What is a Good Metric to Study Generalization of Minimax Learners?

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Abstract

Minimax optimization has served as the backbone of many machine learning (ML) problems. Although the *convergence behavior* of optimization algorithms has been extensively studied in minimax settings, their *generalization* guarantees in the stochastic setting, i.e., how the solution trained on empirical data performs on the unseen testing data, have been relatively underexplored. A fundamental question remains elusive: *What is a good metric to study generalization of minimax learners?* In this paper, we aim to answer this question by first showing that *primal risk*, a universal metric to study generalization in minimization, fails in simple examples of minimax problems. Furthermore, another popular metric, the *primal-dual risk*, also fails to characterize the generalization behavior for minimax problems with nonconvexity, due to non-existence of saddle points. We thus propose a new metric to study generalization of minimax learners: the *primal gap*, to circumvent these issues. Next, we derive generalization bounds for the primal gap in nonconvex-concave settings. As byproducts of our analysis, we also solve two open questions: establishing generalization bounds for primal risk and primal-dual risk in this setting, and in the strong sense, i.e., without assuming that the maximization and expectation can be interchanged. Finally, we leverage this new metric to compare the generalization behavior of two popular algorithms – gradient descent-ascent (GDA) and gradient descent-max (GDMax) in stochastic minimax optimization.

1 Introduction

Stochastic minimax optimization, a classical and fundamental problem in operations research and game theory, involves solving the following problem:

$$\min_{w \in W} \max_{\theta \in \Theta} E_{z \sim P_z}[f(w, \theta; z)].$$

More recently, such minimax formulations have received increasing attention in machine learning, with significant applications in generative adversarial networks (GANs) [Goodfellow et al., 2014], adversarial learning [Madry et al., 2017], and reinforcement learning [Chen and Wang, 2016, Dai et al., 2018]. Most existing works have focused on the *optimization* aspect of the problem, i.e., studying the rates of convergence, robustness, and optimality of several algorithms, in various minimax settings including convex-concave [Nemirovski et al., 2009, Monteiro and Svaiter, 2010], nonconvex-concave [Lin et al., 2020, Rafique et al., 2018], and certain special nonconvex-nonconcave [Nouiehed et al., 2019, Yang et al., 2020] problems.

However, the optimization aspect is not the only venue for understanding the success of minimax optimization in machine learning. In particular, as in classical supervised learning, which is usually studied as a *minimization* problem [Hastie et al., 2009], the out-of-sample *generalization* performance

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is a key metric for evaluating the learned models. The study of generalization guarantees in minimax optimization (and related machine learning problems) has not received significant attention until recently [Arora et al., 2017, Feizi et al., 2020, Yin et al., 2019, Lei et al., 2021, Farnia and Ozdaglar, 2021, Zhang et al., 2021b]. Specifically, existing works along this line have investigated two types of generalization guarantees: *uniform* convergence generalization bounds, and *algorithm-dependent* generalization bounds. The former is more general and irrespective of the optimization algorithms being used, while the latter is usually finer and really explains what happens in practice, when optimization algorithms play an indispensable role. In fact, the former might not be able to explain generalization in deep learning [Nagarajan and Kolter, 2019], making the latter a more favorable metric for understanding the success of minimax optimization in machine learning.

Algorithm-dependent generalization for minimax optimization has been studied recently in [Farnia and Ozdaglar, 2021, Lei et al., 2021, Xing et al., 2021, Yang et al., 2022]. These papers build on the algorithmic stability framework developed in [Bousquet and Elisseeff, 2002]. In particular, these works have studied *primal risk* and/or (variants of) *primal-dual risk* under different convexity and smoothness assumptions of the objective. Primal risk (see formal definition in §2) is a natural extension of risk from minimization problems. Primal-dual risk, on the other hand, is defined similarly but based on the duality gap of the solution, which makes sense when the saddle-point exists (i.e., $\min$ and $\max$ can be interchanged). Based on these metrics, [Farnia and Ozdaglar, 2021, Lei et al., 2021], compare the performance of specific algorithms, e.g., gradient descent-ascent (GDA) and gradient descent-max (GDMax). We provide a more thorough literature review in Appendix A.

Although these metrics are natural extensions of generalization metrics from the *minimization* setting, they might not be the most suitable ones for studying generalization in stochastic *minimax* optimization, especially in the *nonconvex* settings that is pervasive in machine/deep learning applications. In particular, we are interested in the following fundamental question:

What is a good metric to study generalization of minimax learners?

In this paper, we make an initial attempt to answering this question, by identifying the inadequacies of existing metrics, and proposing a new metric, the *primal gap* that overcomes these inadequacies. We then provide generalization bounds for the newly proposed metric, and discuss how it captures information not included in the other existing metrics. We summarize our contributions as follows.

