Stability and Generalization for Markov Chain Stochastic Gradient Methods

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Abstract

Recently there is a large amount of work devoted to the study of Markov chain stochastic gradient methods (MC-SGMs) which mainly focus on their convergence analysis for solving minimization problems. In this paper, we provide a comprehensive generalization analysis of MC-SGMs for both minimization and minimax problems through the lens of algorithmic stability in the framework of statistical learning theory. For empirical risk minimization (ERM) problems, we establish the optimal excess population risk bounds for both smooth and non-smooth cases by introducing on-average argument stability. For minimax problems, we develop a quantitative connection between on-average argument stability and generalization error which extends the existing results for uniform stability [38]. We further develop the first nearly optimal convergence rates for convex-concave problems both in expectation and with high probability, which, combined with our stability results, show that the optimal generalization bounds can be attained for both smooth and non-smooth cases. To the best of our knowledge, this is the first generalization analysis of SGMs when the gradients are sampled from a Markov process.

1 Introduction

Stochastic gradient methods (SGMs) have been the workhorse behind the success of many machine learning (ML) algorithms due to their simplicity and high efficiency. As opposed to the deterministic (full) gradient methods, SGMs only require a small batch of random example(s) to update the model parameters at each iteration, making them amenable for solving large-scale problems.

There are mainly two notable types of SGMs which are inherent for different learning problems. In particular, stochastic gradient descent (SGD) is widely used for solving the empirical risk minimization (ERM) problem and the theoretical convergence has been extensively studied [e.g., 5, 17, 21, 37, 42, 43, 53, 57, 73, 80, 82, 86]. Concomitantly, the minimax problems instantiate many ML problems such as Generative Adversarial Networks (GANs) [2, 30], AUC maximization [29, 45, 81], and algorithmic fairness [16, 41, 52, 51]. Stochastic gradient descent ascent (SGDA) is an off-the-shelf algorithm for solving minimax problems. The convergence of SGDA and its variants is also widely studied in the literature [e.g., 44, 49, 54, 56].

On the other important front, the ultimate goal of learning is to achieve good generalization from the training data to the unknown test data. Along this line, generalization analysis of SGMs has attracted considerable attention using the algorithmic stability approach [11, 24]. In particular, stability and generalization of SGD have been studied using the uniform argument stability [6, 7, 13, 32, 36]

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and on-average stability [39, 40]. In [25, 38, 85], different stability and generalization measures are investigated for SGDA under both convex-concave and non-convex-non-concave settings. A critical assumption in most of the above studies about SGD and SGDA is the *i.i.d. sampling scheme* where the randomly sampled mini-batch or datum at each iteration is i.i.d. drawn from the given training data, guaranteeing that the stochastic gradient is an unbiased estimator of the true gradient.

Markov chain naturally appears in many important problems, such as decentralized consensus optimization, which finds applications in various areas including wireless sensor networks, smart grid implementations and distributed statistical learning [4, 14, 23, 48, 50, 58, 61, 63] as well as pairwise learning [78] which instantiates AUC maximization [1, 29, 46, 81, 87] and metric learning [35, 75, 76, 79]. A common example is a distributed system in which each node stores a subset of the whole data, and one aims to train a global model based on these data. We let a central node that stores all model parameters walk randomly over the system, in which case the samples are accessed according to a Markov chain. Several works studied this kind of model [33, 34, 48, 50, 58]. Markov chains also arise extensively in thermodynamics, statistical mechanics dynamic systems and so on [59, 67]. In addition, it was observed in [69, 78] that SGD with Markov chain sampling (MC-SGD) performs more efficiently than SGD with the common i.i.d. sampling scheme in various cases. Hence, studying the performance of MC-SGMs has certain theoretical and application values. The key difference from the i.i.d. sampling scheme is that the stochastic gradient at each iteration is sampled on the trajectory of a Markov chain, in which the stochastic gradient estimators are neither unbiased nor independent. Recent studies [4, 18, 22, 33, 34, 58, 68] overcame this technical hurdle and provided the convergence rates of MC-SGD. However, to the best of our knowledge, there is no work on the generalization performance of SGMs with Markov sampling.

Main contribution: In this paper, we provide a comprehensive study of the stability and generalization for both SGD and SGDA with Markov sampling in the framework of statistical learning theory [72, 10]. Our main contribution can be summarized as follows.

• We develop stability and generalization results of MC-SGD for solving ERM problems in both smooth and non-smooth cases. In particular, we show that MC-SGD can achieve competitive stability results as SGD with i.i.d. sampling scheme. By trading off the generalization and optimization errors appropriately, we establish the first-ever-known excess generalization bound $\mathcal{O}(1/\sqrt{n})$ for MC-SGD where n is the size of training data. The key idea for handling Markov sampling structure of MC-SGD is to use the concept of on-average argument stability.

• We first establish the connection between on-average argument stability and generalization for minimax optimization algorithms, which extends the existing work on uniform argument stability [38]. We further develop stability bounds of SGDA with Markov sampling (MC-SGDA) for both smooth and non-smooth cases and obtain the nearly optimal convergence rates $\tilde{\mathcal{O}}(1/\sqrt{T})$ for convex-concave problems in the form of both expectation and high probability, where T is the number of iterations, from which its optimal population risk bound is established. Specifically, we consider several measures of generalization performance and show that the optimal population risk bounds $\mathcal{O}(1/\sqrt{n})$ can be derived even in the non-smooth case.

• To the best of our knowledge, this is the first-ever-known work on stability and generalization of SGD and SGDA under the Markov chain setting. Our results show that, despite the stochastic gradient estimator is biased and dependent across iterations due to the Markov sampling scheme, the generalization performance of MC-SGD and MC-SGDA enjoys the same optimal excess generalization rates as the i.i.d. sampling setting.

Organization of the paper: We discuss the related work in Subsection 1.1 and formulate the problem in Section 2. Section 3 presents the stability and generalization results of MC-SGD for both smooth and non-smooth losses. Section 4 develops the first nearly optimal convergence rates for convex-concave problems of MC-SGDA, and show that the optimal risk bounds can be derived in both smooth and non-smooth cases. Section 5 concludes the paper.

1.1 Related Work

In this subsection, we review some further works which are closely related to our paper.

Algorithmic Stability. Algorithmic stability characterizes the sensitivity of a learning algorithm when the inputs to the algorithm are slightly perturbed. The framework of algorithmic stability was established in a seminal paper [11] for the exact minimizer of the ERM problem, where the uniform stability was established for strongly convex objective functions. Recent work [12, 27, 28]

derived sharper generalization bounds for uniformly stable algorithms with high probability. Several other stability measures were later developed for studying the generalization of different learning algorithms including the hypothesis stability [11], on-average stability [64], argument stability [47] and total variation stability [8, 71].

Stability and Generalization Analysis of SGMs. [32] established generalization error bounds of order $\mathcal{O}(1/\sqrt{n})$ in expectation for SGD for convex and smooth problems using uniform stability. The on-average variance of stochastic gradients was used to refine the generalization analysis of SGD for non-convex problems [88]. The results were improved and refined by [36] using a data-dependent notion of algorithmic stability for SGD. [39] introduced on-average argument stability and studied the stability and generalization of SGD for a general class of non-smooth convex losses, i.e., the gradient of the loss function is α-Hölder continuous. They also established fast generalization bounds $\mathcal{O}(1/n)$ for smooth convex losses in a low-noise setting. The same authors also extended the analysis to the non-convex loss functions in [40]. Meanwhile, [6] addressed uniform argument stability of SGD with Lipschitz-continuous convex losses. Optimal generalization bounds were also developed for SGD in different settings [6, 7, 26, 74, 77]. Stability and generalization for SGMs have been studied for pairwise learning [65, 78] where the loss involves a pair of examples. In particular, [78] introduced a simple MC-SGD algorithm for pairwise learning where pairs of examples form a special Markov chain $\{\xi_t = (z_{i_t}, z_{i_{t-1}}) : t \in \mathbb{N}\}$. Here, z_{i_t} and $z_{i_{t-1}}$ are i.i.d. sampled from the training data of size n at time t and $t-1$, respectively. The uniform argument stability and generalization have been established (see more discussion on the difference between our work and [78] in Remark 8 below).

For minimax problems, [85] studied the weak generalization and strong generalization bounds in the strongly-convex-concave setting. [25] established the optimal generalization bounds for proximal point method, while gradient descent ascent (GDA) is not guaranteed to have a vanishing excess risk in convex-concave case. [38] proved that SGDA can achieve the optimal excess risk bounds of order $\mathcal{O}(1/\sqrt{n})$ for both smooth and non-smooth problems in the convex-concave setting. They also extended their work to the nonconvex-nonconcave problems. However, all the above studies the stability and generalization of SGD and SGDA under the assumption of the i.i.d. sampling scheme.

Convergence Analysis of MC-SGMs. The convergence analysis of SGD and its variants when the gradients are sampled from a Markov chain have been studied in different settings [3, 18, 19, 22, 34, 58, 66, 69, 70]. Specifically, [34, 58] studied the Markov subgradient incremental methods in a distributed system under time homogeneous and time non-homogeneous settings, respectively. [22] studied the convergence of stochastic mirror descent under the ergodic assumption. [69] established the convergence rate $\mathcal{O}(1/T^{1-q})$ with some $q \in (1/2, 1)$ for convex problems. They also developed the convergence result for non-convex problems. In addition, decentralized SGD methods with the gradients sampled from a non-reversible Markov chain have been studied in [68]. [18] considered an accelerated ergodic Markov chain SGD for both convex and non-convex problems. [19] further studied the convergence rates without the bounded gradient assumption. All these studies focused on the convergence analysis of MC-SGD for solving the ERM problems.

2 Problem Setting and Target of Analysis

In this section, we introduce the SGD for ERM and SGDA for solving minimax problems with Markov Chain, and describe the target of generalization analysis for both optimization algorithms.

Target of Generalization Analysis. Let $\mathcal{W}$ be a parameter space in $\mathbb{R}^d$ and $\mathcal{D}$ be a population distribution defined on a sample space $\mathcal{Z}$. Let $f : \mathcal{W} \times \mathcal{Z} \to [0, \infty)$ be a loss function. In the standard framework of Statistical Learning Theory (SLT) [10, 72], one aims to minimize the expected population risk, i.e., $F(\mathbf{w}) := \mathbb{E}_z[f(\mathbf{w}; z)]$, where the model parameter $\mathbf{w}$ belongs to $\mathcal{W}$, and the expectation is taken with respect to (w.r.t.) z according to $\mathcal{D}$. However, the population distribution is often unknown. Instead, we have access to a training dataset $S = \{z_i \in \mathcal{Z}\}_{i=1}^n$ with size n, where z_i is independently drawn from $\mathcal{D}$. Then consider the following ERM problem

$$\min_{\mathbf{w} \in \mathcal{W}} \big\{ F_S(\mathbf{w}) := \frac{1}{n} \sum_{i=1}^n f(\mathbf{w}; z_i) \big\}. \tag{1}$$

For a randomized algorithm $\mathcal{A}$ to solve the above problem, let $\mathcal{A}(S)$ be the output of algorithm $\mathcal{A}$ based on the dataset S. Then its statistical generalization performance (prediction ability) is measured by its *excess population risk* $F(\mathcal{A}(S)) - F(\mathbf{w}^*)$, i.e., the discrepancy between the expected risks of the model $\mathcal{A}(S)$ and the best model $\mathbf{w}^* \in \mathcal{W}$. We are interested in studying the excess population risk.

Let $\mathbb{E}_{S,\mathcal{A}}[\cdot]$ denote the expectation w.r.t. both the randomness of data S and the internal randomness of $\mathcal{A}$. To analyze the excess population error, we use the following error decomposition

$$\mathbb{E}_{S,\mathcal{A}}[F(\mathcal{A}(S))] - F(\mathbf{w}^*) = \mathbb{E}_{S,\mathcal{A}}[F(\mathcal{A}(S)) - F_S(\mathcal{A}(S))] + \mathbb{E}_{S,\mathcal{A}}[F_S(\mathcal{A}(S)) - F_S(\mathbf{w}^*)]. \quad (2)$$

The first term is called the generalization error of the algorithm $\mathcal{A}$ measuring the difference between the expected risk and empirical one, for which we will handle using stability analysis as shown soon. The second term is the optimization error, which is induced by running the randomized algorithm $\mathcal{A}$ to minimize the empirical objective. It can be estimated by tools from optimization theory.

As discussed in the introduction, many machine learning problems can be formulated as minimax problems including adversarial learning [30], reinforcement learning [15, 20] and AUC maximization [29, 46, 81, 87]. We are also interested in solving this type of problem. Let $\mathcal{W}$ and $\mathcal{V}$ be parameter spaces in $\mathbb{R}^d$. Let $\mathcal{D}$ be a population distribution defined on a sample space $\mathcal{Z}$, and $f : \mathcal{W} \times \mathcal{V} \times \mathcal{Z} \to [0, \infty)$. We consider the minimax optimization problems: $\min_{\mathbf{w}\in\mathcal{W}} \max_{\mathbf{v}\in\mathcal{V}} \{F(\mathbf{w}, \mathbf{v}) := \mathbb{E}_{\mathbf{z}\sim\mathcal{D}}[f(\mathbf{w}, \mathbf{v}; z)]\}$. In practice, we only have a training dataset $S = \{z_1, \ldots, z_n\}$ independently drawn from $\mathcal{D}$ and hence the minimax problem is reduced to the following empirical version:

$$\min_{\mathbf{w}\in\mathcal{W}} \max_{\mathbf{v}\in\mathcal{V}} \big\{F_S(\mathbf{w}, \mathbf{v}) := \frac{1}{n}\sum_{i=1}^{n} f(\mathbf{w}, \mathbf{v}; z_i)\big\}. \quad (3)$$

Since minimax problems involve the primal variable and dual variable, we have different measures of generalization [38, 85]. For a randomized algorithm $\mathcal{A}(S)$ solving the problem (3), we denote the output of $\mathcal{A}$ as $\mathcal{A}(S) = (\mathcal{A}_{\mathbf{w}}(S), \mathcal{A}_{\mathbf{v}}(S))$ for notation simplicity. Let $\mathbb{E}[\cdot]$ denote the expectation w.r.t. the randomness of both $\mathcal{A}$ and S. We are particularly interested in the following two metrics.

Definition 1 (Weak Primal-Dual (PD) Risk)**.** The weak Primal-Dual population risk of $\mathcal{A}(\mathcal{S})$, denoted by $\triangle^w(\mathcal{A}_{\mathbf{w}}, \mathcal{A}_{\mathbf{v}})$, is defined as $\max_{\mathbf{v}\in\mathcal{V}} \mathbb{E}\big[F(\mathcal{A}_{\mathbf{w}}(\mathcal{S}), \mathbf{v})\big] - \min_{\mathbf{w}\in\mathcal{W}} \mathbb{E}\big[F(\mathbf{w}, \mathcal{A}_{\mathbf{v}}(\mathcal{S}))\big]$. The corresponding (expected) weak PD empirical risk, denoted by $\triangle^w_{\text{emp}}(\mathcal{A}_{\mathbf{w}}, \mathcal{A}_{\mathbf{v}})$, is defined by $\max_{\mathbf{v}\in\mathcal{V}} \mathbb{E}\big[F_{\mathcal{S}}(\mathcal{A}_{\mathbf{w}}(\mathcal{S}), \mathbf{v})\big] - \min_{\mathbf{w}\in\mathcal{W}} \mathbb{E}\big[F_{\mathcal{S}}(\mathbf{w}, \mathcal{A}_{\mathbf{v}}(\mathcal{S}))\big]$. We refer to $\triangle^w(\mathcal{A}_{\mathbf{w}}, \mathcal{A}_{\mathbf{v}}) - \triangle^w_{\text{emp}}(\mathcal{A}_{\mathbf{w}}, \mathcal{A}_{\mathbf{v}})$ as the *weak PD generalization error* of the model $(\mathcal{A}_{\mathbf{w}}(\mathcal{S}), \mathcal{A}_{\mathbf{v}}(\mathcal{S}))$.

Definition 2 (Primal Risk)**.** The primal population and empirical risks of $\mathcal{A}(\mathcal{S})$ are respectively defined by $R(\mathcal{A}_{\mathbf{w}}(\mathcal{S})) = \max_{\mathbf{v}\in\mathcal{V}} F(\mathcal{A}_{\mathbf{w}}(\mathcal{S}), \mathbf{v})$, and $R_{\mathcal{S}}(\mathcal{A}_{\mathbf{w}}(\mathcal{S})) = \max_{\mathbf{v}\in\mathcal{V}} F_{\mathcal{S}}(\mathcal{A}_{\mathbf{w}}(\mathcal{S}), \mathbf{v})$. We refer to $R(\mathcal{A}_{\mathbf{w}}(\mathcal{S})) - R_S(\mathcal{A}_{\mathbf{w}}(\mathcal{S}))$ as the primal generalization error of the model $\mathcal{A}_{\mathbf{w}}(\mathcal{S})$, and $R(\mathcal{A}_{\mathbf{w}}(\mathcal{S})) - \min_{\mathbf{w}\in\mathcal{W}} R(\mathbf{w})$ as the *excess primal population risk*.

SGD and SGDA with Markov Sampling. One often considers SGD to solve the ERM problem (1). Specifically, let $\mathcal{W} \subseteq \mathbb{R}^d$ be convex, $\text{Proj}_{\mathcal{W}}(\cdot)$ denote the projection to $\mathcal{W}$, and $\partial f(\mathbf{w}; z)$ denote a subgradient of $f(\mathbf{w}; z)$ at $\mathbf{w}$. Let $\mathbf{w}_0 \in \mathcal{W}$ be an initial point, and $\{\eta_t\}$ is a stepsize sequence. For any $t \in \mathbb{N}$, the update rule of SGD is given by

$$\mathbf{w}_t = \text{Proj}_{\mathcal{W}}\big(\mathbf{w}_{t-1} - \eta_t \partial f(\mathbf{w}_{t-1}; z_{i_t})\big), \quad (4)$$

where $\{i_t\}$ is generated from $[n] = \{1, 2, \ldots, n\}$ with some sampling scheme. A typically sampling scheme is the uniform i.i.d. sampling, i.e., i_t is drawn randomly from $[n]$ according to a uniform distribution with/without replacement.

In this paper, we are particularly interested in the case when $i_t \in [n]$ is drawn from a *Markov Chain* which is widely used in practice [3, 4, 18, 22, 34, 66, 69, 70]. Let P be an $n \times n$-matrix with real-valued entries. We say a Markov chain $\{X_k\}$ with finite state $[n]$ and transition matrix P is time-homogeneous if, for $k \in \mathbb{N}$, $i, j \in [n]$, and $i_1, \ldots, i_{k-1} \in [n]$, there holds $\Pr(X_{k+1} = j | X_1 = i_1, \ldots, X_k = i) = \Pr(X_{k+1} = j | X_k = i) = [P]_{i,j}$. Likewise, the SGDA algorithm with Markov sampling scheme is defined as follows. Specifically, let $\partial_{\mathbf{w}} f$ and $\partial_{\mathbf{v}} f$ denote the subgradients of f w.r.t. the arguments $\mathbf{w}$ and $\mathbf{v}$, respectively. We initialize $(\mathbf{w}_0, \mathbf{v}_0) \in \mathcal{W} \times \mathcal{V}$, for any $t \in \mathbb{N}$, let $\{i_t\}$ is drawn from $[n]$ according to a Markov Chain. The update rule of SGDA is given by

$$\begin{cases} \mathbf{w}_t = \text{Proj}_{\mathcal{W}}\big(\mathbf{w}_{t-1} - \eta_t \partial_{\mathbf{w}} f(\mathbf{w}_{t-1}, \mathbf{v}_{t-1}; z_{i_t})\big) \\ \mathbf{v}_t = \text{Proj}_{\mathcal{V}}\big(\mathbf{v}_{t-1} + \eta_t \partial_{\mathbf{v}} f(\mathbf{w}_{t-1}, \mathbf{v}_{t-1}; z_{i_t})\big). \end{cases} \quad (5)$$

For brevity, we refer to the above algorithms as Markov chain-SGD (MC-SGD) and Markov chain-SGDA (SGDA), respectively. There are two types of randomness in MC-SGD/MC-SGDA. The first randomness is due to training dataset S which is i.i.d. from the population distribution $\mathcal{D}$. The other randomness arises from the internal randomness of the MC-SGD/MC-SGDA algorithm, i.e., the randomness of the indices $\{i_t\}$, which is a Markov chain.

Remark 1. Convergence analysis mainly considers the empirical optimization gap, i.e., the discrepancy between $F_S(\mathcal{A}(S))$ and $F_S(\mathbf{w}^*)$. Here, we are mainly interested in the generalization error which measures the prediction ability of the trained model on the test (future) data. *As such, the purpose of this paper is to provide a comprehensive generalization analysis of MC-SGD and MC-SGDA in the framework of statistical learning theory.* Specifically, given a finite training data S, let $\mathcal{A}(S)$ be the output of the MC-SGD for solving the ERM problem (1). Our target is to analyze the excess population risk $\mathbb{E}_{S,\mathcal{A}}[F(\mathcal{A}(S))] - F(\mathbf{w}^*)$. Let $\mathcal{A}(S) = (\mathcal{A}_{\mathbf{w}}(S), \mathcal{A}_{\mathbf{v}}(S))$ be the output of MC-SGDA for solving the empirical minimax problem (3), our aim is to analyze the *weak PD population risk* $\triangle^w(\mathcal{A}_{\mathbf{w}}, \mathcal{A}_{\mathbf{v}})$ and the *excess primal population risk* $R(\mathcal{A}_{\mathbf{w}}(\mathcal{S})) - \min_{\mathbf{w}\in\mathcal{W}} R(\mathbf{w})$. In both cases, the generalization analysis will be conducted using the algorithmic stability [11, 32]. As we show soon below, the final rates are obtained through trade-offing the optimization error (convergence rate) and the generalization error (stability results).

Properties of Markov Chain. Denote the probability distribution of X_k as the non-negative row vector $\pi^k = (\pi^k(1), \pi^k(2), \ldots, \pi^k(n))$, i.e., $\Pr(X_k = j) = \pi^k(j)$. Further, we have $\sum_{i=1}^n \pi^k(i) = 1$. For the time-homogeneous Markov chain, it holds $\pi^k = \pi^{k-1}P = \cdots = \pi^1 P^{k-1}$ for all $k \in \mathbb{N}$. Here, π^1 is an initial distribution and P^k denotes the k-th power of P. A Markov chain is irreducible if, for any $i, j \in [n]$, there exists k such that $[P^k]_{i,j} > 0$. That is, the Markov process can go from any state to any other state. State $i \in [n]$ is said to have a period τ if $[P^k]_{i,i} = 0$ whenever k is not a multiple of τ and τ is the greatest integer with this property. If $\tau = 1$ for every state $i \in [n]$, then we say the Markov chain is aperiodic. We say a Markov chain with stationary distribution Π^* is reversible if $\Pi^*(i)[P]_{i,j} = \Pi^*(j)[P]_{j,i}$ for all $i, j \in [n]$.

We need the following assumption for studying optimization error of MC-SGMs.

Assumption 1. Assume the Markov chain $\{i_t\}$ with finite state $[n]$ is time-homogeneous, irreducible and aperiodic. It starts from an initial distribution π^1, and has transition matrix P and stationary distribution Π^* with $\Pi^*(i) = \frac{1}{n}$ for any $i \in [n]$, i.e., $\lim_{k\to\infty} P^k = \frac{1}{n}\mathbf{1}_n\mathbf{1}_n^\top$, where $\mathbf{1}_n \in \mathbf{R}^n$ is the vector with each entry being 1 and $\mathbf{1}_n^\top$ denotes its transpose.

Remark 2. Our assumptions on Markov chains listed above are standard in the literature [18, 34, 50, 69, 68, 78]. For instance, Markov chain-type SGD was proposed for pairwise learning which can apply to various learning task such as AUC maximization and bipartite ranking [1, 83, 87, 29, 46] and metric learning [35, 75, 76, 79]. This pairwise learning algorithm forms pairs of examples following a special Markov chain $\{\xi_t = (z_{i_t}, z_{i_{t-1}}) : t \in \mathbb{N}\}$ where z_{i_t} and $z_{i_{t-1}}$ are i.i.d. sampled from the training data of size n at time t and $t-1$, respectively and, at time t, the model parameter is updated using gradient descent based on ξ_t. As mentioned in Remark 3 of [78], $\{\xi_t : t \in \mathbb{N}\}$ is a Markov Chain satisfying all of our assumptions. Another notable example is the decentralized consensus optimization in a multi-agent network, where the samples are accessed according to a Markov chain and the number of states of the Markov chain equals the number of nodes in the network, which is finite. One always considers the same transition matrix P for each node and assumes the Markov chain is irreducible and aperiodic [50, 84].

3 Results for Markov Chain SGD

In this section, we present the stability and generalization results of MC-SGD. Our analysis requires the following definition and assumptions. Let $G, L > 0$ and $\|\cdot\|_2$ denote the Euclidean norm.

Definition 3. We say f is convex w.r.t. the first argument if, for any $z \in \mathcal{Z}$ and $\mathbf{w}, \mathbf{w}' \in \mathcal{W}$, there holds $f(\mathbf{w}; z) \geq f(\mathbf{w}'; z) + \langle \partial f(\mathbf{w}'; z), \mathbf{w} - \mathbf{w}' \rangle$.

Assumption 2. Assume f is G-Lipschitz continuous, i.e., for any $z \in \mathcal{Z}$ and $\mathbf{w}, \mathbf{w}' \in \mathcal{W}$, there holds $|f(\mathbf{w}; z) - f(\mathbf{w}'; z)| \leq G\|\mathbf{w} - \mathbf{w}'\|_2$.

Assumption 3. Assume f is L-smooth, i.e., for any $z \in \mathcal{Z}$ and $\mathbf{w}, \mathbf{w}' \in \mathcal{W}$, there holds $f(\mathbf{w}; z) - f(\mathbf{w}'; z) \leq \langle \partial f(\mathbf{w}'; z), \mathbf{w} - \mathbf{w}' \rangle + \frac{L}{2}\|\mathbf{w} - \mathbf{w}'\|_2^2$.

