that we want to use it to capture the second order term in the Taylor expansion of regularizer R_ρ when $\rho \to 0$. When the second order term is continuous in x, the definition of $S(x)$ can also be simplified as $R_\rho(x)/\rho^2$. The intuition of the concept of a good limiting regularizer is that, the regularizer should not change very fast, especially in an $O(\rho)$ neighborhood of the minimizer. If so, the minimizer of the regularized loss may be $\Omega(\rho)$ away from any minimizer to reduce the regularizer at the cost of increasing the original loss, which makes the limiting regularizer unable to capture the explicit bias of the regularizer.

Theorem 4.3. *Let U' be any bounded open set such that its closure $\overline{U'}$ is contained in U and that $\overline{U'} \cap \Gamma = \overline{U' \cap \Gamma}$. Then for any family of parametrized regularizers $\{R_\rho\}$ admitting a good limiting*

regularizer on Γ and satisfying Assumption 4.1 and any $\epsilon \geq 0$, there is a $\rho_0 > 0$, such that for all $u \in U'$ and $\rho < \rho_0$, it holds that

$$L(u) + R_\rho(u) \leq \inf_{x \in U'} (L(x) + R_\rho(x)) + \epsilon\rho^2 + o(\rho^2)$$
$$\iff \left(L(u) - \inf_{x \in U'} L(x)\right) + \left|R_\rho(u) - \rho^2 \inf_{x \in U' \cap \Gamma} S(x)\right| \leq \epsilon\rho^2 + o(\rho^2)$$

For the applications we are interested in in this paper, the good limiting regularizer S can be continuously extended to the entire space $\mathbb{R}^D$. In such a case, the implication of "$\Longrightarrow$" of Theorem 4.3 also admits the following alternative form which doesn't involve R_ρ. Corollary 4.4 implies minimizing regularized loss $L(x) + R_\rho(x)$ is equivalent to minimizing the limiting regularizer of $\{R_\rho\}_\rho$, $S(x)$ on the global minimizer manifold Γ.

Corollary 4.4. *Under the setting of Theorem 4.3, let $\overline{S}$ be an continuous extension of S to $\mathbb{R}^d$, if $L(u) + R_\rho(u) \leq \inf_{x \in U'} (L(x) + R_\rho(x)) + \epsilon\rho^2 + o(\rho^2)$, then we have that $L(u) - \inf_{x \in U'} L(x) = O(\rho^2)$ and that $\left|\overline{S}(u) - \inf_{x \in U' \cap \Gamma} \overline{S}(x)\right| = \epsilon + o(1)$.*

Corollary 4.4 suggests a sharp phase transition of the property of the solution of $\min_x L(x) + R_\rho(x)$ when the optimization error drops from $\omega(\rho^2)$ to $O(\rho^2)$. when the optimization error is larger than $\omega(\rho^2)$, no regularization effect happens and any minimizer satisfies the requirement. When the error becomes $O(\rho^2)$, there is a non-trivial restriction on the (extended) limiting regularizer.

Below we show all of worst-, ascent- and average-direction sharpness admit good limiting regularizers. Thus we can apply Corollary 4.4 to characterize their explicit biases, which are all different.

Theorem 4.5. *Worst-direction sharpness $R_\rho^{\max}$ satisfies Assumption 4.1 and admits $\lambda_1(\nabla^2 L(\cdot))/2$ as a good limiting regularizer on Γ.*

Theorem 4.6. *Ascent-direction sharpness R_ρ^{asc} satisfies Assumption 4.1 and admits $\lambda_M(\nabla^2 L(\cdot))/2$ as a good limiting regularizer on Γ.*

Theorem 4.7. *Average-direction sharpness R_ρ^{avg} satisfies Assumption 4.1 and admits $\operatorname{Tr}(\nabla^2 L(\cdot))/(2D)$ as a good limiting regularizer on Γ.*

When R_ρ is continuous at some $x \in \Gamma$, the definition of $S(x)$ can be simplified as $\lim_{\rho \to 0} R_\rho(x)/\rho^2$. Worst- and average- direction sharpness fall into this type and the limiting regularizer can be solved straightforwardly by Taylor expansion, which is well-known in literature (Keskar et al., 2016; Kaur et al., 2022; Zhuang et al., 2022; Orvieto et al., 2022). Theorems 4.5 and 4.7 can be viewed as a restatement of the existing results in our manifold setting.

Our major contribution in this subsection is the analysis for ascent-direction sharpness, which is more tricky as $R_\rho^{\text{asc}}(x) = \infty$ and thus is not continuous for any $x \in \Gamma$. To minimize R_ρ^{asc} around x, we can pick $x' \to x$ to make $\|\nabla L(x)\|_2 \to 0$ but not equal to 0. By (5), we have $R_\rho^{\text{asc}}(x') \approx \rho^2/2 \cdot \nabla L(x')^\top \nabla^2 L(x) \nabla L(x')/\|\nabla L(x')\|^2$. Here the crucial step of the proof is that because of Assumption 3.1, $\nabla L(x)/\|\nabla L(x)\|_2$ must almost lie in the column span of $\nabla^2 L(x)$, and thus implies $\inf_{x'} \nabla L(x')^\top \nabla^2 L(x) \nabla L(x')/\|\nabla L(x')\|^2 \overset{\rho \to 0}{\to} \lambda_M(\nabla^2 L(x))$. The above alignment property between the gradient and the column space of Hessian can be checked directly for any non-negative quadratic function and the maximal Hessian rank assumption in Assumption 3.1 ensures this property extends to general losses.

4.2 SAM Provably Decreases Worst-direction Sharpness Locally

Though ascent-direction sharpness has different explicit bias from worst-direction sharpness, in this subsection we will show that surprisingly, SAM, an heuristic method designed to minimize ascent-direction sharpness, provably decreases worst-direction sharpness. The main result here is an exact characterization of the trajectory of SAM (3) via the following ordinary differential equation (ODE) (6), when learning rate η and perturbation radius ρ are small and the initialization $x(0) = x_{\text{init}}$ is in U. We call the solution of (6) the *limiting flow* of SAM, which is exactly the Riemannian Gradient Flow on the manifold Γ with respect to $\lambda_1(\nabla^2 L(\cdot))$. In other words, the ODE (6) is essentially

a projected gradient descent algorithm with loss $\lambda_1(\nabla^2 L(\cdot))$ on the constraint set Γ and an infinitesimal learning rate.

$$X(\tau) = X(0) - \frac{1}{2}\int_{s=0}^{\tau} P_{X(s),\Gamma}^{\top}\nabla\lambda_1(\nabla^2 L(X(s)))ds, X(0) = \Phi(x_{\text{init}}). \tag{6}$$

Note $\lambda_1(\nabla^2 L(x))$ may not be differentiable at x if $\lambda_1(\nabla^2 L(x)) = \lambda_2(\nabla^2 L(x))$, thus to ensure the (6) is well-defined, we assume there is a positive eigengap for L on Γ. Assuming ODE (6) has a solution till time T_3, we have Theorem 4.9, which is the main theorem of this section.

Assumption 4.8. *For $x \in \Gamma$, there exists a positive eigengap,i.e., $\lambda_1(\nabla^2 L(x)) > \lambda_2(\nabla^2 L(x))$.*

Theorem 4.9 (Main, Theorems C.23 and C.24 stated informally)**.** *Let $\{x(t)\}$ be the iterates of SAM (3) with $x(0) = x_{init} \in U$, then under Assumptions 3.1 and 4.8, for all η, ρ such that $\eta\ln(1/\rho)$ and ρ/η are sufficiently small, the dynamics of SAM can be split into two phases:*

- ***Phase I:*** *SAM follows Gradient Flow with respect to L until entering an $O(\eta\rho)$ neighborhood of the manifold Γ in $\tilde{O}(\frac{1}{\eta})$ steps;*
- ***Phase II:*** *SAM tracks the solution X of (6), the Riemannian Gradient Flow with respect to $\lambda_1(\nabla^2 L(\cdot))$ in the $O(\eta\rho)$ neighborhood in the sense that $\max_{0\le T\le T_3}\|\Phi(x(\lceil T/(\eta\rho^2)\rceil)) - X(T)\| = O((\eta+\rho)\log(1/\eta\rho))$. Moreover, the angle between $\nabla L(x(t))$ and $v_1(\nabla^2 L(x(t)))$ is at most $O(\rho)$.*

Theorem 4.9 shows that SAM decreases the largest eigenvalue of Hessian of loss locally around the manifold of global minimizers. As a corollary of Theorem 4.9, we can also show that the largest eigenvalue of the limiting flow closely tracks the regularized training loss.

Corollary 4.10. *For all $T_3' > 0$, for all ρ, η such that $\eta\ln(1/\rho)$ and ρ/η are sufficiently small we have $\forall T_3' < \eta\rho^2 t \le T_3$, $\|R_\rho^{\max}(x(t)) - \rho^2\lambda_1(\nabla^2 L(X(\eta\rho^2 t))/2\| = \tilde{O}(\eta\rho^2)$*

Recall Theorem 4.6 shows that the largest eigenvalue of Hessian is the limiting regularizer of the *worst-direction sharpness*, leveraging the equivalence relationship in Theorem 4.3, below we show that full-batch SAM provably minimizes *worst-direction sharpness* if we additionally assume the limiting flow converges to a local minimizer of the top eigenvalue of Hessian.

Corollary 4.11. *Define U' as in Theorem 4.3, suppose $X(\infty) = \lim_{t\to\infty} X(t)$ exists and is a minimizer of $\lambda_1(\nabla^2 L(x))$ in $U' \cap \Gamma$, for all $\epsilon > 0$, there exists a constant $T > 0$, then for all ρ, η such that $\eta\ln(1/\rho)$ and ρ/η are sufficiently small we have $L_\rho^{\max}(x(\lceil T/(\eta\rho^2)\rceil)) \le \epsilon\rho^2 + \inf_{x\in U'} L_\rho^{\max}(x)$*

4.3 Proof Sketch for Phase II in Theorem 4.9

Now we sketch the proof for the ODE-based characterization of the trajectory of SAM in Phase II. The framework of the analysis is similar to Arora et al. (2022); Lyu et al. (2022), where the high-level idea is to use $\Phi(x(t))$ as a proxy for $x(t)$ and study the dynamics of $\Phi(x(t))$ via Taylor expansion, which turns out to be dependent on the alignment between the gradient and the eigenvectors of the Hessian. In particular, like Arora et al. (2022); Lyu et al. (2022), we show that the gradient aligns to the top eigenvector of Hessian, and thus encourages the SAM dynamics to reduce the top eigenvalue of the Hessian.

Taylor Expansion on Φ. In Phase II, it can be shown that $\|x(t) - \Phi(x(t))\| = O(\eta\rho)$ holds for every step, this implies $\|x(t+1) - x(t)\|_2 = O(\rho\eta)$. (See Lemma C.12) Therefore we have that

$$\begin{aligned}\Phi(x(t+1)) - \Phi(x(t)) =& -\eta\partial\Phi(x(t))(x(t+1) - x(t)) + O(\eta\|x(t+1) - x(t)\|^2)\\ =& -\eta\partial\Phi(x(t))\nabla L\left(x + \rho\frac{\nabla L(x)}{\|\nabla L(x)\|_2}\right) + O(\eta^3\rho^2)\end{aligned} \tag{7}$$

Now we apply Taylor expansion on $\nabla L\left(x + \rho\frac{\nabla L(x)}{\|\nabla L(x)\|_2}\right)$ around x and get

$$\begin{aligned}&\nabla L\left(x + \rho\frac{\nabla L(x)}{\|\nabla L(x)\|_2}\right)\\ =&\nabla L(x) - \rho\nabla^2 L(x)\frac{\nabla L(x)}{\|\nabla L(x)\|_2} + \frac{\rho^2}{2}\partial^2(\nabla L)(x)\left[\frac{\nabla L(x)}{\|\nabla L(x)\|_2}, \frac{\nabla L(x)}{\|\nabla L(x)\|_2}\right] + O(\rho^3).\end{aligned} \tag{8}$$

Lemma 4.12 (Lemma B.16 Arora et al. (2022)). *For $x \in U$, $\partial\Phi(x)\nabla L(x) = 0$, $\partial\Phi(x)\nabla^2 L(x)\nabla L(x) = -\partial^2\Phi(x)[\nabla L(x), \nabla L(x)]$.*

Now we plug (8) into (7) and simplify the expression using Lemma 4.12. We have that

$$\begin{aligned}\Phi(x(t+1)) - \Phi(x(t)) =& 0 + O(\rho \left\|\partial\Phi(x(t))\nabla^2 L(x(t))\right\| \|\nabla L(x(t))\|_2) \\ &- \frac{\eta\rho^2}{2}\partial\Phi(x)\partial^2(\nabla L)(x)\left[\frac{\nabla L(x)}{\|\nabla L(x)\|_2}, \frac{\nabla L(x)}{\|\nabla L(x)\|_2}\right] + O(\eta^3\rho^2 + \eta\rho^3)\end{aligned} \tag{9}$$

where in the last step we use the property that $\|x(t) - \Phi(x(t))\| = O(\eta\rho)$, which further implies $\|\nabla L(x(t))\|_2 = O(\eta\rho)$ in Phase II (See Lemma C.7).

Lemma 4.13. *For $x \in \Gamma$, $\partial\Phi(x) = P_{x,\Gamma}^\top$, $\partial\Phi(x)\nabla^2 L(x) = 0$, where $P_{x,\Gamma}^\top$ is the orthogonal projection matrix of the tangent space of Γ at x.*

Next we use Lemma 4.13 to further simplify (9). Since the entire phase II happens in an $O(\eta\rho)$-neighborhood of manifold Γ, we have that $\|x(t) - \Phi(x(t))\|_2 = O(\eta\rho)$, thus both $\left\|\partial\Phi(x(t))\nabla^2 L(x(t))\right\|$ and $\|\nabla L(x(t))\|_2$ are $O(\eta\rho)$. So far, the proof is almost completed, with the implicit alignment between gradient and top eigenvector of Hessian being the last missing piece. Suppose we have $\left\|\frac{\nabla L(x)}{\|\nabla L(x)\|_2} - v_1(\nabla^2 L(x))\right\| = O(\rho)$, then it holds that

$$\begin{aligned}\Phi(x(t+1)) - \Phi(x(t)) &= -\frac{\eta\rho^2}{2}\partial\Phi(x)\partial^2(\nabla L)(x)\left[\frac{\nabla L(x)}{\|\nabla L(x)\|_2}, \frac{\nabla L(x)}{\|\nabla L(x)\|_2}\right] + O(\eta^3\rho^2 + \eta\rho^3) \\ &= -\frac{\eta\rho^2}{2}\partial\Phi(x)\partial^2(\nabla L)(x)\left[v_1(\nabla^2 L(x)), v_1(\nabla^2 L(x))\right] + O(\eta^3\rho^2 + \eta\rho^3) \\ &= -\frac{\eta\rho^2}{2}\partial\Phi(x(t))\nabla\lambda_1(\nabla^2 L(x(t))) + O(\eta^3\rho^2 + \eta\rho^3) \\ &= -\frac{\eta\rho^2}{2}\partial\Phi(\Phi(x(t)))\cdot\nabla\lambda_1(\nabla^2 L(x))|_{x=\Phi(x(t))} + O(\eta^3\rho^2 + \eta\rho^3),\end{aligned} \tag{10}$$

where the second to last step we use the following property about the derivative of eigenvalue (Lemma C.33) and the last step is due to Taylor expansion.

Implicit Hessian-gradient Alignment. It remains to explain why the gradient implicitly aligns to the top eigenvector of Hessian, which is the key component of the analysis in Phase II. The proof strategy here is to first show alignment for a quadratic loss function, and then generalize its proof to general loss functions satisfying Assumption 3.1. Below we first give the formal statement of the implicit alignment on quadratic loss Theorem 4.14. Note this alignment property is an implicit property of the SAM algorithm – it is not due to the fact that SAM is an approximation of GD on L_ρ^{asc}, because optimizing L_ρ^{asc} would rather make the gradient align to the smallest eigenvector!

Theorem 4.14. *Suppose A is a positive definite symmetric matrix with unique top eigenvalue. Consider running SAM on loss $L(x) := \frac{1}{2}x^T Ax$ as (11), then for almost every $x(0)$, we have $x(t)$ converges in direction to $v_1(A)$ and $\lim_{t\to\infty}\|x(t)\| = \frac{\eta\rho\lambda_1(A)}{2-\eta\lambda_1(A)}$ with $\eta\lambda_1(A) < 1$.*

$$x(t+1) = x(t) - \eta A\left(x(t) + \rho\frac{Ax(t)}{\|Ax(t)\|}\right), \tag{11}$$

Equivalently, we can reformulate the update rule through the lens of the gradient $\nabla L(x) = Ax$:

$$\nabla L(x(t+1)) = \nabla L(x(t)) - \eta(\nabla^2 L(x(t)))^2\left(\nabla L(x(t)) + \rho\frac{\nabla L(x(t))}{\|\nabla L(x(t)))\|}\right), \tag{12}$$

and the result of Theorem 4.14 becomes the alignment between gradient and the top eigenvector of Hessian. This property can be generalized to the analysis of general loss as the dynamic of SAM near a fixed point on Γ is similar to the quadratic case with small perturbation. To see this, we apply Taylor expansion on the update rule of SAM (3):

$$x(t+1) = x(t) - \eta\nabla L(x(t)) - \eta\rho\nabla^2 L(x(t))\frac{\nabla L(x(t))}{\|\nabla L(x(t))\|_2} + O(\eta\rho^2). \tag{13}$$

Since phase II happens in an $O(\eta\rho)$-neighborhood of manifold Γ, we have $\|x(t+1)-x(t)\|_2 = O(\eta\rho)$. Then by (13) and Taylor expansion on $\nabla L(x(t+1))$ at $x(t)$, we have that

$$\nabla L(x(t+1)) = \nabla L(x(t)) - \nabla^2 L(x(t))\,(x(t+1)-x(t)) + O(\eta^2\rho^2) \tag{14}$$

$$= \nabla L(x(t)) - \eta(\nabla^2 L(x(t)))^2 \left(\nabla L(x(t)) + \rho\frac{\nabla L(x(t))}{\|\nabla L(x(t)))\|}\right) + O(\eta\rho^2) \tag{15}$$

Equation (14) is a $O(\eta\rho^2)$-perturbed version of the update rule in the quadratic case. Note this is a higher order term comparing to the other two terms, which have orders $\Theta(\eta^2\rho)$ and $\Theta(\eta\rho)$ respectively, the implicit alignment between Hessian and gradient happens for the same reason as in the quadratic case. We further show once this alignment happens, it will be kept until the end of our analysis, which is $\Theta(\eta^{-1}\rho^{-2})$ steps.

5 Explicit and Implicit bias in the Stochastic Setting

In practice, people usually use SAM in the stochastic mini-batch setting, and the test accuracy improves as the batch size decreases (Foret et al., 2021). Towards explaining this phenomenon, Foret et al. (2021) argue intuitively that stochastic SAM minimizes stochastic worst-direction sharpness. Given our results in Section 4, it's natural to ask if we can justify the above intuition by showing the implicit Hessian-gradient alignment in the stochastic setting. Unfortunately, such alignment is not possible in the most general setting. For example, take a simple quadratic loss $L(x) = \frac{L_1(x)+L_2(x)}{2}$, where $L_k(x) = 0.5x^\top A_k x$ and A_k is a positive definite matrix for $k = 1, 2$. If A_1 and A_2 have different top eigendirection, then no x can simultaneously satisfy that $\nabla L_k(x) = A_k x$ aligns to the top eigenvector of $\nabla^2 L_k(x) = A_k$. Yet when the batch size is 1, we can prove rigorously that stochastic SAM minimizes stochastic worst-direction sharpness (Section 5.2), which is the main result in this section.

Below we start by introducing our setting for SGD with batch size 1. We still need Assumption 3.1 in this section. We first by analyzing the explicit bias of the stochastic ascent- and worst-direction sharpness in Section 5.1 via the tools developed in Section 4.1. It turns out they are all proportional to the trace of hessian as $\rho \to 0$. In Section 5.2, we show stochastic SAM locally decreases trace of Hessian.

Setting Let $f_k(x)$ be the model output on kth data where f_k is a $\mathcal{C}^4$-smooth function and y_k be the ith label for $l = 1, \ldots, M$. We define the loss on kth data as $L_k(x) = \ell(f_k(x), y_k)$ and the total loss $L = \sum_{k=1}^M L_k/M$, where $\ell(y', y)$ is a $\mathcal{C}^4$-smooth function satisfying the following properties[1]: (1). $\arg\min_{y'\in\mathbb{R}} \ell(y', y) = y$, for any $y \in \mathbb{R}$; (2). $\frac{d^2\ell(y',y)}{d^2y'}|_{y'=y} > 0$, for any $y \in R$; (3). There exists x_0, such that for any $k \in [M]$, it holds that $f_k(x_0) = y_k$.

5.1 Stochastic Worst- and Ascent-direction Sharpness have Same Explicit Bias

Below we specify *stochastic worst-direction sharpness* and *stochastic ascent-direction sharpness* as $\mathbb{E}_k[R^{\max}_{k,\rho}] = \mathbb{E}_k[L^{\max}_{k,\rho}] - L$ and $\mathbb{E}_k[R^{\text{asc}}_{k,\rho}] = \mathbb{E}_k[L^{\text{asc}}_{k,\rho}] - L$. Here $L^{\max}_{k,\rho}$ and $L^{\text{asc}}_{k,\rho}$ is defined as in Equations (1) and (2) with L replaced by L_k. Unlike the full-batch setting, these two sharpness have same explicit bias, or more precisely, they have the same limiting regularizers. We omit the result on the stochastic average-direction sharpness as it is the same as its counterpart in the full-batch case.

Theorem 5.1. *Stochastic worst-direction sharpness* $\mathbb{E}_k[R^{\max}_{k,\rho}]$ *satisfies Assumption 4.1 and admits* $\mathrm{Tr}(\nabla^2 L(\cdot))/2$ *as a good limiting regularizer on* Γ.

Theorem 5.2. *Stochastic ascent-direction sharpness* $\mathbb{E}_k[R^{\text{asc}}_{k,\rho}]$ *satisfies Assumption 4.1 and admits* $\mathrm{Tr}(\nabla^2 L(\cdot))/2$ *as a good limiting regularizer on* Γ.

Unlike in the full-batch setting where the implicit regularizer of ascent-direction sharpness and worst-direction sharpness have different explicit bias, here they are the same because there is no difference between the maximum and minimum of its non-zero eigenvalue for rank-1 Hessian of each individual loss, and that the average of limiting regularizers is equal to the limiting regualrizer of the average regularizers by definition.

[1]Examples include ℓ_2 loss: $\ell(y, y') = 0.5(y - y')^2$.

5.2 STOCHASTIC SAM MINIMIZES STOCHASTIC WORST-DIRECTION SHARPNESS

Stochastic SAM: Recall L_k is the loss on kth data, we use *stochastic SAM* to denote the following update rule, where k_t is sampled i.i.d from uniform distribution on $[M]$.

$$x(t+1) = x(t) - \eta \nabla L_{k_t}\left(x + \rho \frac{\nabla L_{k_t}(x)}{\|\nabla L_{k_t}(x)\|_2}\right), \tag{16}$$

The goal of this section is to show stochastic SAM tracks the following Riemannian gradient flow with respect to $\mathrm{Tr}(\nabla^2 L(\cdot))$ on the manifold for sufficiently small η and ρ,

$$X(\tau) = X(0) - \frac{1}{2}\int_{s=0}^{\tau} P_{X(s),\Gamma}^{\top} \nabla \mathrm{Tr}(X(s)) ds, X(0) = \Phi(x_{\text{init}}). \tag{17}$$

The fundamental difference between stochastic SAM (16) with batch size 1 and that in the general setting is that the rank of the Hessian of each stochastic loss at minimizers is only rank-1, which enforces the gradient $\nabla L_k(x) \approx \nabla^2 L_k(x)(x - \Phi(x))$ to (almost) lie in the direction of the top eigenvalue of the Hessian. Lemma 5.3 formally states this property. For convenience, we denote $\frac{d^2\ell(y',y_k)}{d^2y'}|_{y'=f_k(x)}\|\nabla f_k(x)\|^2, \nabla f_k(x)/\|\nabla f_k(x)\|$ as $\Lambda_k(x), w_k(x)$.

Lemma 5.3. *Under Assumption 3.1, for any $x \in U$ and $p \in \Gamma$,$\nabla^2 L_k(p) = \Lambda_k(p) w_k(p) w_k(p)^T$ and $\exists s \in \{1,-1\} \frac{\nabla L_k(x)}{\|\nabla L_k(x)\|} = s w_k(p) + O(\|x-p\|)$*

With Lemma 5.3, we can show $\Phi(x(t+1)) - \Phi(x(t)) = -\eta\rho^2 P_{t,\Gamma}^{\top}\nabla(\Lambda_k(x))/2 + \tilde{O}(\eta^2\rho^2)$ when $\|x(t+1) - x(t)\| = \tilde{O}(\eta\rho)$, via a similar but slightly more complicated analysis on $\Phi(x(t+1)) - \Phi(x(t))$ as in Section 4.2. As we have $\mathbb{E}[\Lambda_k(x)] = (\sum_k \Lambda_k(x))/M = \mathrm{Tr}(\nabla^2 L(x)), x \in \Gamma$, we have that locally SAM is essentially performing a stochastic projected gradient descent with respect to $\mathrm{Tr}(\nabla^2 L(\cdot))$.