Contributions. First, we introduce an example through which we identify the inadequacies of *primal risk*, a well-studied metric for minimax generalization, in capturing the generalization behavior of *nonconvex-concave* minimax problems. Second, to address the issue, we propose a new metric – the *primal gap*, which provably avoids the issue in the example, and derive its generalization bounds. Next, we leverage this new metric to compare the generalization behavior of GDA and GDMax, two popular algorithms for minimax optimization and GAN training, and answer the question of *when does GDA generalize better than GDMax?* Moreover, we also address two open questions in the literature: establishing generalization bounds for primal risk and primal-dual risk without strong concavity or assuming that the maximization and expectation can be interchanged, while either of these assumptions was needed in the literature [Farnia and Ozdaglar, 2021, Lei et al., 2021, Xing et al., 2021, Yang et al., 2022] (see Section §E due to space limitation). Finally, under certain assumptions of the max learner, our results also generalize to the nonconvex-nonconcave setting.

2 Preliminaries

2.1 Problem formulation

In this paper, we consider the following (stochastic) minimax problem:

$$\min_{w \in W} \max_{\theta \in \Theta} E_{z \sim P_z} f(w, \theta; z). \tag{1}$$

We make the following assumption on the sets W and Θ throughout the paper.

Assumption 1. *W and Θ are convex, closed sets, and we further assume that W is compact with $\|w\| \leq M(W), \forall w \in W$. Here $M(W)$ is a constant dependent on the set W.*

Let $r(w, \theta) = E_{z \sim P_z} f(w, \theta; z)$. For a training dataset $S = \{z_1, \cdots, z_n\}$ with n i.i.d. variables drawn from P_z, we define $r_S(w, \theta) = \frac{1}{n} \sum_{i=1}^{n} f(w, \theta; z_i)$. Next, we define the following quantity:

Reference	Assumption	Metric	Rate
[Farnia and Ozdaglar, 2021]	NC$-\mu-$SC	PR	$L\sqrt{\kappa^2+1}\epsilon$
[Lei et al., 2021]	NC$-\mu-$SC	PR	$L(1+\kappa)\epsilon$
[Lei et al., 2021]	$\mu-$SC-SC	PD	$\sqrt{2}L(1+\kappa)\epsilon$
This work (Theorem 2)	NC-C	PG	$\sqrt{8\ell LC_p^2}\sqrt{\epsilon}+2L_\theta^* C_e/\sqrt{n}$
This work (Lemma 1)	NC-C	PR	$\sqrt{8\ell LC_p^2}\sqrt{\epsilon}$
This work (Theorem 6)	C-C	PD	$L\sqrt{C_p^2\ell}\sqrt{\epsilon}+L\sqrt{(C_p^w)^2\ell}\sqrt{\epsilon}$

Table 1: Generalization bounds for $\epsilon-$ stable algorithms. PR stands for Primal Risk, PD stands for the primal dual gap and PG stands for the primal gap. NC$-\mu-$SC stands for nonconvex-μ strongly concave. $\mu-$SC-SC stands for μ strongly convex-μ strongly concave. NC-C stands for nonconvex-concave. C-C convex-concave. L is the Lipschitz constant of the function f. κ stands for the condition number L/μ. The constants in the in the theorems have been defined in the appropriate sections. Note that there are other results in Farnia and Ozdaglar [2021], Lei et al. [2021] for cases where the expectation and the $\max$ operator can be interchanged. This case is almost identical to the minimization problem and we thus do not include it in the table.

Definition 1 (Primal Risk (Empirical/Population))**.** ***Primal population risk*** *is given by* $r(w) = \max_{\theta\in\Theta} E_{z\sim P_z} f(w,\theta;z)$*, and the* ***primal empirical risk*** *is given by:* $r_S(w) = \max_{\theta\in\Theta} \frac{1}{n}\sum_{i=1}^n f(w,\theta;z_i)$.

Throughout this paper, we use (w_S,θ_S) to denote a solution of the min-max problem: $\min_{w\in W}\max_{\theta\in\Theta} r_S(w,\theta)$. Notice that (w_S,θ_S) need not be a saddle point of r_S. Furthermore, we use (w^*,θ^*) to denote a solution of $\min_{w\in W}\max_{\theta\in\Theta} r(w,\theta)$. Once again, notice that (w^*,θ^*) may not be a saddle point of r.

The goal in Problem (1) is to minimize the primal population risk $r(w)$. Note that this function can be decomposed as

$$r(w) = r_S(w) + (r(w) - r_S(w)). \tag{2}$$

In practice, we only have access to $r_S(w,\theta)$ and our goal is to design algorithms for minimizing $r(w)$ using dataset S. Suppose A is a learning algorithm initialized at $(w,\theta)=(0,0)$. We define (w_S^A,θ_S^A) to be the output of Algorithm A using dataset S.

From Equation (2), it is clear if we ensure $r_S(w_S^A)$ as well as $r(w_S^A)-r_S(w_S^A)$ are small, this would guarantee that $r(w_S^A)$ is small, which is the goal of Problem (1). Note that we can always ensure that $r_S(w_S^A)$ is small by using a good optimization algorithm A (if the problem is tractable). The main goal in the study of generalization is therefore to estimate the generalization error $r(w_S^A)-r_S(w_S^A)$.

Definition 2. *The generalization error for the primal risk is defined as:*

$$\zeta_{gen}^P(A) = E_S E_A[r(w_S^A) - r_S(w_S^A)]. \tag{3}$$

Here the expectations are taken over the randomness in the dataset S, as well as any randomness used in the algorithm A.