3.1 Stability and Generalization of MC-SGD

Let $\mathbf{w}^* = \arg\min_{\mathbf{w}\in\mathcal{W}} F(\mathbf{w})$ be the best model in $\mathcal{W}$ and $\bar{\mathbf{w}}_T = \sum_{j=1}^T \eta_j \mathbf{w}_j / \sum_{j=1}^T \eta_j$ be the output of MC-SGD with T iterations. We will use algorithmic stability to study the generalization errors, which measures the sensitivity of the output model of an algorithm. Below we give the definition of on-average argument stability [39].

Definition 4. (On-average argument stability) Let $S = \{z_1, \ldots, z_n\}$ and $\widetilde{S} = \{\tilde{z}_1, \ldots, \tilde{z}_n\}$ be drawn independently from $\mathcal{D}$. For any $i \in [n]$, define $S^{(i)} = \{z_1, \ldots, z_{i-1}, \tilde{z}_i, z_{i+1}, \ldots, z_n\}$ as the set formed from S by replacing the i-th element with $\tilde{z}_i$. We say a randomized algorithm $\mathcal{A}$ is on-average ϵ-argument-stable if $\mathbb{E}_{S,\widetilde{S},\mathcal{A}}\big[\frac{1}{n}\sum_{i=1}^n \|\mathcal{A}(S) - \mathcal{A}(S^{(i)})\|_2\big] \leq \epsilon$.

To obtain on-average argument stability bounds of MC-SGD, our idea is to first write the stability as a deterministic function according to whether the different data point is selected, and then take the expectation w.r.t. the randomness of the algorithm. The detailed proofs are given in Appendix B.1.

Theorem 1 (Stability bounds)**.** *Suppose f is convex and Assumption 2 holds. Let $\mathcal{W} = \mathbb{R}^d$ and let $\mathcal{A}$ be MC-SGD with T iterations.*

(a) (Smooth case) Suppose Assumption 3 holds and $\eta_j \leq 2/L$. Then $\mathcal{A}$ is on-average ϵ-argument-stable with $\epsilon \leq \frac{2G}{n}\sum_{j=1}^T \eta_j$.

(b) (Non-smooth case) $\mathcal{A}$ is on-average ϵ-argument-stable with $\epsilon \leq 2G\sqrt{\sum_{j=1}^T \eta_j^2} + \frac{4G}{n}\sum_{j=1}^T \eta_j$.

Remark 3. Without any assumption on Markov chain, Theorem 1 shows that argument stability bounds of MC-SGD are in the order of $\mathcal{O}(T\eta/n)$ and $\mathcal{O}(\sqrt{T}\eta + T\eta/n)$ with a constant stepsize η for smooth and non-smooth losses, respectively. Both of them match the corresponding bounds for SGD with i.i.d. sampling [6, 32, 39, 74], which imply that stability of MC-SGD is at least not worse than that of the i.i.d. sampling case. The technical novelty here is to observe that, in the sense of on-average argument stability, we can use the calculation of $\mathbb{E}_{\mathcal{A}}[\sum_{i=1}^n \mathbb{I}_{[i_t=i]}]$ to replace that of $\mathbb{E}_{\mathcal{A}}[\mathbb{I}_{[i_t=i]}]$, where $\mathbb{I}_{[\cdot]}$ is the indicator function. This key step avoids the complicated calculations about $\mathbb{E}_{\mathcal{A}}[\mathbb{I}_{[i_t=i]}]$. Taking the uniform stability as example, we need to consider neighboring datasets differing by the i-th data, and can get $\mathbb{E}_{\mathcal{A}}[\|\mathbf{w}_t - \mathbf{w}_t'\|_2] = \mathcal{O}(\eta\sum_{j=1}^t \mathbb{E}_{\mathcal{A}}[\mathbb{I}_{i_j=i}]) = \mathcal{O}(\eta\sum_{j=1}^t\sum_{k=1}^n [P^{j-1}]_{k,i}\pi^1(k))$, which depends on the transition matrix P and is not easy to control. In contrast, with the on-average stability we get stability bounds depending on $\sum_{i=1}^n \mathbb{I}_{[i_t=i]}$, which is always 1, i.e., the on-average stability allows us to ignore the effect of sampling process.

The following theorem presents generalization bounds for MC-SGD in both smooth and non-smooth cases, which directly follows from Lemma A.4 and Theorem 1.

Theorem 2 (Generalization error bounds)**.** *Suppose f is convex and Assumption 2 holds. Let $\mathcal{W} = \mathbb{R}^d$ and let $\mathcal{A}$ be MC-SGD with T iterations.*

(a) (Smooth case) Suppose Assumption 3 holds and let $\eta_j \equiv \eta \leq 2/L$. Then there holds $\mathbb{E}_{S,\mathcal{A}}[F(\bar{\mathbf{w}}_T) - F_S(\bar{\mathbf{w}}_T)] \leq \frac{2G^2T\eta}{n}$.

(b) (Non-smooth case) If $\eta_j \equiv \eta$, then there holds $\mathbb{E}_{S,\mathcal{A}}[F(\bar{\mathbf{w}}_T) - F_S(\bar{\mathbf{w}}_T)] = \mathcal{O}\big(\sqrt{T}\eta + \frac{T\eta}{n}\big)$.

3.2 Excess Population Risk of MC-SGD

In this subsection, we present excess population risk bounds for MC-SGD in both smooth and non-smooth cases. The proofs are given in Appendix B.3. We use the notation $B \asymp \tilde{B}$ if there exist universal constants $c_1, c_2 > 0$ such that $c_1\tilde{B} \leq B \leq c_2\tilde{B}$. Let $\lambda_i(P)$ be the i-th largest eigenvalue of the transition matrix P and $\lambda(P) = (\max\{|\lambda_2(P)|, |\lambda_n(P)|\} + 1)/2 \in [1/2, 1)$. Let K_P be the mixing time and C_P be a constant depending on P and its Jordan canonical form (detailed expressions are given in Lemma A.1). We assume $\sup_{z\in\mathcal{Z}} f(0; z)$ and $\|\mathbf{w}^*\|_2$ are bounded.

Assumption 4. Assume the Markov chain $\{i_t\}$ is reversible with $P = P^\top$.

Theorem 3 (Excess population risk for smooth losses)**.** *Suppose f is convex and Assumptions 1, 2, 3 and 4 hold. Let $\mathcal{W} \in \mathbb{R}^d$. Let $\mathcal{A}$ be MC-SGD with T iterations, and $\{\mathbf{w}_j\}_{j=1}^T$ be produced by $\mathcal{A}$ with $\mathbf{w}_0 = 0$ and $\eta_j \equiv \eta \leq 2/L$. If we select $T \asymp n$ and $\eta = (T\log(T))^{-1/2}$, then $\mathbb{E}_{S,\mathcal{A}}[F(\bar{\mathbf{w}}_T)] - F(\mathbf{w}^*) = \mathcal{O}\big(\sqrt{\log(n)}/(\sqrt{n}\log(1/\lambda(P)))\big)$.*

Remark 4. A term $K_P/\big(M_0 n^{\frac{3}{4}}\log^{\frac{1}{4}}(n)\big)$ with $M_0 = \min\{\sqrt{n\log(n)}C_P n\lambda(P)^{K_P}, 1\}$ appears in the excess risk bound of MC-SGD (see the proof of Theorem 3), which will be worse than $\sqrt{\log(n)}/\sqrt{n}$ when K_P is large. Note Lemma A.1 implies that this term will disappear if P is symmetric. Hence, we introduce Assumption 4 to get the nearly optimal rate.

Theorem 4 (Excess population risk for non-smooth losses)**.** *Suppose f is convex and Assumptions 1, 2, 4 hold. Let $\mathcal{W} \in \mathbb{R}^d$. Let $\mathcal{A}$ be MC-SGD with T iterations, and $\{\mathbf{w}_j\}_{j=1}^T$ be produced by $\mathcal{A}$ with $\eta_j \equiv \eta$. If we select $T \asymp n^2$ and $\eta = T^{-3/4}$, then $\mathbb{E}_{S,\mathcal{A}}[F(\bar{\mathbf{w}}_T)] - F(\mathbf{w}^*) = \mathcal{O}\big(1/\big(\sqrt{n}\log(1/\lambda(P))\big)\big)$.*

Remark 5. To estimate the excess population risk, we need the convergence rates of MC-SGD which can be found in Appendix B.2. [69] established a convergence rate of $\mathcal{O}(1/T^{1-q})$ with some $q \in (1/2, 1)$ under the bounded parameter domain assumption. We remove this assumption by showing $\|\mathbf{w}_t\|_2^2 = \mathcal{O}(\sum_{k=1}^T \eta_k)$ and obtain the nearly optimal convergence rate $\tilde{\mathcal{O}}(1/\sqrt{T})$ with a careful choice of $\eta = 1/\sqrt{T\log(T)}$. To understand the variation of the algorithm, we present a confidence-based bound for optimization error, which matches the bound in expectation up to a constant factor. We also provide the convergence analysis for non-convex problems in Appendix B.2.

Remark 6. Theorems 3 and 4 show, after carefully selecting the iteration number T and stepsize η, that the excess population risk rate $\mathcal{O}(1/\sqrt{n})$ is achieved in both smooth and non-smooth cases. Note [6, 32, 39] show that the excess population risk rate $\mathcal{O}(1/\sqrt{n})$ is optimal for the i.i.d. sampling case. Therefore, our results for MC-SGD are also optimal since the i.i.d. sampling is a special case of Markov sampling. Our results imply that despite the gradients are biased and dependent across iterations in Markov sampling, the generalization performance of SGD is competitive with the i.i.d. sampling case. Theorems 3 and 4 also show the impact of the smoothness in achieving the optimal rate. The rate for the non-smooth case in Theorem 4 looks slightly better than the smooth case (Theorem 3) with a logarithmic term. However, the optimal rate can be achieved with a linear gradient complexity (i.e., the total number of computing the gradient) for smooth losses, while Theorem 4 implies that gradient complexity $\mathcal{O}(n^2)$ is required for non-smooth losses.

Remark 7. According to Theorems 3 and 4, we can further observe how the transition matrix P affects the excess population risks. Indeed, the excess population risk rates are monotonically increasing w.r.t $\lambda(P)$. Particularly, the closer $\lambda(P)$ is to $1/2$, the better the rate is. Let us consider two extreme examples. Suppose the Markov chain starts from the uniform distribution and has transition matrix $P = \frac{1}{n}\mathbf{1}_n\mathbf{1}_n^T$. MC-SGD degenerates to SGD with i.i.d. sampling in this case. The excess population risk rate $\mathcal{O}(1/\sqrt{n})$ is obtained from Theorem 4 with $\lambda(P) = 1/2$. For a Markov chain moving on a circle (i.e., if the chain is currently at state i, then it goes to states $i+1$, i and $i-1$ with equal probability), we can verify that $\lambda(P) = \mathcal{O}(1 - 1/n^2)$, which implies a bad rate in this case.

Remark 8. [78] proposed a simple MC-SGD algorithm for pairwise learning associated with a pairwise loss $f(\mathbf{w}, z, z')$. Specifically, at iteration t, the algorithm update the model parameter as follows: $\mathbf{w}_t = \mathbf{w}_{t-1} - \eta_t \nabla_{\mathbf{w}} f(\mathbf{w}_{t-1}, z_{i_t}, z_{i_{t-1}})$ where z_{i_t} and $z_{i_{t-1}}$ are i.i.d. sampled from the training data of size n at time t and $t-1$, respectively. In Remark 3 of [78], it was shown that $\{\xi_t = (i_t, i_{t-1}) \in [n] \times [n]\}$ does form a time-homogeneous, irreducible and aperiodic Markov chain. There are two key differences between our work and [78]. Firstly, the work [78] used uniform stability directly due to $\mathbb{E}_{\mathcal{A}}[\mathbb{I}_{i_t=i}] = 1/n$, while this term is not easy to control in our general setting (see Remark 3 for details). To overcome this hurdle, we resort to the on-average stability and show that MC-SGD achieves the optimal excess risk rate. Secondly, the proofs there critically rely on the fact $f(\mathbf{w}_{t-1}; \mathbf{z}_{i_t}, \mathbf{z}_{i_{t-1}}) = f(\mathbf{w}_{t-2}; \mathbf{z}_{i_t}, \mathbf{z}_{i_{t-1}}) + \mathcal{O}(\eta_{t-1})$ and the independence of $\mathbf{w}_{t-2}$ w.r.t. i_t and i_{t-1}. However, these specially tailored techniques for pairwise learning do not apply to the general Markov setting as we considered here.

4 Results for Markov Chain SGDA

In this section, we study the generalization analysis of MC-SGDA for minimax optimization problems. Let $(\bar{\mathbf{w}}_T, \bar{\mathbf{v}}_T)$ be the output of MC-SGDA with T iterations, where

$$\bar{\mathbf{w}}_T = \sum_{j=1}^T \eta_j \mathbf{w}_j \Big/ \sum_{j=1}^T \eta_j \text{ and } \bar{\mathbf{v}}_T = \sum_{j=1}^T \eta_j \mathbf{v}_j \Big/ \sum_{j=1}^T \eta_j. \tag{6}$$

We first introduce some necessary definitions and assumptions.

Definition 5. Let $\rho \geq 0$ and $g : \mathcal{W} \times \mathcal{V} \mapsto \mathbb{R}$. We say g is ρ-strongly-convex-strongly-concave (ρ-SC-SC) if, for any $\mathbf{v} \in \mathcal{V}$, the function $\mathbf{w} \mapsto g(\mathbf{w}, \mathbf{v})$ is ρ-strongly-convex and, for any $\mathbf{w} \in \mathcal{W}$, the function $\mathbf{v} \mapsto g(\mathbf{w}, \mathbf{v})$ is ρ-strongly-concave. We say g is convex-concave if g is 0-SC-SC.

The following two assumptions are standard [25, 85]. Assumption 5 amounts to saying f is Lipschitz continuous w.r.t. both $\mathbf{w}$ and $\mathbf{v}$, while Assumption 6 considers smoothness conditions.

Assumption 5. Assume for all $\mathbf{w} \in \mathcal{W}, \mathbf{v} \in \mathcal{V}$ and $z \in \mathcal{Z}$, $\left\|\partial_{\mathbf{w}} f(\mathbf{w}, \mathbf{v}; z)\right\|_2 \leq G$ and $\left\|\partial_{\mathbf{v}} f(\mathbf{w}, \mathbf{v}; z)\right\|_2 \leq G$.

Assumption 6. For any z, assume the function $(\mathbf{w}, \mathbf{v}) \mapsto f(\mathbf{w}, \mathbf{v}; z)$ is L-smooth, i.e., the following inequality holds for all $\mathbf{w} \in \mathcal{W}, \mathbf{v} \in \mathcal{V}$ and $z \in \mathcal{Z}$

$$\left\|\begin{pmatrix} \partial_{\mathbf{w}} f(\mathbf{w}, \mathbf{v}; z) - \partial_{\mathbf{w}} f(\mathbf{w}', \mathbf{v}'; z) \\ \partial_{\mathbf{v}} f(\mathbf{w}, \mathbf{v}; z) - \partial_{\mathbf{v}} f(\mathbf{w}', \mathbf{v}'; z) \end{pmatrix}\right\|_2 \leq L \left\|\begin{pmatrix} \mathbf{w} - \mathbf{w}' \\ \mathbf{v} - \mathbf{v}' \end{pmatrix}\right\|_2 .$$

4.1 Stability and Generalization Measures

We use algorithmic stability to study the generalization of minimax learners. To this end, we first introduce the stability for minimax optimization problems.

Definition 6 (Argument stability for minimax problems)**.** Let $S, \widetilde{S}$ and $S^{(i)}$ be defined as Definition 4. Let $\mathcal{A}$ be a randomized algorithm and $\epsilon > 0$. We say $\mathcal{A}$ is on-average ϵ-argument-stable for minimax problems if $\frac{1}{n}\sum_{i=1}^{n} \mathbb{E}\big[\|\mathcal{A}_{\mathbf{w}}(S^{(i)}) - \mathcal{A}_{\mathbf{w}}(S)\|_2 + \|\mathcal{A}_{\mathbf{v}}(S^{(i)}) - \mathcal{A}_{\mathbf{v}}(S)\|_2\big] \leq \epsilon$.

The following theorem establishes a connection between stability and generalization. Part (a) shows that on-average argument stability implies generalization measured by the weak PD risk, while Part (b) shows that on-average argument stability guarantees a strong notion of generalization in terms of the primal risk under a strong concavity assumption. Theorem 5 will be proved in Appendix C.1.

Theorem 5 (Generalization via argument stability)**.** *Let $\mathcal{A}$ be a randomized algorithm and $\epsilon > 0$.*

(a) If $\mathcal{A}$ is on-average ϵ-argument-stable and Assumption 5 holds, then there holds $\triangle^{w}(\mathcal{A}_{\mathbf{w}}, \mathcal{A}_{\mathbf{v}}) - \triangle^{w}_{emp}(\mathcal{A}_{\mathbf{w}}, \mathcal{A}_{\mathbf{v}}) \leq G\epsilon$.

(b) If $\mathcal{A}$ is on-average ϵ-argument-stable, the function $\mathbf{v} \mapsto F(\mathbf{w}, \mathbf{v})$ is ρ-strongly-concave and Assumptions 5, 6 hold, then we have $\mathbb{E}_{S,\mathcal{A}}\big[R(\mathcal{A}_{\mathbf{w}}(S)) - R_S(\mathcal{A}_{\mathbf{w}}(S))\big] \leq \big(1 + L/\rho\big)G\epsilon$.

In the following theorem we develop stability bounds for MC-SGDA applied to convex-concave problems. The proof is given in Section C.1 of the Appendix.

Theorem 6 (Stability bounds)**.** *Assume for all z, the function $(\mathbf{w}, \mathbf{v}) \mapsto f(\mathbf{w}, \mathbf{v}; z)$ is convex-concave. Let $\mathcal{W} = \mathbb{R}^d$ and Assumption 5 hold, and let $\mathcal{A}$ be MC-SGDA with T iterations.*

(a) (Smooth case) If Assumption 6 holds and $\sum_{j=1}^{T} \eta_j^2 \leq 1/(2L^2)$, then $\mathcal{A}$ is on-average ϵ-argument stable with $\epsilon \leq 4G\big(\frac{1}{n}\sum_{j=1}^{T}\eta_j^2\big)^{1/2} + \frac{8\sqrt{2}G}{n}\sum_{j=1}^{T}\eta_j$.

(b) (Non-smooth case) $\mathcal{A}$ is on-average ϵ-argument stable with $\epsilon \leq 2G\sqrt{2\sum_{j=1}^{T}\eta_j^2} + \frac{4\sqrt{2}G}{n}\sum_{j=1}^{T}\eta_j$.

Remark 9. For convex-concave and Lipschitz problems, the stability bound of the order $\mathcal{O}(\eta(\sqrt{T} + T/n))$ was established for SGDA with a constant stepsize under the uniformly i.i.d. sampling setting. Under a further smoothness assumption, the stability bound was improved to the order of $O(\eta T/n)$ [38]. Our stability bounds in Theorem 6 match these results up to a constant factor and extend them to the Markov sampling case.

Remark 10. Let $\{(\mathbf{w}_t^{(i)}, \mathbf{v}_t^{(i)})\}$ be the SGDA sequence based on $S^{(i)}$. The existing stability analysis [38] builds a recursive relationship for $\mathbb{E}_{\mathcal{A}}\big[\|\mathbf{w}_t - \mathbf{w}_t^{(i)}\|_2^2 + \|\mathbf{v}_t - \mathbf{v}_t^{(i)}\|_2^2\big]$, which crucially depends on the i.i.d. sampling property of $i_t \in [n]$. This strategy does not apply to MC-SGDA since the conditional expectation over i_t is in a much complex manner due to the Markov Chain sampling. We bypass this difficulty by building a recursive relationship for $\|\mathbf{w}_t - \mathbf{w}_t^{(i)}\|_2^2 + \|\mathbf{v}_t - \mathbf{v}_t^{(i)}\|_2^2$ in terms of a sequence of random variables $\mathbb{I}_{[i_t = i]}$. A key observation is that the effect of randomness would disappear if we consider on-average argument stability since $\sum_{i=1}^{n} \mathbb{I}_{[i_t=i]} = 1$ for any $t \in \mathbb{N}$.

We can combine the stability bounds in Theorem 6 and Theorem 5 to develop generalization bounds. We first establish weak PD risk bounds in Theorem 7, and then move on to primal population risk bounds in Theorem 8. The proofs are given in Section C.1 of the Appendix.

Theorem 7 (Weak PD risk bounds)**.** *Suppose Assumption 5 holds. Assume for all z, the function $(\mathbf{w}, \mathbf{v}) \mapsto f(\mathbf{w}, \mathbf{v}; z)$ is convex-concave. Let $\mathcal{W} = \mathbb{R}^d$ and $\{\mathbf{w}_j, \mathbf{v}_j\}_{j=1}^{T}$ be produced by MC-SGDA with $\eta_j \equiv \eta$. Let $\mathcal{A}$ be defined by $\mathcal{A}_{\mathbf{w}}(S) = \bar{\mathbf{w}}_T$ and $\mathcal{A}_{\mathbf{v}}(S) = \bar{\mathbf{v}}_T$ for $(\bar{\mathbf{w}}_T, \bar{\mathbf{v}}_T)$ in (6). Denote $\epsilon^{w}_{gen} := \triangle^{w}(\bar{\mathbf{w}}_T, \bar{\mathbf{v}}_T) - \triangle^{w}_{emp}(\bar{\mathbf{w}}_T, \bar{\mathbf{v}}_T)$.*

(a) *(Smooth case) If Assumption 6 holds and* $\sum_{j=1}^T \eta_j^2 \leq 1/(2L^2)$, *then* $\epsilon_{gen}^w \leq 4G^2\big(\frac{1}{n}\sum_{j=1}^T \eta_j^2\big)^{1/2} + \frac{8\sqrt{2}G^2}{n}\sum_{j=1}^T \eta_j$.

(b) *(Non-smooth case) The weak PD risk satisfies* $\epsilon_{gen}^w \leq 2\sqrt{2}G^2\big(\sum_{j=1}^T \eta_j^2\big)^{1/2} + \frac{2\sqrt{2}G^2}{n}\sum_{j=1}^T \eta_j$.

Theorem 8 (Primal risk bounds)**.** *Suppose Assumption 5 holds. Assume for all* z, *the function* $(\mathbf{w},\mathbf{v}) \mapsto f(\mathbf{w},\mathbf{v};z)$ *is convex-concave, and the function* $\mathbf{v} \mapsto F(\mathbf{w},\mathbf{v})$ *is* ρ*-strongly-concave. Let* $\mathcal{W} = \mathbb{R}^d$ *and let* $\{\mathbf{w}_j,\mathbf{v}_j\}_{j=1}^T$ *be produced by MC-SGDA with* $\eta_j \equiv \eta$. *Let* $\mathcal{A}$ *be defined by* $\mathcal{A}_{\mathbf{w}}(S) = \bar{\mathbf{w}}_T$ *and* $\mathcal{A}_{\mathbf{v}}(S) = \bar{\mathbf{v}}_T$ *for* $(\bar{\mathbf{w}}_T,\bar{\mathbf{v}}_T)$ *in* (6). *Denote* $\epsilon_{gen}^p := \mathbb{E}_{S,\mathcal{A}}\big[R(\bar{\mathbf{w}}_T) - R_S(\bar{\mathbf{w}}_T)\big]$.

(a) *(Smooth case) If Assumption 6 holds and* $\sum_{j=1}^T \eta_j^2 \leq 1/(2L^2)$, *then* $\epsilon_{gen}^p \leq 4G^2(1 + L/\rho)\big(\big(\frac{1}{n}\sum_{j=1}^T \eta_j^2\big)^{\frac{1}{2}} + \frac{2\sqrt{2}}{n}\sum_{j=1}^T \eta_j\big)$.

(b) *(Non-smooth case) The primal population risk satisfies* $\epsilon_{gen}^p \leq 2\sqrt{2}G^2(1 + L/\rho)\big(\big(\sum_{j=1}^T \eta_j^2\big)^{1/2} + \frac{2}{n}\sum_{j=1}^T \eta_j\big)$.

4.2 Population Risks of MC-SGDA

Now we establish the population risk bounds for MC-SGDA. The following theorem establishes the weak PD population risk of MC-SGDA for both smooth and non-smooth problems. Let $D_{\mathbf{w}}$ and $D_{\mathbf{v}}$ be the diameters of $\mathcal{W}$ and $\mathcal{V}$. The proof for Theorem 9 is provided in Appendix C.3.

Theorem 9 (Weak PD population risk)**.** *Suppose Assumptions 1, 4 and 5 hold. Assume for all* z, *the function* $(\mathbf{w},\mathbf{v}) \mapsto f(\mathbf{w},\mathbf{v};z)$ *is convex-concave. Let* $\{\mathbf{w}_j,\mathbf{v}_j\}_{j=1}^T$ *be produced by MC-SGDA with* $\eta_j \equiv \eta$. *Let* $\mathcal{A}$ *be defined by* $\mathcal{A}_{\mathbf{w}}(S) = \bar{\mathbf{w}}_T$ *and* $\mathcal{A}_{\mathbf{v}}(S) = \bar{\mathbf{v}}_T$ *for* $(\bar{\mathbf{w}}_T,\bar{\mathbf{v}}_T)$ *in* (6).

(a) *(Smooth case) Let Assumption 6 hold. If* $T \asymp n$ *and* $\eta \asymp (T\log(T))^{-\frac{1}{2}}$, *then* $\triangle^w(\bar{\mathbf{w}}_T,\bar{\mathbf{v}}_T) = \mathcal{O}\big(\log(n)/\big(\sqrt{n}\log(1/\lambda(P))\big)\big)$.

(b) *(Non-smooth case) If we select* $T \asymp n^2$ *and* $\eta \asymp T^{-\frac{3}{4}}$, *then we have* $\triangle^w(\bar{\mathbf{w}}_T,\bar{\mathbf{v}}_T) = \mathcal{O}\big(1/\big(\sqrt{n}\log(1/\lambda(P))\big)\big)$.