It still remains to prove stochastic SAM gets $\tilde{O}(\eta\rho)$ close of the manifold, which is addressed by Theorem C.27. Put everything together, we have the following main theorem for this section.

Theorem 5.4. *Let $\{x(t)\}$ be the iterates defined by SAM (16) and $x(0) = x_{init} \in U$, then under Assumption 3.1, for all η and ρ such that $(\eta+\rho)\log(1/\eta\rho)$ is sufficiently small, the dynamics of SAM can be split into two phases:*

- ***Phase I:*** *Stochastic SAM follows Gradient Flow with respect to L until entering an $O(\eta\rho)$ neighborhood of the manifold Γ in $\tilde{O}(\frac{1}{\eta})$ steps, with probability at least $1 - O(\sqrt{\rho})$;*
- ***Phase II:*** *Stochastic SAM tracks the solution X of (17), the Riemannian Gradient Flow with respect to $\mathrm{Tr}(\nabla^2 L(\cdot))$, with time scaling as $\|\Phi(x(\lceil T_3/(\eta\rho^2)\rceil)) - X(T_3)\| = O((\eta+\rho)\log(1/\eta\rho)$.*

Corollaries 5.5 and 5.6 below are stochastic counterparts of Corollaries 4.10 and 4.11, which says that the trace of Hessian of the limiting flow of well-tracks the stochastic worst-direction sharpness, and therefore when the limiting flow converges to a local minimizer of trace of Hessian, stochastic SAM minimizes the stochastic worst-direction sharpness.

Corollary 5.5. *For all $T_3' > 0$, for all ρ, η such that $(\eta+\rho)\log(1/\eta\rho)$ are sufficiently small we have $\forall T_3' \le \eta\rho^2 t \le T_3$, $\|\mathbb{E}_k[R_{k,\rho}^{\max}](x(t)) - \rho^2 \mathrm{Tr}(\nabla^2 L(X(\eta\rho^2 t)))/2\| = \tilde{O}((\eta+\rho)\rho^2)$.*

Corollary 5.6. *Define U' as in Theorem 4.3, suppose $X(\infty) = \lim_{t\to\infty} X(t)$ exists and is a minimizer of $\mathrm{Tr}(\nabla^2 L(x))$ in $U' \cap \Gamma$, for all $\epsilon > 0$, there exists a constant $T > 0$, then for all ρ, η such that $(\eta+\rho)\log(1/\eta\rho)$ are sufficiently small we have $\mathbb{E}_k[L_{k,\rho}^{\max}](\lceil T/(\eta\rho^2)\rceil)) \le \epsilon\rho^2 + \inf_{x\in U'} \mathbb{E}_k[L_{k,\rho}^{\max}](x)$*

6 CONCLUSION

In this work, we have performed a rigorous mathematical analysis of the explicit bias of various notions of sharpness when used as regularizers and the implicit bias of the SAM algorithm. In particular, we show the explicit biases of worst-, ascent- and average-direction sharpness around the manifold of minimizers are minimizing the largest eigenvalue, the smallest nonzero eigenvalue, and the trace of Hessian of the loss function. We show that in the full-batch setting, SAM provably decreases the largest eigenvalue of Hessian, while in the stochastic setting when batch size is 1, SAM provably decreases the trace of Hessian.

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CONTENTS

1 Introduction **1**

2 Related Works **2**

3 Notations and Assumptions **3**

4 Explicit and Implicit Bias in the Full-batch Setting **3**

4.1 Worst- and Ascent-direction Sharpness have Different Explicit Bias 4

4.2 SAM Provably Decreases Worst-direction Sharpness Locally 5

4.3 Proof Sketch for Phase II in Theorem 4.9 6

5 Explicit and Implicit bias in the Stochastic Setting **8**

5.1 Stochastic Worst- and Ascent-direction Sharpness have Same Explicit Bias 8

5.2 Stochastic SAM Minimizes Stochastic Worst-direction Sharpness 9

6 Conclusion **9**

A Additional Related Works **13**

B More Discussions of Manifold Assumption **13**

C Proof **14**

C.1 Proof Setups 14

C.2 Lemma about Φ 15

C.3 Explicit Bias 18

C.4 Full-batch SAM on Quadratic Loss: Proof of Theorem 4.14 20

C.4.1 Preparation Phase 21

C.4.2 Alignment Phase 22

C.4.3 Length Convergence 25

C.5 Full-batch SAM on General Loss: Proof of Theorem 4.9 26

C.5.1 Phase I: Proof of Theorem C.23 27

C.5.2 Phase II: Proof of Theorem C.24 32

C.5.3 Proof of Corollaries 37

C.6 Stochastic SAM: Proof of Theorem 5.4 37

C.6.1 Phase I: Proof of Theorem C.27 38

C.6.2 Phase II: Proof of Theorem C.28 40

C.6.3 Proof of Corollaries 42

C.7 Technical Lemmas 43

A Additional Related Works

Sharpness Minimization as Implicit Bias. Recent theoretical works Blanc et al. (2019); Damian et al. (2021); Li et al. (2021) showed that SGD with label noise is implicitly biased to local minimizers with a smaller trace of Hessian. Arora et al. (2022) showed that normalized GD implicitly decreases the largest eigenvalue of the Hessian. Lyu et al. (2022) showed that GD with weight decay on a scale invariant loss function implicitly decreases the spherical sharpness, *i.e.*, the largest eigenvalue of the Hessian evaluated at the normalized parameter.

In a concurrent work, Bartlett et al. (2022) prove that on quadratic loss, the iterate of SAM (Equation (11)) and its gradient converges to the top eigenvector of Hessian, which is almost the same as our Theorem 4.14. Assuming such alignment for a general loss, the work of Bartlett et al. (2022) shows that the largest eigenvalue of Hessian decreases in the next step. This paper also proves such a Hessian-gradient alignment for general loss functions and an end-to-end theorem showing that the largest eigenvalue of Hessian and worst-direction sharpness decrease along the trajectory of SAM (Theorem 4.9), which are not shown in Bartlett et al. (2022). Moreover, this paper also characterizes implicit bias of stochastic SAM with batch size 1, which is minimizing the average-direction sharpness, while Bartlett et al. (2022) only considers the deterministic case.

Comparison with Arora et al. (2022). Our proof uses similar framework as Arora et al. (2022). However our analysis has its own difficulty for the following reasons. First, Arora et al. (2022) only deal with deterministic case, while our analysis extends to stochastic SAM as well (Section 5). Second, our analysis for the deterministic case is different from that of Arora et al. (2022) in the following two aspects:

1. The alignment analysis is more complicated because we have two hyperparameters,learning rate η and perturbation radius ρ, while Arora et al. (2022) only needs to deal with one hyperparameter, learning rate η.
2. The mechanism of penalizing worst-direction sharpness is different, which can be seen from the dependency of the sharpness-reduction rate over learning rate η. In Arora et al. (2022), normalized GD reduces the sharpness via a second-order effect of GD and thus the sharpness is reduced by $O(\eta^2)$ per step. In our analysis, for fixed small perturbation radius ρ, the sharpness is reduced by $O(\rho^2\eta)$ per step, which is linear in η.

B More Discussions of Manifold Assumption

Validity. Recent empirical studies have shown that there are essentially no barriers in loss landscape between different minimizers, that is, the set of minimizers are path-connected (Draxler et al., 2018; Garipov et al., 2018). Motivated by this empirical discovery, we make the assumption below following Fehrman et al. (2020); Damian et al. (2021); Li et al. (2021), which is theoretically justified by Cooper (2018) under a generic setting.

Importance. The connectivity of the set of local minimizers implied by the manifold assumption above allows us to take limits of perturbation radius $\rho \to 0$ while still yield interesting and insightful implicit bias results. So far almost all analysis of implicit bias for general model parameterizations relies on Taylor expansion, e.g. Blanc et al. (2019); Damian et al. (2021); Li et al. (2021); Arora et al. (2022), so does the derivation of the SAM algorithm (Foret et al., 2020; Wu et al., 2020). Thus it's crucial to consider small perturbation size ρ. On the contrary, if the set of global minimizers are a set of discrete points, then with small perturbation radius ρ, implicit bias of optimizers is not sufficient to drive the iterate from global minimum to the other one.

Limitation. As proved by Cooper (2018), the manifold setting holds generically for regression problems with smooth loss. The manifold assumption doesn't hold for networks with ReLU (which is non-smooth) and classification problems with softmax loss (where an overparametrized network may achieve arbitrarily small but non-zero loss). In the latter case, there may not even exist a global minimizer, not to mention a manifold of minimizers.

C PROOF

C.1 PROOF SETUPS

In this section we provide details of our proof setups, including notations and assumptions/settings.

We first introduce some additional notations that will be used in the proofs. For any subset $S \in \mathbb{R}^D$, we define $\text{Dist}(x, S) \triangleq \inf_{y \in S} \|x - y\|_2$. For any $d > 0$ and any subset $S \in \mathbb{R}^D$, we define $S^d \triangleq \{x \in \mathbb{R}^D \mid \text{Dist}(x, S) \leq d\}$. Our convention is to use K to denote a compact set and U to denote an open set.

Below we restate our main assumption in the full-batch case and related notations in Section 3. Throughout the analysis, we fix our initialization as x_{init}, our loss function as $L : \mathbb{R}^D \to \mathbb{R}$.

Assumption 3.1. *Assume loss $L : \mathbb{R}^D \to \mathbb{R}$ belongs to $\mathcal{C}^4$, and there exists a manifold Γ that is $D - M$ dimensional $\mathcal{C}^2-$submanifold of $\mathbb{R}^D$ for some integer $1 \leq M \leq D$, where for all $x \in \Gamma$, x is a global minimizer of L, $L(x) = 0$ and rank$(\nabla^2 L(x)) = M$.*

Notations for Full-Batch Setting: Given any point $x \in \Gamma$, define $P_{x,\Gamma}$ as the projection operator onto the manifold of the normal space of Γ at x and $P^\top_{x,\Gamma} = I_D - P_{x,\Gamma}$. Given the loss function L, its gradient flow is denoted by mapping $\phi : \mathbb{R}^D \times [0, \infty) \to \mathbb{R}^D$. Here, $\phi(x, \tau)$ denotes the iterate at time τ of a gradient flow starting at x and is defined as the unique solution of $\phi(x, \tau) = x - \int_0^\tau \nabla L(\phi(x, t))dt$, $\forall x \in \mathbb{R}^D$. We further define the limiting map of $\phi(x, \cdot)$ as $\Phi(x) = \lim_{\tau \to \infty} \phi(x, \tau)$, that is, $\Phi(x)$ denotes the convergent point of the gradient flow starting from x. For convenience, we define $\lambda_i(x), v_i(x)$ as $\lambda_i(\nabla^2 L(\Phi(x))), v_i(\nabla^2 L(\Phi(x)))$ whenever the latter is well defined. When $x(t)$ and Γ is clear from context, we also use $\lambda_i(t) := \lambda_i(x(t)), v_i(t) := v_i(x(t)), P^\top_{t,\Gamma} := P^\top_{\Phi(x(t)),\Gamma}, P_{t,\Gamma} := P_{\Phi(x(t)),\Gamma}$.

Definition 3.2 (Attraction Set)**.** *Let U be the attraction set of Γ under gradient flow, that is, a neighborhood of Γ containing all points starting from which gradient flow w.r.t. loss L converges to some point in Γ, or mathematically, $U \triangleq \{x \in \mathbb{R}^D | \Phi(x)$ exists and $\Phi(x) \in \Gamma\}$.*

Below we restate the setting for stochastic loss of batch size one in Section 5.

Setting C.1. *Let $f_k(x)$ be the model output on kth data where f_k is a $\mathcal{C}^4$-smooth function and y_k be the ith label for $l = 1, \ldots, M$. We define the loss on kth data as $L_k(x) = \ell(f_k(x), y_k)$ and the total loss $L = \sum_{k=1}^M L_k/M$, where $\ell(y', y)$ is a $\mathcal{C}^4$-smooth function satisfying the following properties[2]: (1). $\arg\min_{y' \in \mathbb{R}} \ell(y', y) = y$, for any $y \in \mathbb{R}$; (2). $\frac{d^2 \ell(y', y)}{d^2 y'}|_{y'=y} > 0$, for any $y \in R$; (3). There exists x_0, such that for any $k \in [M]$, it holds that $f_k(x_0) = y_k$.*

In our analysis, we prove our main theorems in the stochastic setting under a more general condition than Setting C.1, which is Assumption C.2 (on top of Assumption 3.1). The only usage of Setting C.1 in the proof is Lemma 5.3 and theorem C.26.

Assumption C.2. *Total loss $L = \frac{1}{M} \sum_{k=1}^M L_k$. For each $k \in [M]$, L_k is $\mathcal{C}^4$, and there exists a $(D-1)$-dimensional $\mathcal{C}^2$-submanifold of $\mathbb{R}^D$, Γ_k, where for all $x \in \Gamma_k$, x is a global minimizer of L_k, $L_k(x) = 0$ and rank$(\nabla^2 L_k(x)) = 1$. Moreover, $\Gamma = \cap_{k=1}^M \Gamma_k$ for Γ defined in Assumption 3.1.*

Notations for Stochastic Setting: Since L_k is rank-1 on Γ_k for each $k \in [M]$, we can write it as $L_k(x) = \Lambda_k(x) w_k(x) w_k^\top(x)$ for any $x \in \Gamma$, where w_k is a continuous function on Γ with pointwise unit norm. Given the loss function L_k, its gradient flow is denoted by mapping $\phi_k : \mathbb{R}^D \times [0, \infty) \to \mathbb{R}^D$. Here, $\phi_k(x, \tau)$ denotes the iterate at time τ of a gradient flow starting at x and is defined as the unique solution of $\phi_k(x, \tau) = x - \int_0^\tau \nabla L_k(\phi_k(x, t))dt$, $\forall x \in \mathbb{R}^D$. We further define the limiting map Φ_k as $\Phi_k(x) = \lim_{\tau \to \infty} \phi_k(x, \tau)$, that is, $\Phi_k(x)$ denotes the convergent point of the gradient flow starting from x. Similar to Definition 3.2, we define $U_k = \{x \in \mathbb{R}^D | \Phi(x)$ exists and $\Phi_k(x) \in \Gamma_k\}$ be the attraction set of Γ_i. We have that each U_k is open and Φ_k is $\mathcal{C}^2$ on U_k by Lemma B.15 in Arora et al. (2022).

Definition C.3. *A function L is μ-PL in a set U iff $\forall x \in U$, $\|\nabla L(x)\|_2^2 \geq 2\mu(L(x) - \inf_{x \in U} L(x))$.*

[2]Examples include ℓ_2 loss: $\ell(y, y') = 0.5(y - y')^2$.

Definition C.4. *The spectral 2-norm of a k-order tensor $X_{i_1,\dots,i_k} \in R^{d_1\times\dots\times d_k}$ is defined as*

$$\|X\|_2 = \max_{x_i\in R^{d_i}, \|x_i\|_2=1} X[x_1, \dots, x_k].$$

Lemma C.5 (Arora et al. (2022) Lemma B.2)**.** *Given any compact set $K \subseteq \Gamma$, there exist $r(K), \mu(K), \Delta(K) \in \mathbb{R}^+$ such that*

1. *$K^{r(K)} \cap \Gamma$ is compact.*
2. *$K^{r(K)} \subset U \cap (\cap_k U_k)$.*
3. *L is $\mu(K)$-PL on $K^{r(K)}$.*
4. $\inf_{x\in K^{r(K)}} (\lambda_1(\nabla^2 L(x)) - \lambda_2(\nabla^2 L(x))) \geq \Delta(K) > 0$.
5. $\inf_{x\in K^{r(K)}} \lambda_M(\nabla^2 L(x)) \geq \mu(K) > 0$.
6. $\inf_{x\in K^{r(K)}} \lambda_1(\nabla^2 L_k(x)) \geq \mu(K) > 0$.

Given compact set $K \subset \Gamma$, we further define

$$\zeta(K) = \sup_{x\in K^{r(K)}} \|\nabla^2 L(x)\|_2,\ \nu(K) = \sup_{x\in K^{r(K)}} \|\nabla^3 L(x)\|_2,\ \Upsilon(K) = \sup_{x\in K^{r(K)}} \|\nabla^4 L(x)\|_2,$$
$$\xi(K) = \sup_{x\in K^{r(K)}} \|\nabla^2 \Phi(x)\|_2,\ \chi(K) = \sup_{x\in K^{r(K)}} \|\nabla^3 \Phi(x)\|_2.$$

Similarly, we use notations like $\zeta_k(K), \nu_k(K), \Upsilon_k(K), \xi_k(K), \chi_k(K)$ to denote the counterpart of the above quantities defined for stochastic loss L_k and its limiting map Φ_k for $k \in [M]$.

Lemma C.6 (Arora et al. (2022), Lemma B.5 and B.7)**.** *Given any compact subset $K \subset \Gamma$, let $r(K)$ be defined in Lemma C.5, there exist $0 < h(K) < r(K)$ such that*

1. $\sup_{x\in K^{h(K)}} L(x) - \inf_{x\in K^{h(K)}} L(x) \leq \frac{\mu(K)\rho^2(K)}{8}$.
2. $\forall x \in K^{h(K)}, \Phi(x) \in K^{r(K)/2}$.
3. $\forall x \in K^{h(K)}, \|x - \Phi(x)\|_2 \leq \frac{8\mu(K)^2}{\zeta(K)\nu(K)}$.
4. *The whole segment $\overline{x\Phi(x)}$ lies in $K^{r(K)}$, so does $\overline{x\Phi_k(x)}$, for any $k \in [D]$.*

The proof of the lemmas above can be found in Arora et al. (2022). Readers should note that although Arora et al. (2022) only prove these lemmas when K is a special compact set (the trajectory of an ODE), all the proof does not use any property of K other than it is a compact subset of Γ, and thus our Lemmas C.5 and C.6 hold for general compact subsets of Γ.

In the rest part of the appendix, for convenience we will drop the dependency on K in various constants when there is no ambiguity.

C.2 Lemma about Φ

In this section, we will introduce some geometric lemma about SAM, which will be heavily used in the analysis below.

Lemma C.7. *For $x \in K^h$, we have*

$$\|x - \Phi(x)\| \leq \int_0^\infty \|\frac{d\phi(x,t)}{dt}\| \leq \sqrt{\frac{2(L(x) - L(\Phi(x)))}{\mu}} \leq \frac{\|\nabla L(x)\|}{\mu}$$

Lemma C.8. *For $x \in K^h$, we have*

$$\partial\Phi(x)\nabla L(x) = 0, x \in U$$
$$\partial\Phi(x)\nabla^2 L(x)\nabla L(x) = -\partial^2\Phi(x)[\nabla L(x), \nabla L(x)], x \in U$$
$$\partial\Phi(x)\partial^2(\nabla L)(x)[v_1, v_1] = P^\perp_{X,\Gamma}\nabla(\lambda_1(\nabla^2(L(x)))), x \in \Gamma.$$

Lemma C.9. *At any point $x \in K^h$, we have*

$$\|\nabla L(x) - \nabla^2 L(\Phi(x))(x - \Phi(x))\| \leq \frac{\nu}{2}\|x - \Phi(x)\|^2$$
$$\left|\frac{\|\nabla L(x)\|}{\|\nabla^2 L(\Phi(x))(x - \Phi(x))\|} - 1\right| \leq \frac{2\nu}{\mu}\|x - \Phi(x)\|$$
$$\frac{\nabla L(x)}{\|\nabla L(x)\|} = \frac{\nabla^2 L(\Phi(x))(x - \Phi(x))}{\|\nabla^2 L(\Phi(x))(x - \Phi(x))\|} + O(\frac{\nu}{\mu}\|x - \Phi(x)\|)$$

The proof of above lemmas can be found in Arora et al. (2022).

Lemma C.10. *For $x \in K^h$,*

$$\|\partial\Phi(x)\nabla L_k(x)\| \leq (\nu_k + \zeta_k\xi)\|x - \Phi(x)\|^2$$
$$\|\partial\Phi(x)\nabla^2 L_k(x)\frac{\nabla L_k(x)}{\|\nabla L_k(x)\|}\| \leq (\nu_k + \zeta_k\xi)\|x - \Phi(x)\|$$

Proof. Consider doing Taylor expansion,

$$\begin{aligned}
\|\partial\Phi(x)\nabla L_k(x)\| &\leq \|\partial\Phi(x)\nabla^2 L_k(\Phi(x))(x - \Phi(x))\| + \nu_k\|x - \Phi(x)\|^2 \\
&\leq \|\partial\Phi(\Phi(x))\nabla^2 L_k(\Phi(x))(x - \Phi(x))\| + \nu_k\|x - \Phi(x)\|^2 + \zeta_k\xi\|x - \Phi(x)\|^2 \\
&= \|P^{\top}_{\Phi(\Phi(x)),\Gamma}\nabla^2 L_k(\Phi(x))(x - \Phi(x))\| + \nu_k\|x - \Phi(x)\|^2 + \zeta_k\xi\|x - \Phi(x)\|^2 \\
&= (\nu_k + \zeta_k\xi)\|x - \Phi(x)\|^2
\end{aligned}$$

and

$$\begin{aligned}
\|\partial\Phi(x)\nabla^2 L_k(x)\frac{\nabla L_k(x)}{\|\nabla L_k(x)\|}\| &\leq \|\partial\Phi(x)\nabla^2 L_k(\Phi(x))\frac{\nabla L_k(x)}{\|\nabla L_k(x)\|}\| + \nu_k\|x - \Phi(x)\| \\
&\leq \|\partial\Phi(\Phi(x))\nabla^2 L_k(\Phi(x))\frac{\nabla L_k(x)}{\|\nabla L_k(x)\|}\| + (\nu_k + \zeta_k\xi)\|x - \Phi(x)\| \\
&= (\nu_k + \zeta_k\xi)\|x - \Phi(x)\|
\end{aligned}$$

Here we use Lemma C.6 to ensure the approximation is correct. □

Lemma C.11. *There exists $h_1 > 0$, for $x \in K^h$ and $p \in C, \nabla^2 L_k(p) = \Lambda_k(p)w_k(p)w_k(p)^T$, suppose $\|x - p\| < h_1$, there exists $s \in \{1, -1\}$,*

$$\frac{\nabla L_k(x)}{\|\nabla L_k(x)\|} = sw_k(p) + O(\|x - p\|)$$

Further if we have $|w_k^T(x - p)| \geq \|x - p\|^{3/2}$, then we have $s = sign(w_k^T(x - p))$. This implies

$$\begin{aligned}
\frac{\nabla L_k(x)}{\|\nabla L_k(x)\|}^T(x - p) &\geq sw_k^T(x - p) - O(\|x - p\|^2) \\
&\geq \|w_k^T(x - p)\| - O(\|x - p\|^{3/2})
\end{aligned}$$

Proof. There are two ways we may use to estimate the direction $\frac{\nabla L_k(x)}{\|\nabla L_k(x)\|}$.

First Way According to Lemma C.9,

$$\frac{\nabla L_k(x)}{\|\nabla L_k(x)\|} = \frac{\nabla^2 L_k(\Phi_k(x))(x - \Phi_k(x))}{\|\nabla^2 L_k(\Phi_k(x))(x - \Phi_k(x))\|} + O(\|x - \Phi_k(x)\|)$$

Suppose $\nabla^2 L_k(\Phi_k(x)) = \Lambda_k(\Phi_k(x))w_k(\Phi_k(x))w_k(\Phi_k(x))^T$, then

$$\frac{\nabla L_k(x)}{\|\nabla L_k(x)\|} = w_k(\Phi_k(x)) + O(\|x - \Phi_k(x)\|)$$

Define $\nabla^2 L_k(O) = v_i v_i^T$, using Davis-Kahan Theorem C.31, we would have $\exists s \in \{-1, 1\}$, such that $\|w_k(\Phi_k(x)) - sw_k(p)\| \leq \zeta\|\Phi_k(x) - p\|$

$$\frac{\nabla L_k(x)}{\|\nabla L_k(x)\|} = sw_k(p) + O(\|\Phi_k(x) - p\| + \|x - p\|)$$

According to Lemma C.7, we have $\|x - \Phi_k(x)\| \leq \frac{\|\nabla L_k(x)\|}{\mu} \leq \frac{\zeta\|x-p\|}{\mu}$. This implies,

$$\frac{\nabla L_k(x)}{\|\nabla L_k(x)\|} = sw_k(p) + O(\|x - p\|) \tag{18}$$

Second Way There is another direct way to consider the direction of $\frac{\nabla L_k(x)}{\|\nabla L_k(x)\|}$. Doing a Taylor expansion at O,

$$\nabla L_k(x) = \Lambda_k(x) w_k(p) w_k(p)^T (x-p) + O(\nu\|x-p\|^2).$$

That being said, when $|w_k^T(x-p)| \geq \|x-p\|^{3/2}$, we have

$$\big|\|\nabla L_k(x)\| - \|w_k w_k^T(x-p)\|\big| \leq O(\|x-p\|^2)$$

$$\frac{\big|\|\nabla L_k(x)\| - \|w_k w_k^T(x-p)\|\big|}{\|w_k w_k^T(x-p)\|} \leq O(\frac{\|x-p\|^2}{\|w_k w_k^T(x-p)\|}) = O(\|x-p\|^{1/2})$$

Hence we have

$$\frac{\nabla L_k(x)}{\|\nabla L_k(x)\|} = sign(w_k^T(x-p))w_k + O(\|x-p\|^{1/2}) \tag{19}$$

Comparing (18) and (19), we have there exists h_1, such that if $\|x-p\| \leq h_1$, $s = sign(w_k^T(x-p))$ when $|w_k^T(x-p)| \geq \|x-p\|^{3/2}$. The final inequality is self-explanatory.