This metric has been used to study generalization in stochastic minimization problems, i.e., when the maximization set Θ is a singleton, as well as several recent works in minimax optimization (see [Hardt et al., 2016, Farnia and Ozdaglar, 2021]).

We are interested in when the solution to the empirical problem w_S^A has good *generalization behavior*, i.e., when $E[r(w_S^A) - \min_{w\in W} r(w)]$ is small - w_S^A is an approximate minimizer of the primal population risk r. In the next subsection, we briefly describe why the generalization error of the primal risk $\zeta_{gen}^P(A)$ is a good measure to study generalization behavior in minimization problems.

2.1.1 $\zeta_{gen}^P(A)$ for minimization problems

Consider a minimization problem of the form

$$\min_{w\in W} E_{z\sim P_z}[g(w;z)]. \tag{4}$$

In this case, we define the (minimization) primal risk (population and empirical version respectively) as: $r(w) = E_{z\sim P_z} g(w;z)$, and $r_S(w) = \frac{1}{n}\sum_{i=1}^n g(w;z_i)$. The generalization error $\zeta_{gen}^{P,min}(A)$ for the (minimization) primal risk is the same as in Definition 2 using the (minimization) primal risk.

Assume that the generalization error of the primal risk for an algorithm A is small, say $\zeta_{gen}^{P,min}(A) \leq \epsilon$. This implies that (from Definition 2): $E[r(w_S^A)] \leq E[r_S(w_S^A)] + \epsilon$. Note that the expectation is with respect to S and A. Now, in order to show that w_S^A has good generalization behavior, we first see that:

$$E[r(w_S^A) - \min_{w \in W} r(w)] \leq E[r_S(w_S^A)] + \epsilon - \min_{w \in W} r(w). \tag{5}$$

However, note that for minimization problems, since $E[r_S] = r$, we have [1]: $\min_{w \in W} r(w) \geq E[\min_{w \in W} r_S(w)]$, which gives us:

$$E[r(w_S^A) - \min_{w \in W} r(w)] \leq E[r_S(w_S^A)] + \epsilon - E[\min_{w \in W} r_S(w)] = E[r_S(w_S^A) - \min_{w \in W} r_S(w)] + \epsilon = \epsilon.$$

Therefore, for minimization problems, if the generalization error for primal risk is small, we have good generalization behavior of the solution to the empirical risk minimization. In the next subsection, we highlight some results in the literature which discusses bounds on generalization error of the primal risk. These results depend on the concept of algorithmic stability which we discuss next.

2.2 Stability of algorithms

Stability analysis is a powerful tool to analyse the generalization behavior of algorithms (see [Bousquet and Elisseeff, 2002]). In this section, we will review some definitions and theoretical results about stability bounds existing in the current literature. More specifically, in this paper, we adopt the following definition of stability:

Definition 3. *Suppose that A is a randomized algorithm for solving the minimax problem. We define (w_S^A, θ_S^A) as the output of algorithm A using dataset S. We say S and S' are neighboring dataset if they defer only in one sample. An algorithm A is defined to be ϵ-stable if $\|w_S^A - w_{S'}^A\| \leq \epsilon$, $\|\theta_S^A - \theta_{S'}^A\| \leq \epsilon$ for any neighboring datasets S and S'.*

From [Hardt et al., 2016], we have the following basic result for the generalization error of $r_S(w, \theta)$:

Theorem 1 ([Hardt et al., 2016])**.** *Consider the (stochastic) minimization problem defined in* (4)*. Suppose $g(\cdot; z)$ is L-Lipschitz continuous, i.e., $\|g(w_1; z) - g(w_2; z)\| \leq L\|w_1 - w_2\|, \forall w_1, w_2 \in W$. Then, for an ϵ-stable algorithm A, we have $|E_S E_A[r(w_S^A) - r_S(w_S^A)]| \leq L\epsilon$.*

However, this theorem cannot be directly extended to analyze the generalization behavior of minimax learners because we have an additional maximization step before taking expectation.

In this paper, we first show that good bounds for $\zeta_{gen}^P(A)$ is not sufficient to conclude the generalization behaviour in minimax problems. We then propose a new measure, the primal gap $\zeta_{gen}^{PG}(A)$ which is more insightful to understand generalization behavior in minimax problems. We provide bounds for $\zeta_{gen}^{PG}(A)$ in the nonconvex-concave setting (which includes the more restrictive nonconvex - strongly concave case) and as a byproduct, we also derive bounds for $\zeta_{gen}^P(A)$ for the nonconvex-concave case, which to the best of our knowledge, is an open problem.

3 Primal Gap: A New Metric to Study Generalization

The main idea which leads to the success of $\zeta_{gen}^P(A)$ as a metric to study generalization for minimization learners is that $E[r_S] = r$, which is no longer the case in the minimax case. In fact, in this section, we show that a good bound for the generalization error of primal risk does not imply good generalization behavior in minimax problems. We then propose a new metric, the primal gap, which circumvents these issues and provides insights into the generalization behavior in minimax problems.

3.1 Is $\zeta_{gen}^P(A)$ a good metric?

We provide an example where the generalization error of the primal risk is small, but the final solution to the empirical problem has poor generalization behavior. In this example, the minimizer of $r_S(w)$ is suboptimal for $r(w)$ with high probability, and $E_S[r(w_S) - r(w^*)]$ is large.