Remark 11. The above excess population risk bounds are obtained through the trade-off between the optimization errors (convergence analysis) and stability results of MC-SGDA. The convergence rates $\tilde{\mathcal{O}}(1/\sqrt{T})$ of MC-SGDA for minimax problems in both expectation and high probability are provided in Theorem C.3 and C.4 in Appendix C.2. With gradient complexity $\mathcal{O}(n)$, the minimax optimal excess risk bound $\mathcal{O}(1/\sqrt{n})$ for SGDA with uniform sampling for smooth problems was established in [38]. We show SGDA with Markov sampling can achieve the nearly optimal bound with the same gradient complexity. For non-smooth problems, part (b) shows that the optimal excess risk bound can be exactly achieved with the gradient complexity $\mathcal{O}(n^2)$.

Finally, we establish the following bounds for excess primal population risk under a strong concavity condition on $\mathbf{v} \mapsto F(\mathbf{w},\mathbf{v})$, which measures the performance of the primal variable. The proof for Theorem 10 is provided in Appendix C.3.

Theorem 10 (Excess primal population risk)**.** *Suppose Assumptions 1, 4, 5 and 6 hold. Assume for all* z, *the function* $(\mathbf{w},\mathbf{v}) \mapsto f(\mathbf{w},\mathbf{v};z)$ *is convex-concave. Assume* $\mathbf{v} \mapsto F(\mathbf{w},\mathbf{v})$ *is* ρ*-strongly-concave. Let* $\{\mathbf{w}_j,\mathbf{v}_j\}_{j=1}^T$ *be produced by MC-SGDA with* $\eta_j \equiv \eta$. *Let* $\mathcal{A}$ *be defined by* $\mathcal{A}_{\mathbf{w}}(S) = \bar{\mathbf{w}}_T$ *and* $\mathcal{A}_{\mathbf{v}}(S) = \bar{\mathbf{v}}_T$ *for* $(\bar{\mathbf{w}}_T,\bar{\mathbf{v}}_T)$ *in* (6). *If we choose* $T \asymp n, \eta \asymp (T\log(T))^{-1/2}$, *then* $\mathbb{E}_{S,\mathcal{A}}[R(\bar{\mathbf{w}}_T)] - \min_{\mathbf{w}\in\mathcal{W}} R(\mathbf{w}) = \mathcal{O}\big((L/\rho)\sqrt{\log(n)}/(\sqrt{n}\log(1/\lambda(P)))\big)$.

Remark 12. We show MC-SGDA attains population risk bounds of the order $\tilde{O}(1/\sqrt{n})$ with a linear gradient complexity $\mathcal{O}(n)$, which are minimax optimal up to a logarithmic factor. This implies that considering sampling with a Markov chain does not weaken the learnability. Theorems 9 and 10 also show the effect of P on the population risk rates, i.e., the rates get better as $\lambda(P)$ decreases.

5 Conclusion

We develop the first-ever-known stability and generalization analysis of Markov chain stochastic gradient methods for both minimization and minimax objectives. In particular, we establish the

optimal excess population bounds $\mathcal{O}(1/\sqrt{n})$ for MC-SGD for both smooth and non-smooth cases. We also develop the first nearly optimal convergence rates $\tilde{\mathcal{O}}(1/\sqrt{T})$ for convex-concave problems of MC-SGDA, and show that the optimal risk bounds $\mathcal{O}(1/\sqrt{n})$ can be derived even in the non-smooth case. Although the gradients from Markov sampling are biased and not independent across the iterations, we show the performance of MC-SGMs is competitive compared to SGMs with the classical i.i.d. sampling scheme. An interesting direction is to consider other variants of SGMs with variance reduction techniques and differentially private SGMs under the Markov sampling scheme.

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References

[1] S. Agarwal and P. Niyogi. Generalization bounds for ranking algorithms via algorithmic stability. *Journal of Machine Learning Research*, 10(Feb):441–474, 2009.

[2] M. Arjovsky, S. Chintala, and L. Bottou. Wasserstein generative adversarial networks. In *International conference on machine learning*, pages 214–223. PMLR, 2017.

[3] Y. F. Atchadé, G. Fort, and E. Moulines. On perturbed proximal gradient algorithms. *The Journal of Machine Learning Research*, 18(1):310–342, 2017.

[4] G. Ayache and S. El Rouayheb. Private weighted random walk stochastic gradient descent. *IEEE Journal on Selected Areas in Information Theory*, 2(1):452–463, 2021.

[5] F. Bach and E. Moulines. Non-strongly-convex smooth stochastic approximation with convergence rate O(1/n). In *Advances in Neural Information Processing Systems*, pages 773–781, 2013.

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

[7] R. Bassily, V. Feldman, K. Talwar, and A. G. Thakurta. Private stochastic convex optimization with optimal rates. In *Advances in Neural Information Processing Systems*, pages 11279–11288, 2019.

[8] R. Bassily, K. Nissim, A. Smith, T. Steinke, U. Stemmer, and J. Ullman. Algorithmic stability for adaptive data analysis. *SIAM Journal on Computing*, (50):377–405, 2021.

[9] S. Boucheron, G. Lugosi, and P. Massart. *Concentration Inequalities: A Nonasymptotic Theory of Independence*. Oxford university press, 2013.

[10] O. Bousquet, S. Boucheron, and G. Lugosi. Introduction to statistical learning theory. In *Summer school on machine learning*, pages 169–207. Springer, 2003.

[11] O. Bousquet and A. Elisseeff. Stability and generalization. *The Journal of Machine Learning Research*, 2:499–526, 2002.

[12] O. Bousquet, Y. Klochkov, and N. Zhivotovskiy. Sharper bounds for uniformly stable algorithms. In *Conference on Learning Theory*, pages 610–626. PMLR, 2020.

[13] Z. Charles and D. Papailiopoulos. Stability and generalization of learning algorithms that converge to global optima. In *International Conference on Machine Learning*, pages 744–753, 2018.

[14] J. Chen, Z. J. Towfic, and A. H. Sayed. Dictionary learning over distributed models. *IEEE Transactions on Signal Processing*, 63(4):1001–1016, 2014.

[15] B. Dai, A. Shaw, L. Li, L. Xiao, N. He, Z. Liu, J. Chen, and L. Song. Sbeed: Convergent reinforcement learning with nonlinear function approximation. In *International Conference on Machine Learning*, pages 1125–1134, 2018.

[16] E. Diana, W. Gill, M. Kearns, K. Kenthapadi, and A. Roth. Minimax group fairness: Algorithms and experiments. In *Proceedings of the 2021 AAAI/ACM Conference on AI, Ethics, and Society*, pages 66–76, 2021.

[17] A. Dieuleveut and F. Bach. Nonparametric stochastic approximation with large step-sizes. *The Annals of Statistics*, 44(4):1363–1399, 2016.

[18] T. T. Doan, L. M. Nguyen, N. H. Pham, and J. Romberg. Convergence rates of accelerated markov gradient descent with applications in reinforcement learning. *arXiv preprint arXiv:2002.02873*, 2020.

[19] T. T. Doan, L. M. Nguyen, N. H. Pham, and J. Romberg. Finite-time analysis of stochastic gradient descent under markov randomness. *arXiv preprint arXiv:2003.10973*, 2020.

[20] S. S. Du, J. Chen, L. Li, L. Xiao, and D. Zhou. Stochastic variance reduction methods for policy evaluation. In *International Conference on Machine Learning*, pages 1049–1058, 2017.

[21] J. Duchi and Y. Singer. Efficient online and batch learning using forward backward splitting. In *Advances in Neural Information Processing Systems*, pages 495–503, 2009.

[22] J. C. Duchi, A. Agarwal, M. Johansson, and M. I. Jordan. Ergodic mirror descent. *SIAM Journal on Optimization*, 22(4):1549–1578, 2012.

[23] J. C. Duchi, A. Agarwal, and M. J. Wainwright. Dual averaging for distributed optimization: Convergence analysis and network scaling. *IEEE Transactions on Automatic control*, 57(3):592–606, 2011.

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

[25] F. Farnia and A. Ozdaglar. Train simultaneously, generalize better: Stability of gradient-based minimax learners. In *International Conference on Machine Learning*, pages 3174–3185. PMLR, 2021.

[26] V. Feldman, T. Koren, and K. Talwar. Private stochastic convex optimization: optimal rates in linear time. In *Proceedings of the 52nd Annual ACM SIGACT Symposium on Theory of Computing*, pages 439–449, 2020.

[27] V. Feldman and J. Vondrak. Generalization bounds for uniformly stable algorithms. In *Advances in Neural Information Processing Systems*, pages 9747–9757, 2018.

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

[29] W. Gao, R. Jin, S. Zhu, and Z.-H. Zhou. One-pass auc optimization. In *International Conference on Machine Learning*, pages 906–914, 2013.

[30] I. Goodfellow, J. Pouget-Abadie, M. Mirza, B. Xu, D. Warde-Farley, S. Ozair, A. Courville, and Y. Bengio. Generative adversarial nets. *Advances in Neural Information Processing Systems*, 27:2672–2680, 2014.

[31] M. Hardt and T. Ma. Identity matters in deep learning. *arXiv preprint arXiv:1611.04231*, 2016.

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

[33] B. Johansson, M. Rabi, and M. Johansson. A simple peer-to-peer algorithm for distributed optimization in sensor networks. In *2007 46th IEEE Conference on Decision and Control*, pages 4705–4710. IEEE, 2007.

[34] B. Johansson, M. Rabi, and M. Johansson. A randomized incremental subgradient method for distributed optimization in networked systems. *SIAM Journal on Optimization*, 20(3):1157–1170, 2010.

[35] B. Kulis et al. Metric learning: A survey. *Foundations and Trends® in Machine Learning*, 5(4):287–364, 2013.

[36] I. Kuzborskij and C. Lampert. Data-dependent stability of stochastic gradient descent. In *International Conference on Machine Learning*, pages 2820–2829, 2018.

[37] G. Lan. *First-order and Stochastic Optimization Methods for Machine Learning*. Springer Nature, 2020.

[38] Y. Lei, Z. Yang, T. Yang, and Y. Ying. Stability and generalization of stochastic gradient methods for minimax problems. In *International Conference on Machine Learning*, 2021.

[39] Y. Lei and Y. Ying. Fine-grained analysis of stability and generalization for stochastic gradient descent. In *International Conference on Machine Learning*, pages 5809–5819. PMLR, 2020.

[40] Y. Lei and Y. Ying. Sharper generalization bounds for learning with gradient-dominated objective functions. In *International Conference on Learning Representations*, 2020.

[41] T. Li, M. Sanjabi, A. Beirami, and V. Smith. Fair resource allocation in federated learning. *arXiv preprint arXiv:1905.10497*, 2019.

[42] X. Li and F. Orabona. On the convergence of stochastic gradient descent with adaptive stepsizes. In *The 22nd International Conference on Artificial Intelligence and Statistics*, pages 983–992. PMLR, 2019.

[43] J. Lin and L. Rosasco. Optimal learning for multi-pass stochastic gradient methods. In *Advances in Neural Information Processing Systems*, pages 4556–4564, 2016.

[44] T. Lin, C. Jin, and M. Jordan. On gradient descent ascent for nonconvex-concave minimax problems. In *International Conference on Machine Learning*, pages 6083–6093. PMLR, 2020.

[45] M. Liu, Z. Yuan, Y. Ying, and T. Yang. Stochastic auc maximization with deep neural networks. *arXiv preprint arXiv:1908.10831*, 2019.

[46] M. Liu, X. Zhang, Z. Chen, X. Wang, and T. Yang. Fast stochastic AUC maximization with O(1/n)-convergence rate. In *International Conference on Machine Learning*, pages 3195–3203, 2018.

[47] T. Liu, G. Lugosi, G. Neu, and D. Tao. Algorithmic stability and hypothesis complexity. In *International Conference on Machine Learning*, pages 2159–2167, 2017.

[48] C. G. Lopes and A. H. Sayed. Incremental adaptive strategies over distributed networks. *IEEE Transactions on Signal Processing*, 55(8):4064–4077, 2007.

[49] A. Madry, A. Makelov, L. Schmidt, D. Tsipras, and A. Vladu. Towards deep learning models resistant to adversarial attacks. *arXiv preprint arXiv:1706.06083*, 2017.

[50] X. Mao, K. Yuan, Y. Hu, Y. Gu, A. H. Sayed, and W. Yin. Walkman: A communication-efficient random-walk algorithm for decentralized optimization. *IEEE Transactions on Signal Processing*, 68:2513–2528, 2020.

[51] N. Martinez, M. Bertran, and G. Sapiro. Minimax pareto fairness: A multi objective perspective. In *International Conference on Machine Learning*, pages 6755–6764. PMLR, 2020.

[52] M. Mohri, G. Sivek, and A. T. Suresh. Agnostic federated learning. In *International Conference on Machine Learning*, pages 4615–4625. PMLR, 2019.

[53] A. Nedic and S. Lee. On stochastic subgradient mirror-descent algorithm with weighted averaging. *SIAM Journal on Optimization*, 24(1):84–107, 2014.

[54] A. Nemirovski, A. Juditsky, G. Lan, and A. Shapiro. Robust stochastic approximation approach to stochastic programming. *SIAM Journal on Optimization*, 19(4):1574–1609, 2009.

[55] R. Oldenburger. Infinite powers of matrices and characteristic roots. *Duke Mathematical Journal*, 6(2):357–361, 1940.

[56] H. Rafique, M. Liu, Q. Lin, and T. Yang. Weakly-convex–concave min–max optimization: provable algorithms and applications in machine learning. *Optimization Methods and Software*, pages 1–35, 2021.

[57] A. Rakhlin, O. Shamir, and K. Sridharan. Making gradient descent optimal for strongly convex stochastic optimization. In *Proceedings of the 29th International Coference on International Conference on Machine Learning*, pages 1571–1578, 2012.

[58] S. S. Ram, A. Nedić, and V. V. Veeravalli. Incremental stochastic subgradient algorithms for convex optimization. *SIAM Journal on Optimization*, 20(2):691–717, 2009.

[59] H. E. Rauch, F. Tung, and C. T. Striebel. Maximum likelihood estimates of linear dynamic systems. *AIAA journal*, 3(8):1445–1450, 1965.

[60] R. T. Rockafellar. Monotone operators and the proximal point algorithm. *SIAM Journal on Control and Optimization*, 14(5):877–898, 1976.

[61] A. H. Sayed. Adaptive networks. *Proceedings of the IEEE*, 102(4):460–497, 2014.

[62] M. Schmidt, N. Roux, and F. Bach. Convergence rates of inexact proximal-gradient methods for convex optimization. In *Advances in Neural Information Processing Systems*, 2011.

[63] S. M. Shah and K. E. Avrachenkov. Linearly convergent asynchronous distributed admm via markov sampling. *arXiv preprint arXiv:1810.05067*, 2018.

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

[65] W. Shen, Z. Yang, Y. Ying, and X. Yuan. Stability and optimization error of stochastic gradient descent for pairwise learning. *Analysis and Applications*, pages 1–41, 2019.

[66] S. Smale and D.-X. Zhou. Online learning with markov sampling. *Analysis and Applications*, 7(01):87–113, 2009.

[67] P. Smyth. Hidden markov models for fault detection in dynamic systems. *Pattern recognition*, 27(1):149–164, 1994.

[68] T. Sun and D. Li. Decentralized markov chain gradient descent. *arXiv preprint arXiv:1909.10238*, 2019.

[69] T. Sun, Y. Sun, and W. Yin. On markov chain gradient descent. In *Advances in neural information processing systems*, 2018.

[70] V. B. Tadić and A. Doucet. Asymptotic bias of stochastic gradient search. *The Annals of Applied Probability*, 27(6):3255–3304, 2017.

[71] E. Ullah, T. Mai, A. Rao, R. Rossi, and R. Arora. Machine unlearning via algorithmic stability. *arXiv preprint arXiv:2102.13179*, 2021.

[72] V. Vapnik. *The nature of statistical learning theory*. Springer science & business media, 1999.

[73] S. Vaswani, F. Bach, and M. Schmidt. Fast and faster convergence of sgd for over-parameterized models and an accelerated perceptron. In *The 22nd International Conference on Artificial Intelligence and Statistics*, pages 1195–1204. PMLR, 2019.

[74] P. Wang, Y. Lei, Y. Ying, and H. Zhang. Differentially private sgd with non-smooth losses. *Applied and Computational Harmonic Analysis*, 56:306–336, 2022.

[75] K. Q. Weinberger and L. K. Saul. Distance metric learning for large margin nearest neighbor classification. *Journal of machine learning research*, 10(2), 2009.

[76] E. Xing, M. Jordan, S. J. Russell, and A. Ng. Distance metric learning with application to clustering with side-information. *Advances in neural information processing systems*, 15, 2002.

[77] Z. Yang, Y. Lei, S. Lyu, and Y. Ying. Stability and differential privacy of stochastic gradient descent for pairwise learning with non-smooth loss. In *International Conference on Artificial Intelligence and Statistics*, pages 2026–2034. PMLR, 2021.

[78] Z. Yang, Y. Lei, P. Wang, T. Yang, and Y. Ying. Simple stochastic and online gradient descent algorithms for pairwise learning. *Advances in Neural Information Processing Systems*, 34, 2021.

[79] Y. Ying and P. Li. Distance metric learning with eigenvalue optimization. *The Journal of Machine Learning Research*, 13(1):1–26, 2012.

[80] Y. Ying and M. Pontil. Online gradient descent learning algorithms. *Foundations of Computational Mathematics*, 8(5):561–596, 2008.

[81] Y. Ying, L. Wen, and S. Lyu. Stochastic online auc maximization. *Advances in neural information processing systems*, 29, 2016.

[82] Y. Ying and D.-X. Zhou. Online regularized classification algorithms. *IEEE Transactions on Information Theory*, 52(11):4775–4788, 2006.

[83] Y. Ying and D.-X. Zhou. Online pairwise learning algorithms. *Neural computation*, 28(4):743–777, 2016.

[84] S. Zeng, T. T. Doan, and J. Romberg. Finite-time analysis of decentralized stochastic approximation with applications in multi-agent and multi-task learning. In *2021 60th IEEE Conference on Decision and Control (CDC)*, pages 2641–2646. IEEE, 2021.

[85] J. Zhang, M. Hong, M. Wang, and S. Zhang. Generalization bounds for stochastic saddle point problems. In *International Conference on Artificial Intelligence and Statistics*, pages 568–576. PMLR, 2021.

[86] T. Zhang. Solving large scale linear prediction problems using stochastic gradient descent algorithms. In *International Conference on Machine Learning*, pages 919–926, 2004.

[87] P. Zhao, S. C. Hoi, R. Jin, and T. Yang. Online AUC maximization. In *International Conference on Machine Learning*, pages 233–240, 2011.

[88] Y. Zhou, Y. Liang, and H. Zhang. Generalization error bounds with probabilistic guarantee for SGD in nonconvex optimization. *arXiv preprint arXiv:1802.06903*, 2018.

Checklist

1. For all authors...

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

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

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

4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
   (a) If your work uses existing assets, did you cite the creators? [Yes]
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5. If you used crowdsourcing or conducted research with human subjects...
   (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]
   (b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A]
   (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]

Appendix for "Stability and Generalization of Markov Chain Stochastic Gradient Methods"

A Technical Lemmas

Starting from a deterministic and arbitrary initialization $\mathbf{w}_0$, the iteration of MC-SGMs is illustrated by the following diagram:

$$\begin{array}{ccccccccc} & & z_{i_1} & \longrightarrow & z_{i_2} & \longrightarrow & z_{i_3} & \longrightarrow & \dots \\ & & \downarrow & & \downarrow & & \downarrow & & \\ \mathbf{w}_0 & \longrightarrow & \mathbf{w}_1 & \longrightarrow & \mathbf{w}_2 & \longrightarrow & \mathbf{w}_3 & \longrightarrow & \dots \end{array}$$

The Jordan normal form of transition matrix P [55] is

$$P = U \begin{bmatrix} 1 & & & \\ & J_2 & & \\ & & \ddots & \\ & & & J_m \end{bmatrix} U^{-1},$$

where m is the number of the blocks, $d_i \geq 1$ is the dimension of the i-th block submatrix J_i, $i = 2, 3, \dots, m$, which satisfy $\sum_{i=1}^m d_i = n$, and matrix $J_i := \lambda_i(P) \cdot \mathbf{I}_{d_i} + \mathbf{D}(-1, d_i)$ with $\mathbf{D}(-1, d_i) := \begin{bmatrix} 0 & 1 & & \\ & \ddots & \ddots & \\ & & \ddots & 1 \\ & & & 0 \end{bmatrix}_{d_i \times d_i}$. Here $\mathbf{I}_{d_i}$ is the identity matrix of size d_i. In particular, if P is symmetric, then it is double stochastic and there holds $d_i = 1$ for any $i \in [m]$.

To establish the optimization error for MC-SGMs, we need the following lemma which gives the mixing time of a Markov chain.

Lemma A.1 ([69]). *Suppose Assumption 1 holds. Let $\lambda_i(P)$ be the i-th largest eigenvalue of P, $\lambda(P) = \frac{\max\{|\lambda_2(P)|, |\lambda_n(P)|\}+1}{2} \in [1/2, 1)$, $C_P = \left(\sum_{i=2}^m d_i^2\right)^{1/2} \|U\|_F \|U^{-1}\|_F$ and $K_P = \max\left\{ \max_{1 \leq i \leq m} \left\{ \left\lceil \frac{2d_i(d_i-1)(\log(\frac{2d_i}{|\lambda_2(P)| \cdot \log(\lambda(P)/|\lambda_2(P)|)})-1)}{(d_i+1)\log(\lambda(P)/|\lambda_2(P)|)} \right\rceil \right\}, 0 \right\}$. For any $j \geq K_P$, there holds*

$$\left\|\Pi^* - P^j\right\|_\infty \leq C_P \cdot \left(\lambda(P)\right)^j.$$

In addition, if P is symmetric, then $K_P = 0$ and

$$\left\|\Pi^* - P^j\right\|_\infty \leq n^{3/2} \cdot \left(\lambda(P)\right)^j, \text{ for any } j \geq 0.$$

The following lemma shows the non-expansive behavior for the gradient mapping $\mathbf{w} \mapsto \mathbf{w} - \eta \partial f(\mathbf{w}; z_i)$ associated with a smooth function.

Lemma A.2 ([31]). *Suppose the loss f is convex and L-smooth w.r.t. the first argument. Then for all $\eta \leq 2/L$ and $z \in \mathcal{Z}$ there holds*

$$\|\mathbf{w} - \partial f(\mathbf{w}; z) - \mathbf{w}' + \eta \partial f(\mathbf{w}'; z)\|_2 \leq \|\mathbf{w} - \mathbf{w}'\|_2.$$

Lemma A.3 ([62]). *Assume that the non-negative sequence $\{u_t : t \in \mathbb{N}\}$ satisfies the following recursive inequality for all $t \in \mathbb{N}$,*

$$u_t^2 \leq S_t + \sum_{\tau=1}^{t-1} \alpha_\tau u_\tau.$$

where $\{S_\tau : \tau \in \mathbb{N}\}$ is an increasing sequence, $S_0 \geq u_0^2$ and $\alpha_\tau \geq 0$ for any $\tau \in \mathbb{N}$. Then, the following inequality holds true:

$$u_t \leq \sqrt{S_t} + \sum_{\tau=1}^{t-1} \alpha_\tau.$$

The connection between on-average argument stability for Lipschitz continuous losses and its generalization error has been studied in [39].

Lemma A.4 (Generalization via argument stability)**.** *Let $S, \widetilde{S}$ and $S^{(i)}$ be defined as Definition 4. If $\mathcal{A}$ is on-average ϵ-argument-stable and Assumption 2 holds, then there holds $\big|\mathbb{E}_{S,\mathcal{A}}\big[F(\mathcal{A}(S)) - F_S(\mathcal{A}(S))\big]\big| \leq G\epsilon$.*

Finally, we introduce the following lemma on concentration inequality of martingales.

Lemma A.5 ([9])**.** *Let $z_1, \ldots, z_n$ be a sequence of random variables. Consider a sequence of functionals $\xi_k(z_1, \ldots, z_k)$, $k \in [n]$. Assume $|\xi_k - \mathbb{E}_{z_k}[\xi_k]| \leq b_k$ for each k. Let $\gamma \in (0, 1)$. With probability at least $1 - \gamma$, there holds*

$$\sum_{k=1}^{n} \mathbb{E}_{z_k}[\xi_k] - \sum_{k=1}^{n} \xi_k \leq \Big(2\log(1/\gamma) \sum_{k=1}^{n} b_k^2\Big)^{1/2}.$$

B Proofs of Markov Chain SGD

B.1 Proof of Theorem 1

Proof of Theorem 1. For any $i \in [n]$, define $S^{(i)} = \{z_1, \ldots, z_{i-1}, \tilde{z}_i, z_{i+1}, \ldots, z_n\}$ as the set formed from S by replacing the i-th element with $\tilde{z}_i$. Let $\{\mathbf{w}_t\}$ and $\{\mathbf{w}_t^{(i)}\}$ be produced by MC-SGD based on S and $S^{(i)}$, respectively. For simplicity, we denote by $\delta_t^{(i)} = \|\mathbf{w}_t - \mathbf{w}_t^{(i)}\|_2$ here. Note that the projection step is nonexpansive.

We first prove part (a). Consider the following two cases.