□

We will abuse notation slightly and suppose h_1 in Lemma C.11 satisfies $h_1 \geq h$.

Lemma C.12. *Suppose $x \in K^h$ and $y = x - \eta\nabla L\left(x + \rho\frac{\nabla L(x)}{\|\nabla L(x)\|}\right)$,*

$$\|\nabla L(x)\| \leq \zeta\|x - \Phi(x)\|$$

$$\|\Phi(x) - \Phi(y)\| \leq \xi\eta\rho\|\nabla L(x)\| + \xi\eta\rho^2 + \xi\eta^2\|\nabla L(x)\|^2 + \xi\zeta^2\eta^2\rho^2$$

$$\leq \zeta\xi\eta\rho\|x - \Phi(x)\| + \zeta^2\xi\eta^2\|x - \Phi(x)\|^2 + \xi\eta\rho^2 + \xi\zeta^2\eta^2\rho^2$$

$$\|y - x\| \leq \eta\|\nabla L(x)\| + \eta\zeta\rho$$

Proof. Using Taylor Expansion and Lemma C.6,

$$\|\Phi(y) - \Phi(x)\| \leq \|\partial\Phi(x)(y-x)\| + \xi\|y-x\|^2/2$$

Further

$$y - x = -\eta\nabla L\left(x + \rho\frac{\nabla L(x)}{\|\nabla L(x)\|}\right)$$

$$= -\eta\nabla L(x) - \eta\rho\nabla^2 L(x)\frac{\nabla L(x)}{\|\nabla L(x)\|} - \eta\rho^2\partial\nabla^2 L(x)[\frac{\nabla L(x)}{\|\nabla L(x)\|}, \frac{\nabla L(x)}{\|\nabla L(x)\|}]/2 + O(\eta\rho^3\Upsilon)$$

$$\Rightarrow \|y - x + \eta\nabla L(x) + \eta\rho\nabla^2 L(x)\frac{\nabla L(x)}{\|\nabla L(x)\|} + \eta\rho^2\partial\nabla^2 L(x)[\frac{\nabla L(x)}{\|\nabla L(x)\|}, \frac{\nabla L(x)}{\|\nabla L(x)\|}]/2\| \leq \eta\rho^3\Upsilon$$

This implies

$$\|y - x\| = \eta\|\nabla L\left(x + \rho\frac{\nabla L(x)}{\|\nabla L(x)\|}\right)\| \leq \eta\|\nabla L(x)\| + \eta\zeta\rho$$

$$\|\partial\Phi(x)(y-x)\| \leq \eta\|\partial\Phi(x)\nabla L(x) + \rho\partial\Phi(x)\nabla^2 L(x)\frac{\nabla L(x)}{\|\nabla L(x)\|}\| + \eta\rho^2\xi$$

Using Lemma C.8,

$$\|\partial\Phi(x)(y-x)\| \leq \eta\rho\|\nabla L(x)\|\|\partial^2\Phi(x)\left[\frac{\nabla L(x)}{\|\nabla L(x)\|}, \frac{\nabla L(x)}{\|\nabla L(x)\|}\right]\| + \eta\rho^2\xi$$

$$\leq \xi\eta\rho\|\nabla L(x)\| + \eta\rho^2\xi$$

Putting together we have

$$\|\Phi(x) - \Phi(y)\| \leq \xi\eta\rho\|\nabla L(x)\| + \eta\rho^2\xi + \xi\eta^2\|\nabla L(x)\|^2 + \xi\zeta^2\eta^2\rho^2$$

□

Lemmas in this section will be repeatedly used in our proofs.

C.3 EXPLICIT BIAS

We will first prove the generic Theorem 4.3 and then apply this theorems to characterize a variety of regularizers.

Lemma C.13. *Let U' be any bounded open set such that its closure $\overline{U'} \subseteq U$. Further assume $\overline{U'} \cap \Gamma = \overline{U'} \cap \overline{\Gamma}$, then for all $h_2 > 0, \exists \rho_0 > 0$ if $x \in U', \operatorname{dist}(x, \Gamma) \leq \rho_0 \Rightarrow \operatorname{dist}(x, \overline{U' \cap \Gamma}) \leq h_2$*

Proof. Prove by contradiction. If there exists a list of $\rho_1, ..., \rho_k, ...,$ such that $\rho_k \to 0$ and there exists $x_k \in U'$, such that $\operatorname{dist}(x_k, \Gamma) \leq \rho_k$ and $\operatorname{dist}(x_k, \overline{U'} \cap \Gamma) \geq h_2$. Then consider accumulation point of x_k x^* in $\overline{U'}$. Then we would have $x^* \in \Gamma \cap \overline{U'} = \overline{U' \cap \Gamma}$. □

Lemma C.14. *Let U' be any bounded open set such that its closure $\overline{U'} \subseteq U$. then for all $h_2 > 0, \exists \rho_1 > 0$ if $x \in U', L(x) \leq \rho_1 \Rightarrow \operatorname{dist}(x, \overline{U' \cap \Gamma}) \leq h_2$*

Proof. Prove by contradiction. If there exists a list of $\rho_1, ..., \rho_k, ...,$ such that $\rho_k \to 0$ and there exists $x_k \in U'$, such that $L(x_k) \leq \rho_k$ and $\operatorname{dist}(x_k, \overline{U'} \cap \Gamma) \geq h_2$. Then consider accumulation point of x_k x^* in $\overline{U'}$. Then we would have $x^* \in \Gamma \cap \overline{U'} = \overline{U' \cap \Gamma}$. □

Proof of Theorem 4.3 . We will first prove $\Rightarrow$ side. The proof consists of four steps. Define h as the constant in Lemma C.5 with $K = \overline{U' \cap H}$.

Step 1 Consider $x_0 \in U' \cap \Gamma$, satisfying

$$S(x_0) \leq \inf_{x \in U' \cap \Gamma} S(x) + O(\rho).$$

Then using definition 4.2, we have there exists sufficiently small $\epsilon_\rho < \rho^2$, such that exists $\|x_1 - x_0\| \leq \epsilon_\rho < \rho^2$ and $\|S(x_0) - R_\rho(x_1)/\rho^2\| = O(\rho^2)$. Now that as $x_0 \in U'$, we have for sufficiently small ρ, $x_1 \in U'$. By Lemma C.13, we have for sufficiently small ρ, $\overline{x_0 x_1} \in \overline{U' \cap H}^h$, then consider doing Taylor Expansion, we would have $L(x_1) + R_\rho(x_1) \leq \rho^2 S(x_0) + o(\rho^2)$.

Step 2 Now consider $L(u) + R_\rho(u) \leq \rho^2 \inf_{x \in U' \cap \Gamma} S(x) + \epsilon\rho^2 + o(\rho^2)$. We easily have $L(u) \leq O(\rho^2)$ by Assumption 4.1. By Lemma C.14, we have $\overline{u\Phi(u)} \in K^h$ and that $\|u - \Phi(u)\| = O(\rho)$ by Lemma C.7. This implies $\operatorname{dist}(\overline{U' \cap H}, \Phi(u)) = o(1)$. Notice now, we have shown $R_\rho(u) \leq \rho^2 \inf S(x) + \rho^2\epsilon + o(\rho^2)$

Step 3 Now applying definition of a good limiting regularizer and Finite covering theorem, we have this further implies $S(\Phi(u))\rho^2 \leq R_\rho(u) + o(\rho^2)$. We also have $S(\Phi(u)) \geq \inf_{x \in U' \cap \Gamma} S(x) - o(1)$ as $S \in \mathcal{C}^0$. Finally $R_\rho(u) \geq S(\Phi(u))\rho^2 - o(\rho^2) \geq \rho^2 \inf S(x) - o(\rho^2)$. We also have $L(u) \leq o(\rho^2)$, proving our claim.

For the $\Leftarrow$ side, we need to provide a lower bound for $L(x) + R_\rho(x)$. Define constant C_1 such that for all x, $\|x - \Phi(x)\| \geq C_1\rho$, we have $L(x) \geq (C_{U'} + \inf_{x \in U' \cap \Gamma} S_(x) + 1)\rho^2$ where $C_{U'}$ is the constant in Assumption 4.1. Then we have for x such that $\|x - \Phi(x)\| \geq C_1\rho$, we have $L(x) + R_\rho(x) \geq (\inf_{x \in U' \cap \Gamma} S_(x) + 1)\rho^2$. For $\|x - \Phi(x)\| \leq C_1\rho$, we have by definition of good limiting regularizer and Finite covering theorem, $R_\rho(x) \geq \rho^2 S(\Phi(x)) - o(\rho^2)$. As $\operatorname{dist}\Phi(x), \overline{U' \cap \Gamma} = o(1)$, we have $R_\rho(x) \geq \inf_{x \in U' \cap \Gamma} S(x) - o(\rho^2)$, hence $L(x) + R_\rho(x) \geq \inf_{x \in U' \cap \Gamma} S_(x)\rho^2$. □

Theorem 4.3 implies Corollary C.15 saying that the minimum of the regularized loss is approximately the sum of the minimum of loss and the minimum of limiting regularizer.

Corollary C.15. *Under the setting of Theorem 4.3,*

$$\left| \inf_{x \in U'} (L(x) + R_\rho(x)) - \inf_{x \in U'} L(x) - \rho^2 \inf_{x \in U' \cap \Gamma} S(x) \right| \leq o(\rho^2)$$

Proof of Corollary C.15. In Theorem 4.3, choose $\epsilon = 0$, and choose u such that $L(u) + R_\rho(u) \leq \inf_{x \in U'}(L(x) + R_\rho(x)) + o(\rho^2)$, the result is then clear. □

We will then prove the Corollary 4.4.

Proof of Corollary 4.4. By Theorem 4.3, we have $\|L(u) - \inf_{x\in U'} L(x)\| = O(\rho^2)$. This implies $\|u - \Phi(u)\| = O(\rho)$ and also $\mathrm{dist}(\overline{U' \cap H}, \Phi(u)) = o(1)$.

We also have $\rho^2 S(\Phi(x)) - o(\rho^2) \leq R_\rho(u) \leq \rho^2 \inf_{x\in U'\cap H} S(x)$. We have $\|S(\Phi(x)) - \inf_{x\in U'\cap H} S(x)\| = o(1)$. This further implies $\|\overline{S}(\Phi(x)) - \inf_{x\in U'\cap H} S(x)\| = o(1)$

□

Proof of Theorem 4.5.

Step 1 For assumption 4.1

$$R_\rho^{\max}(p) = \max_{\|v\|_2\leq 1} L(p+\rho v) - L(p) \geq \max_{\|v\|_2\leq 1} \left(\rho\langle \nabla L(p), v\rangle + \rho^2 v^T \nabla^2 L(p) v/2\right) - \Upsilon\rho^3$$
$$\geq -\Upsilon\rho^3 \geq -C\rho^2$$

Step 2 For definition of good limiting regularizer, by Davis-Kahan Theorem and assumption 3.1, $S(x) = \lambda_1(x)/2$ is non-negative and continuous on Γ.
We also have

$$\lim_{\rho\to 0}\lim_{r\to 0}\inf_{\|x'-x\|\leq r} \frac{R_\rho^{\max}(x')}{\rho^2} = \lim_{\rho\to 0}\frac{R_\rho^{\max}(x)}{\rho^2} = \lambda_1(\nabla^2 L(x))/2$$

Further for $x^* \in \Gamma$, consider a sufficiently small open set V containing x^* in which $\|\nabla^3 L\|$ is bounded, for $x \in V \cap \Gamma$, for $\|x' - x\| \leq C\rho$, we have

$$R_\rho^{\max}(x') = \max_{\|v\|_2\leq 1} L(x'+\rho v) - L(x') \geq \max_{\|v\|_2\leq 1} \left(\rho\langle \nabla L(x'), v\rangle + \rho^2 v^T \nabla^2 L(x') v/2\right) - \Upsilon\rho^3$$
$$\geq \rho^2\lambda_1(\nabla^2 L(x'))/2 - \Upsilon\rho^3 \geq \rho^2\lambda_1(\nabla^2 L(x'))/2 - \Upsilon\rho^3 \geq \rho^2\lambda_1(\nabla^2 L(x))/2 - O(\rho^3)$$

On the other hand

$$R_\rho^{\max}(x) = \max_{\|v\|_2\leq 1} L(x+\rho v) - L(x) \geq \rho^2\lambda_1(\nabla^2 L(x))/2 - \Upsilon\rho^3$$

□

Proof of Theorem 4.6.

Step 1 For assumption 4.1

$$R_\rho^{\max}(p) = L(p + \rho\frac{\nabla L\,(p)}{\|\nabla L\,(p)\,\|}) - L(p)$$
$$\geq \left(\rho\|\nabla L\,(p)\,\| + \rho^2(\frac{\nabla L\,(p)}{\|\nabla L\,(p)\,\|})^T\nabla^2 L(p)\frac{\nabla L\,(p)}{\|\nabla L\,(p)\,\|}/2\right) - \Upsilon\rho^3$$
$$\geq -C\rho^2$$

This constant is by taking minimizer of $\lambda_1(\nabla^2 L)$ over $\overline{U'}$.

Step 2 For definition of good limiting regularizer, by Davis-Kahan Theoremm C.31 and assumption 3.1, $S(x) = \lambda_M(x)/2$ is non-negative and continuous on Γ.
Further for $x^* \in \Gamma$, consider a sufficiently small open set V containing x^* in which $\|\nabla^3 L\|$ is bounded, for $x \in V \cap \Gamma$, for $\|x' - x\| \leq C\rho$, then we easily have $\|x' - \Phi(x)\| \leq O(\rho)$, we have

$$R_\rho^{\max}(x') = L(x' + \rho\frac{\nabla L\,(x')}{\|\nabla L\,(x')\,\|}) - L(x')$$
$$\geq \rho\|\nabla L\,(x)\,\| + \rho^2(\frac{\nabla L\,(x')}{\|\nabla L\,(x')\,\|})^T\nabla^2 L(x)\frac{\nabla L\,(x)}{\|\nabla L\,(x)\,\|}/2 - O(\rho^3)$$
$$\geq \rho^2(\frac{\nabla L\,(x)}{\|\nabla L\,(x)\,\|})^T\nabla^2 L(\Phi(x))\frac{\nabla L\,(x)}{\|\nabla L\,(x)\,\|}/2 - O(\rho^3)$$

Using Lemma C.9 and Theorem C.31, we have

$$R_\rho^{\max}(x') \geq \rho^2\lambda_M(\Phi(x)) - O(\rho^3)$$
$$\geq \rho^2\lambda_M(u) - O(\rho^3)$$

We also have

$$\lim_{\rho\to 0}\lim_{r\to 0}\inf_{\|x'-x\|\le r}\frac{R_\rho^{\text{asc}}(x')}{\rho^2}=\lim_{\rho\to 0}\lim_{r\to 0}\inf_{\|x'-x\|\le r}\frac{\rho^2\lambda_M(\Phi(x'))}{2\rho^2}=\lambda_M(\nabla^2 L(x))/2$$

Combining we have $S(x)$ is a good limiting regularizer of $R(x)$.

□

Proof of Theorem 4.7. Step 1 For assumption 4.1

$$\begin{aligned}R_\rho^{\text{avg}}(p)&=\mathbb{E}_{g\sim N(0,I)}L(p+g/\|g\|)-L(p)\\&\ge\left(\rho^2(g/\|g\|)^T\nabla^2 L(p)g/\|g\|\right)/2-\Upsilon\rho^3\\&\ge -C\rho^2\end{aligned}$$

This constant is by taking minimizer of $\text{Tr}(\nabla^2 L)$ over $\overline{U'}$.

Step 2 For definition of good limiting regularizer, by Davis-Kahan Theoremm C.31 and assumption 3.1, $S(x)=\text{Tr}(x)/(2D)$ is non-negative and continuous on Γ.
Further for $x^*\in\Gamma$, consider a sufficiently small open set V containing x^* in which $\|\nabla^3 L\|$ is bounded, for $x\in V\cap\Gamma$, for $\|x'-x\|\le C\rho$, we have

$$\begin{aligned}R_\rho^{\max}(x')&=\mathbb{E}_{g\sim N(0,I)}L(x'+g/\|g\|)-L(x')\\&\ge\left(\rho^2(g/\|g\|)^T\nabla^2 L(x')g/\|g\|\right)/2-O(\rho^3)\\&\ge\rho^2\text{Tr}(\nabla^2 L(x'))/2D-O(\rho^3)\\&\ge\rho^2\text{Tr}(\nabla^2 L(x))/2D-O(\rho^3)\end{aligned}$$

We also have

$$\lim_{\rho\to 0}\lim_{r\to 0}\inf_{\|x'-x\|\le r}\frac{R_\rho^{\text{avg}}(x')}{\rho^2}=\lim_{\rho\to 0}\frac{R_\rho^{\text{avg}}(x)}{\rho^2}=\text{Tr}(\nabla^2 L(x))/2D$$

Combining we have $S(x)$ is a good limiting regularizer of $R(x)$.

□

Proof of Theorem 5.1. By Theorem C.26, Assumption C.2 holds.

Easily deducted from Theorem 4.5 $\Lambda_k(x)$ is a good limiting regularizer for $R_{k,\rho}^{\max}$ on Γ_k. Then as $\Gamma\subset\Gamma_k$, $\Lambda_k(x)$ is a good limiting regularizer for $R_{k,\rho}^{\max}$ on Γ. Hence $S(x)=\sum_k\Lambda_k(x)/2M=\text{Tr}(\nabla^2\text{L(x)})/2$ is a good limiting regularizer of $\mathbb{E}_k[R_{k,\rho}^{\max}](x)$ on Γ.

□

Proof of Theorem 5.2. By Theorem C.26, Assumption C.2 holds.

Easily deducted from Theorem 4.6 $\Lambda_k(x)$ is a good limiting regularizer for $R_{k,\rho}^{\text{asc}}$ on Γ_k as the codimension of Γ_k is 1. Then as $\Gamma\subset\Gamma_k$, $\Lambda_k(x)$ is a good limiting regularizer for $R_{k,\rho}^{\max}$ on Γ.Hence $S(x)=\sum_k\Lambda_k(x)/2M=\text{Tr}(\nabla^2\text{L(x)})/2$ is a good limiting regularizer of $\mathbb{E}_k[R_{k,\rho}^{\text{asc}}](x)$ on Γ. □

C.4 Full-batch SAM on Quadratic Loss: Proof of Theorem 4.14

We first simplify the iterate as

$$x(t+1)=x(t)-\eta Ax(t)-\eta\rho\frac{A^2x(t)}{\|Ax(t)\|}$$

Define $\tilde{x}(t)=\frac{Ax(t)}{\rho}$. We have

$$\tilde{x}(t+1)=\tilde{x}(t)-\eta A\tilde{x}(t)-\eta\frac{A^2\tilde{x}(t)}{\|\tilde{x}(t)\|}\tag{20}$$

Our proof consists of three steps

(1) *Preparation Phase* $\exists T_1, \forall t > T_1, \|P^{(j:D)}\tilde{x}(t)\| \leq \eta\lambda_j^2$

(2) *Alignment Phase* Define $S_1 = \{t | \|\tilde{x}(t)\| \leq \frac{\eta\lambda_1^2}{2-\eta\lambda_1}, t > T_1\}$, suppose $t, t' \in S_1, t \leq t'$, then $|\tilde{x}_1(t)| < |\tilde{x}_1(t')|$ (Lemma C.22) and we have $t \in S_1$ or $t+1 \in S_1$ for $t \geq T_1$(Lemma C.20).

(3) *Length Convergence* $\|\tilde{x}(t)\|$ will converge to $\frac{\eta\lambda_1^2}{2-\eta\lambda_1}$

C.4.1 Preparation Phase

We define $\mathbb{I}_j = \{\tilde{x} | \|P^{(j:D)}\tilde{x}\| \leq \eta\lambda_j^2\}$ and we will prove the following two lemmas. Lemma C.16 will show this is an invariant set for update rule 20 and Lemma C.17 will show that all vectors not in this set will shrink exponentially in norm.

Lemma C.16. *If $\tilde{x}(t) \in \mathbb{I}_j$, using update rule 20, $\tilde{x}(t+1) \in \mathbb{I}_j$*

Proof. We have by update rule 20,

$$P^{(j:D)}\tilde{x}(t+1) = (I - P^{(j:D)}\eta A - \eta\frac{P^{(j:D)}A^2}{\|\tilde{x}(t)\|})P^{(j:D)}\tilde{x}(t)$$

Hence

$$\begin{aligned}\|P^{(j:D)}\tilde{x}(t+1)\| &= \|(I - P^{(j:D)}\eta A - \eta\frac{P^{(j:D)}A^2}{\|\tilde{x}(t)\|})P^{(j:D)}\tilde{x}(t)\| \\ &\leq \|I - P^{(j:D)}\eta A - \eta\frac{P^{(j:D)}A^2}{\|\tilde{x}(t)\|}\|\|P^{(j:D)}\tilde{x}(t)\|\end{aligned}$$

.

We have $\|\tilde{x}(t)\| \leq \frac{\eta\lambda_j^2}{1-\eta\lambda_j}$ by assumption,

$$I(1 - \eta\lambda_j - \eta\frac{\lambda_j^2}{\|P^{(j:D)}\tilde{x}(t)\|}) \prec I(1 - \eta\lambda_j - \eta\frac{\lambda_j^2}{\|\tilde{x}(t)\|}) \prec I - P^{(j:D)}\eta A - \eta\frac{P^{(j:D)}A^2}{\|\tilde{x}(t)\|} \prec I$$

Then we have $\|I - P^{(j:D)}\eta A - \eta\frac{P^{(j:D)}A^2}{\|\tilde{x}(t)\|}\| \leq \max(1, \eta\lambda_j + \eta\frac{\lambda_j^2}{\|P^{(j:D)}\tilde{x}(t)\|} - 1)$

Hence

$$\begin{aligned}\|P^{(j:D)}\tilde{x}(t+1)\| &\leq \max(\|P^{(j:D)}\tilde{x}(t)\|, \eta\lambda_j^2 - (1-\eta\lambda_j)\|P^{(j:D)}\tilde{x}(t)\|) \\ &\leq \eta\lambda_j^2\end{aligned}$$

.

Here the last equation use $1 - \eta\lambda_j \geq 0$. We have by definition $\tilde{x}(t+1) \in \mathbb{I}_j$

□

Lemma C.17. *If $\tilde{x}(t) \notin \mathbb{I}_j$, then $\|P^{(j:D)}\tilde{x}(t+1)\| \leq \max(1 - \eta\lambda_D, \eta\lambda_j)\|P^{(j:D)}\tilde{x}(t)\|$*

Proof.

$$\begin{aligned}\|P^{(j:D)}\tilde{x}(t+1)\| &= \|(I - P^{(j:D)}\eta A - \eta\frac{P^{(j:D)}A^2}{\|\tilde{x}(t)\|})P^{(j:D)}\tilde{x}(t)\| \\ &\leq \|I - P^{(j:D)}\eta A - \eta\frac{P^{(j:D)}A^2}{\|\tilde{x}(t)\|}\|\|P^{(j:D)}\tilde{x}(t)\|\end{aligned}$$

.

We have $\|\tilde{x}(t)\| \geq \|P^{(j:D)}\tilde{x}(t)\| > \eta\lambda_j^2$, hence $\eta\frac{P^{(j:D)}A^2}{\|\tilde{x}(t)\|} \prec \eta\frac{P^{(j:D)}A^2}{\eta\lambda_j^2} \prec I$

This implies

$$-\eta\lambda_j P^{(j:D)} \prec -P^{(j:D)}\eta A \prec I - P^{(j:D)}\eta A - \eta\frac{P^{(j:D)}A^2}{\|\tilde{x}(t)\|} \prec P^{(j:D)}(1 - \eta\lambda_D)$$

Hence we have

$$\|P^{(j:D)}\tilde{x}(t+1)\| \leq \max\left(1-\eta\lambda_D, \eta\lambda_j\right)\|P^{(j:D)}\tilde{x}(t)\|$$

. □

Lemma C.18. *Choosing* $T_1 = \max_j \left(-\log_{\max(1-\eta\lambda_D,\eta\lambda_j)} \max(\frac{\|\tilde{x}(0)\|}{\eta\lambda_j^2}, 1)\right)$, *then* $\forall t \geq T_1, D > j \geq 1, \tilde{x}(t) \in \mathbb{I}_j$

Proof. Proof by contradiction, suppose $\exists j, T > T_1, \tilde{x}(T) \notin \mathbb{I}_j$.

By Lemma C.16, $\forall t < T, \tilde{x}(t) \notin \mathbb{I}_j$.