[1] Here we use the fact that $E_z[\min_x f(x, z)] \leq \min_x E_z[f(x, z)]$.

Example 1 (Analytical example)**.** *Let $y \sim N(0, 1/\sqrt{n})$ be a Gaussian random variable in $\mathbb{R}$. Define the truncated Gaussian variable $z \sim P_z$ as follows: $z = y$ if $|y| < \lambda \log n/\sqrt{n}$ and $z = \lambda \log n/\sqrt{n}$ if $y \geq \lambda \log n/\sqrt{n}$. Let $f(w, \theta; z) = \frac{1}{2}w^2 - \left(\frac{1}{2n^2}\theta^2 - z\theta + 1\right) w$, where $w \in W = [0, 1]$, $\theta \in \Theta = [-\lambda n, \lambda n]$ with a sufficiently large $\lambda > 0$, and $z_i \sim P_z$ be i.i.d truncated Gaussian variables. Then, we have $r_S(w, \theta) = \frac{1}{2}w^2 - \left(\frac{1}{2n^2}\theta^2 - \frac{\sum_{i=1}^n z_i}{n}\theta + 1\right) w$, and*

$$r(w, \theta) = \frac{1}{2}w^2 - \left(\frac{1}{2n^2}\theta^2 + 1\right) w. \tag{6}$$

Note that this leads to the primal population risk function: $r(w) = \frac{1}{2}w^2 - w$.

It is not hard to see that we always have $r_S(w) \geq r(w)$. Note that this means $\zeta^P_{gen}(A) < 0$, and thus we have good generalization of primal risk. However, we can prove that for large enough λ,

$$E_S[r(w_S) - r(w^*)] \geq 0.02. \tag{7}$$

This means that w_S has a constant error compared to w^* in terms of the population risk, despite that the generalization error of the primal risk is small. This phenomenon is due to that $\min_{w \in W} r_S(w) - \min_{w \in W} r(w) > 0$ and hence minimizing $r_S(w)$ is very different from minimizing $r(w)$.

This example shows that the generalization error of primal risk is not a good measure to study generalization in minimax learners. The main drawback is that $\min_w r_S(w)$ and $\min_w r(w)$ can be very different. We now introduce another more practical example, from GAN training, to further illustrate this point.

Example 2 (GAN-training example)**.** *Suppose that we have a real distribution P_r in $\mathbb{R}^d$ which can be represented as $G^*(y)$ with $y \in \mathbb{R}^k$ drawn from a standard Gaussian distribution P_0 and a mapping $G^* : \mathbb{R}^k \to \mathbb{R}^d$. For an arbitrary generator G, we define P_G to be the distribution of the random variable $G(y)$ with $y \sim P_0$. So our goal is to find a generator G such that $P_G = P_r$. The generative adverserial network (GAN) is a popular tool for solving this problem. Consider a Generative Adversarial Network (GAN) with generator G and discriminator D. The goal of GAN training is to find a pair of generator G and a discriminator D that solves the min-max problem:*

$$\begin{aligned}\min_G \max_D \quad & \{E_{x \sim P_r} \Phi(D(x)) + E_{x \sim P_G}[\Phi(1 - D(x))]\} \\ &= \min_G \max_D \quad \{E_{x \sim P_r} \Phi(D(x)) + E_{y \sim P_0}[\Phi(1 - D(G(y)))]\},\end{aligned}$$

where $\Phi : \mathbb{R} \to \mathbb{R}$ is concave, monotonically increasing and $\Phi(u) = -\infty$ for $u \leq 0$. To connect to the minimax formulation in (1)*, we note that $z = (x, y)$, and $P_z = P_r \times P_0$. Also, we denote*

$$r(G, D) = E_{x \sim P_r} \Phi(D(x)) + E_{y \sim P_0}[\Phi(1 - D(G(y)))]$$

to be the population risk. We now give the empirical version of this problem. Let $S_1 = \{x_1, \cdots, x_n\}$ and $S_2 = \{y_1, \cdots, y_n\}$. Let $S = S_1 \cup S_2$ and $r_S(G, D) = \frac{1}{n}\left(\sum_{i=1}^n \Phi(D(x_i) + \Phi(1 - D(G(y_i)))\right)$. We assume that P_{G_w} has the same support set as P_r. Moreover, we assume that $\|w - w^*\| \leq 0.5$ and $G_w(y)$ is 1-Lipschitz w.r.t. w for any y. Then we have (see Theorem B.1 in Arora et al. [2017])

$$E_S[\min_{w \in W} r_S(w) - \min_{w \in W} r(w)] \geq (1 - \delta)\,(2\Phi(1) - 2\Phi(1/2))$$

which is bounded away from 0.

Note that in this example, we also have $E_S[\min_w r_S(w) - \min_w r(w)] > 0$, implying that $\zeta^P_{gen}(A)$ might not be a good metric. To address this issue, we next define a new metric to study the generalization of minimax learners.