Case 1. If $i_t \neq i$, then it follows from the L-smoothness of f and Lemma A.2 that

$$\delta_t^{(i)} \leq \|\mathbf{w}_{t-1} - \eta_t \partial f(\mathbf{w}_{t-1}; z_{i_t}) - \mathbf{w}_{t-1}^{(i)} + \eta_t \partial f(\mathbf{w}_{t-1}^{(i)}; z_{i_t})\|_2 \leq \delta_{t-1}^{(i)}.$$

Case 2. If $i_t = i$, then it follows from the Lipschitz continuity of f that

$$\begin{aligned}\delta_t^{(i)} &\leq \|\mathbf{w}_{t-1} - \eta_t \partial f(\mathbf{w}_{t-1}; z_{i_t}) - \mathbf{w}_{t-1}^{(i)} + \eta_t \partial f(\mathbf{w}_{t-1}^{(i)}; \tilde{z}_{i_t})\|_2 \\ &\leq \delta_{t-1}^{(i)} + \eta_t \|\partial f(\mathbf{w}_{t-1}; z_i) - \partial f(\mathbf{w}_{t-1}^{(i)}; \tilde{z}_i)\|_2 \leq \delta_{t-1}^{(i)} + 2G\eta_t.\end{aligned}$$

Combining the above two cases together, we know

$$\delta_t^{(i)} \leq \delta_{t-1}^{(i)} + 2G\eta_t \mathbb{I}_{[i_t = i]},$$

where $\mathbb{I}_{[i_t=i]}$ is the indicator function, i.e., $\mathbb{I}_{[i_t=1]} = 1$ if $i_t = i$ and 0 else. Now, applying the above inequality recursively we have

$$\delta_t^{(i)} \leq 2G \sum_{j=1}^{t} \eta_j \mathbb{I}_{[i_j = i]},$$

By the convexity of $\|\cdot\|_2$, there holds

$$\|\bar{\mathbf{w}}_t - \bar{\mathbf{w}}_t^{(i)}\|_2 \leq \frac{1}{t} \sum_{j=1}^{t} \delta_j^{(i)} \leq 2G \sum_{j=1}^{t} \eta_j \mathbb{I}_{[i_j = i]}.$$

Taking an average over i yields

$$\frac{1}{n} \sum_{i=1}^{n} \|\bar{\mathbf{w}}_t - \bar{\mathbf{w}}_t^{(i)}\|_2 \leq \frac{2G}{n} \sum_{j=1}^{t} \eta_j \sum_{i=1}^{n} \mathbb{I}_{[i_j = i]} \leq \frac{2G}{n} \sum_{j=1}^{t} \eta_j,$$

where the last inequality used the fact that $\sum_{i=1}^{n} \mathbb{I}_{[i_j=i]} = 1$ for any $j \in [t]$. Taking expectation w.r.t. $\mathcal{A}$, we have

$$\mathbb{E}_{\mathcal{A}}\Big[\frac{1}{n} \sum_{i=1}^{n} \|\bar{\mathbf{w}}_t - \bar{\mathbf{w}}_t^{(i)}\|_2\Big] \leq \frac{2G}{n} \sum_{j=1}^{t} \eta_j,$$

which completes the proof of Part (a).

Now, we turn to the non-smooth case. Similar as before, we consider the following two cases.

Case 1. If $i_t \neq i$, then we have

$$\begin{aligned}
\big(\delta_t^{(i)}\big)^2 &\leq \|\mathbf{w}_{t-1} - \eta_t \partial f(\mathbf{w}_{t-1}; z_{i_t}) - \mathbf{w}_{t-1}^{(i)} + \eta_t \partial f(\mathbf{w}_{t-1}^{(i)}; z_{i_t})\|_2^2 \\
&= \big(\delta_{t-1}^{(i)}\big)^2 + \eta_t^2 \|\partial f(\mathbf{w}_{t-1}; z_{i_t}) - \partial f(\mathbf{w}_{t-1}^{(i)}; z_{i_t})\|_2^2 - 2\eta_t \langle \mathbf{w}_{t-1} - \mathbf{w}_{t-1}^{(i)}, \partial f(\mathbf{w}_{t-1}; z_{i_t}) - \partial f(\mathbf{w}_{t-1}^{(i)}; z_{i_t})\rangle \\
&\leq \big(\delta_{t-1}^{(i)}\big)^2 + 2\eta_t^2 (\|\partial f(\mathbf{w}_{t-1}; z_{i_t})\|_2^2 + \|\partial f(\mathbf{w}_{t-1}^{(i)}; z_{i_t})\|_2^2) \\
&\leq \big(\delta_{t-1}^{(i)}\big)^2 + 4G^2\eta_t^2,
\end{aligned}$$

where in the last second inequality we used $\langle \mathbf{w}_{t-1} - \mathbf{w}_{t-1}^{(i)}, \partial f(\mathbf{w}_{t-1}; z_{i_t}) - \partial f(\mathbf{w}_{t-1}^{(i)}; z_{i_t})\rangle \geq 0$ due to the convexity of f, and the last inequality follows from the Lipschitz continuity of f.

Case 2. If $i_t = i$, then

$$\begin{aligned}
(\delta_t^{(i)})^2 &\leq \|\mathbf{w}_{t-1} - \eta_t \partial f(\mathbf{w}_{t-1}; z_i) - \mathbf{w}_{t-1}^{(i)} + \eta_t \partial f(\mathbf{w}_{t-1}^{(i)}; \tilde{z}_i)\|_2^2 \\
&= (\delta_{t-1}^{(i)})^2 + \eta_t^2 \|\partial f(\mathbf{w}_{t-1}; z_i) - \partial f(\mathbf{w}_{t-1}^{(i)}; \tilde{z}_i)\|_2^2 - 2\eta_t \langle \mathbf{w}_{t-1} - \mathbf{w}_{t-1}^{(i)}, \partial f(\mathbf{w}_{t-1}; z_i) - \partial f(\mathbf{w}_{t-1}^{(i)}; \tilde{z}_i)\rangle \\
&\leq (\delta_{t-1}^{(i)})^2 + 2\eta_t^2 \big(\|\partial f(\mathbf{w}_{t-1}; z_i)\|_2^2 + \|\partial f(\mathbf{w}_{t-1}^{(i)}; \tilde{z}_i)\|_2^2\big) + 2\eta_t \delta_{t-1}^{(i)} \big(\|\partial f(\mathbf{w}_{t-1}; z_i)\|_2 + \|\partial f(\mathbf{w}_{t-1}^{(i)}; \tilde{z}_i)\|_2\big) \\
&\leq (\delta_{t-1}^{(i)})^2 + 4G^2\eta_t^2 + 4G\eta_t \delta_{t-1}^{(i)}, \qquad \text{(B.1)}
\end{aligned}$$

where the last inequality holds since f is G-Lipschitz.

Combining Case 1 and Case 2 together, we have

$$(\delta_t^{(i)})^2 \leq (\delta_{t-1}^{(i)})^2 + 4G^2\eta_t^2 + 4G\eta_t \delta_{t-1}^{(i)} \mathbb{I}_{[i_t = i]}.$$

Note that $\delta_0^{(i)} = \|\mathbf{w}_0 - \mathbf{w}_0^{(i)}\|_2 = 0$, we get the following recursive inequality

$$(\delta_t^{(i)})^2 \leq 4G^2 \sum_{j=1}^t \eta_j^2 + 4G \sum_{j=1}^t \eta_j \delta_{j-1}^{(i)} \mathbb{I}_{[i_j = i]} = 4G^2 \sum_{j=1}^t \eta_j^2 + 4G \sum_{j=1}^{t-1} \eta_{j+1} \delta_j^{(i)} \mathbb{I}_{[i_{j+1} = i]}.$$

Lemma A.3 with $u_t = \delta_t^{(i)}$ implies

$$\delta_t^{(i)} \leq 2G \sqrt{\sum_{j=1}^t \eta_j^2} + 4G \sum_{j=1}^{t-1} \eta_{j+1} \mathbb{I}_{[i_{j+1} = i]}.$$

By the convexity of $\|\cdot\|_2$, it follows

$$\|\bar{\mathbf{w}}_t - \bar{\mathbf{w}}_t^{(i)}\|_2 \leq \frac{1}{t} \sum_{j=1}^t \delta_j^{(i)} \leq 2G \sqrt{\sum_{j=1}^t \eta_j^2} + 4G \sum_{j=1}^{t-1} \eta_{j+1} \mathbb{I}_{[i_{j+1} = i]}.$$

Taking an average over i, we have

$$\begin{aligned}
\frac{1}{n} \sum_{i=1}^n \|\bar{\mathbf{w}}_t - \bar{\mathbf{w}}_t^{(i)}\|_2 &\leq 2G \sqrt{\sum_{j=1}^t \eta_t^2} + \frac{4G}{n} \sum_{j=1}^{t-1} \eta_{j+1} \sum_{i=1}^n \mathbb{I}_{[i_{j+1} = i]} \\
&\leq 2G \sqrt{\sum_{j=1}^t \eta_t^2} + \frac{4G}{n} \sum_{j=1}^t \eta_j,
\end{aligned}$$

where the last inequality used the fact that $\sum_{i=1}^n \mathbb{I}_{[i_{j+1} = i]} = 1$. Taking the expectation w.r.t. $\mathcal{A}$ completes the proof. □

B.2 Optimization Error of MC-SGD for Convex Problems

In this subsection, we establish the convergence rates of MC-SGD for convex and non-convex problems. We consider both upper bounds in expectation and with high probability.

Recall $\mathbf{w}^* = \arg\min_{\mathbf{w}\in\mathcal{W}} F(\mathbf{w})$. Let $\lambda_i(P)$ be the i-th largest eigenvalue of transition matrix P and $\lambda(P) = (\max\{|\lambda_2(P)|, |\lambda_n(P)|\} + 1)/2 \in [1/2, 1)$. Let K_P be the mixing time and C_P be a constant depending on P and its Jordan canonical form (detailed expressions are given in Lemma A.1 in the Appendix).

Theorem B.1 gives optimization error bounds in expectation for MC-SGD in the convex case.

Theorem B.1 (Convex case)**.** *Suppose f is convex and Assumptions 1, 2 hold. Let $\mathcal{A}$ be MC-SGD with T iterations, and $\{\mathbf{w}_j\}_{j=1}^T$ be produced by $\mathcal{A}$ with $\mathbf{w}_0 = 0$ and $\eta_j \equiv \eta \le 2/L$. Let $D_0 = \|\mathbf{w}^*\|_2$, $D = \big((G^2 + 2\sup_{z\in\mathcal{Z}} f(0;z)) \sum_{k=1}^T \eta_k\big)^{1/2} + D_0$ and*

$$k_j = \min\Big\{\max\Big\{\Big\lceil \frac{\log(2C_P Dnj)}{\log(1/\lambda(P))}\Big\rceil, K_P\Big\}, j\Big\}, j \in [T]. \tag{B.2}$$

Then the following inequality holds

$$\mathbb{E}_{\mathcal{A}}[F_S(\bar{\mathbf{w}}_T) - F_S(\mathbf{w}^*)] \le \frac{D_0 + G\big(4D\sum_{j=1}^{K_P-1}\eta_j + \sum_{j=K_P}^T \frac{\eta_j}{j} + G\sum_{j=1}^T (4\eta_j \sum_{k=j-k_j+1}^j \eta_k + \eta_j^2)\big)}{2\sum_{j=1}^T \eta_j}.$$

Furthermore, suppose Assumption 4 holds. Then selecting $\eta_j \equiv \eta = 1/\sqrt{T\log(T)}$ implies $\mathbb{E}_{\mathcal{A}}[F_S(\bar{\mathbf{w}}_T) - F_S(\mathbf{w}^*)] = \mathcal{O}\big(\sqrt{\log(T)}/(\sqrt{T}\log(1/\lambda(P))\big)$.

Remark B.1. For all $j \in [T]$, k_j can be seen as the mixing time such that the distance between the distribution of the current state of the Markov chain and that of the stationary distribution can be controlled by $\mathcal{O}(1/(nj))$.

Now, we give the proof of Theorem B.1.

Proof of Theorem B.1. By the convexity of f and Jensen's inequality,

$$\begin{aligned}
&\Big(\sum_{j=1}^T \eta_j\Big)\mathbb{E}_{\mathcal{A}}[F_S(\bar{\mathbf{w}}_t) - F_S(\mathbf{w}^*)] \\
&\le \sum_{j=1}^T \eta_j \mathbb{E}_{\mathcal{A}}[F_S(\mathbf{w}_j) - F_S(\mathbf{w}^*)] \\
&= \sum_{j=1}^T \eta_j \mathbb{E}_{\mathcal{A}}\big[F_S(\mathbf{w}_j) - F_S(\mathbf{w}_{j-k_j})\big] + \sum_{j=1}^T \eta_j \mathbb{E}_{\mathcal{A}}\big[F_S(\mathbf{w}_{j-k_j}) - F_S(\mathbf{w}^*)\big],
\end{aligned} \tag{B.3}$$

where $k_j = \min\Big\{\max\Big\{\Big\lceil \frac{\log(2C_P Dnj)}{\log(1/\lambda(P))}\Big\rceil, K_P\Big\}, j\Big\}$.

Consider the first term $\sum_{j=1}^T \eta_j \mathbb{E}_{\mathcal{A}}\big[F_S(\mathbf{w}_j) - F_S(\mathbf{w}_{j-k_j})\big]$ in (B.3). By Lipschitz continuity of f, we have

$$\sum_{j=1}^T \eta_j \mathbb{E}_{\mathcal{A}}\big[F_S(\mathbf{w}_j) - F_S(\mathbf{w}_{j-k_j})\big] \le G\sum_{j=1}^T \eta_j \mathbb{E}_{\mathcal{A}}\big[\|\mathbf{w}_j - \mathbf{w}_{j-k_j}\|_2\big] \le G^2 \sum_{j=1}^T \eta_j \sum_{k=j-k_j+1}^j \eta_k, \tag{B.4}$$

where the last inequality used the fact that $\|\mathbf{w}_j - \mathbf{w}_{j-k_j}\|_2 \le \sum_{k=j-k_j+1}^j \eta_k \|\partial f(\mathbf{w}_{k-1}; z_{i_k})\|_2 \le G\sum_{k=j-k_j+1}^j \eta_k$.

Next, we estimate the term $\sum_{j=1}^T \eta_j \mathbb{E}_{\mathcal{A}}[F_S(\mathbf{w}_{j-k_j}) - F(\mathbf{w}^*)]$ in (B.3). Note that

$$\begin{aligned}
&\mathbb{E}_{i_j}[f(\mathbf{w}_{j-k_j}; z_{i_j}) - f(\mathbf{w}^*; z_{i_j}) | \mathbf{w}_0, \ldots, \mathbf{w}_{j-k_j}, z_{i_1}, \ldots, z_{i_{j-k_j}}] \\
&= \sum_{i=1}^n [f(\mathbf{w}_{j-k_j}; z_i) - f(\mathbf{w}^*; z_i)] \cdot \Pr(i_j = i | i_{j-k_j}) \\
&= \sum_{i=1}^n [f(\mathbf{w}_{j-k_j}; z_i) - f(\mathbf{w}^*; z_i)] \cdot [P^{k_j}]_{i_{j-k_j}, i} \\
&= \frac{1}{n} \sum_{i=1}^n [f(\mathbf{w}_{j-k_j}; z_i) - f(\mathbf{w}^*; z_i)] + \sum_{i=1}^n \Big([P^{k_j}]_{i_{j-k_j}, i} - \frac{1}{n} \Big) \cdot [f(\mathbf{w}_{j-k_j}; z_i) - f(\mathbf{w}^*; z_i)] \\
&= \big(F_S(\mathbf{w}_{j-k_j}) - F_S(\mathbf{w}^*) \big) + \sum_{i=1}^n \Big([P^{k_j}]_{i_{j-k_j}, i} - \frac{1}{n} \Big) \cdot [f(\mathbf{w}_{j-k_j}; z_i) - f(\mathbf{w}^*; z_i)]. \qquad \text{(B.5)}
\end{aligned}$$

Rearranging the above equality and taking total expectation give us

$$\begin{aligned}
\mathbb{E}_{\mathcal{A}}[F_S(\mathbf{w}_{j-k_j}) - F_S(\mathbf{w}^*)] =& \mathbb{E}_{\mathcal{A}}[f(\mathbf{w}_{j-k_j}; z_{i_j}) - f(\mathbf{w}^*; z_{i_j})] \\
&+ \mathbb{E}_{\mathcal{A}} \Big[\sum_{i=1}^n \Big(\frac{1}{n} - [P^{k_j}]_{i_{j-k_j}, i} \Big) \big(f(\mathbf{w}_{j-k_j}; z_i) - f(\mathbf{w}^*; z_i) \big) \Big].
\end{aligned}$$

Summing over j yields

$$\begin{aligned}
\sum_{j=1}^T \eta_j \mathbb{E}_{\mathcal{A}}[F_S(\mathbf{w}_{j-k_j}) - F_S(\mathbf{w}^*)] =& \sum_{j=1}^T \eta_j \mathbb{E}_{\mathcal{A}}[f(\mathbf{w}_{j-k_j}; z_{i_j}) - f(\mathbf{w}^*; z_{i_j})] \\
&+ \sum_{j=1}^T \eta_j \mathbb{E}_{\mathcal{A}} \Big[\sum_{i=1}^n \Big(\frac{1}{n} - [P^{k_j}]_{i_{j-k_j}, i} \Big) [f(\mathbf{w}_{j-k_j}; z_i) - f(\mathbf{w}^*; z_i)] \Big]. \qquad \text{(B.6)}
\end{aligned}$$

Now, we estimate the term $\sum_{j=1}^T \eta_j \mathbb{E}_{\mathcal{A}}[f(\mathbf{w}_{j-k_j}; z_{i_j}) - f(\mathbf{w}^*; z_{i_j})]$ in (B.6). According to update rule (4), for any j and $1 \le k_j \le j$

$$\begin{aligned}
&\|\mathbf{w}_j - \mathbf{w}^*\|_2^2 \\
&\le \|\mathbf{w}_{j-1} - \eta_j \partial f(\mathbf{w}_{j-1}; z_{i_j}) - \mathbf{w}^*\|_2^2 \\
&= \|\mathbf{w}_{j-1} - \mathbf{w}^*\|_2^2 - 2\eta_j \langle \mathbf{w}_{j-1} - \mathbf{w}^*, \partial f(\mathbf{w}_{j-1}; z_{i_j}) \rangle + \eta_j^2 \|\partial f(\mathbf{w}_{j-1}; z_{i_j})\|_2^2 \\
&\le \|\mathbf{w}_{j-1} - \mathbf{w}^*\|_2^2 - 2\eta_j \big(f(\mathbf{w}_{j-1}; z_{i_j}) - f(\mathbf{w}^*; z_{i_j}) \big) + G^2 \eta_j^2 \\
&= \|\mathbf{w}_{j-1} - \mathbf{w}^*\|_2^2 - 2\eta_j \big(f(\mathbf{w}_{j-k_j}; z_{i_j}) - f(\mathbf{w}^*; z_{i_j}) \big) + 2\eta_j \big(f(\mathbf{w}_{j-k_j}; z_{i_j}) - f(\mathbf{w}_{j-1}; z_{i_j}) \big) + G^2 \eta_j^2 \\
&\le \|\mathbf{w}_{j-1} - \mathbf{w}^*\|_2^2 - 2\eta_j \big(f(\mathbf{w}_{j-k_j}; z_{i_j}) - f(\mathbf{w}^*; z_{i_j}) \big) + 2G^2 \eta_j \sum_{k=j-k_j+1}^{j} \eta_k + G^2 \eta_j^2,
\end{aligned}$$

where the second inequality is due to the convexity of f, and the last inequality used the fact f is G-Lipschitz and $\|\mathbf{w}_{j-k_j} - \mathbf{w}_{j-1}\|_2 \le \sum_{k=j-k_j+1}^{j} \eta_k \|\partial f(\mathbf{w}_k; z_{i_k})\|_2 \le G \sum_{k=j-k_j+1}^{j} \eta_k$. Taking a summation of the both sides over j and noting $\mathbf{w}_0 = 0$, we get

$$\sum_{j=1}^T \eta_j \big(f(\mathbf{w}_{j-k_j}; z_{i_j}) - f(\mathbf{w}^*; z_{i_j}) \big) \le \frac{\|\mathbf{w}^*\|_2^2 + G^2 \sum_{j=1}^T \big(2\eta_j \sum_{k=j-k_j+1}^{j} \eta_k + \eta_j^2 \big)}{2}. \qquad \text{(B.7)}$$

Then we turn to estimate $\sum_{j=1}^T \eta_j \sum_{i=1}^n \Big(\frac{1}{n} - [P^{k_j}]_{i_{j-k_j}, i} \Big) [f(\mathbf{w}_{j-k_j}; z_i) - f(\mathbf{w}^*; z_i)]$. Recall that $k_j = \min \Big\{ \max \Big\{ \Big\lceil \frac{\log(2C_P Dnj)}{\log(1/\lambda(P))} \Big\rceil, K_P \Big\}, j \Big\}$. For $j \ge K_P$, according to Lemma A.1, we know for any $i, i' \in [n]$

$$\Big| \frac{1}{n} - [P^{k_j}]_{i,i'} \Big| \le C_P \big(\lambda(P) \big)^{k_j} = C_P e^{k_j \log(\lambda(P))} \le \frac{1}{2Dnj}.$$

According to the update rule (4) we know

$$\|\mathbf{w}_t\|_2^2 \leq \|\mathbf{w}_{t-1} - \eta_t \partial f(\mathbf{w}_{t-1}; z_{i_t})\|_2^2 \leq \|\mathbf{w}_{t-1}\|_2^2 + \eta_t^2 \|\partial f(\mathbf{w}_{t-1}; z_{i_t})\|_2^2 - 2\eta_t \langle \partial f(\mathbf{w}_{t-1}; z_{i_t}), \mathbf{w}_{t-1} \rangle.$$

The convexity of f implies

$$\begin{aligned}\eta_t \|\partial f(\mathbf{w}_{t-1}; z_{i_t})\|_2^2 - 2\langle \partial f(\mathbf{w}_{t-1}; z_{i_t}), \mathbf{w}_{t-1} \rangle &\leq \eta_t \|\partial f(\mathbf{w}_{t-1}; z_{i_t})\|_2^2 + 2\Big(f(0; z_{i_t}) - f(\mathbf{w}_{t-1}; z_{i_t})\Big) \\ &\leq G^2 + 2 \sup_{z \in \mathcal{Z}} f(0; z),\end{aligned}$$

where we used $\eta_t < 1$ and Lipschitz continuity and non-negativity of f. Combining the above two inequalities together, we get

$$\|\mathbf{w}_t\|_2^2 \leq \|\mathbf{w}_{t-1}\|_2^2 + \big(G^2 + 2 \sup_{z \in \mathcal{Z}} f(0; z)\big)\eta_t.$$

Applying the above inequality recursively and noting that $\mathbf{w}_0 = 0$, we get

$$\|\mathbf{w}_t\|_2^2 \leq \big(G^2 + 2 \sup_{z \in \mathcal{Z}} f(0; z)\big) \sum_{k=1}^{t-1} \eta_k \leq \big(G^2 + 2 \sup_{z \in \mathcal{Z}} f(0; z)\big) \sum_{k=1}^{T} \eta_k.$$

Recall that $D_0 = \|\mathbf{w}^*\|_2$ and $D = \big((G^2 + 2\sup_{z \in \mathcal{Z}} f(0; z)) \sum_{k=1}^T \eta_k\big)^{1/2} + D_0$, it then follows that

$$\begin{aligned}&\sum_{j=K_P}^{T} \eta_j \sum_{i=1}^{n} \Big(\frac{1}{n} - [P^{k_j}]_{i_{j-k_j}, i}\Big)[f(\mathbf{w}_{j-k_j}; z_i) - f(\mathbf{w}^*; z_i)] \\ &\leq GD \sum_{j=K_P}^{T} \eta_j \sum_{i=1}^{n} \Big|\frac{1}{n} - [P^{k_j}]_{i_{j-k_j}, i}\Big| \leq \sum_{j=K_P}^{T} \frac{G\eta_j}{2j},\end{aligned} \tag{B.8}$$

where the first inequality used $|f(\mathbf{w}_t; z_i) - f(\mathbf{w}^*; z_i)| \leq G\|\mathbf{w}_t - \mathbf{w}^*\|_2 \leq G(\|\mathbf{w}_t\|_2 + \|\mathbf{w}^*\|_2) \leq GD$ for any $t \in [T]$. On the other hand, note that $[P^{k_j}]_{i,i'} \geq 0$ for any $i, i' \in [n]$ and k_j, then

$$\begin{aligned}&\sum_{i=1}^{n} \Big(\frac{1}{n} - [P^{k_j}]_{i_{j-k_j}, i}\Big)[f(\mathbf{w}_{j-k_j}; z_i) - f(\mathbf{w}^*; z_i)] \\ &\leq \sum_{i=1}^{n} \Big(\frac{1}{n} + [P^{k_j}]_{i_{j-k_j}, i}\Big)|f(\mathbf{w}_{j-k_j}; z_i) - f(\mathbf{w}^*; z_i)| \leq 2G\|\mathbf{w}_{j-k_j} - \mathbf{w}^*\|_2 \leq 2GD,\end{aligned}$$

where the last second inequality used Lipschitz continuity of f and $\sum_{j=1}^n [P^x]_{i,j} = 1$ for any fixed $i \in [n]$ and $x \geq 1$. Therefore, there holds

$$\sum_{j=1}^{K_P - 1} \eta_j \sum_{i=1}^{n} \Big(\frac{1}{n} - [P^{k_j}]_{i_{j-k_j}, i}\Big)[f(\mathbf{w}_{j-k_j}; z_i) - f(\mathbf{w}^*; z_i)] \leq 2GD \sum_{j=1}^{K_P - 1} \eta_j.$$

Combining the above inequality and (B.8) together, we get

$$\sum_{j=1}^{T} \eta_j \sum_{i=1}^{n} \Big(\frac{1}{n} - [P^{k_j}]_{i_{j-k_j}, i}\Big)[f(\mathbf{w}_{j-k_j}; z_i) - f(\mathbf{w}^*; z_i)] \leq \sum_{j=K_P}^{T} \frac{G\eta_j}{2j} + 2GD \sum_{j=1}^{K_P - 1} \eta_j. \tag{B.9}$$

Putting (B.7) and (B.9) back into (B.6), we obtain

$$\begin{aligned}&\sum_{j=1}^{T} \eta_j \mathbb{E}_{\mathcal{A}}[F_S(\mathbf{w}_{j-k_j}) - F_S(\mathbf{w}^*)] \\ &\leq \frac{\|\mathbf{w}^*\|_2^2 + 4GD \sum_{j=1}^{K_P - 1} \eta_j}{2} + \frac{G^2 \sum_{j=1}^{T} \big(2\eta_j \sum_{k=j-k_j+1}^{j} \eta_k + \eta_j^2\big)}{2} + \frac{G \sum_{j=K_P}^{T} \eta_j / j}{2}.\end{aligned} \tag{B.10}$$