Then by Lemma C.17,

$$\|P^{(j:D)}\tilde{x}(T)\| \leq (1-\eta\lambda_j)^T\|P^{(j:D)}\tilde{x}(0)\| \leq \max\left(1-\eta\lambda_D, \eta\lambda_j\right)^T\|P^{(j:D)}\tilde{x}(0)\| \leq \eta\lambda_j^2,$$

which is a contradiction.

□

C.4.2 Alignment Phase

Define $\theta(t) = \arccos(\frac{|\langle\tilde{x}(t), e_1\rangle|}{\|\tilde{x}(t)\|})$, $\tilde{x}_i(t) = \langle\tilde{x}, e_i\rangle$

We will first show the following lemma.

Lemma C.19. *When* $\|\tilde{x}(t)\| \leq \frac{\eta\lambda_1^2}{2-\eta\lambda_1}$, *using update rule 20*

$$|\tilde{x}_1(t+1)| > |\tilde{x}_1(t)| \ \& \ \cos(\tilde{x}(t+1)) \geq \cos(\tilde{x}(t))$$

Proof. We have $|\tilde{x}_1(t+1)| = |1-\eta\lambda_1 - \eta\frac{\lambda_1^2}{\|\tilde{x}(t)\|}||\tilde{x}_1(t)|$

We also have $\eta\frac{\lambda_1^2}{\|\tilde{x}(t)\|} > 2-\eta\lambda_1^2$, hence $1-\eta\lambda_1-\eta\frac{\lambda_1^2}{\|\tilde{x}(t)\|} < -1$.

Hence we have $|\tilde{x}_1(t+1)| > |\tilde{x}_1(t)|$

On the other hand, $\|P^{(2:D)}\tilde{x}(t+1)\| \leq \max\left(|1-\eta\lambda_2-\eta\frac{\lambda_2^2}{\|\tilde{x}(t)\|}|, |1-\eta\lambda_D-\eta\frac{\lambda_D^2}{\|\tilde{x}(t)\|}|\right)\|P^{(2:D)}\tilde{x}(t)\|$

Notice that

$$1-\eta\lambda_1-\eta\frac{\lambda_1^2}{\|\tilde{x}(t)\|} < 1-\eta\lambda_2-\eta\frac{\lambda_2^2}{\|\tilde{x}(t)\|} \leq 1-\eta\lambda_D-\eta\frac{\lambda_D^2}{\|\tilde{x}(t)\|} \leq 1-\eta\lambda_D < 1 < \eta\lambda_1+\eta\frac{\lambda_1^2}{\|\tilde{x}(t)\|}-1$$

Hence $\max\left(|1-\eta\lambda_2-\eta\frac{\lambda_2^2}{\|\tilde{x}(t)\|}|, |1-\eta\lambda_D-\eta\frac{\lambda_D^2}{\|\tilde{x}(t)\|}|\right) < |1-\eta\lambda_1-\eta\frac{\lambda_1^2}{\|\tilde{x}(t)\|}|$. □

Lemma C.20. $\|\tilde{x}(t)\| > \frac{\eta\lambda_1^2}{2-\eta\lambda_1}, \tilde{x}(t) \in \cap\mathbb{I}_j$, *then using update rule 20,*

$$\|\tilde{x}(t+1)\| \leq \max(\frac{\eta\lambda_1^2}{2-\eta\lambda_1} - \eta\frac{\lambda_D^4}{2\lambda_1^2}, \eta\lambda_1^2 - (1-\eta\lambda_1)\|\tilde{x}(t)\|)$$

Proof.

$$\begin{aligned}\tilde{x}(t+1) &= (I-\eta A-\eta\frac{A^2}{\|\tilde{x}(t)\|})\tilde{x}(t) \\ &= \frac{1}{\|\tilde{x}(t)\|}\sum_{j=1}^{D}\left((1-\eta\lambda_j)\|\tilde{x}(t)\|-\eta\lambda_j^2\right)\tilde{x}_j(t)e_j\end{aligned}$$

Consider the following three cases.

Case 1 $\forall i, \left|(1-\eta\lambda_1)\|\tilde{x}(t)\| - \eta\lambda_1^2\right| \geq \left|(1-\eta\lambda_i)\|\tilde{x}(t)\| - \eta\lambda_i^2\right|$
In this case, we have $\|\tilde{x}(t+1)\| \leq \left|(1-\eta\lambda_1)\|\tilde{x}(t)\| - \eta\lambda_1^2\right| = \eta\lambda_1^2 - (1-\eta\lambda_1)\|\tilde{x}(t)\|$
A more detailed analysis would show $\|\tilde{x}(t+1)\|$ is upper bounded by

$$\sqrt{\left(\eta\lambda_1^2 - (1-\eta\lambda_1)\|\tilde{x}(t)\|\right)^2 \cos^2(\theta(t)) + \max\{|\eta\lambda_2^2 - (1-\eta\lambda_2)\|\tilde{x}(t)\||, |\eta\lambda_D^2 - (1-\eta\lambda_D)\|\tilde{x}(t)\||\} \sin^2(\theta(t))}$$

Case 2 $\exists i, \left|(1-\eta\lambda_1)\|\tilde{x}(t)\| - \eta\lambda_1^2\right| < \left|(1-\eta\lambda_i)\|\tilde{x}(t)\| - \eta\lambda_i^2\right|$, suppose WLOG, i is the smallest among such index.
As

$$\eta\lambda_i^2 - (1-\eta\lambda_i)\|\tilde{x}(t)\| < \eta\lambda_1^2 - (1-\eta\lambda_1)\|\tilde{x}(t)\| = \left|(1-\eta\lambda_1)\|\tilde{x}(t)\| - \eta\lambda_1^2\right|$$

We have $-\eta\lambda_i^2 + (1-\eta\lambda_i)\|\tilde{x}(t)\| > \eta\lambda_1^2 - (1-\eta\lambda_1)\|\tilde{x}(t)\|$. Equivalently,

$$\|\tilde{x}(t)\| > \frac{\eta\lambda_1^2 + \eta\lambda_i^2}{2 - \eta\lambda_1 - \eta\lambda_i} \tag{21}$$

Combining with $\tilde{x}(t) \in \mathbb{I}_1 \Rightarrow \|\tilde{x}(t)\| \leq \eta\lambda_1^2$, we have $\eta < \frac{\lambda_1 - \lambda_i}{\lambda_1^2}$.
Now consider the following vertors,

$$\begin{aligned}
v^{(1)}(t) &:= (\eta\lambda_1^2 - (1-\eta\lambda_1)\|\tilde{x}(t)\|)\tilde{x}(t) \\
v^{(2)}(t) &:= ((2-\eta\lambda_1-\eta\lambda_i)\|\tilde{x}(t)\| - \eta\lambda_i^2 - \eta\lambda_1^2)P^{(i:D)}\tilde{x}(t) \\
v^{(2+j)}(t) &:= ((\eta\lambda_{i+j-1} - \eta\lambda_{i+j})\|\tilde{x}(t)\| - \eta\lambda_{i+j}^2 + \eta\lambda_{i+j-1}^2)P^{(i+j:D)}\tilde{x}(t), 1 \leq j \leq D-i
\end{aligned}$$

.
Then we have

$$\begin{aligned}
\|\tilde{x}(t+1)\| &= \|\frac{1}{\|\tilde{x}(t)\|}\sum_{j=1}^{D}\left((1-\eta\lambda_j)\|\tilde{x}(t)\| - \eta\lambda_j^2\right)\tilde{x}_j(t)e_j\| \\
&\leq \|\frac{1}{\|\tilde{x}(t)\|}\left(\sum_{j=1}^{i-1}\left(\eta\lambda_1^2 - (1-\eta\lambda_1)\|\tilde{x}(t)\|\right)\tilde{x}_j(t)e_j + \sum_{j=i}^{D}\left((1-\eta\lambda_j)\|\tilde{x}(t)\| - \eta\lambda_j^2\right)\tilde{x}_j(t)e_j\right)\| \\
&= \|\frac{1}{\|\tilde{x}(t)\|}\sum_{j=1}^{D+1-i}\|v^{(j)}\| \\
&\leq \frac{1}{\|\tilde{x}(t)\|}\sum_{j=1}^{D+1-i}\|v^{(j)}\|
\end{aligned}$$

By assumption, we have $\tilde{x}(t) \in \cap\mathbb{I}_j$, hence we have

$$\begin{aligned}
\|v^{(1)}(t)\| &= (\eta\lambda_1^2 - (1-\eta\lambda_1)\|\tilde{x}(t)\|)\|\tilde{x}(t)\| \\
\|v^{(2)}(t)\| &\leq \eta((2-\eta\lambda_1-\eta\lambda_i)\|\tilde{x}(t)\| - \eta\lambda_i^2 - \eta\lambda_1^2)\lambda_i^2 \\
\|v^{(2+j)}(t)\| &\leq \eta((\eta\lambda_{i+j-1} - \eta\lambda_{i+j})\|\tilde{x}(t)\| - \eta\lambda_{i+j}^2 + \eta\lambda_{i+j-1}^2)\lambda_{i+j}^2, 1 \leq j \leq D-i
\end{aligned}$$

Using AM-GM inequality, we have

$$\begin{aligned}
\lambda_{i+j-1}\lambda_{i+j}^2 &\leq \frac{\lambda_{i+j-1}^3 + 2\lambda_{i+j}^3}{3} \\
\lambda_{i+j-1}^2\lambda_{i+j}^2 &\leq \frac{\lambda_{i+j-1}^4 + \lambda_{i+j}^4}{2}
\end{aligned}$$

Hence

$$\begin{aligned}
\|v^{(2+j)}(t)\| &\leq \eta((\eta\lambda_{i+j-1} - \eta\lambda_{i+j})\|\tilde{x}(t)\| - \eta\lambda_{i+j}^2 + \eta\lambda_{i+j-1}^2)\lambda_{i+j}^2 \\
&\leq \eta^2\|\tilde{x}(t)\|\frac{\lambda_{i+j-1}^3 - \lambda_{i+j}^3}{3} + \eta^2\frac{\lambda_{i+j-1}^4 - \lambda_{i+j}^4}{2}, 1 \leq j \leq D-i \\
\sum_{j=1}^{D-i}\|v^{(2+j)}(t)\| &\leq \eta^2\|\tilde{x}(t)\|\frac{\lambda_i^3 - \lambda_D^3}{3} + \eta^2\frac{\lambda_i^4 - \lambda_D^4}{2}
\end{aligned}$$

So,

$$
\begin{aligned}
\|\tilde{x}(t+1)\| &\leq \frac{1}{\|\tilde{x}(t)\|} \sum_{j=1}^{D+1-i} \|v^{(i)}\| \\
&\leq \eta\lambda_1^2 + \eta\lambda_i^2(2-\eta\lambda_1-\eta\lambda_i) + \eta^2\frac{\lambda_i^3-\lambda_D^3}{3} - (1-\eta\lambda_1)\|\tilde{x}(t)\| \\
&- \eta^2\lambda_i^2(\lambda_i^2+\lambda_1^2)\frac{1}{\|\tilde{x}(t)\|} + \eta^2\frac{\lambda_i^4-\lambda_1^4}{2}\frac{1}{\|\tilde{x}(t)\|} \\
&\leq \eta\lambda_1^2 + \eta\lambda_i^2(2-\eta\lambda_1-\frac{2}{3}\eta\lambda_i) - (1-\eta\lambda_1)\|\tilde{x}(t)\| - \eta^2\lambda_i^2(\frac{1}{2}\lambda_i^2+\lambda_1^2)\frac{1}{\|\tilde{x}(t)\|} - \eta^2\frac{\lambda_D^4}{2\|\tilde{x}(t)\|} \\
&\leq \eta\lambda_1^2 + \eta\lambda_i^2(2-\eta\lambda_1-\frac{2}{3}\eta\lambda_i) - (1-\eta\lambda_1)\|\tilde{x}(t)\| - \eta^2\lambda_i^2(\frac{1}{2}\lambda_i^2+\lambda_1^2)\frac{1}{\|\tilde{x}(t)\|} - \eta\frac{\lambda_D^4}{2\lambda_1^2}
\end{aligned}
$$

We further discuss three cases

Case 2.1 $\eta\lambda_i\sqrt{\frac{\frac{1}{2}\lambda_i^2+\lambda_1^2}{1-\eta\lambda_1}} < \frac{\eta\lambda_1^2+\eta\lambda_i^2}{2-\eta\lambda_1-\eta\lambda_i}$.

In this case we have $\|\tilde{x}(t)\| > \frac{\eta\lambda_1^2+\eta\lambda_i^2}{2-\eta\lambda_1-\eta\lambda_i} > \eta\lambda_i\sqrt{\frac{\frac{1}{2}\lambda_i^2+\lambda_1^2}{1-\eta\lambda_1}}$,then

$$
\begin{aligned}
\|\tilde{x}(t+1)\| &\leq \eta\lambda_1^2 + \eta\lambda_i^2(2-\eta\lambda_1-\frac{2}{3}\eta\lambda_i) - (1-\eta\lambda_1)\|\tilde{x}(t)\| - \eta^2\lambda_i^2(\frac{1}{2}\lambda_i^2+\lambda_1^2)\frac{1}{\|\tilde{x}(t)\|} - \eta\frac{\lambda_D^4}{2\lambda_1^2} \\
&\leq \eta\lambda_1^2 + \eta\lambda_i^2(2-\eta\lambda_1-\frac{2}{3}\eta\lambda_i) - (1-\eta\lambda_1)\frac{\eta\lambda_1^2+\eta\lambda_i^2}{2-\eta\lambda_1-\eta\lambda_i} \\
&- \eta^2\lambda_i^2(\frac{1}{2}\lambda_i^2+\lambda_1^2)\frac{2-\eta\lambda_1-\eta\lambda_i}{\eta\lambda_1^2+\eta\lambda_i^2} - \eta\frac{\lambda_D^4}{2\lambda_1^2} \\
&\leq \frac{\eta\lambda_1^2}{2-\eta\lambda_1} - \eta\frac{\lambda_D^4}{2\lambda_1^2}
\end{aligned}
$$

The second line is because $(1-\eta\lambda_1)\|\tilde{x}(t)\|+\eta^2\lambda_i^2(\frac{1}{2}\lambda_i^2+\lambda_1^2)\frac{1}{\|\tilde{x}(t)\|}$ monotonously increase w.r.t $\|\tilde{x}(t)\|$ when $\|\tilde{x}(t)\| > \eta\lambda_i\sqrt{\frac{\frac{1}{2}\lambda_i^2+\lambda_1^2}{1-\eta\lambda_1}}$. The last line is due to technical lemma Lemma C.35.

Case 2.2 $\eta\lambda_1^2 \geq \eta\lambda_i\sqrt{\frac{\frac{1}{2}\lambda_i^2+\lambda_1^2}{1-\eta\lambda_1}} \geq \frac{\eta\lambda_1^2+\eta\lambda_i^2}{2-\eta\lambda_1-\eta\lambda_i}$.

$$
\begin{aligned}
\|\tilde{x}(t+1)\| &\leq \eta\lambda_1^2 + \eta\lambda_i^2(2-\eta\lambda_1-\frac{2}{3}\eta\lambda_i) - (1-\eta\lambda_1)\|\tilde{x}(t)\| - \eta^2\lambda_i^2(\frac{1}{2}\lambda_i^2+\lambda_1^2)\frac{1}{\|\tilde{x}(t)\|} - \eta\frac{\lambda_D^4}{2\lambda_1^2} \\
&\leq \eta\lambda_1^2 + \eta\lambda_i^2(2-\eta\lambda_1-\frac{2}{3}\eta\lambda_i) - 2\eta\lambda_i\sqrt{(\lambda_1^2+\frac{1}{2}\lambda_i^2)(1-\eta\lambda_1)} - \eta\frac{\lambda_D^4}{2\lambda_1^2} \\
&\leq \frac{\eta\lambda_1^2}{2-\eta\lambda_1} - \eta\frac{\lambda_D^4}{2\lambda_1^2}
\end{aligned}
$$

The second line is because of AM-GM inequality. The last line is due to technical lemma Lemma C.37.

Case 2.3 $\eta\lambda_1^2 < \eta\lambda_i\sqrt{\frac{\frac{1}{2}\lambda_i^2+\lambda_1^2}{1-\eta\lambda_1}}$.

In this case we have $\|\tilde{x}(t)\| < \eta\lambda_1^2 < \eta\lambda_i\sqrt{\frac{\frac{1}{2}\lambda_i^2+\lambda_1^2}{1-\eta\lambda_1}}$, then

$$
\begin{aligned}
\|\tilde{x}(t+1)\| &\leq \eta\lambda_1^2 + \eta\lambda_i^2(2-\eta\lambda_1-\frac{2}{3}\eta\lambda_i) - (1-\eta\lambda_1)\|\tilde{x}(t)\| - \eta^2\lambda_i^2(\frac{1}{2}\lambda_i^2+\lambda_1^2)\frac{1}{\|\tilde{x}(t)\|} - \eta\frac{\lambda_D^4}{2\lambda_1^2} \\
&\leq \eta\lambda_1^2 + \eta\lambda_i^2(2-\eta\lambda_1-\frac{2}{3}\eta\lambda_i) - (1-\eta\lambda_1)\eta\lambda_1^2 - \eta\lambda_i^2(\frac{1}{2}\lambda_i^2+\lambda_1^2)\frac{1}{\lambda_1^2} - \eta\frac{\lambda_D^4}{2\lambda_1^2} \\
&\leq \frac{\eta\lambda_1^2}{2-\eta\lambda_1} - \eta\frac{\lambda_D^4}{2\lambda_1^2}
\end{aligned}
$$

The second line is because $(1-\eta\lambda_1)\|\tilde{x}(t)\|+\eta^2\lambda_i^2(\frac{1}{2}\lambda_i^2+\lambda_1^2)\frac{1}{\|\tilde{x}(t)\|}$ monotonously decrease w.r.t $\|\tilde{x}(t)\|$ when $\|\tilde{x}(t)\| < \eta\lambda_i\sqrt{\frac{\frac{1}{2}\lambda_i^2+\lambda_1^2}{1-\eta\lambda_1}}$. The last line is due to technical lemma Lemma C.36.

□

Lemma C.21. *If* $\|\tilde{x}(t)\| \leq \frac{\eta\lambda_1^2}{2-\eta\lambda_1}, \tilde{x}(t) \in \cap \mathbb{I}_j$, *then* $\|\tilde{x}(t+1)\| \leq \eta\lambda_1^2 - (1-\eta\lambda_1)\|\tilde{x}(t)\|$

Proof. This can be directly inferred from the proof of lemma C.19 □

Lemma C.22. *Define* $S_1 = \{t | \|\tilde{x}(t)\| \leq \frac{\eta\lambda_1^2}{2-\eta\lambda_1}, t > T_1\}$, *suppose* $t, t' \in S_1, t \leq t'$, *then* $|\tilde{x}_1(t)| < |\tilde{x}_1(t')|$

Proof. For $t \in S_1$, by Lemma C.20, $t+1 \in S_1$ or $t+1 \notin S_1, t+2 \in S_1$.

Case 1 $t+1 \in S_1$, we can use Lemma C.19 to show $|\tilde{x}_1(t)| < |\tilde{x}_1(t+1)|$.
Case 2 $t+1 \notin S_1, t+2 \in S_1$.

$$|\tilde{x}_1(t+2)| = \frac{(\eta\lambda_1^2 - (1-\eta\lambda_1)\|\tilde{x}(t)\|)(\eta\lambda_1^2 - (1-\eta\lambda_1)\|\tilde{x}(t+1)\|)}{\|\tilde{x}(t)\|\|\tilde{x}(t+1)\|}|\tilde{x}(t)|$$

We only need to prove

$$\begin{aligned}
&(\eta\lambda_1^2 - (1-\eta\lambda_1)\|\tilde{x}(t)\|)(\eta\lambda_1^2 - (1-\eta\lambda_1)\|\tilde{x}(t+1)\|) > \|\tilde{x}(t)\|\|\tilde{x}(t+1)\| \\
\iff &\eta^2\lambda_1^4 - \eta\lambda_1^2(1-\eta\lambda_1)(\|\tilde{x}(t)\| + \|\tilde{x}(t+1)\|) + (-2\eta\lambda_1 + \eta^2\lambda_1^2)\|\tilde{x}(t)\|\|\tilde{x}(t+1)\| \geq 0 \\
\iff &\eta^2\lambda_1^4 - \eta\lambda_1^2(1-\eta\lambda_1)\|\tilde{x}(t)\| \geq \left((2\eta\lambda_1 - \eta^2\lambda_1^2)\|\tilde{x}(t)\| + \eta\lambda_1^2(1-\eta\lambda_1)\right)\|\tilde{x}(t+1)\|
\end{aligned}$$

Now using Lemma C.21, we only need to prove,

$$\eta^2\lambda_1^4 - \eta\lambda_1^2(1-\eta\lambda_1)\|\tilde{x}(t)\| \geq \left((2\eta\lambda_1 - \eta^2\lambda_1^2)\|\tilde{x}(t)\| + \eta\lambda_1^2(1-\eta\lambda_1)\right)\left(\eta\lambda_1^2 - (1-\eta\lambda_1)\|\tilde{x}(t)\|\right)$$

Through some calculation, this is equivalent to

$$((2-\eta\lambda_1)\|\tilde{x}(t)\| - \eta\lambda_1^2)((1-\eta\lambda_1)\|\tilde{x}(t)\| - \eta\lambda_1^2) \geq 0$$

which holds for $\|\tilde{x}(t)\| \leq \frac{\eta\lambda_1^2}{2-\eta\lambda_1}$.

Concluding the two cases and use induction, we can get the desired result.

□

C.4.3 Length Convergence

As Lemma C.22 show, $\|\tilde{x}_1(t)\|$ increase monotonously for $t \in S_1$. We can inferred from Lemma C.20, S_1 is infinite.

$\forall\epsilon > 0, \exists T_\epsilon$ satisfies $\forall t, t' \in S_1, t' > t > T_\epsilon, \frac{\|\tilde{x}_1(t')\|}{\|\tilde{x}_1(t)\|} < 1+\epsilon$.

Then $\forall t > T_\epsilon$, we have

$$1+\epsilon \geq \frac{\|\tilde{x}_1(t+1)\|}{\|\tilde{x}_1(t)\|} = \frac{\eta\lambda_1^2 - (1-\eta\lambda_1)\|\tilde{x}(t)\|}{\|\tilde{x}(t)\|}$$

or

$$\begin{aligned}
1+\epsilon \geq \frac{\|\tilde{x}_1(t+2)\|}{\|\tilde{x}_1(t)\|} &= \frac{(\eta\lambda_1^2 - (1-\eta\lambda_1)\|\tilde{x}(t)\|)(\eta\lambda_1^2 - (1-\eta\lambda_1)\|\tilde{x}(t+1)\|)}{\|\tilde{x}(t)\|\|\tilde{x}(t+1)\|} \\
&\geq \frac{(\eta\lambda_1^2 - (1-\eta\lambda_1)\|\tilde{x}(t)\|)\left(\eta\lambda_1^2 - (1-\eta\lambda_1)\left(\eta\lambda_1^2 - (1-\eta\lambda_1)\|\tilde{x}(t)\|\right)\right)}{\|\tilde{x}(t)\|\left(\eta\lambda_1^2 - (1-\eta\lambda_1)\|\tilde{x}(t)\|\right)} \\
&= \frac{\eta\lambda_1^2 - (1-\eta\lambda_1)\left(\eta\lambda_1^2 - (1-\eta\lambda_1)\|\tilde{x}(t)\|\right)}{\|\tilde{x}(t)\|}
\end{aligned}$$

Hence $\|\tilde{x}(t)\| \geq \min\left(\frac{\eta\lambda_1^2}{2-\eta\lambda_1^2+\epsilon}, \frac{\eta^2\lambda_1^3}{(2-\lambda_1\eta)\lambda_1\eta+\epsilon}\right), \forall t > T_\epsilon, t \in S_1$.

As $\forall t \notin S_1, t > T_\epsilon$ we have $\|\tilde{x}(t)\| \geq \eta\lambda_i\sqrt{\frac{\frac{1}{2}\lambda_i^2+\lambda_1^2}{1-\eta\lambda_1}}$.

Hence we have $\forall t > T_\epsilon, \|\tilde{x}(t)\| \geq \min\left(\frac{\eta\lambda_1^2}{2-\eta\lambda_1^2+\epsilon}, \frac{\eta^2\lambda_1^3}{(2-\lambda_1\eta)\lambda_1\eta+\epsilon}\right)$

Further by Lemma C.21, we can prove $\forall t > T_\epsilon + 1, \|\tilde{x}(t)\| \leq \eta\lambda_1^2 - (1-\eta\lambda_1)\min\left(\frac{\eta\lambda_1^2}{2-\eta\lambda_1^2+\epsilon}, \frac{\eta^2\lambda_1^3}{(2-\lambda_1\eta)\lambda_1\eta+\epsilon}\right)$.

Combining both bound, we have $\lim_{t\to\infty}\|\tilde{x}(t)\| = \frac{\eta\lambda_1^2}{2-\eta\lambda_1}$.

Notice that $\|P^{(2:D)}\tilde{x}(t+1)\| \leq \max\left(|1-\eta\lambda_2-\eta\frac{\lambda_2^2}{\|\tilde{x}(t)\|}|, |1-\eta\lambda_D-\eta\frac{\lambda_D^2}{\|\tilde{x}(t)\|}|\right)\|P^{(2:D)}\tilde{x}(t)\|$.