3.2 Primal gap

The empirical and population versions of the primal gap are defined as follows:

Definition 4 (Primal gap (empirical/population))**.** *The **population primal gap** is defined as $\Delta(w) = r(w) - \min_{w \in W} r(w)$, and the **empirical primal gap** is defined as $\Delta_S(w) = r_S(w) - \min_{w \in W} r_S(w)$.*

Notice that these two primal gaps can always take 0 at $w_S = \arg\min_{w\in W} r_S(w)$ and $w^* = \arg\min_{w\in W} r(w)$ respectively even if the saddle point of problem 2 does not exist. Next, we define the expected generalization error of this primal gap as follows:

Definition 5. *The generalization error for the primal gap is defined as*

$$\zeta_{gen}^{PG}(A) = E_S E_A[\Delta(w_S^A) - \Delta_S(w_S^A)].$$

Next, we provide bounds on $\zeta_{gen}^{PG}(A)$ for stable algorithms A, and show that in Example 1, $\zeta_{gen}^{PG}(A)$ cannot be small (unlike $\zeta_{gen}^{P}(A)$).

3.3 Relationship between generalization and stability

We provide bounds for the generalization error of the primal gap (Definition 5) for $\epsilon-$stable algorithms A. We will focus on the nonconvex-concave case where the following assumptions are made throughout the rest of the paper.

Assumption 2. *The function f in Problem* (1) *is nonconvex-concave, i.e. $f(w,\cdot;z)$ is a concave function for all $w \in W$ and for all z.*

Next we define the notion of *capacity*, which will play a key role in the bounds we derive for $\zeta_{gen}^{PG}(A)$.

Definition 6 (Capacity)**.** *For any $w \in W$ and any constraint set Θ, we define*

$$\Theta(w) = \arg\max_{\theta\in\Theta} r(w,\theta) \qquad \Theta_S(w) = \arg\max_{\theta\in\Theta} r_S(w).$$

We define the capacities C_e and C_p as:

$$C_e(\Theta) = \max_S \max_{w\in W} \mathrm{dist}(0,\Theta_S(w)) \qquad C_p(\Theta) = \max_{w\in W} \mathrm{dist}(0,\Theta(w)).$$

For the specific constraint set in Problem 1, we denote the capacities as C_e and C_p respectively.

The norm of the parameter is usually viewed as the metric for the complexity of learning models. In fact, the norm of the optimal solution determines the Rademacher complexity of the function class in statistical learning theory [Vapnik, 1999]. Moreover, in deep learning, minimum-norm solution of overparameterized neural networks is well-known to enjoy better generalization performance [Zhang et al., 2021a]. Hence, we view the capacity constant C_e and C_p as natural metrics to capture the model complexity for the best response of the max learner, when using the empirical data set and population data respectively.

Now, we are ready to discuss the relationship between the stability bound and the generalization error of algorithms in nonconvex-concave minimax problems. All proofs have been deferred to the appendix. We make the following assumptions throughout the paper:

Assumption 3. *The gradient of f is ℓ-Lipschitz-continuous for all z, i.e.,*

$$\|\nabla f(w_1,\theta_1;z) - \nabla f(w_2,\theta_2;z)\| \le \ell(\|w_1-w_2\| + \|\theta_1-\theta_2\|), \forall w_1,w_2 \in W, \quad \forall \theta_1,\theta_2 \in \Theta.$$

Moreover, fixing $w \in W$, the partial gradient $\nabla_\theta f(w,\cdot;z)$ is $\ell_{\theta\theta}$-Lipschitz continuous with respect to θ for all z, i.e., $\|\nabla_\theta f(w,\theta_1;z) - \nabla_\theta f(w,\theta_2;z)\| \le \ell_{\theta\theta}\|\theta_1-\theta_2\|, \forall w \in W, \quad \forall \theta_1,\theta_2 \in \Theta$.

Assumption 4. *For any $\Theta_1 \subseteq \Theta$, we assume that f is $L(\Theta_1)$-Lipschitz-continuous with respect to $w \in W, \theta \in \Theta_1$ for all z, i.e., $\|f(w_1,\theta_1;z) - f(w_2,\theta_2;z)\| \le L(\Theta_1)(\|w_1-w_2\| + \|\theta_1-\theta_2\|), \quad \forall w_1,w_2 \in W, \forall \theta_1,\theta_2 \in \Theta_1$, and the gradient $\nabla f(w,\theta;z)$ is uniformly bounded as $\|\nabla_{w,\theta} f(w,\theta;z)\| \le L(\Theta_1)$ for all z and $w \in W, \theta \in \Theta_1$. Moreover, $f(w^*,\cdot;z)$ is L_θ^* Lipschitz continuous with respect to θ where $w^* \in \arg\min_{w\in W} r(w)$. We also define $L := L(B(0,2C_p+1)\cap\Theta)$ and $L_r := L(B(0,r)\cap\Theta)$, where $B(v,r)$ denotes the l_2-ball with radius r centered at v.*

Note that we can decompose the generalization error of the primal gap as follows:

$$\begin{aligned}\zeta_{gen}^{PG}(A) &:= E_S E_A[\Delta(w_S^A) - \Delta_S(w_S^A)] = E_S E_A[r(w_S^A) - r_S(w_S^A)] + E_S[\min_{w\in W} r_S(w) - \min_{w\in W} r(w)] \\ &= \zeta_{gen}^{P}(A) + E_S[\min_{w\in W} r_S(w) - \min_{w\in W} r(w)].\end{aligned}$$

Next, we provide a bound on the generalization error for the primal risk $\zeta_{gen}^{P}(A)$. To the best of our knowledge, this is the first bound for $\zeta_{gen}^{P}(A)$ in the nonconvex-concave setting.