Now, plugging (B.4) and (B.10) back into (B.3), we have

$$\mathbb{E}_{\mathcal{A}}[F_S(\bar{\mathbf{w}}_t) - F_S(\mathbf{w}^*)] \leq \frac{\|\mathbf{w}^*\|_2^2 + 4GD\sum_{j=1}^{K_P-1}\eta_j + G^2\sum_{j=1}^{T}\left(4\eta_j\sum_{k=j-k_j+1}^{j}\eta_k + \eta_j^2\right)}{2\sum_{j=1}^{T}\eta_j} + \frac{G\sum_{j=K_P}^{T}\eta_j/j}{2\sum_{j=1}^{T}\eta_j}.$$

Furthermore, choosing $\eta_j \equiv \eta = \frac{1}{\sqrt{T\log(T)}}$ and noting $D = \mathcal{O}(\sqrt{\eta T}) = \mathcal{O}\big((T/\log(T))^{1/4}\big)$, we have

$$\begin{aligned}\mathbb{E}_{\mathcal{A}}[F_S(\bar{\mathbf{w}}_T) - F_S(\mathbf{w}^*)] &= \mathcal{O}\big(\frac{1 + K_P\eta^{\frac{3}{2}}\sqrt{T} + T\eta^2 + \sum_{j=1}^{T}k_j\eta^2}{T\eta}\big) \\ &= \mathcal{O}\Big(\frac{\sqrt{\log(T)}\big(1 + \sum_{j=1}^{T}k_j\eta^2\big)}{\sqrt{T}} + \frac{K_P\sqrt{\eta}}{\sqrt{T}}\Big).\end{aligned} \tag{B.11}$$

Recall that $k_j = \min\Big\{\max\Big\{\Big\lceil\frac{\log(2C_PDnj)}{\log(1/\lambda(P))}\Big\rceil, K_P\Big\}, j\Big\}$. Let $K = \frac{1}{2C_PDn\lambda(P)^{K_P}}$. If $j \leq K$, we have $k_j \leq K_P$ and

$$\sum_{j=1}^{K}k_j\eta^2 \leq KK_P\eta^2 = \frac{K_P}{T^{\frac{5}{4}}\log^{\frac{3}{4}}(T)2C_Pn\lambda(P)^{K_P}}.$$

If $j > K$, there holds $k_j \leq \Big\lceil\frac{\log(2C_PDnj)}{\log(1/\lambda(P))}\Big\rceil$. Then we have

$$\begin{aligned}\sum_{j=K+1}^{T}k_j\eta^2 &\leq \frac{1}{\log(1/\lambda(P))}\Big[\sum_{j=K+1}^{T}\log(2C_PD)\eta^2 + \sum_{j=K+1}^{T}\log(n)\eta^2 + \sum_{j=K+1}^{T}\log(j)\eta^2\Big] + T\eta^2 \\ &= \mathcal{O}\Big(\frac{\log(n) + \log(T)}{\log(1/\lambda(P))\log(T)} + 1\Big) = \mathcal{O}\Big(\frac{1}{\log(1/\lambda(P))}\Big).\end{aligned}$$

Here, we use a reasonable assumption $n = \mathcal{O}(T)$. Combining the above two cases, we get

$$\sum_{j=1}^{T}k_j\eta^2 = \mathcal{O}\Big(\frac{K_P}{T^{\frac{5}{4}}\log^{\frac{3}{4}}(T)C_Pn\lambda(P)^{K_P}} + \frac{1}{\log(1/\lambda(P))}\Big). \tag{B.12}$$

Putting (B.12) back into (B.11) yields

$$\mathbb{E}_{\mathcal{A}}[F_S(\bar{\mathbf{w}}_T) - F_S(\mathbf{w}^*)] = \mathcal{O}\Big(\frac{\sqrt{\log(T)}}{\sqrt{T}\log(1/\lambda(P))} + \frac{K_P}{T^{\frac{3}{4}}\log^{\frac{1}{4}}(T)\min\{\sqrt{T\log(T)}C_Pn\lambda(P)^{K_P}, 1\}}\Big).$$

Note Assumption 4 implies $K_P = 0$, then

$$\mathbb{E}_{\mathcal{A}}[F_S(\bar{\mathbf{w}}_T) - F_S(\mathbf{w}^*)] = \mathcal{O}\Big(\frac{\sqrt{\log(T)}}{\sqrt{T}\log(1/\lambda(P))}\Big),$$

which completes the proof. □

To understand the variation of the algorithm, we present a confidence-based bound for optimization error, which matches the bound in expectation up to a constant factor.

Theorem B.2 (High-probability bound)**.** *Suppose f is convex and Assumptions 1, 2 and 4 hold. Let $\mathcal{A}$ be MC-SGD with T iterations and $\{\mathbf{w}_j\}_{j=1}^{T}$ be produced by $\mathcal{A}$ with $\eta_j \equiv \eta = 1/\sqrt{T\log(T)}$. Assume $\sup_{z\in\mathcal{Z}} f(\mathbf{w}; z) \leq B$ for some $B > 0$. Let $\gamma \in (0, 1)$, then with probability at least $1 - \gamma$*

$$F_S(\bar{\mathbf{w}}_T) - F_S(\mathbf{w}^*) = \mathcal{O}\Big(\frac{\sqrt{\log(T)}\big(\frac{1}{\log(1/\lambda(P))} + B\sqrt{\log(\frac{1}{\gamma})}\big)}{\sqrt{T}}\Big).$$

Proof of Theorem B.2. We decompose the optimization error as follows

$$\begin{aligned}\sum_{j=1}^{T}\eta_j[F_S(\bar{\mathbf{w}}_t)-F_S(\mathbf{w}^*)] &\le \sum_{j=1}^{T}\eta_j[F_S(\mathbf{w}_j)-F_S(\mathbf{w}_{j-k_j})]+\sum_{j=1}^{T}\eta_j[F_S(\mathbf{w}_{j-k_j})-F_S(\mathbf{w}^*)]\\ &\le G\sum_{j=1}^{T}\eta_j\|\mathbf{w}_j-\mathbf{w}_{j-k_j}\|_2+\sum_{j=1}^{T}\eta_j[F_S(\mathbf{w}_{j-k_j})-F_S(\mathbf{w}^*)]\\ &\le G^2\sum_{j=1}^{T}\eta_j\sum_{k=j-k_j+1}^{j}\eta_k+\sum_{j=1}^{T}\eta_j[F_S(\mathbf{w}_{j-k_j})-F_S(\mathbf{w}^*)], \quad \text{(B.13)}\end{aligned}$$

where the last second inequality used the Lipschitz continuity of f and the last inequality follows from the update rule (4).

Consider the second term in (B.13). Let $\xi_j=\eta_j[f(\mathbf{w}_{j-k_j};z_{i_j})-f(\mathbf{w}^*;z_{i_j})]$. Observe that $|\xi_j-\mathbb{E}_{i_j}[\xi_j]|\le 2B\eta_j$. Then, applying Lemma A.5 implies, with probability at least $1-\gamma$, that

$$\sum_{j=1}^{T}\mathbb{E}_{i_j}[\xi_j]-\sum_{j=1}^{T}\xi_j\le 2B\Big(2\sum_{j=1}^{T}\eta_j^2\log(1/\gamma)\Big)^{1/2}. \quad \text{(B.14)}$$

Note (B.5) implies

$$\begin{aligned}&\sum_{j=1}^{T}\eta_j[F_S(\mathbf{w}_{j-k_j})-F_S(\mathbf{w}^*)]+\sum_{j=1}^{T}\eta_j\sum_{i=1}^{n}\Big([P^{k_j}]_{i_{j-k_j},i}-\frac{1}{n}\Big)[f(\mathbf{w}_{j-k_j};z_i)-f(\mathbf{w}^*;z_i)]\\ &=\sum_{j=1}^{T}\mathbb{E}_{i_j}[\eta_j f(\mathbf{w}_{j-k_j};z_{i_j})-f(\mathbf{w}^*;z_{i_j})|\mathbf{w}_0,\ldots,\mathbf{w}_{j-k_j},z_{i_1},\ldots,z_{i_{j-k_j}}],\end{aligned}$$

which combines with (B.14) yields

$$\begin{aligned}&\sum_{j=1}^{T}\eta_j[F_S(\mathbf{w}_{j-k_j})-F_S(\mathbf{w}^*)]+\sum_{j=1}^{T}\eta_j\sum_{i=1}^{n}\Big([P^{k_j}]_{i_{j-k_j},i}-\frac{1}{n}\Big)[f(\mathbf{w}_{j-k_j};z_i)-f(\mathbf{w}^*;z_i)]\\ &\le\sum_{j=1}^{T}\eta_j[f(\mathbf{w}_{j-k_j};z_{i_j})-f(\mathbf{w}^*;z_{i_j})]+2B\Big(2\sum_{j=1}^{T}\eta_j^2\log(1/\gamma)\Big)^{1/2}.\end{aligned}$$

Putting (B.7) and (B.9) back into the above inequality, we obtain

$$\begin{aligned}&\sum_{j=1}^{T}\eta_j[F_S(\mathbf{w}_{j-k_j})-F_S(\mathbf{w}^*)]\\ &\le\sum_{j=1}^{T}\eta_j\sum_{i=1}^{n}\Big(\frac{1}{n}-[P^{k_j}]_{i_{j-k_j},i}\Big)[f(\mathbf{w}_{j-k_j};z_i)-f(\mathbf{w}^*;z_i)]\\ &\quad+\sum_{j=1}^{T}\eta_j[f(\mathbf{w}_{j-k_j};z_{i_j})-f(\mathbf{w}^*;z_{i_j})]+2B\Big(2\sum_{j=1}^{T}\eta_j^2\log(1/\gamma)\Big)^{1/2}\\ &\le\frac{C+G^2\sum_{j=1}^{T}\big(2\eta_j\sum_{k=j-k_j+1}^{j}\eta_k+\eta_j^2\big)}{2}+\frac{G\sum_{j=K_P}^{T}\eta_j/j+4B\Big(2\sum_{j=1}^{T}\eta_j^2\log(1/\gamma)\Big)^{1/2}}{2},\end{aligned} \quad \text{(B.15)}$$

where $C=\|\mathbf{w}^*\|_2^2+4GD\sum_{j=1}^{K_P-1}\eta_j$.

Now, plugging (B.15) back into (B.13), with probability at least $1-\gamma$, there holds

$$\begin{aligned}\sum_{j=1}^{T}\eta_j[F_S(\bar{\mathbf{w}}_t)-F_S(\mathbf{w}^*)]\le&\frac{C+G^2\sum_{j=1}^{T}\big(4\eta_j\sum_{k=j-k_j+1}^{j}\eta_k+\eta_j^2\big)}{2}\\ &+\frac{G\sum_{j=K_P}^{T}\eta_j/j+4B\Big(2\sum_{j=1}^{T}\eta_j^2\log(1/\gamma)\Big)^{1/2}}{2}.\end{aligned}$$

By Jensen's inequality, there holds

$$F_S(\bar{\mathbf{w}}_t) - F_S(\mathbf{w}^*) \leq \frac{C + G^2 \sum_{j=1}^T \big(4\eta_j \sum_{k=j-k_j+1}^j \eta_k + \eta_j^2\big)}{2\sum_{j=1}^T \eta_j} + \frac{G\sum_{j=K_P}^T \eta_j/j + 4B\Big(2\sum_{j=1}^T \eta_j^2 \log(1/\gamma)\Big)^{1/2}}{2\sum_{j=1}^T \eta_j}.$$

Similar as the discussion in Theorem B.1, by choosing $\eta_j \equiv \eta = 1/\sqrt{T\log(T)}$, there holds

$$F_S(\bar{\mathbf{w}}_T) - F_S(\mathbf{w}^*) = \mathcal{O}\Big(\frac{\sqrt{\log(T)}\big(\log^{-1}(1/\lambda(P)) + B\sqrt{\log(1/\gamma)}\big)}{\sqrt{T}} + \frac{K_P}{T^{\frac{3}{4}}\log^{\frac{1}{4}}(T)\min\{\sqrt{T\log(T)}C_P n\lambda(P)^{K_P}, 1\}}\Big)\Big).$$

If we further assume the Markov chain is reversible with $P = P^\top$, then we have

$$F_S(\bar{\mathbf{w}}_T) - F_S(\mathbf{w}^*) = \mathcal{O}\Big(\frac{\sqrt{\log(T)}\big(\frac{1}{\log(1/\lambda(P))} + B\sqrt{\log(\frac{1}{\gamma})}\big)}{\sqrt{T}}\Big).$$

The proof is completed. □

The following theorem provides the convergence analysis for non-convex problems. Since the convergence in terms of objective values cannot be given, we only measure the convergence rate in terms of gradient norm. The proof follows from [69].

Theorem B.3 (Non-convex case)**.** *Suppose Assumptions 1, 2 and 3 hold. Let $\mathcal{A}$ be MC-SGD with T iterations and $\{\mathbf{w}_j\}_{j=1}^T$ be produced by $\mathcal{A}$. Let D be the diameter of $\mathcal{W}$, and*

$$k_j = \min\Big\{\max\Big\{\Big\lceil\frac{\log(2C_P Dnj)}{\log(1/\lambda(P))}\Big\rceil, K_P\Big\}, j\Big\}, j \in [T].$$

Then

$$\min_{1\leq j\leq T} \mathbb{E}_{\mathcal{A}}\big[\|\partial F_S(\mathbf{w}_j)\|_2^2\big] \leq \frac{C + \sum_{j=K_P}^T \eta_j/j}{2\sum_{j=1}^T \eta_j} + \frac{G^2 L \sum_{j=1}^T (\eta_j^2 + k_j \sum_{k=j-k_j}^j \eta_k^2 + 6\eta_j \sum_{k=j-k_j}^j \eta_k)}{2\sum_{j=1}^T \eta_j},$$

where $C = 2(F_S(\mathbf{w}_0) + 2G^2 \sum_{j=1}^{K_P-1} \eta_j)$. Furthermore, suppose Assumption 4 holds. Selecting $\eta_j \equiv \eta = 1/\big(\log(T)\sqrt{T}\big)$ implies $\min_{1\leq j\leq T} \mathbb{E}_{\mathcal{A}}\big[\|\partial F_S(\mathbf{w}_j)\|_2^2\big] = \mathcal{O}\big(\log(T)/(\sqrt{T}\log^2(1/(\lambda(P)))\big)$.

Proof of Theorem B.3. Let $k_j = \min\Big\{\max\Big\{\Big\lceil\frac{\log(2C_P Dnj)}{\log(1/\lambda(P))}\Big\rceil, K_P\Big\}, j\Big\}$. Consider the following decomposition

$$\sum_{j=1}^T \eta_j \mathbb{E}_{\mathcal{A}}\big[\|\partial F_S(\mathbf{w}_j)\|_2^2\big] = \sum_{j=1}^T \eta_j \mathbb{E}_{\mathcal{A}}\big[\|\partial F_S(\mathbf{w}_j)\|_2^2 - \|\partial F_S(\mathbf{w}_{j-k_j})\|_2^2\big] + \sum_{j=1}^T \eta_j \mathbb{E}_{\mathcal{A}}\big[\|\partial F_S(\mathbf{w}_{j-k_j})\|_2^2\big]. \tag{B.16}$$

Note that

$$\begin{aligned}
&\sum_{j=1}^T \eta_j \mathbb{E}_{\mathcal{A}}\big[\|\partial F_S(\mathbf{w}_j)\|_2^2 - \|\partial F_S(\mathbf{w}_{j-k_j})\|_2^2\big] \\
&\leq \sum_{j=1}^T \eta_j \mathbb{E}_{\mathcal{A}}\big[\big(\|\partial F_S(\mathbf{w}_j)\|_2 + \|\partial F_S(\mathbf{w}_{j-k_j})\|_2\big)\big(\|\partial F_S(\mathbf{w}_j)\|_2 - \|\partial F_S(\mathbf{w}_{j-k_j})\|_2\big)\big] \\
&\leq 2G\sum_{j=1}^T \eta_j \mathbb{E}_{\mathcal{A}}[\|\partial F_S(\mathbf{w}_j) - \partial F_S(\mathbf{w}_{j-k_j})\|_2] \leq 2GL\sum_{j=1}^T \eta_j \mathbb{E}_{\mathcal{A}}\big[\|\mathbf{w}_j - \mathbf{w}_{j-k_j}\|_2\big] \\
&\leq 2G^2 L \sum_{j=1}^T \eta_j \sum_{k=j-k_j}^j \eta_k,
\end{aligned} \tag{B.17}$$

where the second inequality used the fact that f is G-Lipschitz, the third inequality follows from the smoothness of f, and the last inequality used the update rule (4). The first term in (B.16) is bounded.

Now, we turn to estimate the second term in (B.16). Note that

$$\begin{aligned}
&\mathbb{E}_{i_j}\big[\langle \partial f(\mathbf{w}_{j-k_j}; z_{i_j}), \partial F_S(\mathbf{w}_{j-k_j})\rangle | \mathbf{w}_0, \ldots, \mathbf{w}_{j-k_j}, i_1, \ldots, i_{j-k_j}\big] \\
&= \sum_{i=1}^{n} \langle \partial f(\mathbf{w}_{j-k_j}; z_i), \partial F_S(\mathbf{w}_{j-k_j})\rangle \cdot \Pr(i_j = i | i_{j-k_j}) \\
&= \sum_{i=1}^{n} \langle \partial f(\mathbf{w}_{j-k_j}; z_i), \partial F_S(\mathbf{w}_{j-k_j})\rangle \cdot [P^{k_j}]_{i_{j-k_j}, i} \\
&= \frac{1}{n}\sum_{i=1}^{n} \langle \partial f(\mathbf{w}_{j-k_j}; z_i), \partial F_S(\mathbf{w}_{j-k_j})\rangle + \sum_{i=1}^{n}\Big([P^{k_j}]_{i_{j-k_j}, i} - \frac{1}{n}\Big)\langle \partial f(\mathbf{w}_{j-k_j}; z_i), \partial F_S(\mathbf{w}_{j-k_j})\rangle \\
&= \|\partial F_S(\mathbf{w}_{j-k_j})\|_2^2 + \sum_{i=1}^{n}\Big([P^{k_j}]_{i_{j-k_j}, i} - \frac{1}{n}\Big)\langle \partial f(\mathbf{w}_{j-k_j}; z_i), \partial F_S(\mathbf{w}_{j-k_j})\rangle. \qquad \text{(B.18)}
\end{aligned}$$

Taking total expectations on both sides and summing over j yields

$$\begin{aligned}
\sum_{j=1}^{T} \eta_j \mathbb{E}_{\mathcal{A}}\big[\|\partial F_S(\mathbf{w}_{j-k_j})\|_2^2\big] =& \sum_{j=1}^{T} \eta_j \mathbb{E}_{\mathcal{A}}\big[\langle \partial f(\mathbf{w}_{j-k_j}; z_{i_j}), \partial F_S(\mathbf{w}_{j-k_j})\rangle\big] \\
&+ \sum_{j=1}^{T} \eta_j \mathbb{E}_{\mathcal{A}}\Big[\sum_{i=1}^{n}\Big(\frac{1}{n} - [P^{k_j}]_{i_{j-k_j}, i}\Big)\langle \partial f(\mathbf{w}_{j-k_j}; z_i), \partial F_S(\mathbf{w}_{j-k_j})\rangle\Big]. \qquad \text{(B.19)}
\end{aligned}$$

Consider the first term in (B.19). By the smoothness of f, we have

$$\begin{aligned}
F_S(\mathbf{w}_j) &\le F_S(\mathbf{w}_{j-1}) + \langle \mathbf{w}_j - \mathbf{w}_{j-1}, \partial F_S(\mathbf{w}_{j-1})\rangle + \frac{L}{2}\|\mathbf{w}_j - \mathbf{w}_{j-1}\|_2^2 \\
&\le F_S(\mathbf{w}_{j-1}) + \langle \mathbf{w}_j - \mathbf{w}_{j-1}, \partial F_S(\mathbf{w}_{j-k_j})\rangle + \langle \mathbf{w}_j - \mathbf{w}_{j-1}, \partial F_S(\mathbf{w}_{j-1}) - \partial F_S(\mathbf{w}_{j-k_j})\rangle \\
&\quad + \frac{L}{2}\|\mathbf{w}_j - \mathbf{w}_{j-1}\|_2^2 \\
&\le F_S(\mathbf{w}_{j-1}) + \langle \mathbf{w}_j - \mathbf{w}_{j-1}, \partial F_S(\mathbf{w}_{j-k_j})\rangle + \frac{1}{2}\|\mathbf{w}_j - \mathbf{w}_{j-1}\|_2^2 \\
&\quad + \frac{1}{2}\|\partial F_S(\mathbf{w}_{j-1}) - \partial F_S(\mathbf{w}_{j-k_j})\|_2^2 + \frac{LG^2\eta_j^2}{2} \\
&\le F_S(\mathbf{w}_{j-1}) + \langle \mathbf{w}_j - \mathbf{w}_{j-1}, \partial F_S(\mathbf{w}_{j-k_j})\rangle + \frac{(L+1)G^2\eta_j^2}{2} + \frac{L^2\|\mathbf{w}_j - \mathbf{w}_{j-k_j}\|_2^2}{2} \\
&\le F_S(\mathbf{w}_{j-1}) + \langle \mathbf{w}_j - \mathbf{w}_{j-1}, \partial F_S(\mathbf{w}_{j-k_j})\rangle + \frac{(L+1)G^2\eta_j^2}{2} + \frac{G^2L^2k_j\sum_{k=j-k_j}^{j}\eta_k^2}{2},
\end{aligned}$$

where the third inequality used $ab \le a^2/2 + b^2/2$, and the last inequality follows from $\|\mathbf{w}_j - \mathbf{w}_{j-k_j}\|_2^2 = \|\sum_{k=j-k_j}^{j}\eta_k \partial f(\mathbf{w}_{k-1}; z_{i_{k-1}})\|_2^2 \le k_j G^2 \sum_{k=j-k_j}^{j}\eta_k^2$. Rearrangement of the above inequality and taking expectation over $\mathcal{A}$ give us

$$\begin{aligned}
\mathbb{E}_{\mathcal{A}}[\langle \mathbf{w}_{j-1} - \mathbf{w}_j, \partial F_S(\mathbf{w}_{j-k_j})\rangle] \le& \mathbb{E}_{\mathcal{A}}[F_S(\mathbf{w}_{j-1}) - F_S(\mathbf{w}_j)] + \frac{(L+1)G^2\eta_j^2}{2} \\
&+ \frac{G^2L^2k_j\sum_{k=j-k_j}^{j}\eta_k^2}{2}. \qquad \text{(B.20)}
\end{aligned}$$

Note that

$$
\begin{aligned}
&\mathbb{E}_{\mathcal{A}}\big[\langle \mathbf{w}_{j-1} - \mathbf{w}_j, \partial F_S(\mathbf{w}_{j-k_j})\rangle\big] \\
&= \eta_j \mathbb{E}_{\mathcal{A}}\big[\langle \partial f(\mathbf{w}_{j-1}; z_{i_j}), \partial F_S(\mathbf{w}_{j-k_j})\rangle\big] \\
&= \eta_j \mathbb{E}_{\mathcal{A}}\big[\langle \partial f(\mathbf{w}_{j-k_j}; z_{i_j}), \partial F_S(\mathbf{w}_{j-k_j})\rangle\big] + \eta_j \mathbb{E}\big[\langle \partial f(\mathbf{w}_{j-1}; z_{i_j}) - \partial f(\mathbf{w}_{j-k_j}; z_{i_j}), \partial F_S(\mathbf{w}_{j-k_j})\rangle\big] \\
&\geq \eta_j \mathbb{E}_{\mathcal{A}}\big[\langle \partial f(\mathbf{w}_{j-k_j}; z_{i_j}), \partial F_S(\mathbf{w}_{j-k_j})\rangle\big] - G^2 L \eta_j \sum_{k=j-k_j}^{j} \eta_k.
\end{aligned}
$$

Combining (B.20) with the above inequality together, we obtain

$$
\begin{aligned}
&\eta_j \mathbb{E}_{\mathcal{A}}\big[\langle \partial f(\mathbf{w}_{j-k_j}; z_{i_j}), \partial F_S(\mathbf{w}_{j-k_j})\rangle\big] \\
&\leq \mathbb{E}_{\mathcal{A}}[F_S(\mathbf{w}_{j-1}) - F_S(\mathbf{w}_j)] + \frac{G^2 L(\eta_j^2 + L k_j \sum_{k=j-k_j}^{j} \eta_k^2 + 2\eta_j \sum_{k=j-k_j}^{j} \eta_k) + G^2 \eta_j^2}{2}.
\end{aligned} \tag{B.21}
$$

Summing over j yields

$$
\begin{aligned}
&\sum_{j=1}^{T} \eta_j \mathbb{E}_{\mathcal{A}}[\langle \partial f(\mathbf{w}_{j-k_j}; z_{i_j}), \partial F_S(\mathbf{w}_{j-k_j})\rangle] \\
&\leq F_S(\mathbf{w}_0) + \frac{G^2 L \sum_{j=1}^{T}(\eta_j^2 + k_j \sum_{k=j-k_j}^{j} \eta_k^2 + 2\eta_j \sum_{k=j-k_j}^{j} \eta_k) + G^2 \sum_{j=1}^{T} \eta_j^2}{2}.
\end{aligned} \tag{B.22}
$$

Now, we consider the second term in (B.19). Similar as the proof of Theorem B.1, it is easy to obtain the following bound by using Lemma A.1

$$
\begin{aligned}
&\sum_{j=1}^{T} \eta_j \mathbb{E}_{\mathcal{A}}\Big[\sum_{i=1}^{n} \Big(\frac{1}{n} - [P^{k_j}]_{i_{j-k_j}, i}\Big) \langle \partial f(\mathbf{w}_{j-k_j}; z_{i_j}), \partial F_S(\mathbf{w}_{j-k_j})\rangle\Big] \\
&\leq G^2 \sum_{j=1}^{K_P - 1} \eta_j \sum_{i=1}^{n} \Big(\frac{1}{n} + [P^{k_j}]_{i_{j-k_j}, i}\Big) + G^2 \sum_{j=K_P}^{T} \eta_j \sum_{i=1}^{n} \Big|\frac{1}{n} - [P^{k_j}]_{i_{j-k_j}, i}\Big| \\
&\leq 2G^2 \sum_{j=1}^{K_P - 1} \eta_j + \sum_{j=K_P}^{T} \eta_j / 2j.
\end{aligned} \tag{B.23}
$$