When $\|\tilde{x}(t)\| > \frac{\eta\lambda_2^2}{2-\eta\lambda_2-\delta}$,

$$-1+\delta \leq 1-\eta\lambda_2-\eta\frac{\lambda_2^2}{\|\tilde{x}(t)\|} \leq 1-\eta\lambda_D-\eta\frac{\lambda_D^2}{\|\tilde{x}(t)\|} \leq 1-\eta\lambda_D$$
$$\|P^{(2:D)}\tilde{x}(t+1)\| \leq \max(1-\eta\lambda_D, 1-\delta)\|P^{(2:D)}\tilde{x}(t)\|$$

Hence for sufficiently large t, $\|P^{(2:D)}\tilde{x}(t)\|$ shrinks exponentially, showing that $\lim_{t\to\infty}\|\tilde{x}_1(t)\| = \frac{\eta\lambda_1^2}{2-\eta\lambda_1}$

C.5 Full-batch SAM on General Loss: Proof of Theorem 4.9

To prove the theorem, we will separate the dynamic of SAM on general loss L to two phases.

Define

$$R_j(x) = \sqrt{\sum_{i=j}^{M}\lambda_i^2(x)\langle v_i(x), x-\Phi(x)\rangle^2} - \eta\rho\lambda_j(x), j\in[M], x\in U,$$

which is the length projection of $x-\Phi(x)$ on button$-k$ eigenspace of $\nabla^2 L(\Phi(x))$. We will provide a fine-grained convergence bound on $R_j(x)$.

Theorem C.23 (Phase I). *Let $\{x(t)\}$ be the iterates defined by SAM (3) and $x(0) = x_{init} \in U$, then under Assumption 3.1 there exists a constant T_1, such that for any $T_1' > T_1$, it holds for all η, ρ such that $(\eta+\rho)\log(1/\eta\rho)$ is sufficiently small, we have*

$$\max_{T_1\log(1/\eta\rho)\leq\eta t\leq T_1'\log(1/\eta\rho)}\max_{j\in[M]} R_j(x) = O(\eta\rho^2)$$
$$\max_{T_1\log(1/\eta\rho)\leq\eta t\leq T_1'\log(1/\eta\rho)}\|\Phi(x(t))-\Phi(x_{init})\| = O((\eta+\rho)\log(1/\eta\rho))$$

Theorem C.23 implies SAM will converge to an $O(\eta\rho)$ neighbor of Γ. Notice in the time frame defined by Theorem C.23, $x(t)$ effectively operates at a local regime around $\Phi(\lceil -T_1\log\eta\rho/\eta\rceil)$, this allows us to approximate L with the quadratic Taylor expansion of L at $\Phi(\lceil -T_1\log\eta\rho/\eta\rceil)$ and give us the following theorem.

Theorem C.24 (Phase II). *Let $\{x(t)\}$ be the iterates defined by SAM (3) under Assumptions 3.1 and 4.8, further assuming that (1) $\max_j R_j(x(0)) = O(\eta\rho^2)$, (2) $\|\Phi(x(0))-\Phi(x_{init})\| = O((\eta+\rho)\log(1/\eta\rho))$ and (3) $|\langle x(0)-\Phi(x(0)), v_1(x(0))\rangle| \geq \Omega(\rho^2)$, then there exists constant $T_2 > 0$, for any $T_3 > 0$ till which solution of (6) exists, for all η, ρ such that $\eta\ln(1/\rho)$ and ρ/η is sufficiently small,*

$$\max_{t\leq T_3/\eta\rho^2}\|\Phi(x(t))-X(\eta\rho^2 t)\| = O((\eta+\rho)\log(1/\eta\rho))$$
$$\min_{T_2\log(1/\rho)/\eta\leq t\leq T_3/\eta\rho^2}|\langle x(t)-\Phi(x(t)), v_1(x(t))\rangle| = \Theta(\eta\rho)$$
$$\max_{T_2\log(1/\rho)/\eta\leq t\leq T_3/\eta\rho^2}\max_{j\in[2:M]}|\langle x(t)-\Phi(x(t)), v_j(x(t))\rangle| = O(\eta\rho^2)$$

In this section we will define K as $\{X(t)\}$ where X is the solution of (6).

C.5.1 PHASE I: PROOF OF THEOREM C.23

The proof of Theorem C.23 is further split into three subphases.

In **Subphase A**, we will show that the trajectory of SAM will track gradient flow to the working zone K^h. This subphase will take time $O(\frac{1}{\eta})$ for sufficiently small η and ρ. At the end of this subphase $x(t) - \Phi(x(t)) = O(1), \Phi(x(t)) - \Phi(x(0)) = O(\eta + \rho)$.

In **Subphase B**, we will show that in the working zone, the loss will continue to decrease until $\|\nabla L\| = O(\rho)$. This will take time $O(\frac{-\log \rho}{\eta})$ for sufficiently small η and ρ. At the end of this subphase $x(t) - \Phi(x(t)) = O(\rho), \Phi(x(t)) - \Phi(x(0)) = O(-(\eta + \rho)\log \rho)$.

In **Subphase C**, we will show that $R_j(x)$ will shrink exponentially to $O(\eta\rho^{3/2})$ and $x(t)$ will stay in the invariant sets $I_j = \{R_j(x) \leq O(\eta\rho^{3/2})\}$.

Subphase A We know $\exists T_0, \|\Phi(x_{\text{init}}, T_0) - \Phi(x_{\text{init}})\| \leq \frac{h}{4}, L(\Phi(x_{\text{init}}, T_0)) < \frac{h^2\mu}{16}$. Using standard approximation theory, $\exists \eta_0, \rho_0 > 0$, such that

$$\eta < \eta_0, \rho < \rho_0 \Rightarrow \|x(\frac{T_0}{\eta}) - \Phi(x_{\text{init}}, T_0)\| \leq O(\eta + \rho),$$
$$L(x(\frac{T_0}{\eta})) \leq \frac{h^2\mu}{8}$$

This further implies

$$\begin{aligned}\|\Phi(x(\frac{T_0}{\eta})) - \Phi(x_{\text{init}})\| &= \|\Phi(x(\frac{T_0}{\eta})) - \Phi(\Phi(x_{\text{init}}, T_0))\| \\ &\leq O(\|x(\frac{T_0}{\eta}) - \Phi(x_{\text{init}}, T_0)\|) \\ &\leq O(\eta + \rho)\end{aligned}$$

Subphase B Define

$$D(x) = \|\Phi(x) - \Phi(x(\frac{T_0}{\eta}))\|$$

In this subphase, we will track the descent of loss to show that $\exists t$, such that

$$\begin{aligned}\|\nabla(L(x(t)))\| &\leq 4\zeta\rho \\ \|\Phi(x(t)) - \Phi(x_{\text{init}})\| &\leq O(-(\eta + \rho)\log \rho)\end{aligned}$$

for sufficiently small η. We require $\eta \leq \frac{1}{2\zeta}$. We assume $\inf_{x \in U} L(x) = 0$.

We also requires $-\eta \log \rho$ being sufficiently small, i.e ρ is not too small compared to η. So that

$$\begin{aligned}\log_{1-\frac{\eta\mu}{8}}(\frac{64\zeta^2\rho^2}{h^2})(2\eta\rho\zeta^2 h + 2\eta^2\zeta^4 h^2) &\leq \frac{-\log \frac{64\zeta^2\rho^2}{h^2}}{\frac{\eta\mu}{8}}(2\eta\rho\zeta^2 h + 2\eta^2\zeta^4 h^2) \\ &\leq -1024 \log \rho(2\rho\zeta^2 h + 2\eta\zeta^4 h^2) \\ &\leq \frac{h}{8}\end{aligned}$$

We will prove the following proposition,

$$\begin{aligned}&\|\nabla L(x)\| \geq 4\zeta\rho, t \leq \frac{T_0}{\eta} + \log_{1-\frac{\eta\mu}{8}}(\frac{64\zeta^2\rho^2}{h^2}) \\ &L(x(t)) \leq \frac{h^2\mu}{8}, D(x(t)) \leq (2\eta\rho\zeta^2 h + 2\eta^2\zeta^4 h^2)(t - \frac{T_0}{\eta}) \\ \Rightarrow &L(x(t+1)) \leq (1 - \frac{\eta\mu}{8})L(x(t)), D(x(t+1)) \leq (2\eta\rho\zeta^2 h + 2\eta^2\zeta^4 h^2)(t + 1 - \frac{T_0}{\eta})\end{aligned}$$

Proof. By lemma C.8, we have

$$\|x(t) - \Phi(x(t))\| \leq \sqrt{\frac{2L(x(t))}{\mu}} \leq \frac{h}{2}$$

Further, given the choice of η, ρ, $\|\Phi(x(t)) - \Phi(x_{\text{init}})\| \leq \frac{h}{4}$.

Hence we have $x(t) \in K^{\frac{3h}{4}}$. By Lemma C.12. we have $\overline{x(t)x(t+1)} \subset K^h$

Under update rule (3), using the smoothness of L, we have

$$\begin{aligned} L(x(t+1)) &= L(x(t) - \eta \nabla L\left(x(t) + \rho \frac{\nabla L\left(x(t)\right)}{\|\nabla L\left(x(t)\right)\|}\right)) \\ &\leq L(x(t)) - \eta \left\langle \nabla L\left(x(t)\right), \nabla L\left(x(t) + \rho \frac{\nabla L\left(x(t)\right)}{\|\nabla L\left(x(t)\right)\|}\right)\right\rangle + \frac{\zeta \eta^2 \|\nabla L\left(x(t) + \rho \frac{\nabla L(x(t))}{\|\nabla L(x(t))\|}\right)\|^2}{2} \end{aligned}$$

□

We have that

$$\|\nabla L\left(x(t) + \rho \frac{\nabla L\left(x(t)\right)}{\|\nabla L\left(x(t)\right)\|}\right) - \nabla L\left(x(t)\right)\| \leq \zeta \rho$$

Hence

$$L(x(t+1)) \leq L(x(t)) - \eta \|\nabla L\left(x(t)\right)\|^2 + \eta \zeta \rho \|\nabla L\left(x(t)\right)\| + \zeta \eta^2 \|\nabla L\left(x(t)\right)\|^2 + \zeta^3 \eta^2 \rho^2 33$$

By induction hypothesis, we have

$$\begin{aligned} \zeta \eta^2 \|\nabla L\left(x(t)\right)\|^2 &\leq \frac{1}{2} \eta \|\nabla L\left(x(t)\right)\|^2 \\ \eta \zeta \rho \|\nabla L\left(x(t)\right)\| &\leq \frac{1}{4} \eta \|\nabla L\left(x(t)\right)\|^2 \\ \zeta^3 \eta^2 \rho \leq \zeta^2 \eta \rho^2 &\leq \frac{1}{16} \eta \|\nabla L\left(x(t)\right)\|^2 \end{aligned}$$

Hence as $\overline{x(t+1)x(t)} \in K^h$

$$\begin{aligned} L(x(t+1)) &\leq L(x(t)) - \frac{1}{16} \eta \|\nabla L\left(x(t)\right)\|^2 \\ &\leq L(x(t)) - \frac{\eta \mu}{8} L(x(t)) \end{aligned}$$

This implies

$$L(x(t+1)) \leq (1 - \frac{\eta \mu}{8}) L(x(t))$$

Using Lemma C.7

$$\begin{aligned} \|\Phi(x(t+1)) - \Phi(x(t))\| &\leq \zeta \eta \rho \|\nabla L\left(x\right)\| + \eta \rho^2 \nu + \zeta^2 \eta^2 \|\nabla L\left(x\right)\|^2 + \zeta^3 \eta^2 \rho^2 \\ &\leq \eta \rho \zeta^2 h + \eta \rho^2 \nu + \eta^2 \zeta^4 h^2 + \eta^2 \rho^2 \zeta^3 \\ &\leq 2 \eta \rho \zeta^2 h + 2 \eta^2 \zeta^4 h^2 \end{aligned}$$

The induction is complete.

Now define t_1 the minimal $t \geq \frac{T_0}{\eta}$, such that $\|\nabla L(x(t))\| \leq 4\zeta\rho$.

If $t_1 > \frac{T_0}{\eta} + \log_{1-\frac{\eta\mu}{8}}(\frac{64\zeta^2\rho^2}{h^2})$, then by the induction,

$$\begin{aligned} L(\frac{T_0}{\eta} + \log_{1-\frac{\eta\mu}{8}}(\frac{64\zeta^2\rho^2}{h^2})) &\leq (1-\frac{\eta\mu}{8})^{\log_{1-\frac{\eta\mu}{8}}(\frac{64\zeta^2\rho^2}{h^2}} L(\frac{T_0}{\eta}) \\ &\leq \frac{64\zeta^2\rho^2}{h^2} L(\frac{T_0}{\eta}) \\ &\leq 8\zeta^2\rho^2\mu \\ \Rightarrow \nabla L\left(\frac{T_0}{\eta} + \log_{1-\frac{\eta\mu}{8}}(\frac{64\zeta^2\rho^2}{h^2})\right) &\leq 4\zeta\rho. \end{aligned}$$

This is a contradiction.

Subphase C Recall the definition of $R_j(x)$,

$$R_j(x) = \sqrt{\sum_{i=j}^{M} \lambda_i^2(x)\langle v_i(x), x-\Phi(x)\rangle^2 - \eta\rho\lambda_j^2(x)}$$

In this subphase, we will show that $R_j(x)$ will shrink exponentially to $O(\eta\rho^2)$ and $x(t)$ will stay in the invariant sets $I_j = \{R_j(x) \leq O(\eta\rho^2 + (\eta\rho)^{3/2})\}$.

Define $\hat{x}(t) = x(t) - \Phi(x(t)), A(t) = \nabla^2 L\left(\Phi(x(t))\right), \tilde{x}(t) = A(t)\hat{x}(t)$

We will prove the induction hypothesis for $t_1 \leq t \leq t_1 + 10\log_{1-\eta\mu}\frac{\eta\mu^3}{4\zeta^2}$,

$$\begin{aligned} \|\tilde{x}(t)\| \geq \eta\lambda_1(t)^2 &\Rightarrow \|\tilde{x}(t+1)\| \leq (1-\eta\mu)\|\tilde{x}(t)\| \\ \|\tilde{x}(t)\| \leq \eta\lambda_1(t)^2\mu &\Rightarrow \|\tilde{x}(t+1)\| \leq \eta\rho\lambda_1^2(t) + 2c_1\eta\rho^2 \end{aligned}$$

As we have $\|\tilde{x}(t_1)\| = \|A(t_1)\hat{x}(t_1)\| \leq \frac{\zeta}{\mu}\|\nabla L\left(x(t_1)\right)\| \leq \frac{4\zeta^2\rho}{\mu}$.

Combining with the induction hypothesis, we have $\|\tilde{x}(t)\| \leq \frac{4\zeta^2\rho}{\mu}$.

Then we have,

$$\begin{aligned} \|\Phi(x(t+1)) - \Phi(x(t))\| &\leq \zeta\eta\rho\|\nabla L\left(x(t)\right)\| + \eta\rho^2\nu + \zeta^2\eta^2\|\nabla L\left(x(t)\right)\|^2 + \zeta^3\eta^2\rho^2 \\ &\leq \zeta^2\eta\rho\|x(t) - \Phi(x(t))\| + \zeta^4\eta^2\|x(t) - \Phi(x(t))\|^2 + \eta\rho^2\nu + \zeta^3\eta^2\rho^2 \\ &\leq \frac{\zeta\eta\rho}{\mu}\|\tilde{x}(t)\| + \frac{\zeta^4\eta^2}{\mu^2}\|\tilde{x}(t)\|^2 + \eta\rho^2\nu + \zeta^3\eta^2\rho^2 \\ &\leq c_0\eta\rho^2 \end{aligned}$$

As $t_1 \leq t \leq t_1 + 10\log_{1-\eta\mu}\frac{\eta\mu^3}{4\zeta^2} \leq t_1 + 10\frac{-\log\frac{\eta\mu^3}{4\zeta^2}}{\eta\mu}$, this implies

$$\begin{aligned} \|\Phi(x(t)) - \Phi(x(t_1))\| &\leq O(-\rho^2\log\eta) \\ \|\Phi(x(t)) - \Phi(x_{\text{init}})\| &\leq O(-(\eta+\rho)\log\rho) \end{aligned}$$

We have $x(t) \in K^{\frac{h}{2}}$ Using Lemma C.12, we conclude that $\overline{x(t)x(t+1)} \subset K^h$.

$$\|\left(x(t+1) - x(t)\right) + \left(\eta\nabla L\left(x(t)\right) + \eta\rho\nabla^2 L\left(x(t)\right)\frac{\nabla L\left(x(t)\right)}{\|\nabla L\left(x(t)\right)\|}\right)\| \leq \nu\rho^2\eta$$

Now Using Lemma C.9, we have

$$\|(x(t+1) - x(t)) + \eta\nabla^2 L\left(\Phi(x(t))\right)\left(x(t) - \Phi(x(t))\right) + \eta\rho\nabla^2 L\left(x(t)\right)\frac{\nabla L\left(x(t)\right)}{\|\nabla L\left(x(t)\right)\|}\| \leq \nu\rho^2\eta + \nu\eta\|x(t) - \Phi(x(t))\|^2$$

Further we have

$$\|\frac{\nabla L\left(x(t)\right)}{\|\nabla L\left(x(t)\right)\|}-\frac{\nabla^2 L\left(\Phi(x(t))\right)\left(x(t)-\Phi(x(t))\right)}{\|\nabla L\left(x(t)\right)\|}\|\leq\frac{\nu\|x(t)-\Phi(x(t))\|^2}{2\|\nabla L\left(x(t)\right)\|}\leq\frac{\nu\|x(t)-\Phi(x(t))\|}{2\mu}$$

$$\|\frac{\nabla^2 L\left(\Phi(x(t))\right)\left(x(t)-\Phi(x(t))\right)}{\|\nabla L\left(x(t)\right)\|}-\frac{\nabla^2 L\left(\Phi(x(t))\right)\left(x(t)-\Phi(x(t))\right)}{\|\nabla^2 L\left(\Phi(x(t))\right)\left(x(t)-\Phi(x(t))\right)\|}\|\leq\frac{4v}{3\mu}\|x(t)-\Phi(x(t))\|$$

Hence

$$\begin{aligned}&\|(x(t+1)-x(t))+\eta\nabla^2 L\left(\Phi(x(t))\right)\left(x(t)-\Phi(x(t))\right)+\eta\rho\nabla^2 L\left(x(t)\right)\frac{\nabla^2 L\left(\Phi(x(t))\right)\left(x(t)-\Phi(x(t))\right)}{\|\nabla^2 L\left(\Phi(x(t))\right)\left(x(t)-\Phi(x(t))\right)\|}\|\\&\leq\nu\rho^2\eta+\nu\eta\|x(t)-\Phi(x(t))\|^2+\eta\rho\frac{2\zeta\nu}{\mu}\|x(t)-\Phi(x(t))\|\end{aligned}$$

Hence,

$$\begin{aligned}&\|(x(t+1)-x(t))+\eta\nabla^2 L\left(\Phi(x(t))\right)\left(x(t)-\Phi(x(t))\right)+\eta\rho\nabla^2 L\left(\Phi(x(t))\right)\frac{\nabla^2 L\left(\Phi(x(t))\right)\left(x(t)-\Phi(x(t))\right)}{\|\nabla^2 L\left(\Phi(x(t))\right)\left(x(t)-\Phi(x(t))\right)\|}\|\\&\leq\nu\rho^2\eta+\nu\eta\|x(t)-\Phi(x(t))\|^2+\eta\rho\frac{2\zeta\nu}{\mu}\|x(t)-\Phi(x(t))\|+\nu\eta\rho\|x(t)-\Phi(x(t))\|\end{aligned}$$

This implies,

$$\begin{aligned}&\|A(t)\left((x(t+1)-x(t))+\eta\tilde{x}(t)+\eta\rho A(t)\frac{\tilde{x}(t)}{\|\tilde{x}(t)\|}\right)\|\\&\leq\zeta\nu\rho^2\eta+\zeta\nu\eta\|x(t)-\Phi(x(t))\|^2+\zeta\eta\rho\frac{2\zeta\nu}{\mu}\|x(t)-\Phi(x(t))\|+\zeta\nu\eta\rho\|x(t)-\Phi(x(t))\|\end{aligned}$$

Also by Lemma C.12

$$\begin{aligned}&\|A(t)(x(t+1)-x(t))-\tilde{x}(t+1)+\tilde{x}(t)\|\\&=\|A(t)(x(t+1)-x(t))-A(t+1)x(t+1)+A(t)x(t)+A(t+1)\Phi(x(t+1))-A(t)\Phi(x(t))\|\\&=\|(A(t)-A(t+1))(x(t+1)-\Phi(x(t+1)))+A(t)(\Phi(x(t+1))-\Phi(x(t)))\|\\&\leq\nu\|\Phi(x(t+1))-\Phi(x(t))\|\|x(t+1)-\Phi(x(t+1))\|+\zeta\|\Phi(x(t+1))-\Phi(x(t))\|\\&\leq(\nu h+\zeta)\|\Phi(x(t+1))-\Phi(x(t))\|\\&\leq(\nu h+\zeta)(\zeta\eta\rho\|\nabla L\left(x\right)\|+\eta\rho^2\nu+\zeta^2\eta^2\|\nabla L\left(x\right)\|^2+\zeta^3\eta^2\rho^2)\end{aligned}$$

Combining with induction hypothesis, we know exists constant c_1, such that

$$\|\tilde{x}(t+1)-\tilde{x}(t)+\eta A(t)\tilde{x}(t)+\eta\rho A^2(t)\frac{\tilde{x}(t)}{\|\tilde{x}(t)\|}\|\leq c_1\eta\rho^2$$

We first bound $\|\tilde{x}(t)\|$, as in quadratic case, if $\|\tilde{x}(t)\|>\eta\rho\lambda_1^2(t)$, we would have

$$\begin{aligned}\|\tilde{x}(t)-\eta A(t)\tilde{x}(t)-\eta\rho A^2(t)\frac{\tilde{x}(t)}{\|\tilde{x}(t)\|}\|&\leq\|\tilde{x}(t)\|\|I-\eta A(t)-\eta\rho A^2(t)\frac{1}{\|\tilde{x}(t)\|}\|\\&\leq\|\tilde{x}(t)\|\max\{\eta\lambda_1,1-\eta\lambda_D-\eta\rho\lambda_D^2\frac{1}{\|x(t)\|}\}\\&\leq\max\{(1-\eta\lambda_D)\|\tilde{x}(t)\|-\eta\rho\lambda_D^2,\eta\lambda_1\|\tilde{x}(t)\|\}\end{aligned}$$

Choosing ρ small enough, we have

$$\|\tilde{x}(t+1)\|\leq\max\{1-\eta\lambda_D,2\eta\lambda_1\}\|\tilde{x}(t)\|\leq(1-\eta\mu)\|\tilde{x}(t)\|$$

If$\|\tilde{x}(t)\| \leq \eta\rho\lambda_1^2(t)$

$$\begin{aligned}\|\tilde{x}(t+1)\| &\leq \eta\rho\lambda_1^2(t) + c_1\eta\rho^2 \\ &\leq \eta\rho\lambda_1^2(t+1) + 2c_1\eta\rho^2\end{aligned}$$

Here we use

$$\max_i \|\lambda_i(t) - \lambda_i(t+1)\| \leq \|A(t+1) - A(t)\|_2 \leq c_0\kappa\eta\rho^2$$

Now define t_2 the minimal $t \geq t_1$, such that $\|\tilde{x}(t)\| \leq \eta\rho\lambda_1^2(t)$.

If $t_2 > t_1 + \log_{1-\eta\mu}(\frac{\eta\mu^3}{4\zeta^2})$, then by the induction,

$$\begin{aligned}\|\tilde{x}(t_1 + \log_{1-\eta\mu}(\frac{\eta\mu^3}{4\zeta^2}) + 1)\| &\leq (1-\eta\mu)^{\log_{1-\eta\mu}(\frac{\eta\mu^3}{4\zeta^2})}\|\tilde{x}(t_1)\| \\ &\leq \frac{\eta\mu^3}{4\zeta^2}\|\tilde{x}(t_1)\| \\ &\leq \frac{\eta\mu^3}{4\zeta^2}\zeta\|x(t_1) - \Phi(x(t_1)\| \\ &\leq \frac{\eta\mu^2}{4\zeta}\|\nabla L(t_1)\| \\ &\leq \mu^2\eta\rho \\ &\leq \lambda_1^2(t_1 + \log_{1-\eta\mu}(\frac{\eta\mu^3}{4\zeta^2}) + 1)\eta\rho\end{aligned}$$

This is a contradiction.