Lemma 1. *The generalization error of the primal risk of an $\epsilon-$stable algorithm A for a min-max problem with concave maximization problem can be bounded by* $\zeta_{gen}^{P}(A) \leq \sqrt{8C_p^2 \ell L} \cdot \sqrt{\epsilon}$.

Since we already have the generalization error for the primal risk $E_S E_A[r(w_S^A) - r_S(w_S^A)]$ from Lemma 1, we only need to estimate

$$E_S E_A[\min_{w \in W} r_S(w) - \min_{w \in W} r(w)] = E_S[\min_{w \in W} r_S(w) - \min_{w \in W} r(w)] \qquad \text{[Primal Min Error]}. \quad (8)$$

The following theorem gives the generalization bound of the primal gap using the upper bound from Lemma 1 and bounding the Primal Min Error in Equation (8).

Theorem 2. *Suppose algorithm A is ϵ-stable. The generalization bound of the primal gap is given by*

$$\zeta_{gen}^{PG}(A) \leq \sqrt{8\ell L C_p^2 \epsilon} + 2L_\theta^* C_e/\sqrt{n}.$$

Note that the first term is from the generalization of the primal risk, as shown in Lemma 1, and the second term is an upper bound for the Primal Min Error in Equation (8).

3.4 Revisiting Example 1

Recall Example 1 in the Section 3.1. In this example, we have that the primal risk generalizes well, but the solution w_S does not, thereby indicating that the generalization error of the primal risk may not be a good metric to study generalization behavior of minimax problem. First, as shown in the appendix (Proposition 4), we have

$$E_S[\min_{w \in W} r_S(w) - \min_{w \in W} r(w)] \geq 0.005. \quad (9)$$

On the other hand, it is easy to compute that $L_\theta^* = \lambda \log n/\sqrt{n}$ and $C_e = \lambda n$. Therefore, by Theorem 2, we have an upper bound for the primal min error (see Equation (8)): $E_S[\min_{w \in W} r_S(w) - \min_{w \in W} r(w)] \leq 2L_\theta^* C_e/\sqrt{n} = 2\log n$, which is tight up to a log factor according to (9). Therefore, the primal gap has a constant generalization error which is consistent with the observation that the solution to the empirical problem does not have good generalization behavior.

3.5 Nonconvex-nonconcave case

We briefly note that our results above for the nonconvex-concave case can also be generalized to nonconvex-nonconcave case, under certain assumptions of the max learner.

Theorem 3 (Nonconvex-nonconcave case)**.** *Suppose that for any fixed w, gradient ascent with diminishing stepsizes $1/\ell_{\theta\theta} t$ for the empirical risk $r_S(w, \cdot)$ has convergence rate $r_S(w) - r_S(w, \theta^t) \leq \ell_{\theta\theta} C_p^2/2$. Also, for any fixed w, gradient ascent with diminishing stepsizes $1/L_\theta^* t$ for the population risk $r(w, \cdot)$ has convergence rate $r(w) - r(w, \theta^t) \leq \ell_{\theta\theta} C_e^2/2$. Then, the results in Lemma 1 and Theorem 2 still hold.*

In particular, we assume that the maximization problem can be solved by gradient ascent for any w efficiently, which appears to be the case in many problems, e.g., training deep overparameterized neural networks [Du et al., 2019], and robust least squares problems [El Ghaoui and Lebret, 1997].

4 Comparison of GDA and GDMax

In Section 3.3, we provide generalization bounds for the primal gap for any $\epsilon-$ stable algorithm. In this section, we focus on two algorithms in particular – GDA and GDMax. These two algorithms are described in Algorithms 1 and 2 in Appendix D.

We note that though analyzing the optimization properties of GDA/stochastic GDA for solving the empirical minimax problem is an important topic, our focus in this paper is on studying the generalization behavior of these algorithms. We assume that the empirical version of minimax problem we consider can be solved by GDA and GDMax, i.e., we assume that GDA and GDMax satisfy the following assumption:

Assumption 5. *Let A be an minmax learner, such as GDA or GDMax. Then we assume that A has the following convergence rate: $E_A[r_S(w^t) - \min_{w\in W} r_S(w)] \leq (\phi_A(M(W)) + \phi_A(C_e))/\psi_A(t)$, where $M(W)$ is the maximum of the norms of w, $\phi_A(s)$, $\psi_A(s)$ are nonnegative, increasing functions that tend to infinity as $s \to \infty$.*

For simplicity, throughout this section, we assume that $\|f(w, \theta; z)\| \leq 1$ for all w, θ, and z.

The next theorem provides a bound for the population primal gap $\Delta(w_S^A) := r(w_S^A) - \min_{w\in W} r(w)$. Note that the goal of any algorithm is to make this gap as small as possible.