Plugging (B.22) and (B.23) back into (B.19), we have

$$
\begin{aligned}
&\sum_{j=1}^{T} \eta_j \mathbb{E}_{\mathcal{A}}\big[\|\partial F_S(\mathbf{w}_{j-k_j})\|_2^2\big] \\
&\leq \frac{2(F_S(\mathbf{w}_0) + 2G^2 \sum_{j=1}^{K_P - 1} \eta_j) + \sum_{j=K_P}^{T} \eta_j / j + G^2 \sum_{j=1}^{T} \eta_j^2}{2} \\
&\quad + \frac{G^2 L \sum_{j=1}^{T}(\eta_j^2 + L k_j \sum_{k=j-k_j}^{j} \eta_k^2 + 2\eta_j \sum_{k=j-k_j}^{j} \eta_k)}{2}.
\end{aligned} \tag{B.24}
$$

Finally, putting (B.17) and (B.24) back into (B.16), we obtain

$$
\begin{aligned}
\sum_{j=1}^{T} \eta_j \min_{1 \leq j \leq T} \mathbb{E}_{\mathcal{A}}\big[\|\partial F_S(\mathbf{w}_j)\|_2^2\big] &\leq \sum_{j=1}^{T} \eta_j \mathbb{E}_{\mathcal{A}}\big[\|\partial F_S(\mathbf{w}_j)\|_2^2\big] \\
&\leq \frac{2(F_S(\mathbf{w}_0) + 2G^2 \sum_{j=1}^{K_P - 1} \eta_j) + \sum_{j=K_P}^{T} \eta_j / j + G^2 \sum_{j=1}^{T} \eta_j^2}{2} \\
&\quad + \frac{G^2 L \sum_{j=1}^{T}(\eta_j^2 + L k_j \sum_{k=j-k_j}^{j} \eta_k^2 + 6\eta_j \sum_{k=j-k_j}^{j} \eta_k)}{2}.
\end{aligned}
$$

Dividing both sides of the above inequality by $\sum_{j=1}^T \eta_j$ yields

$$\min_{1\le j\le T} \mathbb{E}_{\mathcal{A}}\big[\|\partial F_S(\mathbf{w}_j)\|_2^2\big] \le \frac{2(F_S(\mathbf{w}_0) + 2G^2\sum_{j=1}^{K_P-1}\eta_j) + \sum_{j=K_P}^T \eta_j/j + \sum_{j=1}^T G^2\eta_j^2}{2\sum_{j=1}^T \eta_j} + \frac{G^2 L\sum_{j=1}^T(\eta_j^2 + Lk_j\sum_{k=j-k_j}^j \eta_k^2 + 6\eta_j\sum_{k=j-k_j}^j \eta_k)}{2\sum_{j=1}^T \eta_j}.$$

If we set $\eta_j \equiv \eta = \frac{1}{\sqrt{T}\log(T)}$, then

$$\min_{1\le j\le T} \mathbb{E}_{\mathcal{A}}\big[\|\partial F_S(\mathbf{w}_j)\|_2^2\big] = \mathcal{O}\Big(\frac{K_P}{T} + \frac{1}{T\eta} + \eta + \frac{\sum_{j=1}^T k_j^2\eta^2}{T\eta}\Big) = \mathcal{O}\Big(\frac{K_P}{T} + \frac{\log(T)\big(1+\sum_{j=1}^T k_j^2\eta^2\big)}{\sqrt{T}}\Big).$$

It suffices to estimate $\sum_{j=1}^T k_j^2\eta^2$. Recall that $k_j = \min\Big\{\max\Big\{\Big\lceil \frac{\log(2C_P Dnj)}{\log(1/\lambda(P))}\Big\rceil, K_P\Big\}, j\Big\}$. Let $K = \frac{1}{2C_P Dn\lambda(P)^{K_P}}$. If $j \le K$, we have $k_j \le K_P$ and

$$\sum_{j=1}^K k_j^2\eta^2 \le KK_P^2\eta^2 = \frac{K_P^2}{T\log(T)2C_P Dn\lambda(P)^{K_P}}.$$

If $j > K$, there holds $k_j \le \Big\lceil \frac{\log(2C_P Dnj)}{\log(1/\lambda(P))}\Big\rceil$. Then with a reasonable assumption $n = \mathcal{O}(T)$ we have

$$\begin{aligned}\sum_{j=K+1}^T k_j^2\eta^2 &\le \frac{6}{\log^2(1/\lambda(P))}\Big[\sum_{j=K+1}^T \big(\log(2C_P D)\big)^2\eta^2 + \sum_{j=K+1}^T \log^2(n)\eta^2 + \sum_{j=K+1}^T \log^2(j)\eta^2\Big] \\ &\quad + 2T\eta^2 \\ &= \mathcal{O}\Big(\frac{1}{\log^2(1/\lambda(P))}\Big).\end{aligned}$$

Combining the above two cases together yields

$$\sum_{j=1}^T k_j^2\eta^2 = \mathcal{O}\Big(\frac{K_P^2}{T\log(T)C_P n\lambda(P)^{K_P}} + \frac{1}{\log^2(1/\lambda(P))}\Big).$$

Therefore,

$$\min_{1\le j\le T} \mathbb{E}_{\mathcal{A}}\big[\|\partial F_S(\mathbf{w}_j)\|_2^2\big] = \mathcal{O}\Big(\frac{K_P}{T} + \frac{\log(T)}{\sqrt{T}}\big(\frac{K_P^2}{T\log(T)C_P n\lambda(P)^{K_P}} + \frac{1}{\log^2(1/\lambda(P))}\big)\Big).$$

The stated bound then follows from $K_P = 0$. □

B.3 Proofs of Theorem 3 and Theorem 4

Proof of Theorem 3. Let $\eta_j \equiv \eta$. According to Part (a) in Theorem 2 and (B.11), we know

$$\begin{aligned}\mathbb{E}_{S,\mathcal{A}}[F(\bar{\mathbf{w}}_T) - F_S(\mathbf{w}^*)] &= \mathbb{E}_{S,\mathcal{A}}[F(\bar{\mathbf{w}}_T) - F_S(\bar{\mathbf{w}}_T)] + \mathbb{E}_{\mathcal{A}}[F_S(\bar{\mathbf{w}}_T) - F_S(\mathbf{w}^*)] \\ &= \mathcal{O}\Big(\frac{T\eta}{n} + \frac{1 + \big(T + \sum_{j=1}^T k_j\big)\eta^2}{T\eta} + \frac{K_P\sqrt{\eta}}{\sqrt{T}}\Big).\end{aligned}$$

Setting $\eta = \frac{1}{\sqrt{T\log(T)}}$ and choosing $T \asymp n$, we have

$$\begin{aligned}&\mathbb{E}_{S,\mathcal{A}}[F(\bar{\mathbf{w}}_T) - F_{S,\mathcal{A}}(\mathbf{w}^*)] \\ &= \mathcal{O}\Big(\frac{\sqrt{T}}{n} + \frac{\sqrt{\log(T)}}{\sqrt{T}\log(1/\lambda(P))} + \frac{K_P}{T^{\frac{3}{4}}\log^{\frac{1}{4}}(T)\min\{\sqrt{T\log(T)}C_P n\lambda(P)^{K_P}\}}\Big) \\ &= \mathcal{O}\Big(\frac{\sqrt{\log(n)}}{\sqrt{n}\log(1/\lambda(P))} + \frac{K_P}{n^{\frac{3}{4}}\log^{\frac{1}{4}}(n)\min\{\sqrt{n\log(n)}C_P n\lambda(P)^{K_P}, 1\}}\Big),\end{aligned}$$

where the first equality follows from Eq.(B.12). Note that $K_P = 0$ when $P = P^\top$, we immediately obtain

$$\mathbb{E}_{S,\mathcal{A}}[F(\bar{\mathbf{w}}_T) - F_{S,\mathcal{A}}(\mathbf{w}^*)] = \mathcal{O}\Big(\frac{\sqrt{\log(n)}}{\sqrt{n}\log(1/\lambda(P))}\Big).$$

□

Proof of Theorem 4 . Part (b) in Theorem 2 and (B.11) implies

$$\begin{aligned}\mathbb{E}_{S,\mathcal{A}}[F(\bar{\mathbf{w}}_T) - F_S(\mathbf{w}^*)] &= \mathbb{E}_{S,\mathcal{A}}[F(\bar{\mathbf{w}}_T) - F_S(\bar{\mathbf{w}}_T)] + \mathbb{E}_{\mathcal{A}}[F_S(\bar{\mathbf{w}}_T) - F_S(\mathbf{w}^*)] \\ &= \mathcal{O}\big(\sqrt{T}\eta + \frac{T\eta}{n} + \frac{1 + (T + \sum_{j=1}^T k_j)\eta^2}{T\eta} + \frac{K_P\sqrt{\eta}}{\sqrt{T}}\big). \end{aligned} \tag{B.25}$$

Selecting $\eta = T^{-\frac{3}{4}}$. Similar as the discussion in Theorem B.1, we know

$$\begin{aligned}\sum_{j=1}^T k_j\eta^2 &= \sum_{j=1}^K k_j\eta^2 + \sum_{j=K+1}^T k_j\eta^2 \\ &\le KK_P\eta^2 + \frac{1}{\log(1/\lambda(P))}\big(\sum_{j=K+1}^T \log(2C_PD)\eta^2 + \sum_{j=K+1}^T \log(n)\eta^2 + \sum_{j=K+1}^T \log(j)\eta^2\big) \\ &\quad + T\eta^2 \\ &= \mathcal{O}\Big(\frac{\log(T)}{\sqrt{T}\log(1/\lambda(P))} + \frac{K_P}{T^{13/8}C_Pn\lambda(P)^{K_P}}\Big),\end{aligned}$$

where $K = \frac{1}{2C_PDn\lambda(P)^{K_P}}$ and $D = \mathcal{O}(\sqrt{\eta T})$. Note transition matrix P is symmetric implies $K_P = 0$. Plugging the above estimation with $K_P = 0$ back into (B.25) and choosing $T \asymp n^2$, we get

$$\mathbb{E}_{S,\mathcal{A}}[F(\bar{\mathbf{w}}_T)] - F(\mathbf{w}^*) = \mathcal{O}\Big(\frac{1}{\sqrt{n}\log(1/\lambda(P))}\Big).$$

The above results The proof is completed. □

C Proofs of Markov Chain SGDA

In this section, we present the proof on MC-SGDA. Let $(\mathbf{w}^*, \mathbf{v}^*)$ be a saddle point of F, i.e., for any $\mathbf{w} \in \mathcal{W}, \mathbf{v} \in \mathcal{V}$, there holds $F(\mathbf{w}^*, \mathbf{v}) \le F(\mathbf{w}^*, \mathbf{v}^*) \le F(\mathbf{w}, \mathbf{v}^*)$.

C.1 Proofs of Theorem 5-Theorem 8

We first prove Theorem 5 on the connection between stability and generalization for minimax problems.

Proof of Theorem 5. We follow the argument in [38] to prove Theorem 5. For any function $g, \tilde{g}$, we have the basic inequalities

$$\begin{aligned}&\sup_{\mathbf{w}} g(\mathbf{w}) - \sup_{\mathbf{w}} \tilde{g}(\mathbf{w}) \le \sup_{\mathbf{w}} \big(g(\mathbf{w}) - \tilde{g}(\mathbf{w})\big) \\ &\inf_{\mathbf{w}} g(\mathbf{w}) - \inf_{\mathbf{w}} \tilde{g}(\mathbf{w}) \le \sup_{\mathbf{w}} \big(g(\mathbf{w}) - \tilde{g}(\mathbf{w})\big).\end{aligned} \tag{C.1}$$

According to Eq. (C.1), we know

$$\begin{aligned}\triangle^w(\mathcal{A}_{\mathbf{w}}(S), \mathcal{A}_{\mathbf{v}}(S)) - \triangle^w_{emp}(\mathcal{A}_{\mathbf{w}}(S), \mathcal{A}_{\mathbf{v}}(S)) \le &\sup_{\mathbf{v}' \in \mathcal{V}} \mathbb{E}[F(\mathcal{A}_{\mathbf{w}}(S), \mathbf{v}') - F_S(\mathcal{A}_{\mathbf{w}}(S), \mathbf{v}')] \\ &+ \sup_{\mathbf{w}' \in \mathcal{W}} \mathbb{E}[F_S(\mathbf{w}', \mathcal{A}_{\mathbf{v}}(S)) - F(\mathbf{w}', \mathcal{A}_{\mathbf{v}}(S))].\end{aligned}$$

Recall that $S = \{z_1, \ldots, z_n\}$, $\tilde{S} = \{\tilde{z}_1, \ldots, \tilde{z}_n\}$ and $S^{(i)} = \{z_1, \ldots, z_{i-1}, \tilde{z}_i, z_{i+1}, \ldots, z_n\}$. According to the symmetry between z_i and $\tilde{z}_i$ we know

$$\begin{aligned}
\mathbb{E}[F(\mathcal{A}_{\mathbf{w}}(S), \mathbf{v}') - F_S(\mathcal{A}_{\mathbf{w}}(S), \mathbf{v}')] &= \frac{1}{n}\sum_{i=1}^n \mathbb{E}[F(\mathcal{A}_{\mathbf{w}}(S^{(i)}), \mathbf{v}')] - \mathbb{E}[F_S(\mathcal{A}_{\mathbf{w}}(S), \mathbf{v}')] \\
&= \frac{1}{n}\sum_{i=1}^n \mathbb{E}\big[f(\mathcal{A}_{\mathbf{w}}(S^{(i)}), \mathbf{v}'; z_i) - f(\mathcal{A}_{\mathbf{w}}(S), \mathbf{v}'; z_i)\big] \\
&\leq \frac{G}{n}\sum_{i=1}^n \mathbb{E}\big[\|\mathcal{A}_{\mathbf{w}}(S^{(i)}) - \mathcal{A}_{\mathbf{w}}(S)\|_2\big],
\end{aligned}$$

where the second identity holds since z_i is not used to train $\mathcal{A}_{\mathbf{w}}(S^{(i)})$ and the last inequality holds due to the Lipschitz continuity of f. In a similar way, we can prove

$$\mathbb{E}[F_S(\mathbf{w}', \mathcal{A}_{\mathbf{v}}(S)) - F(\mathbf{w}', \mathcal{A}_{\mathbf{v}}(S))] \leq \frac{G}{n}\sum_{i=1}^n \mathbb{E}\big[\|\mathcal{A}_{\mathbf{v}}(S^{(i)}) - \mathcal{A}_{\mathbf{v}}(S)\|_2\big].$$

As a combination of the above three inequalities we get

$$\triangle^w(\mathcal{A}_{\mathbf{w}}(S), \mathcal{A}_{\mathbf{v}}(S)) - \triangle_S^w(\mathcal{A}_{\mathbf{w}}(S), \mathcal{A}_{\mathbf{v}}(S)) \leq \frac{G}{n}\sum_{i=1}^n \mathbb{E}\Big[\|\mathcal{A}_{\mathbf{w}}(S^{(i)}) - \mathcal{A}_{\mathbf{w}}(S)\|_2 + \|\mathcal{A}_{\mathbf{v}}(S^{(i)}) - \mathcal{A}_{\mathbf{v}}(S)\|_2\Big].$$

This proves Part (a). Part (b) was proved in [38]. The proof is completed. □

To prove our stability bounds, we first introduce two useful lemmas. The first lemma is due to [60], while the second lemma is elementary.

Lemma C.1 ([60]). *Let f be ρ-SC-SC with $\rho \geq 0$. For any $(\mathbf{w}, \mathbf{v})$ and $(\mathbf{w}', \mathbf{v}')$, then*

$$\left\langle \begin{pmatrix} \mathbf{w} - \mathbf{w}' \\ \mathbf{v} - \mathbf{v}' \end{pmatrix}, \begin{pmatrix} \partial_{\mathbf{w}} f(\mathbf{w}, \mathbf{v}) - \partial_{\mathbf{w}} f(\mathbf{w}', \mathbf{v}') \\ \partial_{\mathbf{v}} f(\mathbf{w}', \mathbf{v}') - \partial_{\mathbf{v}} f(\mathbf{w}, \mathbf{v}) \end{pmatrix} \right\rangle \geq \rho \left\| \begin{pmatrix} \mathbf{w} - \mathbf{w}' \\ \mathbf{v} - \mathbf{v}' \end{pmatrix} \right\|_2^2. \tag{C.2}$$

Lemma C.2. *Let $b, c \geq 0$. If $x^2 \leq bx + c$, then $x \leq b + \sqrt{c}$.*

Proof of Theorem 6. For any $i \in [n]$, define $S^{(i)} = \{z_1, \ldots, z_{i-1}, \tilde{z}_i, z_{i+1}, \ldots, z_n\}$ as the set formed from S by replacing the i-th element with $\tilde{z}_i$. Let $(\mathbf{w}_t^{(i)}, \mathbf{v}_t^{(i)})$ be produced by MC-SGDA based on $S^{(i)}$ for $i \in [n]$. Note that the projection step is nonexpansive.

We first prove Part (a). We consider two cases at the t-th iteration.

Case 1. If $i_t \neq i$, then it follows from the L-smoothness of f and Lemma C.1 with $\rho = 0$ that

$$\begin{aligned}
&\left\| \begin{pmatrix} \mathbf{w}_t - \mathbf{w}_t^{(i)} \\ \mathbf{v}_t - \mathbf{v}_t^{(i)} \end{pmatrix} \right\|_2^2 \\
&\leq \left\| \begin{pmatrix} \mathbf{w}_{t-1} - \eta_t \partial_{\mathbf{w}} f(\mathbf{w}_{t-1}, \mathbf{v}_{t-1}; z_{i_t}) - \mathbf{w}_{t-1}^{(i)} + \eta_t \partial_{\mathbf{w}} f(\mathbf{w}_{t-1}^{(i)}, \mathbf{v}_{t-1}^{(i)}; z_{i_t}) \\ \mathbf{v}_{t-1} + \eta_t \partial_{\mathbf{v}} f(\mathbf{w}_{t-1}, \mathbf{v}_{t-1}; z_{i_t}) - \mathbf{v}_{t-1}^{(i)} - \eta_t \partial_{\mathbf{v}} f(\mathbf{w}_{t-1}^{(i)}, \mathbf{v}_{t-1}^{(i)}; z_{i_t}) \end{pmatrix} \right\|_2^2 \\
&= \left\| \begin{pmatrix} \mathbf{w}_{t-1} - \mathbf{w}_{t-1}^{(i)} \\ \mathbf{v}_{t-1} - \mathbf{v}_{t-1}^{(i)} \end{pmatrix} \right\|_2^2 + \eta_t^2 \left\| \begin{pmatrix} \partial_{\mathbf{w}} f(\mathbf{w}_{t-1}, \mathbf{v}_{t-1}; z_{i_t}) - \partial_{\mathbf{w}} f(\mathbf{w}_{t-1}^{(i)}, \mathbf{v}_{t-1}^{(i)}; z_{i_t}) \\ \partial_{\mathbf{v}} f(\mathbf{w}_{t-1}, \mathbf{v}_{t-1}; z_{i_t}) - \partial_{\mathbf{v}} f(\mathbf{w}_{t-1}^{(i)}, \mathbf{v}_{t-1}^{(i)}; z_{i_t}) \end{pmatrix} \right\|_2^2 \\
&\quad - 2\eta_t \left\langle \begin{pmatrix} \mathbf{w}_{t-1} - \mathbf{w}_{t-1}^{(i)} \\ \mathbf{v}_{t-1} - \mathbf{v}_{t-1}^{(i)} \end{pmatrix}, \begin{pmatrix} \partial_{\mathbf{w}} f(\mathbf{w}_{t-1}, \mathbf{v}_{t-1}; z_{i_t}) - \partial_{\mathbf{w}} f(\mathbf{w}_{t-1}^{(i)}, \mathbf{v}_{t-1}^{(i)}; z_{i_t}) \\ \partial_{\mathbf{v}} f(\mathbf{w}_{t-1}^{(i)}, \mathbf{v}_{t-1}^{(i)}; z_{i_t}) - \partial_{\mathbf{v}} f(\mathbf{w}_{t-1}, \mathbf{v}_{t-1}; z_{i_t}) \end{pmatrix} \right\rangle \\
&\leq (1 + L^2\eta_t^2) \left\| \begin{pmatrix} \mathbf{w}_{t-1} - \mathbf{w}_{t-1}^{(i)} \\ \mathbf{v}_{t-1} - \mathbf{v}_{t-1}^{(i)} \end{pmatrix} \right\|_2^2.
\end{aligned} \tag{C.3}$$

Case 2. If $i_t = i$, then it follows from the Lipschitz continuity of f that

$$\begin{aligned}
&\left\|\begin{pmatrix}\mathbf{w}_t - \mathbf{w}_t^{(i)}\\ \mathbf{v}_t - \mathbf{v}_t^{(i)}\end{pmatrix}\right\|_2^2\\
\leq&\left\|\begin{pmatrix}\mathbf{w}_{t-1} - \eta_t\nabla_{\mathbf{w}} f(\mathbf{w}_{t-1},\mathbf{v}_{t-1};z_i) - \mathbf{w}_{t-1}^{(i)} + \eta_t\nabla_{\mathbf{w}} f(\mathbf{w}_{t-1}^{(i)},\mathbf{v}_{t-1}^{(i)};\tilde{z}_i)\\ \mathbf{v}_{t-1} + \eta_t\nabla_{\mathbf{v}} f(\mathbf{w}_{t-1},\mathbf{v}_{t-1};z_i) - \mathbf{v}_{t-1}^{(i)} - \eta_t\nabla_{\mathbf{v}} f(\mathbf{w}_{t-1}^{(i)},\mathbf{v}_{t-1}^{(i)};\tilde{z}_i)\end{pmatrix}\right\|_2^2\\
=&\left\|\begin{pmatrix}\mathbf{w}_{t-1} - \mathbf{w}_{t-1}^{(i)}\\ \mathbf{v}_{t-1} - \mathbf{v}_{t-1}^{(i)}\end{pmatrix}\right\|_2^2 + \eta_t^2\left\|\begin{pmatrix}\partial_{\mathbf{w}} f(\mathbf{w}_{t-1},\mathbf{v}_{t-1};z_i) - \partial_{\mathbf{w}} f(\mathbf{w}_{t-1}^{(i)},\mathbf{v}_{t-1}^{(i)};\tilde{z}_i)\\ \partial_{\mathbf{v}} f(\mathbf{w}_{t-1},\mathbf{v}_{t-1};z_i) - \partial_{\mathbf{v}} f(\mathbf{w}_{t-1}^{(i)},\mathbf{v}_{t-1}^{(i)};\tilde{z}_i)\end{pmatrix}\right\|_2^2\\
&+ 2\eta_t\left\|\begin{pmatrix}\mathbf{w}_{t-1} - \mathbf{w}_{t-1}^{(i)}\\ \mathbf{v}_{t-1} - \mathbf{v}_{t-1}^{(i)}\end{pmatrix}\right\|_2\left\|\begin{pmatrix}\partial_{\mathbf{w}} f(\mathbf{w}_{t-1},\mathbf{v}_{t-1};z_i) - \partial_{\mathbf{w}} f(\mathbf{w}_{t-1}^{(i)},\mathbf{v}_{t-1}^{(i)};\tilde{z}_i)\\ \partial_{\mathbf{v}} f(\mathbf{w}_{t-1}^{(i)},\mathbf{v}_{t-1}^{(i)};\tilde{z}_i) - \partial_{\mathbf{v}} f(\mathbf{w}_{t-1},\mathbf{v}_{t-1};z_i)\end{pmatrix}\right\|_2\\
\leq&\left\|\begin{pmatrix}\mathbf{w}_{t-1} - \mathbf{w}_{t-1}^{(i)}\\ \mathbf{v}_{t-1} - \mathbf{v}_{t-1}^{(i)}\end{pmatrix}\right\|_2^2 + 8\eta_t^2G^2 + 4\sqrt{2}G\eta_t\left\|\begin{pmatrix}\mathbf{w}_{t-1} - \mathbf{w}_{t-1}^{(i)}\\ \mathbf{v}_{t-1} - \mathbf{v}_{t-1}^{(i)}\end{pmatrix}\right\|_2
\end{aligned}\tag{C.4}$$

We can combine the above two inequalities together and get the following inequality

$$\begin{aligned}
\left\|\begin{pmatrix}\mathbf{w}_t - \mathbf{w}_t^{(i)}\\ \mathbf{v}_t - \mathbf{v}_t^{(i)}\end{pmatrix}\right\|_2^2 \leq&(1+L^2\eta_t^2)\left\|\begin{pmatrix}\mathbf{w}_{t-1} - \mathbf{w}_{t-1}^{(i)}\\ \mathbf{v}_{t-1} - \mathbf{v}_{t-1}^{(i)}\end{pmatrix}\right\|_2^2 + 8\eta_t^2G^2\mathbb{I}_{[i_t=i]}\\
&+ 4\sqrt{2}G\eta_t\left\|\begin{pmatrix}\mathbf{w}_{t-1} - \mathbf{w}_{t-1}^{(i)}\\ \mathbf{v}_{t-1} - \mathbf{v}_{t-1}^{(i)}\end{pmatrix}\right\|_2\mathbb{I}_{[i_t=i]}.
\end{aligned}$$