Following the induction, we further have for $t_2 \leq t \leq t_1 + T_1' \log_{1-\eta\mu}(\frac{\eta\mu^3}{4\zeta^2})$,

$$\|x(t)\| \leq \eta\rho\lambda_1^2(t+1) + 2c_1\eta\rho^2$$

We will now use a quantization technique separating $[M]$ into disjoint continuous subset $S_1, ..., S_p$ such that $\forall i \neq j$,

$$\min_{k\in s_k, l\in S_j} |\lambda_k(t) - \lambda_l(t)| \geq \rho$$

We would have

$$\min_{k\in s_k, l\in S_j} |\lambda_k(t+1) - \lambda_l(t+1)| \geq \rho - 8\nu\eta\rho^2 \geq 0.99\rho$$

We would then have for $t \geq t_2$ (analogous to proof in Section C.4.1)

If $\sqrt{\sum_{i=j}^p \|P_{S^{(i)}}^{(t)}\tilde{x}(t)\|^2} > \max_{k\in S_j} \lambda_k^2(t)\eta\rho$

$$\sqrt{\sum_{i=j}^p \|P_{S^{(i)}}^{(t)}\tilde{x}(t+1)\|^2} \leq \max\{(1-\eta\lambda_D(t+1)\|\sum_{i=j}^p P_{S^{(i)}}^{(t)}\tilde{x}(t)\| - \eta\rho\lambda_D(t+1)^2, \eta\max_{k\in S_j}\lambda_k(t+1)\|\sum_{i=j}^p P_{S^{(i)}}^{(t)}\tilde{x}(t)\|\} + c_1\eta\rho$$

If $\sqrt{\sum_{i=j}^p \|P_{S^{(i)}}^{(t)}\tilde{x}(t)\|^2} \leq \max_{k\in S_j} \lambda_k^2(t)\eta\rho$

$$\begin{aligned}\sqrt{\sum_{i=j}^p \|P_{S^{(i)}}^{(t)}\tilde{x}(t+1)\|^2} &\leq \max_{k\in S_j}\lambda_k^2(t)\eta\rho + c_1\eta\rho^2 \\ &\leq \max_{k\in S_j}\lambda_k^2(t+1)\eta\rho + 2c_1\eta\rho^2\end{aligned}$$

Further we have $\|P_{s_k}^{(t)} - P_{s_k}^{(t+1)}\| \leq O(\nu\eta\rho)$ by the Lemma C.29

So we have

If $\sqrt{\sum_{i=j}^{p} \|P_{S^{(i)}}^{(t)} \tilde{x}(t)\|^2} > \max_{k\in S_j} \lambda_k^2(t)\eta\rho$

$$\sqrt{\sum_{i=j}^{p} \|P_{S^{(i)}}^{(t+1)} \tilde{x}(t+1)\|^2} \leq \max\{(1-\eta\lambda_D)\|\sum_{i=j}^{p} P_{S^{(i)}}^{(t)} \tilde{x}(t)\| - \eta\rho\lambda_D^2, \eta \max_{k\in S_j} \lambda_k \|\sum_{i=j}^{p} P_{S^{(i)}}^{(t)} \tilde{x}(t)\|\} + c_1\eta\rho^2$$

If $\sqrt{\sum_{i=j}^{p} \|P_{S^{(i)}}^{(t)} \tilde{x}(t)\|^2} \leq \max_{k\in S_j} \lambda_k^2(t)\eta\rho$

$$\begin{aligned}\sqrt{\sum_{i=j}^{p} \|P_{S^{(i)}}^{(t+1)} \tilde{x}(t+1)\|^2} &\leq \max_{k\in S_j} \lambda_k^2(t)\eta\rho + c_1\eta\rho^2 + O(\eta\rho^2) \\ &\leq \max_{k\in S_j} \lambda_k^2(t+1)\eta\rho + 2c_1\eta\rho^2 + O(\eta\rho^2)\end{aligned}$$

Finally taking into quantization error, as all the eigenvalue in the same group at most differ $D\rho$, we would have

If $R_k(x(t)) \geq 0$

$$\begin{aligned}R_k(x(t+1)) + \lambda_k^2(t+1)\eta\rho &\leq (1-\eta\lambda_D)R_k(x(t)) \\ &\leq (1-\eta\mu)(R_k(x(t)) + \lambda_k^2(t)\eta\rho)\end{aligned}$$

If $R_k(x(t)) < 0$

$$R_k(x(t+1)) \leq O(\eta\rho^2)$$

Similar to the proof of existence of t_2, we can show the existence of $t_3 \leq t_2 + \log_{1-\eta\mu}(\frac{\eta\mu^3}{4\zeta^2})$, such that for $t_3 \leq t \leq t_3 + T_1' \log_{1-\eta\mu}(\frac{\eta\mu^3}{4\zeta^2})$,

$$\max_j R_j(t) \leq O(\eta\rho^2)$$

C.5.2 Phase II: Proof of Theorem C.24

The proof consists of two subphase.

In **subphase A**, we will show $x(t) - \Phi(x(t))$ aligns with $v_1(t)$ in $O(\log(1/\rho)/\eta)$ steps.

In **subphase B**, we will show that the alignment continues to hold and $x(t)$ moves as a time-rescaled version of solution of Equation (6).

Subphase A This proof is analogous to Section C.4.2. To maintain consistency with previous section, we abuse notation and change the starting step to t_3. The time frame we are discussing is $t_3 \leq t \leq t_3 + T_1' \log_{1-\eta\mu}(\frac{\eta\mu^3}{4\zeta^2})$.

First Induction We will inductively prove $\|x_1(t)\|$ is $\Omega(\rho^2)$ and that there exists step t_4 for $t_4 \leq t \leq t_3 + T_1' \log_{1-\eta\mu}(\frac{\eta\mu^3}{4\zeta^2})$ that $x_1(t) \geq \frac{1}{4}\left(\frac{\eta\lambda_1^2}{2-\eta\lambda_1} + 3\frac{\eta\lambda_2^2}{2-\eta\lambda_2}\right)\rho - O(\eta\rho^2)$

For step t, we fixed the quadratic function as $\langle x - \Phi(x(t)), \nabla^2 L\left(\Phi(x(t))\right)(x - \Phi(x(t))\rangle$,

Define $\bar{x} = \frac{\nabla^2 L(\Phi(x(t)))(x-\Phi(x(t))}{\rho}$, $A = \nabla^2 L(t)$

We have for $t \leq t_4 - 1$, $\|\bar{x}_1(t)\| \leq \frac{1}{2}\left(\frac{\eta\lambda_1^2}{2-\eta\lambda_1} + \frac{\eta\lambda_2^2}{2-\eta\lambda_2}\right)$.

By assumption, we have $\|\bar{x}_1(t)\| \geq \Omega(\rho)$.

We have

$$\|(x(t+1)-x(t))+\eta\nabla^2 L\left(\Phi(x(t))\right)(x(t)-\Phi(x(t)))+\eta\rho\nabla^2 L\left(\Phi(x(t))\right)\frac{\nabla^2 L\left(\Phi(x(t))\right)(x(t)-\Phi(x(t)))}{\|\nabla^2 L\left(\Phi(x(t))\right)(x(t)-\Phi(x(t)))\|}\|$$
$$\leq \nu\rho^2\eta+\nu\eta\|x(t)-\Phi(x(t))\|^2+\eta\rho\frac{2\zeta\nu}{\mu}\|x(t)-\Phi(x(t))\|+\nu\eta\rho\|x(t)-\Phi(x(t))\|$$
$$\leq c_2\eta\rho^2$$

Further we have, there exists constant c_4 such that

$$\begin{aligned}&\|(x(t+1)-x(t))+\eta\rho\bar{x}(t)+\eta\rho A\frac{\bar{x}(t)}{\|\bar{x}(t)\|}\|\\ \leq& c_2\eta\rho^2+c_3\|\Phi(x(t))-\Phi(x(t_3))\|\\ \leq& -\frac{c_4}{\zeta}\eta\rho^2\log\rho\end{aligned}$$

Now we have

$$\|\bar{x}(t+1)-\bar{x}(t)+\eta A\bar{x}(t)+\eta A^2\frac{\bar{x}(t)}{\|\bar{x}(t)\|}\|\leq -c_4\eta\rho\log\rho$$

So here our goal is to discuss the dynamics of the following perturbed version of quadratic SAM.

$$\|\bar{x}(t+1)-\bar{x}(t)+\eta A\bar{x}(t)+\eta A^2\frac{\bar{x}(t)}{\|\bar{x}(t)\|}\|\leq -c_4\eta\rho\log\rho$$
$$\|P^{(j:D)}\bar{x}(t)\|-\lambda_j^2\eta\leq c_5(\eta\rho+\eta^{3/2}\rho^{1/2})$$

Define $\hat{x}(t+1)$,

$$\hat{x}(t+1)=\bar{x}(t)-\eta A\bar{x}(t)-\eta A^2\frac{\bar{x}(t)}{\|\bar{x}(t)\|}$$

In the quadratic case, we have Lemma C.20 to show $\|\tilde{x}(t)\|$ can't stay greater $\frac{\eta\lambda_1^2}{2-\eta\lambda_1}$ for two steps. Hence here we have if $\|\bar{x}(t)\|\geq\frac{\eta\lambda_1^2}{2-\eta\lambda_1}$, then $\|\hat{x}(t+1)\|\leq\frac{\eta\lambda_1^2}{2-\eta\lambda_1}-O(\eta)$, which leads $\|\bar{x}(t+1)\|\leq\|\hat{(}x(t+1))\|+\tilde{O}(\eta\rho)\leq\frac{\eta\lambda_1^2}{2-\eta\lambda_1}$. Here we can in fact prove a more subtle version of this lemma showing,

Lemma C.25.

$$\exists C_1(\lambda_1,\lambda_2,\lambda_D),C_2(\lambda_1,\lambda_2,\lambda_D)<1,\|\bar{x}(t)\|\geq C_1\frac{\eta\lambda_1^2}{2-\eta\lambda_1}\Rightarrow\|\bar{x}(t+1)\|\leq C_2\frac{\eta\lambda_1^2}{2-\eta\lambda_1}$$

Proof. If

$$\|\bar{x}(t)\|\geq\frac{\eta\lambda_1^4}{\lambda_1^2(1-\eta\lambda_D)+(\lambda_1^2-\lambda_D^2)(1-\eta\lambda_1)}$$

Using Lemma C.20, we have

$$\|\hat{x}(t)\|\leq\max(\frac{\eta\lambda_1^2}{2-\eta\lambda_1}-\eta\frac{\lambda_D^4}{2\lambda_1^2},\eta\lambda_1^2-(1-\eta\lambda_1)\|\tilde{x}(t)\|)\leq c_6(\lambda_1,\lambda_D)\frac{\eta\lambda_1^2}{2-\eta\lambda_1}$$
$$c_6(\lambda_1,\lambda_D)<1$$

If

$$\|\bar{x}(t)\| \leq \frac{\eta\lambda_1^4}{\lambda_1^2(1-\eta\lambda_D)+(\lambda_1^2-\lambda_D^2)(1-\eta\lambda_1)}$$

Then we have

$$\frac{-\eta\lambda_D^2+(1-\eta\lambda_D)\|\bar{x}(t)\|}{\eta\lambda_1^2-(1-\eta\lambda_1)\|\bar{x}(t)\|} \leq \frac{\lambda_1^2-\lambda_D^2}{\lambda_1^2}$$
$$\frac{\eta\lambda_2^2-(1-\eta\lambda_2)\|\bar{x}(t)\|}{\eta\lambda_1^2-(1-\eta\lambda_1)\|\bar{x}(t)\|} \leq \frac{\lambda_2^2}{\lambda_1^2}$$

This implies,

$$\|\hat{x}(t+1)\| \leq (\eta\lambda_1^2-(1-\eta\lambda_1)\|\bar{x}(t)\|)\sqrt{\frac{\|\bar{x}_1^2(t)\|}{\|\bar{x}(t)\|^2}+(1-\frac{\|\bar{x}_1^2(t)\|}{\|\bar{x}(t)\|^2})\max\{\frac{\lambda_1^2-\lambda_D^2}{\lambda_1^2},\frac{\lambda_2^2}{\lambda_1^2}\}}$$

As we suppose

$$\|\bar{x}_1(t)\| \leq \frac{1}{2}\left(\frac{\eta\lambda_1^2}{2-\eta\lambda_1}+\frac{\eta\lambda_2^2}{2-\eta\lambda_2}\right)$$
$$\|\bar{x}(t)\| \geq \frac{\eta\lambda_1^2}{2-\eta\lambda_1}$$

This implies

$$\frac{\|\bar{x}_1(t)\|}{\|\bar{x}(t)\|} \leq \frac{\lambda_1^2+\lambda_2^2}{2\lambda_1^2}$$

Combining we have

$$\|\hat{x}(t+1)\| \leq c_7(\lambda_1,\lambda_2,\lambda_D)(\eta\lambda_1^2-(1-\eta\lambda_1)\|\bar{x}(t)\|)$$
$$c_7(\lambda_1,\lambda_2,\lambda_D) < 1$$

This implies

$$\|\bar{x}(t)\| \geq \frac{c_6\eta\lambda_1^2-\frac{c_5+1}{\frac{\eta\lambda_1^2}{2-\eta\lambda_1}}}{c_6(1-\lambda_1)}$$
$$\Rightarrow \|\hat{x}(t+1)\| \leq \max\{c_7,\frac{c_6+1}{2}\}\frac{\eta\lambda_1^2}{2-\eta\lambda_1}$$

As $\exists c_8$,

$$\|\hat{x}(t+1)-\bar{x}(t+1)\| \leq c_8\eta\rho$$

. We can conclude that

$$\exists C_1(\lambda_1,\lambda_2,\lambda_D), C_2(\lambda_1,\lambda_2,\lambda_D) < 1, \|\bar{x}(t)\| \geq C_1\frac{\eta\lambda_1^2}{2-\eta\lambda_1} \Rightarrow \|\bar{x}(t+1)\| \leq C_2\frac{\eta\lambda_1^2}{2-\eta\lambda_1}$$

□

Define $T = \{t|\|\bar{x}(t)\| \leq \frac{1}{2}\left(\frac{\eta\lambda_1^2}{2-\eta\lambda_1}+\frac{\eta\lambda_2^2}{2-\eta\lambda_2}\right)\}$, $S = \{t|\|\bar{x}(t)\| \leq \frac{\eta\lambda_1^2}{2-\eta\lambda_1}\}$,

For $s \in S, n(s) := \min_{j>s}\{j \in S\}$.

We will show when $\|\bar{x}_1(t)\| \leq \frac{1}{2}\left(\frac{\eta\lambda_1^2}{2-\eta\lambda_1}+\frac{\eta\lambda_2^2}{2-\eta\lambda_2}\right)$,

$$\exists c_4(\lambda_1,\lambda_2,\lambda_D) > 1, \|\bar{x}_1(n(s))\| \geq c_4\|\bar{x}_1(s)\| \text{ or } \|\bar{x}_1(n(n(s)))\| \geq c_4\|\bar{x}_1(s)\|$$

Define $\underline{x}(t+1) = \hat{x}(t) - \eta A\hat{x}(t) - \eta A^2\frac{\hat{x}(t)}{\|\hat{x}(t)\|}$

Consider two cases

Case 1 $\|\bar{x}(s)\| \leq C_1 \frac{\eta\lambda_1^2}{2-\eta\lambda_1}$

$$\begin{aligned}
\frac{\|\hat{x}_1(s+1)\|}{\|\bar{x}_1(t)\|} &= \frac{\eta\lambda_1^2 - (1-\eta\lambda_1)\|\bar{x}(t)\|}{\|\bar{x}(t)\|} \geq \frac{(2-C_1) - \eta\lambda_1 + C_1\eta\lambda_1}{C_1} \geq \frac{1}{C_1} \\
\frac{\|\underline{x}_1(s+2)\|}{\|\bar{x}_1(s)\|} &= \frac{(\eta\lambda_1^2 - (1-\eta\lambda_1)\|\bar{x}(s)\|)(\eta\lambda_1^2 - (1-\eta\lambda_1)\|\hat{x}(s+1)\|)}{\|\bar{x}(s)\|\|\hat{x}(s+1)\|} \\
&\geq \frac{(\eta\lambda_1^2 - (1-\eta\lambda_1)\|\bar{x}(s)\|)\left(\eta\lambda_1^2 - (1-\eta\lambda_1)\left(\eta\lambda_1^2 - (1-\eta\lambda_1)\|\bar{x}(s)\|\right)\right)}{\|\bar{x}(s)\|\left(\eta\lambda_1^2 - (1-\eta\lambda_1)\|\bar{x}(s)\|\right)} \\
&= \frac{\eta\lambda_1^2 - (1-\eta\lambda_1)\left(\eta\lambda_1^2 - (1-\eta\lambda_1)\|\bar{x}(s)\|\right)}{\|\bar{x}(s)\|} \geq (1-\eta\lambda_1)^2 + \frac{(2-\eta\lambda_1)}{C} \\
&\geq 1 + C_3\eta
\end{aligned}$$

Here we require $C_3 \geq 0$ As $n(s) = s+1$ or $n(s) = s+2$ and we have

$$\begin{aligned}
\|\underline{x} - \bar{x}\| &\leq c_9\eta\rho \\
\|\hat{x} - \bar{x}\| &\leq c_8\eta\rho
\end{aligned}$$

Also

$$|\bar{x}_1(s)| \geq \Omega(\rho)$$

We have

$$\|\bar{x}_1(n(s))\| \geq (1 + C_3\eta/2)\|\bar{x}_1(s)\|$$

Case 2 $\|\bar{x}(s)\| > C_1 \frac{\eta\lambda_1^2}{2-\eta\lambda_1}$, then $\|\bar{x}(s+1)\| \leq C_2 \frac{\eta\lambda_1^2}{2-\eta\lambda_1}$, $n(s) = s+1$
Similar to case 1 We have $\|\hat{x}_1(s+1)\| \geq \|\tilde{x}_1(s)\|$
So in fact we have $\bar{x}_1(n(s)) \geq \bar{x}_1(s) - O(\eta\rho)$, suppose $\frac{\bar{x}_1(t_3)}{\rho}$ is a sufficiently large constant, then we can assume $|\bar{x}_1(n(s))| \geq (1 - C_3\eta/8)|\bar{x}_1(s)|$.
As $\|\bar{x}(n(s))\| \leq C_2 \frac{\eta\lambda_1^2}{2-\eta\lambda_1}$, similar to case 1, $\|\bar{x}_1(n(n(s)))\| \geq (1 + C_3\eta/2)\|\bar{x}_1(n(s))\| \geq (1 + C_3\eta/2)\|\bar{x}_1(s)\|$

In conclusion, if $\|\bar{x}_1(s)\| \leq \frac{1}{2}\left(\frac{\eta\lambda_1^2}{2-\eta\lambda_1} + \frac{\eta\lambda_2^2}{2-\eta\lambda_2}\right)$, we would have

$$\exists c_4(\lambda_1, \lambda_2, \lambda_D) > 0, \|\bar{x}_1(n(s))\| \geq (1 + c_4\eta)\|\bar{x}_1(s)\| \text{ or } \|\bar{x}_1(n(n(s)))\| \geq (1 + c_4\eta)\|\bar{x}_1(s)\|$$

This implies $\exists t_4 \leq t_3 - 4(\log\rho)/(c_4\eta)$, such that

$$\|\bar{x}_1(t_4)\| \geq \frac{1}{2}\left(\frac{\eta\lambda_1^2}{2-\eta\lambda_1} + \frac{\eta\lambda_2^2}{2-\eta\lambda_2}\right)$$

As we have $\|\bar{x}_1(n(t))\| \geq \|\bar{x}_1(t)\| - \max\{c_8, c_9\}(\eta\rho + \eta^{3/2}\rho^{1/2})$ for $\|\bar{x}_1(t)\| \geq \frac{1}{2}\left(\frac{\eta\lambda_1^2}{2-\eta\lambda_1} + \frac{\eta\lambda_2^2}{2-\eta\lambda_2}\right)$, we would have

$$\|\bar{x}(t)\| \geq \|\bar{x}_1(t))\| \geq \frac{1}{4}\left(\frac{\eta\lambda_1^2}{2-\eta\lambda_1} + 3\frac{\eta\lambda_2^2}{2-\eta\lambda_2}\right)$$

for $t_3 + T_1' \log_{1-\eta\mu}(\frac{\eta\mu^3}{4\zeta^2}) \geq t \geq t_4$ and the first induction is complete.

SECOND INDUCTION Define $\hat{x}$ and $\bar{x}$ as before.

This implies for $t \geq t_4$,

$$-1 + c_{10}(\lambda_1, \lambda_2) \leq 1 - \eta\lambda_2 - \eta\frac{\lambda_2^2}{\|\tilde{x}(t)\|} \leq 1 - \eta\lambda_D - \eta\frac{\lambda_D^2}{\|\tilde{x}(t)\|} \leq 1 - \frac{\lambda_D^2}{2\lambda_1^2}$$

$$\|P^{(2:D)}\hat{x}(t+1)\| \leq \max(1 - \frac{\lambda_D^2}{2\lambda_1^2}, 1 - c_{10}(\lambda_1, \lambda_2))\|P^{(2:D)}\bar{x}(t)\|$$

As $\|P^{(2:D)}\bar{x}(t)\| \leq 2\lambda_2^2\eta$ We can inductively show that for $t \geq t_4 + \log_{\max(1-\frac{\lambda_D^2}{2\lambda_1^2}, 1-c_{10}(\lambda_1,\lambda_2))} \frac{\rho^2}{\zeta^2}$ iteration, $\|P^{(2:D)}\bar{x}(t+1)\| \leq 2c_5(\eta\rho)$

Now as we have

$$\begin{aligned}\|P^{(2:D)}(t) - P^{(2:D)}(t+1)\| &\leq O(\nu\rho^2)\\ \|v_1(t) - v_1(t+1)\| &\leq O(\nu\rho^2)\\ \|\lambda_1(t) - \lambda_1(t+1)\| &\leq O(\nu\rho^2)\end{aligned}$$

This implies we have for $t \geq t_4 + O(\log_{\max(1-\frac{\lambda_D^2}{2\lambda_1^2}, 1-c_{10}(\lambda_1,\lambda_2))} \frac{\rho^2}{\zeta^2})$

$$\begin{aligned}\|\tilde{x}(t)\| \geq \|\tilde{x}_1(t)\| &\geq \frac{1}{2}\left(\frac{\eta\lambda_1^2(t)}{2-\eta\lambda_1(t)} + \frac{\eta\lambda_2^2(t)}{2-\eta\lambda_2(t)}\right)\rho - O(\eta\rho^2)\\ \|P^{(2:D)}(t)\tilde{x}(t)\| &\leq O(\eta\rho^2)\end{aligned}$$

Subphase B We are now ready to show that $\Phi(x(t))$ will track the solution of (6). The main principal of this proof have been introduced in Section 4.3.

To simplify our writing define $\theta(t) = \arccos(\langle v_1, \frac{\nabla L(x)}{\|\nabla L(x)\|}\rangle)$

We can inductively prove the following statement

$$\begin{aligned}\|\Phi(x(t)) - X(\eta\rho^2 t)\| &\leq O(-(\eta+\rho)\log\rho)\\ \|x(t) - \Phi(x(t))\| &= \Theta(\frac{\eta\rho\lambda_1(t)}{2-\eta\lambda_1(t)})\\ \|\bar{x}_1(t)\| &\geq \frac{1}{2}\left(\frac{\eta\lambda_1^2(t)}{2-\eta\lambda_1(t} + \frac{\eta\lambda_2^2(t)}{2-\eta\lambda_2(t)}\right)\rho - O(\eta\rho^2)\\ \|P^{(2:D)}(t)\bar{x}(t)\| &\leq O(\eta\rho^2)\end{aligned}$$

The initial condition is satisfied by assumption.

We have

$$\|\partial\Phi(x(t))(x(t+1)-x(t)) - \eta\rho\partial\Phi(x)\nabla^2 L(x)\frac{\nabla L(x)}{\|\nabla L(x)\|} - \eta\rho^2\partial\Phi(x)\partial\nabla^2 L(x)[\frac{\nabla L(x)}{\|\nabla L(x)\|}, \frac{\nabla L(x)}{\|\nabla L(x)\|}]/2\| \leq \eta\rho^3\Upsilon$$

Using Lemma C.8, we have

$$\eta\rho\partial\Phi(x)\nabla^2 L(x)\frac{\nabla L(x)}{\|\nabla L(x)\|} = \eta\rho\|\nabla L(x)\|\|\partial^2\Phi(x)\left[\frac{\nabla L(x)}{\|\nabla L(x)\|}, \frac{\nabla L(x)}{\|\nabla L(x)\|}\right]/2\| \leq \eta\rho\kappa\|\nabla L(x)\|$$

This implies,

$$\|\partial\Phi(x(t))(x(t+1)-x(t)) - \eta\rho^2\partial\Phi(x)\partial\nabla^2 L(x)[\frac{\nabla L(x)}{\|\nabla L(x)\|}, \frac{\nabla L(x)}{\|\nabla L(x)\|}]/2\| \leq \eta\rho^3\Gamma + \eta\rho\kappa\|\nabla L(x)\|.$$

Further

$$\begin{aligned}&\|\Phi(x(t+1)) - \Phi(x(t)) - \eta\rho^2\partial\Phi(x)\partial\nabla^2 L(\Phi(x))[\frac{\nabla L(x)}{\|\nabla L(x)\|}, \frac{\nabla L(x)}{\|\nabla L(x)\|}]/2\|\\ \leq&\eta\rho^3\Gamma + \eta\rho\kappa\|\nabla L(x)\| + \eta\rho^2\nu\|x-\Phi(x)\| + \frac{1}{2}\zeta\|x(t+1)-x(t)\|^2\end{aligned}$$

By induction we have $0 \leq t \leq \frac{T_3}{\eta\rho^2}$, we have $\|x - \Phi(x)\| = \Theta(\eta\rho), \theta = O(\rho)$

So we have

$$\|\Phi(x(t+1)) - \Phi(x(t)) - \eta\rho^2\partial\Phi(x)\partial\nabla^2 L(\Phi(x))[\frac{\nabla L(x)}{\|\nabla L(x)\|}, \frac{\nabla L(x)}{\|\nabla L(x)\|}]/2\| \leq O(\eta\rho^3 + \eta^2\rho^2)$$

Further we have

$$\|\eta\rho^2\partial\Phi(x)\partial\nabla^2 L\left(\Phi(x)\right)[\frac{\nabla L\left(x\right)}{\|\nabla L\left(x\right)\|},\frac{\nabla L\left(x\right)}{\|\nabla L\left(x\right)\|}]/2-\eta\rho^2\partial\Phi(x)\partial\nabla^2 L\left(\Phi(x)\right)[v_1(t),v_1(t)]/2$$
$$\leq\eta\rho^2(O(\zeta\theta)+O(\frac{\nu\zeta\|x-\Phi(x(t))\|}{\mu}))\leq O(\eta\rho^3)$$

We have

$$\partial\Phi(x)\partial\nabla^2 L\left(\Phi(x)\right)[v_1(t),v_1(t)]=P_{X,\Gamma}^{\perp}\nabla(\lambda_1(\nabla^2(\Phi(L(x))))$$

This implies

$$\|\Phi(x(t+1))-\Phi(x(t))+\eta\rho^2P_{X,\Gamma}^{\perp}\nabla(\lambda_1(\nabla^2(\Phi(L(x))))/2\|\leq O(\eta\rho^3+\eta^2\rho^2)$$

Hence we can perform the induction and the accumulated approximation error will be of order $O(\rho+\eta)$.