For an algorithm A and subsets $W_0 \subseteq W, \Theta_0 \subseteq \Theta$, we define $A(W_0, \Theta_0)$ as the algorithm which restricts Algorithm A to solve (1) under constraint sets W_0 and Θ_0. Specifically, $A(W, \Theta)$ is just A.

Theorem 4. *Let $w_S^{A,t}, \theta_S^{A,t}$ be the t-th iterate generated by algorithm A using dataset S. Assume that $\{\theta_S^{A,t}\} \subseteq \Theta_0 = \Theta_\theta^A$ for $t \leq T$ with probability $1 - \delta$ (due to the randomness in S) and $B(0, C_p) \subseteq \Theta_\theta^A$. Here $B(v, r)$ denotes the l_2-ball with radius r centered at v. Let $A_0 = A(W, \Theta_0)$. Then after T iterations of algorithm A, the population primal gap can be bounded as:*

$$E_S[r(w_S^{A,T}) - \min_{w\in W} r(w)] \leq (\phi_{A_0}(M_w) + \phi_{A_0}(C_e(\Theta_\theta^A)))/\psi_{A_0}(T) + \zeta_{gen}^P(A_0) + L_\theta^* C_e(\Theta_\theta^A)/\sqrt{n} + \delta,$$

where $\zeta_{gen}^P(A_0) = E_S E_A[r(w_S^{A_0,T}) - r_S(w_S^{A_0,T})]$ is the generalizationerror of the primal risk of Algorithm A_0.

Remark 1. *Theorem 4 builds a closer connection between generalization behavior and the dynamics of minimax learner A. More restricted the the max learner is, better the the generalization behavior. We make this clear in the comparison of GDA and GDMax by analyzing the three terms in Theorem 4.*

4.1 Analyzing the term $\zeta_{gen}^P(A_0)$

First, we study the generalization bound of the primal risk, i.e., ζ_{gen}^P in Theorem 4. For GDA, we can estimate ζ_{gen}^P by using Lemma 1. Therefore, it suffices to estimate the stability of GDA. We do this in the following lemma:

Lemma 2. *Let $c_0 = \max\{\alpha_0, \beta_0\}$, If we use diminishing stepsizes $\alpha_t = \alpha_0/t$ and $\beta_t = \beta_0/t$ for GDA for T iterations, we have the stability bound $\epsilon^{GDA} \leq L_{\Theta_\theta^{GDA}} T^{c_0\ell}/(n\ell)$.*

We can bound $\zeta_{gen}^P(A_0)$ for GDA by substituting the stability bound 2 in Lemma 1.

Proposition 1. *Let $c_0 = \max\{\alpha_0, \beta_0\}$ and assume that $f(\cdot, \cdot; z)$ is $L_{\Theta_\theta^{GDA}}$-Lipschitz-continuous inside the set $W \times \Theta_\theta^{GDA}$. For GDA with diminishing stepsizes $\alpha_0/t, \beta_0/t$ run for T iterations (denoted by GDA_T), the generalization error of the primal risk can be bounded by:*

$$\zeta_{gen}^P(GDA_T) \leq (L_{\Theta_\theta^{GDA}})^{3/2} \sqrt{8C_p^2/\ell} \sqrt{T^{c_0\ell}/n}.$$

However for GDMax, we can not compute a uniform stability bound that vanishes as n goes to infinity. In fact, we can show from the following simple example that ζ_{gen}^P(GDMax) can be a constant independent of n, which means that for the case where $r(w, \theta)$ is nonconvex-concave, the generalization bound for primal risk of GDMax can be undesirable.

Example 3 (Constant generalization error of primal risk for GDMax)**.** *Consider a dataset S with n elements. Define the objective function: $f(w, \theta; z) = \left(\frac{w}{n^2} - z\right)\theta - \frac{\theta^2}{2n}$, where $w \in W = [-n\sqrt{n}, n\sqrt{n}]$, $\theta \in \Theta = \mathbb{R}$ and z is drawn from the uniform distribution over $\{-1/\sqrt{n}, 1/\sqrt{n}\}$. We have*

$$r_S(w) = \frac{n^2}{2}\left(\frac{w}{n^2} - \frac{1}{n}\sum_{i=1}^n z_i\right)^2,$$

and $r(w) = \frac{w^2}{2n^2}$. Therefore, $\min_{w\in W} r(w) = 0$. From the definition of the function f and the sets W and Θ, we have $\ell = 1/n^2$, $L = \mathcal{O}(1/\sqrt{n})$.

Note that one step of GDMax can attain the minimizer of $r_S(w)$ (since it is a one dimensional quadratic problem), i.e., $w_S = n\sum_{i=1}^n z_i$ and $r_S(w_S) = 0$. Furthermore, we have $E_S r(w_S) = E[\frac{(\sum_{i=1}^n z_i)2}{2}] = 1/2 > 0$. Therefore, ζ_{gen}^P(GDMax) $= E[r(w_S) - r_S(w_S)] = 1/2 > 0$ cannot be made small.

Therefore, from Proposition 1 and Example 3, we see that the bound for the expected Population primal gap contains the term ζ_{gen}^P which cannot be bounded for GDMax, whereas can be bounded for GDA which leads us to conclude that GDA generalizes better than GDMax for such problems. However, it is possible to bound $\zeta_{gen}^P(\text{GDMax})$ in certain problems, and in this case the two other terms in Theorem 4 become crucial. We analyze them next.