We can apply the above inequality recursively and derive

$$\begin{aligned}
\left\|\begin{pmatrix}\mathbf{w}_t - \mathbf{w}_t^{(i)}\\ \mathbf{v}_t - \mathbf{v}_t^{(i)}\end{pmatrix}\right\|_2^2 \leq&L^2\sum_{j=1}^{t-1}\eta_j^2\left\|\begin{pmatrix}\mathbf{w}_j - \mathbf{w}_j^{(i)}\\ \mathbf{v}_j - \mathbf{v}_j^{(i)}\end{pmatrix}\right\|_2^2 + 8G^2\sum_{j=1}^{t}\eta_j^2\mathbb{I}_{[i_j=i]}\\
&+ 4\sqrt{2}G\sum_{j=1}^{t}\eta_j\left\|\begin{pmatrix}\mathbf{w}_{j-1} - \mathbf{w}_{j-1}^{(i)}\\ \mathbf{v}_{j-1} - \mathbf{v}_{j-1}^{(i)}\end{pmatrix}\right\|_2\mathbb{I}_{[i_j=i]}
\end{aligned}$$

For simplicity, we let

$$\delta_t^{(i)} = \max_{j\in[t]}\left\|\begin{pmatrix}\mathbf{w}_j - \mathbf{w}_j^{(i)}\\ \mathbf{v}_j - \mathbf{v}_j^{(i)}\end{pmatrix}\right\|_2.\tag{C.5}$$

Then we have

$$\begin{aligned}
\big(\delta_t^{(i)}\big)^2 \leq& L^2\big(\delta_t^{(i)}\big)^2\sum_{j=1}^{t-1}\eta_j^2 + 8G^2\sum_{j=1}^{t}\eta_j^2\mathbb{I}_{[i_j=i]} + 4\sqrt{2}G\delta_t^{(i)}\sum_{j=1}^{t}\eta_j\mathbb{I}_{[i_j=i]}\\
\leq& \frac{\big(\delta_t^{(i)}\big)^2}{2} + 8G^2\sum_{j=1}^{t}\eta_j^2\mathbb{I}_{[i_j=i]} + 4\sqrt{2}G\delta_t^{(i)}\sum_{j=1}^{t}\eta_j\mathbb{I}_{[i_j=i]},
\end{aligned}$$

where we have used $\sum_{j=1}^t \eta_j^2 \leq 1/(2L^2)$. It then follows that

$$\big(\delta_t^{(i)}\big)^2 \leq 16G^2\sum_{j=1}^{t}\eta_j^2\mathbb{I}_{[i_j=i]} + 8\sqrt{2}G\delta_t^{(i)}\sum_{j=1}^{t}\eta_j\mathbb{I}_{[i_j=i]}.$$

We can apply Lemma C.2 with $x = \delta_t^{(i)}$ to show that

$$\left\|\begin{pmatrix}\mathbf{w}_t - \mathbf{w}_t^{(i)}\\ \mathbf{v}_t - \mathbf{v}_t^{(i)}\end{pmatrix}\right\|_2 \leq \delta_t^{(i)} \leq 4G\Big(\sum_{j=1}^{t}\eta_j^2\mathbb{I}_{[i_j=i]}\Big)^{\frac{1}{2}} + 8\sqrt{2}G\sum_{j=1}^{t}\eta_j\mathbb{I}_{[i_j=i]}.$$

It then follows from the concavity of the function $x \mapsto \sqrt{x}$ that

$$\begin{aligned}\frac{1}{n}\sum_{i=1}^n \left\| \begin{pmatrix} \mathbf{w}_t - \mathbf{w}_t^{(i)} \\ \mathbf{v}_t - \mathbf{v}_t^{(i)} \end{pmatrix} \right\|_2 &\leq \frac{4G}{n}\sum_{i=1}^n \Big(\sum_{j=1}^t \eta_j^2 \mathbb{I}_{[i_j=i]}\Big)^{\frac{1}{2}} + \frac{8\sqrt{2}G}{n}\sum_{i=1}^n\sum_{j=1}^t \eta_j \mathbb{I}_{[i_j=i]} \\ &\leq 4G\Big(\frac{1}{n}\sum_{i=1}^n\sum_{j=1}^t \eta_j^2 \mathbb{I}_{[i_j=i]}\Big)^{\frac{1}{2}} + \frac{8\sqrt{2}G}{n}\sum_{i=1}^n\sum_{j=1}^t \eta_j \mathbb{I}_{[i_j=i]} \\ &= 4G\Big(\frac{1}{n}\sum_{j=1}^t \eta_j^2\Big)^{\frac{1}{2}} + \frac{8\sqrt{2}G}{n}\sum_{j=1}^t \eta_j,\end{aligned}$$

where we have used the identity $\sum_{i=1}^n \mathbb{I}_{[i_j=i]} = 1$. Finally, the convexity of the norm implies

$$\begin{aligned}\frac{1}{n}\sum_{i=1}^n \left\| \begin{pmatrix} \bar{\mathbf{w}}_T - \bar{\mathbf{w}}_T^{(i)} \\ \bar{\mathbf{v}}_T - \bar{\mathbf{v}}_T^{(i)} \end{pmatrix} \right\|_2 &\leq \frac{4G}{n}\sum_{i=1}^n \Big(\sum_{j=1}^t \eta_j^2 \mathbb{I}_{[i_j=i]}\Big)^{\frac{1}{2}} + \frac{8\sqrt{2}G}{n}\sum_{i=1}^n\sum_{j=1}^t \eta_j \mathbb{I}_{[i_j=i]} \\ &\leq 4G\Big(\frac{1}{n}\sum_{i=1}^n\sum_{j=1}^t \eta_j^2 \mathbb{I}_{[i_j=i]}\Big)^{\frac{1}{2}} + \frac{8\sqrt{2}G}{n}\sum_{i=1}^n\sum_{j=1}^t \eta_j \mathbb{I}_{[i_j=i]} \\ &= 4G\Big(\frac{1}{n}\sum_{j=1}^t \eta_j^2\Big)^{\frac{1}{2}} + \frac{8\sqrt{2}G}{n}\sum_{j=1}^t \eta_j,\end{aligned}$$

The proof of part (a) is completed.

We now move to the nonsmooth case. In a similar way, we consider the following two cases.

Case 1. If $i_t \neq i$, analogous to Eq. (C.3), we can use the Lipschitz continuity of f to derive

$$\left\| \begin{pmatrix} \mathbf{w}_t - \mathbf{w}_t^{(i)} \\ \mathbf{v}_t - \mathbf{v}_t^{(i)} \end{pmatrix} \right\|_2^2 \leq \left\| \begin{pmatrix} \mathbf{w}_{t-1} - \mathbf{w}_{t-1}^{(i)} \\ \mathbf{v}_{t-1} - \mathbf{v}_{t-1}^{(i)} \end{pmatrix} \right\|_2^2 + 8G^2\eta_t^2.$$

Case 2. For the case $i_t = i$, we have Eq. (C.4).

We can combine the above two cases together and derive

$$\left\| \begin{pmatrix} \mathbf{w}_t - \mathbf{w}_t^{(i)} \\ \mathbf{v}_t - \mathbf{v}_t^{(i)} \end{pmatrix} \right\|_2^2 \leq \left\| \begin{pmatrix} \mathbf{w}_{t-1} - \mathbf{w}_{t-1}^{(i)} \\ \mathbf{v}_{t-1} - \mathbf{v}_{t-1}^{(i)} \end{pmatrix} \right\|_2^2 + 8G^2\eta_t^2 + 4\sqrt{2}G\eta_t \left\| \begin{pmatrix} \mathbf{w}_{t-1} - \mathbf{w}_{t-1}^{(i)} \\ \mathbf{v}_{t-1} - \mathbf{v}_{t-1}^{(i)} \end{pmatrix} \right\|_2 \mathbb{I}_{[i_t=i]}.$$

We apply the above inequality recursively and derive

$$\left\| \begin{pmatrix} \mathbf{w}_t - \mathbf{w}_t^{(i)} \\ \mathbf{v}_t - \mathbf{v}_t^{(i)} \end{pmatrix} \right\|_2^2 \leq 8G^2\sum_{j=1}^t \eta_j^2 + 4\sqrt{2}G\sum_{j=1}^t \eta_j \left\| \begin{pmatrix} \mathbf{w}_{j-1} - \mathbf{w}_{j-1}^{(i)} \\ \mathbf{v}_{j-1} - \mathbf{v}_{j-1}^{(i)} \end{pmatrix} \right\|_2 \mathbb{I}_{[i_j=i]}$$

Let $\delta_t^{(i)}$ be defined in Eq. (C.5). It then follows that

$$\big(\delta_t^{(i)}\big)^2 \leq 8G^2\sum_{j=1}^t \eta_j^2 + 4\sqrt{2}G\delta_t^{(i)}\sum_{j=1}^t \eta_j \mathbb{I}_{[i_j=i]}.$$

We can apply Lemma C.2 with $x = \delta_t^{(i)}$ to show that

$$\left\| \begin{pmatrix} \mathbf{w}_t - \mathbf{w}_t^{(i)} \\ \mathbf{v}_t - \mathbf{v}_t^{(i)} \end{pmatrix} \right\|_2 \leq \delta_t^{(i)} \leq 2\sqrt{2}G\Big(\sum_{j=1}^t \eta_j^2\Big)^{\frac{1}{2}} + 4\sqrt{2}G\sum_{j=1}^t \eta_j \mathbb{I}_{[i_j=i]}.$$

We can take an average over i to derive

$$\begin{aligned}\frac{1}{n}\sum_{i=1}^n \left\| \begin{pmatrix} \mathbf{w}_t - \mathbf{w}_t^{(i)} \\ \mathbf{v}_t - \mathbf{v}_t^{(i)} \end{pmatrix} \right\|_2 &\leq \frac{2\sqrt{2}G}{n}\sum_{i=1}^n \Big(\sum_{j=1}^t \eta_j^2\Big)^{\frac{1}{2}} + \frac{4\sqrt{2}G}{n}\sum_{i=1}^n\sum_{j=1}^t \eta_j \mathbb{I}_{[i_j=i]} \\ &= 2\sqrt{2}G\Big(\sum_{j=1}^t \eta_j^2\Big)^{\frac{1}{2}} + \frac{4\sqrt{2}G}{n}\sum_{j=1}^t \eta_j.\end{aligned}$$

It follows from the convexity of a norm that

$$\frac{1}{n}\sum_{i=1}^{n}\left\|\begin{pmatrix}\bar{\mathbf{w}}_T-\bar{\mathbf{w}}_T^{(i)}\\ \bar{\mathbf{v}}_T-\bar{\mathbf{v}}_T^{(i)}\end{pmatrix}\right\|_2 \leq \frac{2\sqrt{2}G}{n}\sum_{i=1}^{n}\Big(\sum_{j=1}^{t}\eta_j^2\Big)^{\frac{1}{2}}+\frac{4\sqrt{2}G}{n}\sum_{i=1}^{n}\sum_{j=1}^{t}\eta_j\mathbb{I}_{[i_j=i]}$$
$$=2\sqrt{2}G\Big(\sum_{j=1}^{t}\eta_j^2\Big)^{\frac{1}{2}}+\frac{4\sqrt{2}G}{n}\sum_{j=1}^{t}\eta_j.$$

The proof is completed. □

Now, we can combine the stability bounds in Theorem 6 and Theorem 5 to develop generalization bounds for weak PD risk bounds and primal population risk bounds.

Proof of Theorem 7. (a) Note Theorem 6 shows, for smooth case, that MC-SGDA is on-average ϵ-argument stable with $\epsilon \leq 4G\big(\frac{1}{n}\sum_{j=1}^{T}\eta_j^2\big)^{1/2}+\frac{8\sqrt{2}G}{n}\sum_{j=1}^{T}\eta_j$. We can combine the above stability bound with Part (a) in Theorem 5 and get the desired result. Part (b) can be proved in a similar way by combining Part (b) in Theorem 6 and Part (a) in Theorem 5. □

Proof of Theorem 8. (a) For smooth case, Theorem 6 implies that MC-SGDA is on-average ϵ-argument stable with $\epsilon \leq 4G\big(\frac{1}{n}\sum_{j=1}^{T}\eta_j^2\big)^{1/2}+\frac{8\sqrt{2}G}{n}\sum_{j=1}^{T}\eta_j$. Plugging this stability bound back into Part (b) in Theorem 5 yields the desired result. Part (b) can be directly proved by combining Part (b) in Theorem 6 and Part (b) in Theorem 5. □

C.2 Optimization Error for MC-SGDA

We now develop convergence rates on MC-SGDA for convex-concave problems. We consider bounds both in expectation and with high probability. To this aim, we decompose $\max_{\mathbf{v}\in\mathcal{V}}F_S(\bar{\mathbf{w}}_T,\mathbf{v})-\min_{\mathbf{w}\in\mathcal{W}}F_S(\mathbf{w},\bar{\mathbf{v}}_T)$ into two parts: $\frac{1}{T}\sum_{j=1}^{T}F_S(\mathbf{w}_j,\mathbf{v}_j)-\min_{\mathbf{w}\in\mathcal{W}}F_S(\mathbf{w},\bar{\mathbf{v}}_T)$ and $\max_{\mathbf{v}\in\mathcal{V}}F_S(\bar{\mathbf{w}}_T,\mathbf{v})-\frac{1}{T}\sum_{j=1}^{T}F_S(\mathbf{w}_j,\mathbf{v}_j)$, which are estimated separately.

Theorem C.3. *Suppose Assumptions 1 and 5 hold. Assume for all z, the function $(\mathbf{w},\mathbf{v})\mapsto f(\mathbf{w},\mathbf{v};z)$ is convex-concave. Let $\mathcal{A}$ be MC-SGDA with T iterations, and $\{\mathbf{w}_j,\mathbf{v}_j\}_{j=1}^{T}$ be the sequence produced by MC-SGDA with $\eta_j\equiv\eta$. Let $D_{\mathbf{w}}$ and $D_{\mathbf{v}}$ be the diameter of $\mathcal{W}$ and $\mathcal{V}$ respectively, and $D=D_{\mathbf{w}}+D_{\mathbf{v}}$. For any $j\in[T]$, let*

$$k_j=\min\Big\{\max\Big\{\Big\lceil\frac{\log(2C_PDnj^2)}{\log(1/\lambda(P))}\Big\rceil,K_P\Big\},j\Big\}. \tag{C.6}$$

Then the following inequality holds

$$\mathbb{E}_{\mathcal{A}}\big[\max_{\mathbf{v}\in\mathcal{V}}F_S(\bar{\mathbf{w}}_T,\mathbf{v})-\min_{\mathbf{w}\in\mathcal{W}}F_S(\mathbf{w},\bar{\mathbf{v}}_T)\big]\leq G^2\eta+\frac{D^2}{2T\eta}$$
$$+\frac{2GK_PD+12G^2\eta\sum_{j=1}^{T}k_j+G\sum_{j=K_P}^{T}1/j^2}{T}.$$

Furthermore, suppose Assumption 4 holds. Then selecting $\eta\asymp(T\log(T))^{-1/2}$ implies

$$\mathbb{E}_{\mathcal{A}}\big[\max_{\mathbf{v}\in\mathcal{V}}F_S(\bar{\mathbf{w}}_T,\mathbf{v})-\min_{\mathbf{w}\in\mathcal{W}}F_S(\mathbf{w},\bar{\mathbf{v}}_T)\big]=\mathcal{O}\big(\sqrt{\log(T)}/\big(\sqrt{T}\log(1/\lambda(P))\big)\big).$$

Proof of Theorem C.3. To estimate $\mathbb{E}_{\mathcal{A}}\big[\max_{\mathbf{v}\in\mathcal{V}}F_S(\bar{\mathbf{w}}_T,\mathbf{v})-\min_{\mathbf{w}\in\mathcal{W}}F_S(\mathbf{w},\bar{\mathbf{v}}_T)\big]$, we use the following decomposition

$$\mathbb{E}_{\mathcal{A}}\big[\max_{\mathbf{v}\in\mathcal{V}}F_S(\bar{\mathbf{w}}_T,\mathbf{v})-\min_{\mathbf{w}\in\mathcal{W}}F_S(\mathbf{w},\bar{\mathbf{v}}_T)\big]$$
$$=\mathbb{E}_{\mathcal{A}}\Big[\frac{1}{T}\sum_{j=1}^{T}F_S(\mathbf{w}_j,\mathbf{v}_j)-\min_{\mathbf{w}\in\mathcal{W}}F_S(\mathbf{w},\bar{\mathbf{v}}_T)\Big]+\mathbb{E}_{\mathcal{A}}\Big[\max_{\mathbf{v}\in\mathcal{V}}F_S(\bar{\mathbf{w}}_T,\mathbf{v})-\frac{1}{T}\sum_{j=1}^{T}F_S(\mathbf{w}_j,\mathbf{v}_j)\Big]. \tag{C.7}$$

Consider the first term in (C.7). Let $k_j = \min\Big\{\max\Big\{\Big\lceil \frac{\log(2C_P(D_{\mathbf{w}}+D_{\mathbf{v}})nj^2)}{\log(1/\lambda(P))}\Big\rceil, K_P\Big\}, j\Big\}$ and $\mathbf{w}_S^* = \arg\min_{\mathbf{w}\in\mathcal{W}} F_S(\mathbf{w}, \bar{\mathbf{v}}_T)$. The concavity of $F_S(\mathbf{w}, \cdot)$ implies

$$
\begin{aligned}
&\mathbb{E}_{\mathcal{A}}\Big[\frac{1}{T}\sum_{j=1}^{T} F_S(\mathbf{w}_j, \mathbf{v}_j) - F_S(\mathbf{w}_S^*, \bar{\mathbf{v}}_T)\Big] \\
&\le \mathbb{E}_{\mathcal{A}}\Big[\frac{1}{T}\sum_{j=1}^{T} \big(F_S(\mathbf{w}_j, \mathbf{v}_j) - F_S(\mathbf{w}_S^*, \mathbf{v}_j)\big)\Big] \\
&= \mathbb{E}_{\mathcal{A}}\Big[\frac{1}{T}\sum_{j=1}^{T} \big(F_S(\mathbf{w}_j, \mathbf{v}_j) - F_S(\mathbf{w}_{j-k_j}, \mathbf{v}_j)\big)\Big] + \mathbb{E}_{\mathcal{A}}\Big[\frac{1}{T}\sum_{j=1}^{T} \big(F_S(\mathbf{w}_{j-k_j}, \mathbf{v}_j) - F_S(\mathbf{w}_{j-k_j}, \mathbf{v}_{j-k_j})\big)\Big] \\
&+ \mathbb{E}_{\mathcal{A}}\Big[\frac{1}{T}\sum_{j=1}^{T} \big(F_S(\mathbf{w}_{j-k_j}, \mathbf{v}_{j-k_j}) - F_S(\mathbf{w}_S^*, \mathbf{v}_{j-k_j})\big)\Big] + \mathbb{E}_{\mathcal{A}}\Big[\frac{1}{T}\sum_{j=1}^{T} \big(F_S(\mathbf{w}_S^*, \mathbf{v}_{j-k_j}) - F_S(\mathbf{w}_S^*, \mathbf{v}_j)\big)\Big] \\
&\le \frac{3G^2\eta}{T}\sum_{j=1}^{T} k_j + \mathbb{E}_{\mathcal{A}}\Big[\frac{1}{T}\sum_{j=1}^{T} \big(F_S(\mathbf{w}_{j-k_j}, \mathbf{v}_{j-k_j}) - F_S(\mathbf{w}_S^*, \mathbf{v}_{j-k_j})\big)\Big], \qquad \text{(C.8)}
\end{aligned}
$$

where the last inequality used the Lipschitz continuity of $f(\cdot, \mathbf{v}; z)$ and $f(\mathbf{w}, \cdot; z)$ and the fact that $\|\mathbf{w}_j - \mathbf{w}_{j-k_j}\|_2 \le G\eta k_j$ and $\|\mathbf{v}_j - \mathbf{v}_{j-k_j}\|_2 \le G\eta k_j$.

Now, we turn to estimate the term $\mathbb{E}_{\mathcal{A}}\big[\frac{1}{T}\sum_{j=1}^{T}\big(F_S(\mathbf{w}_{j-k_j}, \mathbf{v}_{j-k_j}) - F_S(\mathbf{w}_S^*, \mathbf{v}_{j-k_j})\big)\big]$. Note that

$$
\begin{aligned}
&\mathbb{E}_{i_j}\big[f(\mathbf{w}_{j-k_j}, \mathbf{v}_{j-k_j}; z_{i_j}) - f(\mathbf{w}_S^*, \mathbf{v}_{j-k_j}; z_{i_j}) | (\mathbf{w}_0, \mathbf{v}_0), \ldots, (\mathbf{w}_{j-k_j}, \mathbf{v}_{j-k_j}), z_{i_1}, \ldots, z_{i_{j-k_j}}\big] \\
&= \sum_{i=1}^{n} \big[f(\mathbf{w}_{j-k_j}, \mathbf{v}_{j-k_j}; z_i) - f(\mathbf{w}_S^*, \mathbf{v}_{j-k_j}; z_i)\big] \cdot [P^{k_j}]_{i_{j-k_j}, i} \\
&= \big(F_S(\mathbf{w}_{j-k_j}, \mathbf{v}_{j-k_j}) - F_S(\mathbf{w}_S^*, \mathbf{v}_{j-k_j})\big) \\
&\quad + \sum_{i=1}^{n} \Big([P^{k_j}]_{i_{j-k_j}, i} - \frac{1}{n}\Big) \cdot \big[f(\mathbf{w}_{j-k_j}, \mathbf{v}_{j-k_j}; z_i) - f(\mathbf{w}_S^*, \mathbf{v}_{j-k_j}; z_i)\big]. \qquad \text{(C.9)}
\end{aligned}
$$

Summing over j and taking total expectation we have

$$
\begin{aligned}
&\sum_{j=1}^{T} \mathbb{E}_{\mathcal{A}}\big[F_S(\mathbf{w}_{j-k_j}, \mathbf{v}_{j-k_j}) - F_S(\mathbf{w}_S^*, \mathbf{v}_{j-k_j})\big] \\
&= \sum_{j=1}^{T} \mathbb{E}_{\mathcal{A}}\big[f(\mathbf{w}_{j-k_j}, \mathbf{v}_{j-k_j}; z_{i_j}) - f(\mathbf{w}_S^*, \mathbf{v}_{j-k_j}; z_{i_j})\big] \\
&\quad + \sum_{j=1}^{T} \mathbb{E}_{\mathcal{A}}\Big[\sum_{i=1}^{n} \Big(\frac{1}{n} - [P^{k_j}]_{i_{j-k_j}, i}\Big) \cdot \big[f(\mathbf{w}_{j-k_j}, \mathbf{v}_{j-k_j}; z_i) - f(\mathbf{w}_S^*, \mathbf{v}_{j-k_j}; z_i)\big]\Big]. \qquad \text{(C.10)}
\end{aligned}
$$

Similar to before, according to MC-SGDA update rule (5), for any j and $1 \le k_j \le j$

$$
\begin{aligned}
&\|\mathbf{w}_j - \mathbf{w}_S^*\|_2^2 \\
&\le \|\mathbf{w}_{j-1} - \eta\partial_{\mathbf{w}} f(\mathbf{w}_{j-1}, \mathbf{v}_{j-1}; z_{i_j}) - \mathbf{w}_S^*\|_2^2 \\
&= \|\mathbf{w}_{j-1} - \mathbf{w}_S^*\|_2^2 - 2\eta\langle \mathbf{w}_{j-1} - \mathbf{w}_S^*, \partial_{\mathbf{w}} f(\mathbf{w}_{j-1}, \mathbf{v}_{j-1}; z_{i_j})\rangle + \eta^2\|\partial_{\mathbf{w}} f(\mathbf{w}_{j-1}, \mathbf{v}_{j-1}; z_{i_j})\|_2^2 \\
&\le \|\mathbf{w}_{j-1} - \mathbf{w}_S^*\|_2^2 - 2\eta\big(f(\mathbf{w}_{j-1}, \mathbf{v}_{j-1}; z_{i_j}) - f(\mathbf{w}_S^*, \mathbf{v}_{j-1}; z_{i_j})\big) + G^2\eta^2 \\
&= \|\mathbf{w}_{j-1} - \mathbf{w}_S^*\|_2^2 - 2\eta\big(f(\mathbf{w}_{j-k_j}, \mathbf{v}_{j-k_j}; z_{i_j}) - f(\mathbf{w}_S^*, \mathbf{v}_{j-k_j}; z_{i_j})\big) \\
&\quad + 2\eta\big(f(\mathbf{w}_{j-k_j}, \mathbf{v}_{j-k_j}; z_{i_j}) - f(\mathbf{w}_{j-k_j}, \mathbf{v}_{j-1}; z_{i_j}) + f(\mathbf{w}_{j-k_j}, \mathbf{v}_{j-1}; z_{i_j}) - f(\mathbf{w}_{j-1}, \mathbf{v}_{j-1}; z_{i_j})\big) \\
&\quad + 2\eta\big(f(\mathbf{w}_S^*, \mathbf{v}_{j-1}; z_{i_j}) - f(\mathbf{w}_S^*, \mathbf{v}_{j-k_j}; z_{i_j})\big) + G^2\eta^2 \\
&\le \|\mathbf{w}_{j-1} - \mathbf{w}_S^*\|_2^2 - 2\eta\Big(f(\mathbf{w}_{j-k_j}, \mathbf{v}_{j-k_j}; z_{i_j}) - f(\mathbf{w}_S^*, \mathbf{v}_{j-k_j}; z_{i_j})\Big) + 6G^2\eta^2 k_j + G^2\eta^2,
\end{aligned}
$$

where the second inequality is due to the convexity of $f(\cdot, \mathbf{v}; z)$, and the last inequality used the fact that $\|\mathbf{w}_{j-k_j} - \mathbf{w}_{j-1}\|_2 \leq G\eta k_j$ and $\|\mathbf{v}_{j-k_j} - \mathbf{v}_{j-1}\|_2 \leq G\eta k_j$. Rearranging the above inequality and taking a summation of both sides over j, we get

$$\sum_{j=1}^{T} \Big(f(\mathbf{w}_{j-k_j}, \mathbf{v}_{j-k_j}; z_{i_j}) - f(\mathbf{w}_S^*, \mathbf{v}_{j-k_j}; z_{i_j}) \Big) \leq \frac{D_{\mathbf{w}}^2 + 6G^2\eta^2 \sum_{j=1}^{T} k_j + TG^2\eta^2}{2\eta}. \quad \text{(C.11)}$$