C.5.3 Proof of Corollaries

Proof of Corollary 4.10. We will do a Taylor expansion on $L_\rho^{\max}(x)$. By Theorem C.23 and C.24, for $t>T_3'/\eta\rho^2$, we have $\|X(\eta\rho^2 t)-x(t)\|=\tilde{O}(\eta+\rho)$ and $\|x(t)-\Phi(x(t))\|=O(\eta\rho)$

$$R_\rho^{\max}(x)=\max_v \rho v^T\nabla L(x)+\rho^2 v^T\nabla^2 L(x)v/2+O(\rho^3)$$

Then as $\|v^T\nabla L(x)\|=O(\eta\rho)$, this implies

$$\begin{aligned}R_\rho^{\max}(x)&=\rho^2\max_v v^T\nabla^2 L(x)v/2+O(\eta^2\rho^2+\rho^3)\\&=\rho^2\max_v v^T\nabla^2 L(X(\eta\rho^2 t))v/2+\tilde{O}(\eta\rho^2)\\&=\rho^2\lambda_1(X(\eta\rho^2 t))/2+\tilde{O}(\eta\rho^2)\end{aligned}$$

□

Proof of Corollary 4.11. Choose T such that $X(T)$ is sufficiently close to $X(\infty)$, such that $\lambda_1(X(T))\leq\lambda_1(X(\infty))+2\epsilon$

By corollary 4.10, we have $\|R_\rho^{\max}(x(\lceil T/(\eta\rho^2)\rceil))-\rho^2\lambda_1(X(T))/2\|\leq\tilde{O}(\eta\rho^2)$. This further implies $\|R_\rho^{\max}(x(\lceil T/(\eta\rho^2)\rceil))-\rho^2\lambda_1(X(\infty))/2\|\leq\epsilon\rho^2+\tilde{O}(\eta\rho^2)$. We also have $\|L(x(\lceil T/(\eta\rho^2)\rceil))\|=O(\eta^2\rho^2)$. Then we can leverage Theorem 4.3 and Theorem 4.5 to get the desired bound. □

C.6 Stochastic SAM: Proof of Theorem 5.4

We will first prove Lemma 5.3,

Proof of Lemma 5.3. Note that $\frac{d\ell(y',y_k)}{dy'}|_{y'=f_k(p)}=0$, we have $\nabla^2 L_k(p)=\Lambda_k(p)w_k(p)w_k(p)^T$. Also note $\nabla L_k(x)/\|\nabla L_k(x)\|=\text{sign}(\frac{d\ell(y',y_k)}{dy'}|_{y'=f_k(x)})\nabla f_k(x)/\|\nabla f_k(x)\|$. By Assumption 3.1, $\nabla^2 L(p)=\sum_k\nabla^2 L_k(p)/M=\sum_k\Lambda_k(p)w_k(p)w_k(p)^T/M$ has rank M , this implies $\forall k,\nabla f_k(p)\neq 0$, hence $\nabla f_k(x)/\|\nabla f_k(x)\|$ is in C^1 near p and we have proved our claim. □

We will prove under a more general assumption.

Assumption C.2. *Total loss $L=\frac{1}{M}\sum_{k=1}^M L_k$. For each $k\in[M]$, L_k is $\mathcal{C}^4$, and there exists a $(D-1)$-dimensional $\mathcal{C}^2$-submanifold of $\mathbb{R}^D$, Γ_k, where for all $x\in\Gamma_k$, x is a global minimizer of L_k, $L_k(x)=0$ and rank$(\nabla^2 L_k(x))=1$. Moreover, $\Gamma=\cap_{k=1}^M\Gamma_k$ for Γ defined in Assumption 3.1.*

We have U_k is open and Φ_k is in $\mathcal{C}^3$ on U_k.(from Lemma B.15 Arora et al. (2022))

Theorem C.26 shows that Setting in Theorem 5.4 satisfies assumption C.2.

Theorem C.26. *Suppose $L(x) = \sum_{k=1}^{M} L_k(x)/M$ and manifold Γ satisfy Assumption 3.1, and that $f_k(x) = y_k$ for every $x \in \Gamma, k \in [M]$. Then there exists $(D-1)$-dimensional $\mathcal{C}^2$ submanifolds of $\mathbb{R}^D$, such that $\cap_{k=1}^{M} \Gamma_k = \Gamma$ and for every $x \in \Gamma_k$ and $k \in [M]$, $f_k(x) = y_k$, that is, Γ_k is a manifold of global minimizers of L_k.*

Proof of Theorem C.26. By standard calculus, for $x \in \Gamma$, we have $\nabla^2 L(x) = \sum_{k=1}^{M} w_k w_k^T/M$. By Assumption 3.1,$\nabla^2 L(x)$ is full rank, this implies $w_k \neq 0$. Then we have in an open set $V(x)$ containing x, $\nabla f_k(x) \neq 0$. Then consider $V = \cup_{x \in \Gamma} V(x)$, which is an open set and in which $\nabla f_k \neq 0$. Now apply preimage theorem, we would have $\Gamma_k = \{x \in V | f_k(x) \neq y_k\}$ forms C^2 dimensional sub-manifolds. We also easily have $\cap \Gamma_k = \Gamma$ from definitions. □

The following theorems shows that stochastic SAM (16) essentially minimize trace of Hessian of loss. Analogous to the full-batch setting, we will split the trajectory into two phase.

Theorem C.27 (Phase I)**.** *Let $\{x(t)\}$ be the iterates defined by SAM (3) and $x(0) = x_{init} \in U$, then under Assumption 3.1 and C.2 there exists a constant T_1, it holds for sufficiently small $-(\eta + \rho)\log(\eta\rho)$, we have with probability $1 - O(\sqrt{\rho})$, $\min_{-T_1 \log \rho/\eta \geq t} \|x(t) - \Phi(x(t))\| = O(-(\eta\rho + \rho^2)\log \eta\rho)$ and $\max_{-T_1 \log \rho/\eta \geq t} \|\Phi(x_{init}) - \Phi(x(t))\| = O(-(\eta + \rho)\log(\eta\rho))$.*

Theorem C.27 shows that SAM will converges to an $\tilde{O}(\eta\rho)$ neighborhood of the manifold without getting far away from $\Phi(x(0))$, where we can perform a local analysis on the trajectory of $\Phi(x(t))$.

Under Assumptions 3.1 and C.2, we have $\mathrm{Tr}(\nabla^2 L_k(x)) = \lambda_1(\nabla^2 L_k(x))$ is differentiable for $x \in \Gamma_i$. Hence $\mathrm{Tr}(\nabla^2 L(x)) = \sum_i \mathrm{Tr}(\nabla^2 L_k(x))$ is also differentiable and we have (17) is well defined for some finite time T_2.

Theorem C.28 (Phase II)**.** *Let $\{x(t)\}$ be the iterates defined by SAM (16) under Assumptions 3.1 and C.2, assuming (1) $\forall t, k, L_k(x(t)) \neq 0$, (2) $\|x(0) - \Phi(x(0))\| = O(-(\eta\rho + \rho^2)\log \eta\rho)$ and (3) $\|\Phi(x_{init}) - \Phi(x(0))\| = O(-(\eta + \rho)\log(\eta\rho))$, then for any $T_2 > 0$ till which solution of (17) exists, for sufficiently small $-(\eta + \rho)\log(\eta\rho)$, we have with probability $1 - O(\eta\rho)$, for all $\eta\rho^2 t < T_2$, $\|\Phi(x(t)) - X(\eta\rho^2 t)\| = O(-(\eta + \rho)\log \eta\rho)$ and $\|x(t) - \Phi(x(t))\| = O(-(\eta\rho + \rho^2)\log \eta\rho)$.*

In this section we will define K as $\{X(t)\}$ where X is the solution of (17).

We will prove these theorems respectively in the following sections.

C.6.1 Phase I: Proof of Theorem C.27

We will now discuss the convergence of 1-SAM to the manifold of minimizer. We will separate the dynamics into the following phase. Define ϕ as the gradient flow projection as in deterministic case.

Subphase A Gradient flow approximation, using standard approximation, we can show that $x(t)$ with high probability falls into a region K^h where the loss satisfies PL condition.

Subphase B After reaching the region, a detailed analysis will show that loss continue to decrease until $\|x(t) - \Phi(x(t))\| = \tilde{O}(\rho)$.

Subphase C Consider a quadratic approximation and we will get with high probability $x(t)$ will falls into $O(\eta\rho + \rho^2)$ neighbor of $\Phi(x(t))$.

Subphase A This is analogous to Subphase A in Section C.5.1 and we can suppose $\exists t_1, x(t_1) \in K^h$

Subphase B Define event $A(t)$ as $\{\nabla L(x(\tau)) \geq 4\zeta\rho, \forall \tau \leq t\}$.

We have if $\|\nabla L\left(x(t)\right)\| \geq 4\zeta\rho$

$$\begin{aligned}
\mathbb{E}[L(x(t+1))|x(t)] &= \mathbb{E}\left[L\left(x(t) - M\eta\nabla L_k[x(t) + \rho\frac{\nabla L_k\left(x(t)\right)}{\|\nabla L_k\left(x(t)\right)\|}]\right)|x(t)\right] \\
&\leq \mathbb{E}\left[L(x(t)) - M\eta\left\langle\nabla L\left(x(t)\right), \nabla L_k[x(t) + \rho\frac{\nabla L_k\left(x(t)\right)}{\|\nabla L_k\left(x(t)\right)\|}]\right\rangle\right] \\
&+ \mathbb{E}\left[\frac{\zeta M\eta^2}{2}\|\nabla L_k[x(t) + \rho\frac{\nabla L_k\left(x(t)\right)}{\|\nabla L_k\left(x(t)\right)\|}]\|^2\right] \\
&\leq L(x(t)) - M\eta\|\nabla L\left(x(t)\right)\|^2 + M\eta\rho\zeta\|\nabla L\left(x(t)\right)\| + \zeta M\eta^2\mathbb{E}[\|\nabla L_k(x(t))\|^2] + \zeta^3 M\eta^2\rho^2 \\
&\leq L(x(t)) - \frac{M\eta}{2}\|\nabla L\left(x(t)\right)\|^2 \\
&\leq L(x(t)) - \frac{M\eta\mu}{2}L(x(t))
\end{aligned}$$

We have

$$\mathbb{E}[L(x(t+1))\mathbf{1}A(t+1)] \leq \mathbb{E}[L(x(t+1))\mathbf{1}A(t)] \leq (1 - \frac{M\eta\mu}{2})\mathbb{E}[L(x(t))\mathbf{1}A(t)].$$

We can then conclude that with $t_2 = \frac{2\log\frac{h^2}{16\rho^2\mu M\eta}}{M\eta\mu} + t_1$

$$16\zeta^2\rho^2\mu\mathbb{P}\left(A(t_2+1)\right) \leq \mathbb{E}[L(x(t_2+1))\mathbf{1}A(t_2+1)] \leq (1 - \frac{M\eta\mu}{2})^{t_2-t_1}L(x(t_1)) \leq \zeta^2h^2(1 - \frac{M\eta\mu}{2})^{t_2-t_1}$$

We have

$$\mathbb{P}\left(A(t_2+1)\right) \leq M\eta$$

With an abuse of notation, suppose $\nabla L\left(x(t_2)\right) \leq 4\zeta\rho$, which implies $\|x(t_2) - \Phi(x(t_2))\| = O(\rho)$.

Subphase C After $\|\nabla L\left(x(t_2)\right)\| \leq 4\zeta\rho$, it becomes difficult to prove the loss continue to decrease. We proceed by consider a quadratic approximation. Now consider

$$\begin{aligned}
x(t+1) &= x(t) - M\eta\nabla L_k\left(x(t) + \rho\frac{\nabla L_k\left(x(t)\right)}{\|\nabla L_k\left(x(t)\right)\|}\right) \\
&= x(t) - M\eta\nabla L_k\left(x(t)\right) - M\eta\rho\nabla^2 L_k(x(t))\frac{\nabla L_k\left(x(t)\right)}{\|\nabla L_k\left(x(t)\right)\|} + O(M\eta\rho^2) \\
&= x(t) - M\eta\nabla L_k\left(x(t)\right) - M\eta\rho\Lambda_k w_k w_k^T\frac{\nabla L_k\left(x(t)\right)}{\|\nabla L_k\left(x(t)\right)\|} + O(M\eta\rho^2)
\end{aligned}$$

Iteratively define $t_{2,j}$, for $1 \leq j \leq 3$, $t_{2,1} = t_2$.

For $j \leq 2$, inductively suppose $\|x(t_{2,j}) - \Phi(x(t_{2,j}))\| \leq O(\rho^{(j+1)/2} + M\eta\rho)$, let $p_j = \Phi(x(t_{2,j}))$, further assume $\nabla L_k(\Phi(x(t_{2,j}))) = v_i v_i^T$. Further suppose N as the normal space of Γ at p_j and T as the tangent space. Define P_N and P_T as projection to the space.

We have $\|P_T(x(t_{2,j}) - p_j)\| = O((x(t_{2,j}) - p_j)^2)$.

Consider $t_{2,j} \leq t \leq t_{2,j} + \frac{\rho^{\frac{j-2}{2}}}{M\eta}$

Define event $A_j(t) = \{\|x(\tau) - p_j\| \geq \rho^{(j+2)/2}|\forall\tau \leq t\}$

We have $\|P_N(x(t) - p_j)\| = O(\rho^{k+1} + M\eta\rho^2(t - t_{2,j})) \leq O(\rho^{(j+2)/2})$

Under $A_j(t)$, we would have $\|P_T(x(t) - p_j)\| = O(\|x(t) - p_j\|)$

By Lemma C.11, we have

$$\frac{\nabla L_k\left(x(t)\right)}{\|\nabla L_k\left(x(t)\right)\|} = s_k(t)w_k + O(\|x(t) - p_j\|)$$

We also have

$$s_k(t) \neq sign(w_k^T(x(t)-p_j)) \Rightarrow \|w_k^T(x(t)-p_j)\| \leq \|x(t)-p_j\|^{3/2}$$

Now by Taylor Expansion,

$$\begin{aligned} x(t+1)-p_j &= (x(t)-p_j) - M\eta\Lambda_k w_k w_k^T(x(t)-p_j) + O(M\eta\|x(t)-p_j\|^2) \\ &\quad - M\eta\rho\Lambda_k s_k(t) w_k w_k^T w_k + O(M\eta\rho\|x(t)-p_j\|) + O(M\eta\rho^2) \\ &= (x(t)-p_j) - M\eta\Lambda_k w_k w_k^T(x(t)-p_j) - M\eta\rho\Lambda_k s_k(t) w_k w_k^T w_k + O(M\eta\rho^2) \end{aligned}$$

We then have

$$\begin{aligned} \mathbb{E}[\|x(t+1)-p_j\|^2|x(t)] &= \|x(t)-p_j\|^2 + 2\eta^2\sum_k \Lambda_k^2|w_k^T(x(t)-p_j)|^2 + \eta^2\rho^2\sum_k \Lambda_k^2 + O(M\eta\rho^2\|x(t)-p_j\|) \\ &\quad - \eta\sum_k \Lambda_k|w_k^T(x(t)-p_j)|^2 - \eta\rho\sum_k \Lambda_k s_k(t) w_k^T(x(t)-p_j) \end{aligned}$$

We lower bound $\sum_k \Lambda_k s_k(t) v_i^T(x(t)-p_j)$ again by Lemma C.11, there exists C such that

$$\begin{aligned} \sum_k \|v_i\| s_k(t) v_i^T(x(t)-p_j) &\geq \sum_k \|v_i^T(x(t)-p_j)\| - 2\kappa\sum_k \|v_i\|\|x(t)-p_j\|^{3/2} \\ &\geq C\|x(t)-p_j\|. \end{aligned}$$

and

$$\begin{aligned} \mathbb{E}[\|x(t+1)-p_j\|^2|x(t)] &\leq \|x(t)-p_j\|^2 + 2\eta^2 C_1\|x(t)-p_j\|^2 + \eta^2\rho^2 C_1 + \eta\rho^2 C_1\|x(t)-p_j\| \\ &\quad - \eta C\|x(t)-p_j\|^2 - 3\eta\rho C\|x(t)-p_j\| \\ &\leq \|x(t)-p_j\|^2 - 2\eta\rho C\|x(t)-p_j\| + \eta^2\rho^2 C_1 \end{aligned}$$

Hence we have if $\|x(t)-p_j\| \geq O(\eta\rho)$

$$\mathbb{E}[\|x(t+1)-p_j\||x(t)] \leq \|x(t)-p_j\| - \alpha\eta\rho.$$

which implies,

$$\mathbb{E}[\|x(t+1)-p_j\|\mathbf{1}A_j(t+1)] \leq \mathbb{E}[\|x(t+1)-p_j\|\mathbf{1}A_j(t)] \leq \mathbb{E}[\|x(t)-p_j\|\mathbf{1}A_j(t)] - \alpha\eta\rho P(A_j(t))$$

Hence

$$\alpha\rho^{j/2}P(A_j(t_{2,j}+\frac{\rho^{(j-2)/2}}{\eta}) \leq \alpha\eta\rho\sum_{t=t_{2,j}}^{t=t_{2,j}+\frac{\rho^{(j-2)/2}}{\eta}} P(A_j(t)) \leq \|x(t_{2,j})-\Phi(x(t_{2,j}))\| = O(\rho^{(j+1)/2})$$

Hence with probability $O(\sqrt{\rho})$, there exists $t_{2,j+1}$, such that $\|x(t_{2,j+1})-p_j\| \leq O(\rho^{(j+2)/2})$, which further implies $\|x(t_{2,j+1})-\Phi(x(t_{2,j+1}))\| \leq O(\rho^{(j+2)/2})$ using Lemma C.7.

Define $t_3 = t_{2,3}$

C.6.2 Phase II: Proof of Theorem C.28

We will inductively prove the following claim holds with probability $1-O(\eta\rho)$,

$$\begin{aligned} \|\Phi(x(t)) - X(\eta\rho^2 t)\| &\leq O((\eta+\rho)\log(1/\rho)) \\ \|x(t)-\Phi(x(t))\| &= O(\rho(\eta+\rho)\log(1/\rho)) \end{aligned}$$

To be more precise, the induction mainly consists of two parts. The first part shows that $x(t)$ will stay close to the manifold with large probability and the second part shows the direction $\Phi(x(t))$ moves.

To be more succinct with previous section, we abuse notation and suppose the iteration starts at t_3.

Part I: Convergence Near Manifold We have $\|x(t_3) - \Phi(x(t_3))\| = O(\eta\rho + \rho^2)$. By induction hypothesis, we have $x(t) \in K^h$.

According to Lemma C.10

$$\|\Phi(x(t+1)) - \Phi(x(t))\| = O(\eta\rho^2)$$

Using the same argument in previous section, we have for sufficienly large constant A, if $A(\eta\rho + \rho^2)\log(1/\eta\rho) \geq \|x(t) - \Phi(x(t))\| \geq A(\eta\rho + \rho^2)$, then there exists constant α, B independent of A,

$$\mathbb{E}[\|x(t+1) - \Phi(x(t+1))\| | x(t)] \leq \|x(t) - \Phi(x(t))\| - \alpha\eta\rho$$
$$\|(x(t+1) - \Phi(x(t+1))) - (x(t) - \Phi(x(t)))\| \leq B\eta\rho$$

.

We then have

$$Pr(y(t+1) \geq A(\eta\rho + \rho^2)\log(1/\eta\rho)) = \sum_{\tau=t_3}^{t} Pr(y(t+1) \geq A(\eta\rho + \rho^2)\log(1/\eta\rho) \text{ and } y(\tau) < A(\eta\rho + \rho^2) \text{ and } \forall t+1 \geq \tau' \geq \tau+1, y(\tau') > A(\eta\rho + \rho^2)$$

We then consider each term,

$$\begin{aligned}
&Pr(y(t+1) \geq A(\eta\rho + \rho^2)\log(1/\eta\rho) \text{ and } y(\tau) < A(\eta\rho + \rho^2) \text{ and } \forall t+1 \geq \tau' \geq \tau+1, y(\tau') > A(\eta\rho + \rho^2)) \\
\leq & Pr(y(t+1) \geq A(\eta\rho + \rho^2)\log(1/\eta\rho) \text{ and } \forall t+1 \geq \tau' \geq \tau+1, y(\tau') > A(\eta\rho + \rho^2) \\
&|A(\eta\rho + \rho^2) < y(\tau+1) < (A+B)(\eta\rho + \rho^2))
\end{aligned}$$

Define a coupled process $\tilde{y}(\tau+1) = y(\tau+1)$ and

$$\tilde{y}(\tau') = \begin{cases} \|x(\tau') - \Phi(x(\tau'))\|, & \text{if } \tilde{y}(\tau'-1) = \|x(\tau'-1) - \Phi(x(\tau'-1))\| > A(\eta\rho + \rho^2) \\ \tilde{y}(\tau'-1) - \alpha\eta\rho, & \text{if otherwise} \end{cases}$$

Then clearly

$$\begin{aligned}
&Pr(y(t+1) \geq A(\eta\rho + \rho^2)\log(1/\eta\rho) \text{ and } \forall t+1 \geq \tau' \geq \tau+1, y(\tau') > A(\eta\rho + \rho^2) \\
&|A(\eta\rho + \rho^2) < y(\tau+1) < (A+B)(\eta\rho + \rho^2)) \leq Pr(\tilde{y}(t+1) \geq A(\eta\rho + \rho^2)\log(1/\eta\rho))
\end{aligned}$$

We have

$$|\tilde{y}(t+1) - \tilde{y}(t)| \leq B\eta\rho$$
$$\mathbb{E}[\tilde{y}(t+1)] - \mathbb{E}[\tilde{y}(t)] \leq -\alpha\eta\rho$$

Now applying Azuma-Hoeffding bound(Lemma C.32), we have

$$\begin{aligned}
P(\tilde{y}(t+1) \geq \tilde{y}(\tau+1) - \alpha\eta\rho(t-\tau) + h) &\leq P(\tilde{y}(t+1) \geq \mathbb{E}[\tilde{y}(t+1)] + h) \\
&\leq exp(-\frac{2h^2}{(t-\tau)B^2\eta^2\rho^2})
\end{aligned}$$

Choosing $h = \alpha\eta\rho(t-\tau) - y(\tau+1) + A(\eta\rho + \rho^2)\log(1/\eta\rho)$

$$\begin{aligned}
P(\tilde{y}(t+1) \geq A(\eta\rho + \rho^2)\log(1/\eta\rho)) &\leq exp(-2\frac{(\alpha\eta\rho(t-\tau) - y(\tau+1) + A(\eta\rho + \rho^2)\log(1/\eta\rho))^2}{(t-\tau)B^2\eta^2\rho^2}) \\
&\leq exp(-2\frac{(\alpha\eta\rho(t-\tau) - A(\eta\rho + \rho^2) + A(\eta\rho + \rho^2)\log(1/\eta\rho))^2}{(t-\tau)B^2\eta^2\rho^2}) \\
&\leq exp(-2\frac{(\alpha\eta\rho(t-\tau) - A(\eta\rho + \rho^2)\log(\eta\rho)/2)^2}{(t-\tau)B^2\eta^2\rho^2}) \\
&= exp(-2\frac{(\alpha(t-\tau) - A\log(\eta\rho)/2)^2}{(t-\tau)B^2}) \\
&\leq exp(-2\frac{\sqrt{A\alpha}}{B^2}\log(\eta\rho)) = \eta^{10}\rho^{10}
\end{aligned}$$