4.2 Analyzing the other two terms of Theorem 4

As shown in Example 1, sometimes the GDMax can have a good generalization bound of the primal risk. Therefore, we need to analyze the other two terms in Theorem 4, i.e., $(\phi_A(M_w) + \phi_A(C_e(\Theta_\theta^A)))/\psi_A(T)$ and $L_\theta^* C_e(\Theta_\theta^A)/\sqrt{n}$. For these two terms, since L_θ^* is fixed, the constant $C_e(\Theta_\theta^A)$ is the key term which differentiates the performance of different algorithms.

By definition, the constant $C_e(\Theta_\theta^{GDMax})$ for GDMax is nearly C_e (See Definition 6). Therefore, the population primal gap after T steps of GDMax is dominated by C_e if C_e is large. However, the set Θ_θ^{GDA} for GDA can be much smaller than Θ, which implies that $C_e(\Theta_\theta^{GDA})$ can be much smaller than C_e. This phenomenon can be seen from Example 1: If we perform one step of GDMax with primal stepsize 1, we can attain $w^1 = w_S$. Then $E_S[r(w_S^1) - \min_{w\in W} r(w)] \geq 0.005$ from (7). For GDA, we can see that $w^1 = 1$ after one step of GDA with stepsize 1. Therefore, GDA generalizes better than GDMax. Generally, we have the following estimate of $C_e(\Theta_\theta^{GDA})$.

Lemma 3. *Let $L_0 = \max_z \|\nabla f(w_0, \theta_0; z)\|$. Let $c_0 = \max\{\alpha_0, \beta_0\}$, If we use diminishing stepsizes $\alpha_t = \alpha_0/t$ and $\beta_t = \beta_0/t$ for GDA, then after T steps we have $\|\theta^t\| \leq T^{c_0\ell} L_0/\ell$ for $t \in [T]$.*

Therefore, if C_e is much larger than C_p, using GDA with $C_p \leq T^{c_0\ell} L_0/\ell \leq C_e$ is better than GDMax. We make this more concrete in the context of GAN training next.

4.3 GAN training

We now study the specific case of GAN training to explore why GDA generalizes better than GDMax. Specifically, we revisit Example 2, and consider a special case: D is restricted to be a linear function with respect to θ. Define the descriminator $D(x) = \Phi^T(x)v + b_0$, where $\Phi(x) = [\Phi_1(x), \cdots, \Phi_m(x)]^T \in \mathbb{R}^m$ is the feature matrix and $b_0 \in \mathbb{R}$. Also suppose that G is parametrized by w and $G^* = G_{w^*}$. Then the GAN problem can be written as $\min_{w\in W} \max_{\theta\in\Theta}\ r(w, \theta)$, where

$$r(w, \theta) = E_{x\sim P_r}[\phi(v^T\Phi(x) + b_0)] + E_{y\sim P_0}[\phi(1 - v^T\Phi(G_w(y)) - b_0)].$$

Here $\theta = (v, b_0)$. Assume that $\sigma_{\max}\left(E_{x\sim P_{G_w}} \Phi(x)\Phi^T(x)\right) \leq \sigma_{\max}/\sqrt{m}$, where $\sigma_{\max}(\cdot)$ denotes the largest singular value of a matrix. Also, we assume that $|\phi'(\lambda)| \leq L_\phi$ for any $\lambda \in [0, 1]$. Therefore, we have $\|\nabla_\theta f(w, \theta; z)\| \approx L_\phi \sigma_{\max}$.

Lemma 4. *Suppose $\Phi(x)$ is sub-Gaussian and the matrix $Q_S = [\Phi(x_1)\ \ \Phi(x_2) \cdots\ \ \Phi(x_n)\ \ \Phi(G_w(y_1))\ \ \cdots\ \ \Phi(G_w(y_n))]$ is full rank with probability 1. Then with probability at least $1 - C\delta$, we have $\|\theta_S(w^*)\| \geq \Omega(\sqrt{n})$, where $\theta_S(w^*) \in \arg\max_{\theta\in\Theta} r_S(w^*, \theta)$.*

Now, for $\theta = \arg\max_{\theta\in\Theta} r(w^*, \theta)$, it can be easily seen that $v = 0, b_0 = 1/2$ in this case. Therefore, $C_p \approx 1/2$. Finally, combining the previous discussion on GDA in Lemma 3, and using the fact that C_e is large from Lemma 4, we see from Theorem 4 that GDA can generalize better than GDMax. More detailed discuss of the GAN-training example and Lemma 4 can be found in Section D.

5 Conclusion

In this paper, we first demonstrate the shortcomings of two popular metrics - the primal risk, and the primal dual gap, which are used to study generalization of minimax learners. We then propose a new metric, the primal gap, which overcomes these shortcomings and captures the generalization behavior of algorithms that solve minimax problems. Finally, we use this newly proposed metric to study the generalization behavior of two different algorithms – GDA and GDMax, and study cases where GDA has a better generalization behavior than GDMax.

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   (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]
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