Now, we consider the second term in (C.10). Recall that $k_j = \min\Big\{ \max\Big\{ \Big\lceil \frac{\log(2C_P(D_{\mathbf{w}}+D_{\mathbf{v}})nj^2)}{\log(1/\lambda(P))} \Big\rceil, K_P \Big\}, j \Big\}$. If $j \geq K_P$, then according to Lemma A.1, for any $i, i' \in [n]$ we have

$$\Big| \frac{1}{n} - [P^{k_j}]_{i,i'} \Big| \leq \frac{1}{2(D_{\mathbf{w}} + D_{\mathbf{v}})nj^2}.$$

Combining this with Assumption 5 we get

$$\begin{aligned} &\sum_{j=K_P}^{T} \sum_{i=1}^{n} \Big(\frac{1}{n} - [P^{k_j}]_{i_{j-k_j},i} \Big) \cdot \big[f(\mathbf{w}_{j-k_j}, \mathbf{v}_{j-k_j}; z_i) - f(\mathbf{w}_S^*, \mathbf{v}_{j-k_j}; z_i) \big] \\ &\leq GD_{\mathbf{w}} \sum_{j=K_P}^{T} \sum_{i=1}^{n} \Big| [P^{k_j}]_{i_{j-k_j},i} - \frac{1}{n} \Big| \leq G \sum_{j=K_P}^{T} \frac{1}{2j^2}. \end{aligned} \quad \text{(C.12)}$$

For $j < K_P$, there holds

$$\sum_{j=1}^{K_P} \sum_{i=1}^{n} \Big(\frac{1}{n} - [P^{k_j}]_{i_{j-k_j},i} \Big) \cdot \big[f(\mathbf{w}_{j-k_j}, \mathbf{v}_{j-k_j}; z_i) - f(\mathbf{w}_S^*, \mathbf{v}_{j-k_j}; z_i) \big] \leq 2GK_P D_{\mathbf{w}}, \quad \text{(C.13)}$$

where we use $\sum_{i=1}^{n} [P^{k_j}]_{i_{j-k_j},i} = 1$ and the Lipschitz continuity of $f(\cdot, \mathbf{v})$. Combining (C.12) and (C.13) together, we get

$$\begin{aligned} &\sum_{j=1}^{T} \sum_{i=1}^{n} \Big(\frac{1}{n} - [P^{k_j}]_{i_{j-k_j},i} \Big) \cdot \big[f(\mathbf{w}_{j-k_j}, \mathbf{v}_{j-k_j}; z_i) - f(\mathbf{w}_S^*, \mathbf{v}_{j-k_j}; z_i) \big] \\ &\leq 2GK_P D_{\mathbf{w}} + G \sum_{j=K_P}^{T} \frac{1}{2j^2}. \end{aligned} \quad \text{(C.14)}$$

Putting (C.11) and (C.14) back into (C.10), we obtain

$$\begin{aligned} &\sum_{j=1}^{T} \mathbb{E}_{\mathcal{A}} \big[F_S(\mathbf{w}_{j-k_j}, \mathbf{v}_{j-k_j}) - F_S(\mathbf{w}_S^*, \mathbf{v}_{j-k_j}) \big] \\ &\leq \frac{D_{\mathbf{w}}^2 + 6G^2\eta^2 \sum_{j=1}^{T} k_j + TG^2\eta^2}{2\eta} + 2GK_P D_{\mathbf{w}} + G \sum_{j=K_P}^{T} \frac{1}{2j^2}. \end{aligned}$$

Finally, plugging the above inequality back into (C.8), we have

$$\begin{aligned} &\mathbb{E}_{\mathcal{A}} \Big[\frac{1}{T} \sum_{j=1}^{T} F_S(\mathbf{w}_j, \mathbf{v}_j) - \min_{\mathbf{w} \in \mathcal{W}} F_S(\mathbf{w}, \bar{\mathbf{v}}_T) \Big] \\ &\leq \frac{6G^2\eta \sum_{j=1}^{T} k_j}{T} + \frac{2GK_P D_{\mathbf{w}} + G \sum_{j=K_P}^{T} \frac{1}{2j^2}}{T} + \frac{D_{\mathbf{w}}^2}{2T\eta} + \frac{G^2\eta}{2}. \end{aligned}$$

In a similar way, we can show

$$\begin{aligned} &\mathbb{E}_{\mathcal{A}} \Big[\max_{\mathbf{v} \in \mathcal{V}} F_S(\bar{\mathbf{w}}_T, \mathbf{v}) - \frac{1}{T} \sum_{j=1}^{T} F_S(\mathbf{w}_j, \mathbf{v}_j) \Big] \\ &\leq \frac{6G^2\eta \sum_{j=1}^{T} k_j}{T} + \frac{2GK_P D_{\mathbf{v}} + G \sum_{j=K_P}^{T} \frac{1}{2j^2}}{T} + \frac{D_{\mathbf{v}}^2}{2T\eta} + \frac{G^2\eta}{2}. \end{aligned}$$

Combining the above two bounds together, we get

$$\mathbb{E}_{\mathcal{A}}\Big[\max_{\mathbf{v}\in\mathcal{V}} F_S(\bar{\mathbf{w}}_T,\mathbf{v}) - \min_{\mathbf{w}\in\mathcal{W}} F_S(\mathbf{w},\bar{\mathbf{v}}_T)\Big]$$
$$\leq G^2\eta + \frac{(D_{\mathbf{w}}+D_{\mathbf{v}})^2}{2T\eta} + \frac{2GK_P(D_{\mathbf{w}}+D_{\mathbf{v}}) + 12G^2\eta\sum_{j=1}^T k_j + G\sum_{j=K_P}^T \frac{1}{j^2}}{T}.$$

The first part of theorem is proved. Now, we turn to the second part of theorem. Let $K = \frac{1}{\sqrt{2C_P(D_{\mathbf{w}}+D_{\mathbf{v}})n\lambda(P)^{K_P}}}$ and $\eta \asymp 1/\sqrt{T\log(T)}$. If $j < K$, we have

$$\sum_{j=1}^{K-1} k_j\eta^2 \leq KK_P\eta^2 = \frac{K_P}{T\log(T)\sqrt{2C_P(D_{\mathbf{w}}+D_{\mathbf{v}})n\lambda(P)^{K_P}}}.$$

If $j \geq K$, there holds

$$\sum_{j=K}^T k_j\eta^2 \leq \frac{1}{\log(1/\lambda(P))}\Big[\sum_{j=K}^T \log(2C_P(D_{\mathbf{w}}+D_{\mathbf{v}}))\eta^2 + \sum_{j=K}^T \log(n)\eta^2 + 2\sum_{j=K}^T \log(j)\eta^2\Big] + T\eta^2$$
$$= \mathcal{O}\Big(\frac{1}{\log(1/\lambda(P))}\Big).$$

Combining the above two cases together, we get

$$\sum_{j=1}^T k_j\eta^2 = \mathcal{O}\Big(\frac{K_P}{T\log(T)\sqrt{C_Pn\lambda(P)^{K_P}}} + \frac{1}{\log(1/\lambda(P))}\Big). \tag{C.15}$$

Then we obtain

$$\mathbb{E}_{\mathcal{A}}\Big[\max_{\mathbf{v}\in\mathcal{V}} F_S(\bar{\mathbf{w}}_T,\mathbf{v}) - \min_{\mathbf{w}\in\mathcal{W}} F_S(\mathbf{w},\bar{\mathbf{v}}_T)\Big]$$
$$= \mathcal{O}\Big(\frac{K_P}{T} + \frac{1+\sum_{j=1}^T k_j\eta^2}{T\eta} + \eta\Big)$$
$$= \mathcal{O}\Big(\frac{\sqrt{\log(T)}}{\sqrt{T}\log(1/\lambda(P))} + \frac{K_P}{T\min\{1,\sqrt{C_Pn\lambda(P)^{K_P}T\log(T)}\}}\Big).$$

Note Assumption 4 implies $K_P = 0$. Then we get

$$\mathbb{E}_{\mathcal{A}}\Big[\max_{\mathbf{v}\in\mathcal{V}} F_S(\bar{\mathbf{w}}_T,\mathbf{v}) - \min_{\mathbf{w}\in\mathcal{W}} F_S(\mathbf{w},\bar{\mathbf{v}}_T)\Big] = \mathcal{O}\Big(\frac{\sqrt{\log(T)}}{\sqrt{T}\log(1/\lambda(P))}\Big).$$

This completes the proof. □

Theorem C.4 (High-probability bound)**.** *Suppose Assumptions 1, 4 and 5 hold. Assume for all z, the function $(\mathbf{w},\mathbf{v}) \mapsto f(\mathbf{w},\mathbf{v};z)$ is convex-concave. Let $\{\mathbf{w}_j,\mathbf{v}_j\}_{j=1}^T$ be produced MC-SGDA with $\eta_j \equiv \eta \asymp 1/\sqrt{T\log(T)}$. Assume $\sup_{z\in\mathcal{Z}} f(\mathbf{w},\mathbf{v};z) \leq B$ with some $B > 0$ for any $\mathbf{w}\in\mathcal{W}$ and $\mathbf{v}\in\mathcal{V}$. Let $\gamma \in (0,1)$. Then with probability $1-\gamma$*

$$\max_{\mathbf{v}\in\mathcal{V}} F_S(\bar{\mathbf{w}}_T,\mathbf{v}) - \min_{\mathbf{w}\in\mathcal{W}} F_S(\mathbf{w},\bar{\mathbf{v}}_T) = \mathcal{O}\Big(\frac{\sqrt{\log(T)}}{\sqrt{T}}\Big(\frac{1}{\log(1/\lambda(P))} + B\sqrt{\log(1/\gamma)}\Big)\Big).$$

Proof of Theorem C.4. Note that

$$\max_{\mathbf{v}\in\mathcal{V}} F_S(\bar{\mathbf{w}}_T,\mathbf{v}) - \min_{\mathbf{w}\in\mathcal{W}} F_S(\mathbf{w},\bar{\mathbf{v}}_T)$$
$$= \Big[\frac{1}{T}\sum_{j=1}^T F_S(\mathbf{w}_j,\mathbf{v}_j) - \min_{\mathbf{w}\in\mathcal{W}} F_S(\mathbf{w},\bar{\mathbf{v}}_T)\Big] + \Big[\max_{\mathbf{v}\in\mathcal{V}} F_S(\bar{\mathbf{w}}_T,\mathbf{v}) - \frac{1}{T}\sum_{j=1}^T F_S(\mathbf{w}_j,\mathbf{v}_j)\Big]. \tag{C.16}$$

Consider the first term in (C.16). Let $k_j = \min\left\{\max\left\{\left\lceil \frac{\log(2C_P(D_{\mathbf{w}}+D_{\mathbf{v}})nj^2)}{\log(1/\lambda(P))}\right\rceil, K_P\right\}, j\right\}$ and $\mathbf{w}_S^* = \arg\min_{\mathbf{w}\in\mathcal{W}} F_S(\mathbf{w}, \bar{\mathbf{v}}_T)$. Similar to (C.8), we can show

$$\frac{1}{T}\sum_{j=1}^{T} F_S(\mathbf{w}_j, \mathbf{v}_j) - F_S(\mathbf{w}_S^*, \bar{\mathbf{v}}_T) \leq \frac{3G^2\eta}{T}\sum_{j=1}^{T} k_j + \frac{1}{T}\sum_{j=1}^{T}\big(F_S(\mathbf{w}_{j-k_j}, \mathbf{v}_{j-k_j}) - F_S(\mathbf{w}_S^*, \mathbf{v}_{j-k_j})\big). \tag{C.17}$$

Let $\xi_j = f(\mathbf{w}_{j-k_j}, \mathbf{v}_{j-k_j}; z_{i_j}) - f(\mathbf{w}_S^*, \mathbf{v}_{j-k_j}; z_{i_j})$. Observe that $|\xi_j - \mathbb{E}_{i_j}[\xi_j]| \leq 2B$. Then, applying Lemma A.5 implies, with probability at least $1-\gamma/2$, that

$$\sum_{j=1}^{T}\mathbb{E}_{i_j}[\xi_j] - \sum_{j=1}^{T}\xi_j \leq 2B\sqrt{2T\log(2/\gamma)}. \tag{C.18}$$

Combining (C.9) and (C.18) together, we get

$$\begin{aligned}
&\sum_{j=1}^{T}[F_S(\mathbf{w}_{j-k_j}, \mathbf{v}_{j-k_j}) - F_S(\mathbf{w}_S^*, \mathbf{v}_{j-k_j})] + \sum_{j=1}^{T}\sum_{i=1}^{n}\big([P^{k_j}]_{i_{j-k_j},i} - \frac{1}{n}\big)[f(\mathbf{w}_{j-k_j}, \mathbf{v}_{j-k_j}; z_i) - f(\mathbf{w}_S^*, \mathbf{v}_{j-k_j}; z_i)] \\
&= \sum_{j=1}^{T}\mathbb{E}_{i_j}[f(\mathbf{w}_{j-k_j}, \mathbf{v}_{j-k_j}; z_{i_j}) - f(\mathbf{w}_S^*, \mathbf{v}_{j-k_j}; z_{i_j}) | \{\mathbf{w}_0, \mathbf{v}_0\}, \ldots, \{\mathbf{w}_{j-k_j}, \mathbf{v}_{j-k_j}\}, z_{i_1}, \ldots, z_{i_{j-k_j}}] \\
&\leq \sum_{j=1}^{T}[f(\mathbf{w}_{j-k_j}, \mathbf{v}_{j-k_j}; z_{i_j}) - f(\mathbf{w}_S^*, \mathbf{v}_{j-k_j}; z_{i_j})] + 2B\sqrt{2T\log(2/\gamma)}
\end{aligned}$$

with probability at least $1-\gamma/2$. Putting (C.11) and (C.14) back into the above inequality, we obtain

$$\begin{aligned}
&\sum_{j=1}^{T}[F_S(\mathbf{w}_{j-k_j}, \mathbf{v}_{j-k_j}) - F_S(\mathbf{w}_S^*, \mathbf{v}_{j-k_j})] \\
&\leq \sum_{j=1}^{T}\sum_{i=1}^{n}\Big(\frac{1}{n} - [P^{k_j}]_{i_{j-k_j},i}\Big)[f(\mathbf{w}_{j-k_j}, \mathbf{v}_{j-k_j}; z_i) - f(\mathbf{w}_S^*, \mathbf{v}_{j-k_j}; z_i)] \\
&\quad + \sum_{j=1}^{t}[f(\mathbf{w}_{j-k_j}, \mathbf{v}_{j-k_j}; z_{i_j}) - f(\mathbf{w}_S^*, \mathbf{v}_{j-k_j}; z_{i_j})] + 2B\sqrt{2T\log(2/\gamma)} \\
&\leq \frac{D_{\mathbf{w}}^2 + 6G^2\eta^2\sum_{j=1}^{T}k_j + TG^2\eta^2}{2\eta} + 2GK_PD_{\mathbf{w}} + G\sum_{j=K_P}^{T}\frac{1}{2j^2} + 2B\sqrt{2T\log(2/\gamma)}.
\end{aligned} \tag{C.19}$$

Now, plugging (C.19) back into (C.17), with probability at least $1-\gamma/2$, there holds

$$\begin{aligned}
&\frac{1}{T}\sum_{j=1}^{T}F_S(\mathbf{w}_j, \mathbf{v}_j) - \min_{\mathbf{w}\in\mathcal{W}}F_S(\mathbf{w}, \bar{\mathbf{v}}_T) \\
&\leq \frac{6G^2\eta\sum_{j=1}^{T}k_j + 2GK_PD_{\mathbf{w}} + G\sum_{j=K_P}^{T}\frac{1}{2j^2}}{T} + \frac{D_{\mathbf{w}}^2}{2T\eta} + \frac{G^2\eta}{2} + \frac{2B\sqrt{2\log(\frac{2}{\gamma})}}{\sqrt{T}}.
\end{aligned}$$

In a similar way, we can show, with probability at least $1-\gamma/2$, that

$$\begin{aligned}
&\max_{\mathbf{v}\in\mathcal{V}}F_S(\bar{\mathbf{w}}_T, \mathbf{v}) - \frac{1}{T}\sum_{j=1}^{T}F_S(\mathbf{w}_j, \mathbf{v}_j) \\
&\leq \frac{6G^2\eta\sum_{j=1}^{T}k_j + 2GK_PD_{\mathbf{v}} + G\sum_{j=K_P}^{T}\frac{1}{2j^2}}{T} + \frac{D_{\mathbf{v}}^2}{2T\eta} + \frac{G^2\eta}{2} + \frac{2B\sqrt{2\log(\frac{2}{\gamma})}}{\sqrt{T}}.
\end{aligned}$$

Combining the above two inequalities together, with probability at least $1-\gamma$, we get

$$\max_{\mathbf{v}\in\mathcal{V}} F_S(\bar{\mathbf{w}}_T,\mathbf{v}) - \min_{\mathbf{w}\in\mathcal{W}} F_S(\mathbf{w},\bar{\mathbf{v}}_T)$$
$$\leq \frac{12G^2\eta\sum_{j=1}^T k_j + 2GK_P(D_{\mathbf{w}}+D_{\mathbf{v}}) + G\sum_{j=K_P}^T \frac{1}{j^2}}{T} + \frac{(D_{\mathbf{w}}+D_{\mathbf{v}})^2}{2T\eta} + G^2\eta + \frac{4B\sqrt{2\log(\frac{2}{\gamma})}}{\sqrt{T}}.$$

Further, if we select $\eta \asymp 1/\sqrt{T\log(T)}$, according to Eq.(C.15) we have

$$\begin{aligned}
&\max_{\mathbf{v}\in\mathcal{V}} F_S(\bar{\mathbf{w}}_T,\mathbf{v}) - \min_{\mathbf{w}\in\mathcal{W}} F_S(\mathbf{w},\bar{\mathbf{v}}_T)\\
&= \mathcal{O}\Big(\frac{K_P}{T} + \eta + \frac{1+\sum_{j=1}^T k_j\eta^2}{T\eta} + \frac{B\sqrt{\log(1/\gamma)}}{\sqrt{T}}\Big)\\
&= \mathcal{O}\Big(\frac{\sqrt{\log(T)}}{\sqrt{T}}\Big(\frac{1}{\log(1/\lambda(P))} + B\sqrt{\log(1/\gamma)}\Big) + \frac{K_P}{T\min\{1,\sqrt{C_P n\lambda(P)^{K_P}T\log(T)}\}}\Big)\\
&= \mathcal{O}\Big(\frac{\sqrt{\log(T)}}{\sqrt{T}}\Big(\frac{1}{\log(1/\lambda(P))} + B\sqrt{\log(1/\gamma)}\Big)\Big),
\end{aligned}$$

where in the last equality we used $K_P = 0$ due to $P = P^\top$. This completes the proof. □

C.3 Proofs of Theorem 9 and Theorem 10

Proof of Theorem 9. We can choose η such that $T\eta^2 \leq 1/(2L^2)$ and therefore Theorem 7 applies. According to part (a) of Theorem 7 we have

$$\triangle^w(\bar{\mathbf{w}}_T,\bar{\mathbf{v}}_T) - \triangle^w_{\text{emp}}(\bar{\mathbf{w}}_T,\bar{\mathbf{v}}_T) \leq \frac{4G^2\sqrt{T}\eta}{\sqrt{n}} + \frac{8\sqrt{2}G^2T\eta}{n}.$$

Combining the above inequality with Theorem C.3 together, we get

$$\begin{aligned}
&\triangle^w(\bar{\mathbf{w}}_T,\bar{\mathbf{v}}_T) = \triangle^w(\bar{\mathbf{w}}_T,\bar{\mathbf{v}}_T) - \triangle^w_{\text{emp}}(\bar{\mathbf{w}}_T,\bar{\mathbf{v}}_T)\\
&\leq \frac{4G^2\sqrt{T}\eta}{\sqrt{n}} + \frac{8\sqrt{2}G^2T\eta}{n} + G^2\eta + \frac{D^2}{2T\eta} + \frac{2GK_PD + 12G^2\eta\sum_{j=1}^T k_j + G\sum_{j=K_P}^T 1/j^2}{T}
\end{aligned}$$

where $D = D_{\mathbf{w}} + D_{\mathbf{v}}$. If we choose $T \asymp n$ and $\eta \asymp (T\log(T))^{-\frac{1}{2}}$, according to (C.15) we get

$$\triangle^w(\bar{\mathbf{w}}_T,\bar{\mathbf{v}}_T) = \mathcal{O}\Big(\frac{\log(n)}{\sqrt{n}\log(1/\lambda(P))} + \frac{K_P}{n\min\{1, n\sqrt{\log(n)C_P\lambda(P)^{K_P}}\}}\Big).$$

Note Assumption 4 implies $K_P = 0$, the proof of part (a) is completed.

Part (b) can be proved in a similar way (e.g., by combining part (b) of Theorem 7 and Theorem C.3 together). We omit the proof for brevity. □

Proof of Theorem 10. We use the following decomposition

$$\begin{aligned}
R(\bar{\mathbf{w}}_T) - R(\mathbf{w}^*) =& \Big(R(\bar{\mathbf{w}}_T) - R_S(\bar{\mathbf{w}}_T)\Big) + \Big(R_S(\bar{\mathbf{w}}_T) - F_S(\mathbf{w}^*,\bar{\mathbf{v}}_T)\Big)\\
&+ \Big(F_S(\mathbf{w}^*,\bar{\mathbf{v}}_T) - F(\mathbf{w}^*,\bar{\mathbf{v}}_T)\Big) + \Big(F(\mathbf{w}^*,\bar{\mathbf{v}}_T) - R(\mathbf{w}^*)\Big).
\end{aligned}$$

Note that $F(\mathbf{w}^*,\bar{\mathbf{v}}_T) \leq F(\mathbf{w}^*,\mathbf{v}^*)$. Then we have

$$\begin{aligned}
R(\bar{\mathbf{w}}_T) - R(\mathbf{w}^*) \leq& \Big(R(\bar{\mathbf{w}}_T) - R_S(\bar{\mathbf{w}}_T)\Big) + \Big(R_S(\bar{\mathbf{w}}_T) - F_S(\mathbf{w}^*,\bar{\mathbf{v}}_T)\Big)\\
&+ \Big(F_S(\mathbf{w}^*,\bar{\mathbf{v}}_T) - F(\mathbf{w}^*,\bar{\mathbf{v}}_T)\Big).
\end{aligned}$$

Taking the expectation on both sides gives

$$\begin{aligned}
\mathbb{E}_{S,\mathcal{A}}[R(\bar{\mathbf{w}}_T) - R(\mathbf{w}^*)] \leq& \mathbb{E}_{S,\mathcal{A}}[R(\bar{\mathbf{w}}_T) - R_S(\bar{\mathbf{w}}_T)] + \mathbb{E}_{S,\mathcal{A}}[R_S(\bar{\mathbf{w}}_T) - F_S(\mathbf{w}^*,\bar{\mathbf{v}}_T)]\\
&+ \mathbb{E}_{S,\mathcal{A}}[F_S(\mathbf{w}^*,\bar{\mathbf{v}}_T) - F(\mathbf{w}^*,\bar{\mathbf{v}}_T)]. \qquad \text{(C.20)}
\end{aligned}$$

According to part (a) of Theorem 8 we know

$$\mathbb{E}_{S,\mathcal{A}}[R(\bar{\mathbf{w}}_T) - R_S(\bar{\mathbf{w}}_T)] \leq 4G^2(1+L/\rho)\Big(\frac{\sqrt{T}\eta}{\sqrt{n}} + \frac{2\sqrt{2}T\eta}{n}\Big).$$

Similarly, the stability bound in Theorem 6 also implies

$$\mathbb{E}_{S,\mathcal{A}}[F_S(\mathbf{w}^*, \bar{\mathbf{v}}_T) - F(\mathbf{w}^*, \bar{\mathbf{v}}_T)] \leq 4G^2(1+L/\rho)\Big(\frac{\sqrt{T}\eta}{\sqrt{n}} + \frac{2\sqrt{2}T\eta}{n}\Big).$$

According to Theorem C.3, we know

$$\begin{aligned}\mathbb{E}_{S,\mathcal{A}}[R_S(\bar{\mathbf{w}}_T) - F_S(\mathbf{w}^*, \bar{\mathbf{v}}_T)] &\leq \mathbb{E}_{\mathcal{A}}\big[\max_{\mathbf{v}\in\mathcal{V}} F_S(\bar{\mathbf{w}}_T, \mathbf{v}) - \min_{\mathbf{w}\in\mathcal{W}} F_S(\mathbf{w}, \bar{\mathbf{v}}_T)\big] \\ &\leq G^2\eta + \frac{D^2}{2T\eta} + \frac{2GK_PD + 12G^2\eta\sum_{j=1}^T k_j + G\sum_{j=K_P}^T 1/j^2}{T},\end{aligned}$$

where $D = D_{\mathbf{w}} + D_{\mathbf{v}}$. Putting the above three inequalities back into Eq. (C.20), we obtain

$$\begin{aligned}\mathbb{E}_{S,\mathcal{A}}[R(\bar{\mathbf{w}}_T) - R(\mathbf{w}^*)] \leq& 8G^2(1+L/\rho)\Big(\frac{\sqrt{T}\eta}{\sqrt{n}} + \frac{2\sqrt{2}T\eta}{n}\Big) + G^2\eta + \frac{D^2}{2T\eta} \\ &+ \frac{2GK_PD + 12G^2\eta\sum_{j=1}^T k_j + G\sum_{j=K_P}^T 1/j^2}{T}.\end{aligned}$$

If we choose $T \asymp n$ and $\eta \asymp (T\log(T))^{-1/2}$, combining the above estimation with (C.15) implies

$$\mathbb{E}_{S,\mathcal{A}}[R(\bar{\mathbf{w}}_T) - R(\mathbf{w}^*)] = \mathcal{O}\Big(\frac{(L/\rho)\log(n)}{\sqrt{n}\log(\lambda(P))} + \frac{K_P}{n\min\{1, n\sqrt{\log(n)C_P\lambda(P)^{K_P}}\}}\Big).$$

The above result combines with $K_P = 0$ complete the proof. □