We then have

$$Pr(y(t+1) \geq A(\eta\rho + \rho^2)\log(1/\eta\rho)) \leq \eta^{10}\rho^{10}(t - t_3) \leq \eta^8\rho^8$$

Part II: Direction of $\Phi(x(t+1)) - \Phi(x(t))$ We shall do a Taylor expansion and show that

$$\begin{aligned} x(t+1) &= x(t) - \eta\nabla L_k\left(x(t) + \rho\frac{\nabla L_k(x(t))}{\|\nabla L_k(x(t))\|}\right) \\ &= x(t) - \eta\nabla L_k(x(t)) - \eta\rho\nabla^2 L_k(x(t))\frac{\nabla L_k(x(t))}{\|\nabla L_k(x(t))\|} \\ &- \eta\rho^2\partial^2(\nabla L_k)[\frac{\nabla L_k(x(t))}{\|\nabla L_k(x(t))\|}, \frac{\nabla L_k(x(t))}{\|\nabla L_k(x(t))\|}]/2 + O(\eta\rho^3) \end{aligned}$$

Now by induction we have,

$$\|x(t) - \Phi(x(t))\| = \tilde{O}(\eta\rho + \rho^2)$$

, then by Lemma C.12, it implies

$$\|x(t+1) - x(t)\| = O(\eta\rho)$$

Then we have

$$\|\Phi(x(t+1)) - \Phi(x(t)) - \partial\Phi(x(t))(x(t+1) - x(t))\| \leq \xi\|x(t+1) - x(t)\|^2 = O(\eta^2\rho^2)$$

Using Lemma C.10, we have

$$\begin{aligned} \|\eta\partial\Phi(x(t))\nabla L_k(x(t))\| &= O(\eta\|x(t) - \Phi(x(t))\|^2) = O(\eta^3\rho^2 + \eta\rho^4) \\ \|\eta\rho\partial\Phi(x(t))\nabla^2 L_k(x(t))\frac{\nabla L_k(x(t))}{\|\nabla L_k(x(t))\|}\| &= O(\eta\rho\|x(t) - \Phi(x(t))\|) = \tilde{O}(\eta^2\rho^2 + \eta\rho^3) \end{aligned}$$

Hence

$$\|\Phi(x(t+1)) - \Phi(x(t)) + \eta\rho^2\partial\Phi(x(t))\partial^2(\nabla L_k)[\frac{\nabla L_k(x(t))}{\|\nabla L_k(x(t))\|}, \frac{\nabla L_k(x(t))}{\|\nabla L_k(x(t))\|}]/2\| = \tilde{O}(\eta^2\rho^2 + \eta\rho^3)$$

Notice finally that by Lemma C.11

$$\begin{aligned} \partial\Phi(x(t))\partial^2(\nabla L_k)[\frac{\nabla L_k(x(t))}{\|\nabla L_k(x(t))\|}, \frac{\nabla L_k(x(t))}{\|\nabla L_k(x(t))\|}] &= \partial\Phi(\Phi(x(t)))\partial^2(\nabla L_k)[w_k, w_k] + O(\|x(t) - \Phi(x(t))\|) \\ &= P_{x,\Gamma}^\top\Phi(x(t))\nabla(\lambda_1(\nabla^2 L_k(\Phi(x(t))))) + O(\|x(t) - \Phi(x(t))\|) \end{aligned}$$

Hence we have

$$\Phi(x(t+1)) - \Phi(x(t)) = -\eta\rho^2 P_{x,\Gamma}^\top\Phi(x(t))\nabla(\lambda_1(\nabla^2 L_k(\Phi(x(t)))))/2 + \tilde{O}(\eta^2\rho^2 + \eta\rho^3)$$

Notice finally,

$$\mathbb{E}_k[MP_{x,\Gamma}^\top\Phi(x(t))\nabla(\lambda_1(\nabla^2 L_k(\Phi(x(t)))))] = P_{x,\Gamma}^\top\Phi(x(t))\nabla(\mathrm{Tr}(\nabla^2 L(\Phi(x(t)))))$$

Together with standard concentration bound, we would have $x(t)$ follows the Riemannian gradient flow on Γ for loss

$$\mathbb{E}_i\lambda_1\left(\nabla^2 L_k(\Phi(x(t)))\right) = \mathbb{E}_i\mathrm{Tr}\left(\nabla^2 L_k(\Phi(x(t)))\right) = \mathrm{Tr}\nabla^2 L(\Phi(x(t))).$$

C.6.3 Proof of Corollaries

Proof of Corollary 5.5. We will do a Taylor expansion on $\mathbb{E}_k[L_{k,\rho}^{\max}](x)$. By Theorem C.27 and C.28, for $t > \eta\rho^2 T_3'$, we have $\|X(\eta\rho^2 t) - x(t)\| = \tilde{O}(\eta + \rho)$ and $\|x(t) - \Phi(x(t))\| = \tilde{O}(\eta\rho + \rho^2)$

$$\mathbb{E}_k[R_{k,\rho}^{\max}](x) = \max_v \mathbb{E}_k[\rho v^T\nabla L_k(x) + \rho^2 v^T\nabla^2 L_k(x)v/2] + O(\rho^3)$$

Then as $L_k(x) = \tilde{O}(\eta^2\rho^2 + \rho^4)$ and $\|v^T \nabla L_k(x)\| = \tilde{O}(\eta\rho + \rho^2)$, this implies

$$\begin{aligned}\mathbb{E}_k[R^{\max}_{k,\rho}](x) &= \rho^2 \mathbb{E}_k \max_v v^T \nabla^2 L(x) v/2 + \tilde{O}(\eta^2\rho^2 + \rho^3) \\ &= \rho^2 \mathbb{E}_k \max_v v^T \nabla^2 L(X(\eta\rho^2 t)) v/2 + \tilde{O}(\eta\rho^2 + \rho^3) \\ &= \rho^2 \mathrm{Tr}(X(\eta\rho^2 t))/2 + \tilde{O}(\eta\rho^2)\end{aligned}$$

□

Proof of Corollary 5.6. Choose T such that $X(T)$ is sufficiently close to $X(\infty)$, such that $\mathrm{Tr}(X(T)) \leq \mathrm{Tr}(X(\infty)) + 2\epsilon$

By corollary 5.5, we have $\|\mathbb{E}_k[R^{\max}_{k,\rho}](x(\lceil T/(\eta\rho^2)\rceil)) - \rho^2 \mathrm{Tr}(X(T))/2\| \leq \tilde{O}(\eta\rho^2)$. This further implies $\|\mathbb{E}_k[R^{\max}_{k,\rho}](x(\lceil T/(\eta\rho^2)\rceil)) - \rho^2 \mathrm{Tr}(X(\infty))/2\| \leq \epsilon\rho^2 + \tilde{O}(\eta\rho^2)$. We also have $\|L(x(\lceil T/(\eta\rho^2)\rceil))\| = O(\eta^2\rho^2)$. Then we can leverage Theorem 4.3 and Theorem 5.1 to get the desired bound. □

C.7 Technical Lemmas

Lemma C.29 (Cor. 4.3.15, Horn & Johnson (2012))**.** *Let $\Sigma, \hat{\Sigma} \in R^{D\times D}$ be symmetric and non-negative with eigenvalues $\lambda_1 \geq ... \geq \lambda_D$ and $\hat{\lambda}_1 \geq ... \geq \hat{\lambda}_D$, then for any i,*

$$|\hat{\lambda}_i - \lambda_i| \leq \|\Sigma - \hat{\Sigma}\|_2$$

Definition C.30 (Unitary invariant norms)**.** *A matrix norm $\|\cdot\|_*$ on the space of matrices in $\mathbb{R}^{p\times d}$ is unitary invariant if for any matrix $K \in \mathbb{R}^{p\times d}$, $\|UKW\|_* = \|K\|_*$ for any unitary matrices $U \in \mathbb{R}^{p\times p}, W \in \mathbb{R}^{d\times d}$.*

Theorem C.31. *[Davis-Kahan $\sin(\theta)$ theorem, Davis & Kahan (1970)] Let $\Sigma, \hat{\Sigma} \in \mathbb{R}^{p\times p}$ be symmetric, with eigenvalues $\lambda_1 \geq \ldots \geq \lambda_p$ and $\hat{\lambda}_1 \geq \ldots \geq \hat{\lambda}_p$ respectively. Fix $1 \leq r \leq s \leq p$, let $d := s - r + 1$ and let $V = (v_r, v_{r+1}, \ldots, v_s) \in \mathbb{R}^{p\times d}$ and $\hat{V} = (\hat{v}_r, \hat{v}_{r+1}, \ldots, \hat{v}_s) \in \mathbb{R}^{p\times d}$ have orthonormal columns satisfying $\Sigma v_j = \lambda_j v_j$ and $\hat{\Sigma}\hat{v}_j = \hat{\lambda}_j \hat{v}_j$ for $j = r, r+1, \ldots, s$. Define $\Delta := \min\left\{\max\{0, \lambda_s - \hat{\lambda}_{s+1}\}, \max\{0, \hat{\lambda}_{r-1} - \lambda_r\}\right\}$, where $\hat{\lambda}_0 := \infty$ and $\hat{\lambda}_{p+1} := -\infty$, we have for any unitary invariant norm $\|\cdot\|_*$,*

$$\Delta \cdot \|\sin\Theta(\hat{V}, V)\|_* \leq \|\hat{\Sigma} - \Sigma\|_*.$$

Here $\Theta(\hat{V}, V) \in \mathbb{R}^{d\times d}$, with $\Theta(\hat{V}, V)_{j,j} = \arccos\sigma_j$ for any $j \in [d]$ and $\Theta(\hat{V}, V)_{i,j} = 0$ for all $i \neq j \in [d]$. $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_d$ denotes the singular values of $\hat{V}^\top V$. $[\sin\Theta]_{ij}$ is defined as $\sin(\Theta_{ij})$.

Lemma C.32 (Azuma-Hoeffding Bound)**.** *Suppose Z_n is a super-martingale, suppose $-\alpha \leq Z_{i+1} - Z_i \leq \beta$, then for all $n > 0, a > 0$, we have*

$$P(|Z_n - Z_0| \geq a) \leq 2exp(-a^2/(2N(\alpha+\beta)^2))$$

Lemma C.33 (Magnus (1985))**.** *Let $A : \mathbb{R}^D \to \mathbb{R}^{D\times D}$ be any $\mathcal{C}^1$ symmetric matrix function and $x^* \in \mathbb{R}^D$ satisfying $\lambda_1(A(x^*)) > \lambda_2(A(x^*))$ and v_1 be the top eigenvector of $A(x^*)$. It holds that $\nabla\lambda_1(A(x))|_{x=x^*} = \nabla(v_1^\top A(x) v_1)|_{x=x^*}$.*

We then present some of the technical lemmas we required to prove Lemma C.20.

Lemma C.34. *If $0 < c < \frac{b-a}{b^2}, a\sqrt{\frac{a^2+2b^2}{2(1-cb)}} \geq \frac{a^2+b^2}{2-ca-cb}$, then $a > \frac{1}{2}b, cb \leq \frac{1}{2}$*

Proof. Notice that

$$ca\sqrt{\frac{a^2+b^2}{1-cb}} \geq ca\sqrt{\frac{a^2+2b^2}{2(1-cb)}} \geq \frac{cb^2+ca^2}{2-cb-ca} \geq \frac{cb^2+ca^2}{2-cb}$$

.

So

$$\sqrt{1-cb}+\frac{1}{\sqrt{1-cb}}\geq\sqrt{1+\frac{b^2}{a^2}}$$

As $c<\frac{b-a}{b^2}$, we have $1>1-cb>\frac{a}{b}$.

So

$$\sqrt{\frac{a}{b}}+\sqrt{\frac{b}{a}}\geq\sqrt{1+\frac{b^2}{a^2}}$$

The above inequality implies $a\geq\frac{1}{2}b$. As $c<\frac{b-a}{b^2}$,$cb\leq\frac{1}{2}$

□

Lemma C.35. *When* $0<a<b, 0<c<\frac{b-a}{b^2}$*, we have*

$$cb^2+ca^2(2-cb-\frac{2}{3}ca)-(1-cb)\frac{c(a^2+b^2)}{2-ca-cb}-ca^2(\frac{1}{2}a^2+b^2)\frac{2-ca-cb}{(a^2+b^2)}\leq\frac{cb^2}{2-cb}$$

Proof. Equivalently, we are going to prove

$$(1-cb)b^2\left(\frac{1}{2-ca-cb}-\frac{1}{2-cb}\right)+a^2\frac{1-cb}{2-ca-cb}+a^2(\frac{1}{2}a^2+b^2)\frac{2-ca-cb}{(a^2+b^2)}\geq a^2(2-cb-\frac{2}{3}ca)$$

Further simplifying, we only need to prove

$$\frac{(1-cb)cab^2}{(2-cb)(2-ca-cb)}+a^2\frac{1-cb}{2-ca-cb}\geq\frac{1}{3}ca^3+\frac{a^4}{2(a^2+b^2)}(2-ca-cb)$$

We have the following auxiliary inequalities,

$$(1-cb)b>a$$
$$\frac{1-cb}{2-ca-cb}=\frac{1}{\frac{a+b}{b}+\frac{b-a}{1-cb}}\geq\frac{1}{\frac{a+b}{b}+\frac{b^2-ab}{a}}=\frac{ab}{a^2+b^2}\geq\frac{a^2}{a^2+b^2}$$

Using the above anxiliary inequalities we have

$$\begin{aligned}
&\frac{(1-cb)cab^2}{(2-cb)(2-ca-cb)}+a^2\frac{1-cb}{2-ca-cb}\geq\frac{1}{3}ca^3+\frac{a^4}{2(a^2+b^2)}(2-ca-cb)\\
\Leftarrow&\frac{ca^2b}{(2-cb)(2-ca-cb)}+\left(1-\frac{1}{2}(2-ca-cb)\right)\frac{a^2(1-cb)}{2-ca-cb}\geq\frac{1}{3}ca^3\\
\Leftarrow&\frac{ca^2b}{(2-cb)(2-ca-cb)}+\frac{ca^2(a+b)(1-cb)}{2(2-ca-cb)}\geq\frac{1}{3}ca^3\\
\Leftarrow&\frac{ca^2b}{(2-cb)(2-ca-cb)}+\frac{ca^2b(1-cb)}{2(2-ca-cb)}\geq\frac{1}{3}ca^2b\\
\Leftarrow&\frac{1}{(2-cb)^2}+\frac{1-cb}{2(2-cb)}\geq\frac{1}{3}\\
\Leftarrow&3(1-cb)(2-cb)+6\geq2(2-cb)^2\\
\Leftarrow&(cb)^2-cb+4\geq0
\end{aligned}$$

□

Lemma C.36. *When* $0<a<b, 0<c<\frac{b-a}{b^2}, a\sqrt{\frac{a^2+2b^2}{2(1-cb)}}\geq\frac{a^2+b^2}{2-ca-cb}$*, we have*

$$cb^2+ca^2(2-cb-\frac{2}{3}ca)-(1-cb)cb^2-ca^2(\frac{1}{2}a^2+b^2)\frac{1}{b^2}\leq\frac{cb^2}{2-cb}$$

Proof. Equivalently, we are going to prove,

$$cb^3 + a^2(2 - cb - \frac{2}{3}ca) \leq \frac{b^2}{2-cb} + \frac{a^2(\frac{1}{2}a^2 + b^2)}{b^2}$$
$$\iff cb^3 + a^2(1 - cb - \frac{2}{3}ca) \leq \frac{b^2}{2-cb} + \frac{a^4}{2b^2}$$

We have the auxiliary inequality $\frac{1}{2-cb} > \frac{1}{2} + \frac{cb}{4}$.

Hence

$$cb^3 + a^2(1 - cb - \frac{2}{3}ca) \leq \frac{b^2}{2-cb} + \frac{a^4}{2b^2}$$
$$\Leftarrow cb^3 + a^2(1 - cb - \frac{2}{3}ca) \leq \frac{b^2}{2} + \frac{a^4}{2b^2} + \frac{cb^3}{4}$$
$$\Leftarrow c(\frac{3b^3}{4} - ba^2 - \frac{2}{3}a^3) \leq \frac{b^2}{2} + \frac{a^4}{2b^2} - a^2$$

Case 1 If $\frac{3b^3}{4} - ba^2 - \frac{2}{3}a^3 \leq 0$, then

$$c(\frac{3b^3}{4} - ba^2 - \frac{2}{3}a^3) \leq 0 \leq \frac{b^2}{2} + \frac{a^4}{2b^2} - a^2$$

Case 2 If $\frac{3b^3}{4} - ba^2 - \frac{2}{3}a^3 > 0$, then

$$c(\frac{3b^3}{4} - ba^2 - \frac{2}{3}a^3) \leq \frac{b^2}{2} + \frac{a^4}{2b^2} - a^2$$
$$\Leftarrow \frac{b-a}{b^2}(\frac{3b^3}{4} - ba^2 - \frac{2}{3}a^3) \leq \frac{(b^2-a^2)^2}{2b^2}$$
$$\Leftarrow 2(\frac{3b^3}{4} - ba^2 - \frac{2}{3}a^3) \leq (b-a)(b+a)^2$$
$$\Leftarrow 2(b^3 - ba^2) - (b-a)(b+a)^2 \leq \frac{b^3}{2} + \frac{4a^3}{3}$$
$$\Leftarrow (b-a)(2b(a+b) - (a+b)^2) \leq \frac{b^3}{2} + \frac{4a^3}{3}$$
$$\Leftarrow (b-a)^2(b+a) \leq \frac{b^3}{2} + \frac{4a^3}{3}$$

Using Lemma C.34,$a > \frac{b}{2}$,$(b-a)^2(b+a) = (b^2-a^2)(b-a) \leq b^2(b-a) \leq \frac{b^3}{2}$

□

Lemma C.37. *When* $0 \leq a \leq b, 0 \leq c \leq \frac{b-a}{b^2}, b^2 \geq a\sqrt{\frac{a^2+2b^2}{2(1-cb)}} \geq \frac{a^2+b^2}{2-ca-cb}$, *we have*

$$cb^2 + ca^2(2 - cb - \frac{2}{3}ca) - 2ca\sqrt{(b^2 + \frac{1}{2}a^2)(1-cb)} \leq \frac{cb^2}{2-cb}$$

Proof. Define

$$F(a) := a^2(2 - cb - \frac{2}{3}ca) - 2a\sqrt{(b^2 + \frac{1}{2}a^2)(1-cb)}$$
$$S_a(c,b) := \{a | 0 \leq a \leq b, 0 < c \leq \frac{b-a}{b^2}, b^2 \geq a\sqrt{\frac{a^2+2b^2}{2(1-cb)}} \geq \frac{a^2+b^2}{2-ca-cb}\}$$
$$a_{min}(c,b) := \inf S_a(c,b)$$
$$a_{max}(c,b) := \sup S_a(c,b) \leq b - cb^2$$

Here we suppose WLOG $S_a(c,b) \neq \phi$.

Consider

$$\frac{dF(a)}{da} = 2a(2 - cb - \frac{2}{3}ca) - \frac{2}{3}ca^2 - 2\sqrt{(b^2 + \frac{1}{2}a^2)(1 - cb)} - a^2\sqrt{\frac{1 - cb}{b^2 + \frac{1}{2}a^2}}$$

$$\frac{d^2F(a)}{da^2} = 2(2 - cb - \frac{2}{3}ca) - \frac{4}{3}ca - \frac{4}{3}ca - a\sqrt{\frac{1 - cb}{b^2 + \frac{1}{2}a^2}} - 2a\sqrt{\frac{1 - cb}{b^2 + \frac{1}{2}a^2}} + \frac{a^3}{2(b^2 + \frac{1}{2}a^2)^{\frac{3}{2}}}\sqrt{1 - cb}$$

$$\geq 4 - 2cb - 4ca - 3a\sqrt{\frac{1 - cb}{b^2 + \frac{1}{2}a^2}}$$

Define $u := cb, v := \frac{a}{b}$, then $u + v \leq 1$.

$$\begin{aligned}\frac{d^2F(a)}{da^2} &\geq 4 - 2u - 4uv - 3\sqrt{1 - u}\frac{1}{\sqrt{\frac{1}{2} + \frac{1}{v^2}}} \\ &\geq 4 - 2u - 4u(1 - u) - 3\sqrt{1 - u}\frac{1}{\sqrt{\frac{1}{2} + \frac{1}{(1-u)^2}}} \\ &\geq 4u^2 - 6u + 4 - 3\sqrt{1 - u}\frac{(1 - u)}{\sqrt{\frac{(1-u)^2}{2} + 1}}\end{aligned}$$

As $\sqrt{\frac{(1-u)^2}{2} + 1} \geq \sqrt{\frac{(1-u)^2+1}{2}} \geq (1 - u)$,we have

$$\frac{d^2F(a)}{da^2} \geq 4u^2 - 6u + 4 - 3(1 - u) = 4u^2 + 1 - 3u > 0$$

The above inequality shows that $F(a)$ is convex w.r.t to a for $a_{min}(c, b) \leq a \leq a_{max}(c, b)$.

Hence $F(a) \leq \max\left(F(a_{min}(c, b)), F(a_{max}(c, b))\right)$

Part 1 We abuse the notation and use a_{min} a shorthand for $a_{min}(c, b)$.

We have $a_{min}\sqrt{\frac{a_{min}^2+2b^2}{2(1-cb)}} = \frac{a_{min}^2+b^2}{2-ca_{min}-cb}$. This implies

$$2a_{min}\sqrt{(b^2 + \frac{1}{2}a_{min}^2)(1 - cb)} = (1 - cb)\frac{(a_{min}^2 + b^2)}{2 - ca_{min} - cb} + a_{min}^2(\frac{1}{2}a_{min}^2 + b^2)\frac{2 - ca_{min} - cb}{(a_{min}^2 + b^2)}$$

Hence using Lemma C.20,

$$\begin{aligned}F(a_{min}) &= a_{min}^2(2 - cb - \frac{2}{3}ca_{min}) - (1 - cb)\frac{c(a_{min}^2 + b^2)}{2 - ca_{min} - cb} - ca_{min}^2(\frac{1}{2}a_{min}^2 + b^2)\frac{2 - ca_{min} - cb}{(a_{min}^2 + b^2)} \\ &\leq \frac{1}{c}(\frac{cb^2}{2 - cb} - cb^2)\end{aligned}$$

Part 2 We abuse the notation and use a_{max} a shorthand for $a_{max}(c, b)$.

It's not easy to see which boundary condition a_{max} satisfy, hence we will discuss by cases.

Case 1 $a_{max}\sqrt{\frac{a_{max}^2+2b^2}{2(1-cb)}} = \frac{a_{max}^2+b^2}{2-ca_{max}-cb}$, in this case we simply redo the calculation in Part 1.

Case 2 $b^2 = a_{max}\sqrt{\frac{a_{max}^2+2b^2}{2(1-cb)}}$. This implies

$$2a_{max}\sqrt{(b^2 + \frac{1}{2}a_{max}^2)(1 - cb)} = (1 - cb)b^2 + a_{max}^2(\frac{1}{2}a_{max}^2 + b^2)\frac{1}{b^2}$$

Hence using Lemma C.36,

$$\begin{aligned}F(a_{max}) &= a_{max}^2(2 - cb - \frac{2}{3}ca_{max}) - (1 - cb)cb^2 - ca_{max}^2(\frac{1}{2}a_{max}^2 + b^2)\frac{1}{b^2} \\ &\leq \frac{1}{c}(\frac{cb^2}{2 - cb} - cb^2)\end{aligned}$$

Case 3 $cb^2 = b - a_{max}$ As $1 - cb = \frac{a_{max}}{b}$ and $b^2 \geq a_{max}\sqrt{\frac{b(a_{max}^2+2b^2)}{2a_{max}}}$.
This implies $a_{max}^3 + 2a_{max}b^2 - 2b^3 \leq 0 \Rightarrow a_{max} < \frac{9}{10}b$.
Define $v := \frac{a_{max}}{b}, cb = 1 - v$
Then by Lemma C.34, $\frac{1}{2} \leq v \leq \frac{9}{10}$

$$\begin{aligned} F(a_{max}) &= a_{max}^2(2 - cb - \frac{2}{3}ca_{max}) - 2a_{max}\sqrt{(b^2 + \frac{1}{2}a_{max}^2)(1 - cb)} \\ &= b^2\left(v^2(2 - (1 - v) - \frac{2}{3}(1 - v)v) - 2v\sqrt{(1 + \frac{v^2}{2})v}\right) \end{aligned}$$

We will prove the following inequality,

$$v^2(2 - (1 - v) - \frac{2}{3}(1 - v)v) - 2v\sqrt{(1 + \frac{v^2}{2})v} \leq \frac{1}{2 - cb} - 1 = \frac{-v}{1 + v}$$

In fact we can directly show

$$\begin{aligned} & v^2(1 + v) + \frac{v}{1 + v} \leq 2v\sqrt{(1 + \frac{v^2}{2})v} \\ \iff & v(1 + v) + \frac{1}{1 + v} \leq 2\sqrt{(1 + \frac{v^2}{2})v} \end{aligned}$$

for $v \in [0.5, 0.9]$.

Hence we have

$$\begin{aligned} F(a) &\leq \max\left(F(a_{min}(c, b)), F(a_{max}(c, b))\right) \\ &\leq \frac{1}{c}(\frac{cb^2}{2 - cb} - cb^2) \end{aligned}$$

□