An SDE Framework for Adversarial Training, with Convergence and Robustness Analysis

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Abstract

Adversarial training has gained great popularity as one of the most effective defenses for deep neural networks against adversarial perturbations on data points. Consequently, research interests have grown in understanding the convergence and robustness of adversarial training. This paper considers the min-max game of adversarial training by alternating stochastic gradient descent. It approximates the training process with a continuous-time stochastic-differential-equation (SDE). In particular, the error bound and convergence analysis is established.

This SDE framework allows direct comparison between adversarial training and stochastic gradient descent; and confirms analytically the robustness of adversarial training from a (new) gradient-flow viewpoint. This analysis is then corroborated via numerical studies.

To demonstrate the versatility of this SDE framework for algorithm design and parameter tuning, a stochastic control problem is formulated for learning rate adjustment, where the advantage of adaptive learning rate over fixed learning rate in terms of training loss is demonstrated through numerical experiments.

1 Introduction

Deep neural networks (DNNs) trained by gradient-based methods have enjoyed substantial successes in many applications. Their performance, however, can significantly deteriorate by small and human imperceptible adversarial perturbations [24]. Such vulnerability of DNNs raises security concerns of their practicability in safety-critical applications.

Adversarial training, proposed in [19], is one of the most promising defenses for deep neural network against adversarial perturbation. Recent empirical studies such as [5] and [2] have demonstrated its effectiveness and robustness of neural networks in many practical applications.

The idea of adversarial training [19] is to formulate a min-max game between a neural network learner and an adversary who is allowed to perturb the normal inputs. Algorithmically speaking, in each round, the adversary generates new adversarial examples against the current neural network via projected gradient descent (PGD), in response the learner takes a gradient step to decrease its loss. (See Algorithm 1 for more details.)

Given the popularity of adversarial training, considerable effort has been made to further improve its performance. [27] and [11] use Lipschitz regularizations for better generalization performance of trained models. [30] designs a computationally efficient variant of adversarial training based on the Pontryagin Maximum Principle from robust controls. [31] suggests an early-stopped PGD for generating adversarial examples. To improve robustness, [20] generalizes the standard PGD procedure to incorporate multiple perturbation models into a single attack.

Parallel to these empirical successes, there are growing research interests in analyzing convergence and robustness properties of adversarial training [19]. [26] considers quantitatively evaluating the convergence quality of adversarial examples found by the adversary, in order

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to ensure the convergence and the robustness. [12] and [32] study the convergence and the robustness of adversarial training on over-parameterized neural networks. [23] provides convergence analysis of adversarial training by combining techniques from robust optimal controls and inexact oracle methods from optimization. [10] investigates the non-concave landscape of the adversary for a two-layer neural network with a quadratic loss function. [28] studies the adversarially robust generalization problem via Rademacher complexity, and [8] characterizes the generalization gap in terms of the number of training samples for Gaussian and Bernoulli models. Finally, [22] explores the tradeoff between the robustness and the accuracy in linear models.

Our work. This paper considers the min-max game of adversarial training by alternating stochastic gradient descent. It approximates the training process with a continuous-time stochastic-differential-equation (SDE) dynamic. In particular,

• the approximation error bound between the continuous-time SDE dynamic and discrete-time adversarial training is established;
• the convergence of adversarial training is established via studies of the invariant measure of the SDE;
• this SDE framework allows direct comparison between adversarial training and stochastic gradient descent (SGD), and confirms analytically the robustness of adversarial training from a (new) gradient-flow viewpoint. This analysis is then corroborated via numerical studies;
• and furthermore, the versatility of this SDE framework for algorithm design and parameter tuning is demonstrated through a stochastic control problem formulated for learning rate adjustment, where the advantage of adaptive learning rate over fixed learning rate in terms of training loss is illustrated through numerical experiments.

Related works in SDE modeling of stochastic algorithm. The idea of approximating discrete-time stochastic gradient algorithms (SGAs) by continuous-time SDE dynamics can be dated back to [21] and [17]. This SDE framework has recently been extended to various settings of SGAs. For instance, [16] and [1] introduce the SDE approximations of accelerated mirror descent, and asynchronous SGD, respectively. [6] designs an entropy-regularized training algorithm motivated by the SDE approximation. [7] builds the connection between SGD and variational inference by considering the evolution of training parameters. [4] studies the training process of generative adversarial networks (GANs) via SDE approximations and analyzes the convergence and loss functions of GANs training.

Organization. Section 2 presents the problem set-up for adversarial training. Section 3 establishes the continuous-time SDE approximation for adversarial training, with error bound and robustness analysis. Section 4 establishes the convergence of adversarial training via the invariant measure of the SDE. Section 5 formulates the learning rate tuning problem in adversarial training as a stochastic control problem, with explicit solutions for linear models. Finally, Section 6 compares theoretical results with numerical experiments.

2 Problem Setting

Adversarial training. Given a data set \( \{x_i\}_{i=1}^N \subset \mathbb{R}^d \) with \( d, N \in \mathbb{Z}^+ \), and a constraint set \( \Delta \in \mathbb{R}^d \), the adversarial training problem is to find an appropriate model parameter \( \hat{\theta} \in \mathbb{R}^d \) and small perturbations \( \delta_i \) to solve the following min-max optimization problem:

\[
\min_{\theta \in \mathbb{R}^d} \max_{\delta_i \in \Delta, i=1,...,N} \frac{1}{N} \sum_{i=1}^N L(\theta, x_i + \delta_i). \tag{2.1}
\]
Here \( L(\cdot, \cdot) \) is a loss function, and \( \delta_i \) is a perturbation on the \( i \)-th data point \( x_i \) within the constraint set \( \Delta \). A common choice for \( \Delta \) is \( \{ \delta \in \mathbb{R}^d : \| \delta \|_p \leq \epsilon \} \) for \( p = 1, 2, \infty \) and some given \( \epsilon > 0 \). The notation \( d_\theta \) emphasizes the dimension of a given parameter space for \( \theta \).

One of the established approaches is to compute (2.1) by performing a gradient ascent on the perturbation parameter \( \delta \) and a gradient descent on the model parameter \( \theta \). Such an alternating optimization algorithm is called projected-gradient-descent (PGD) adversarial training [19], shown in Algorithm 1. More specifically, in the inner loop, the most powerful adversarial attack \( \delta \) to the input data batch is obtained via the multi-step projected gradient ascent; in the outer loop, \( \theta \) is updated by the one-step gradient descent, based on the perturbed batch of data.

Algorithm 1 Projected Gradient Descent (PGD) Adversarial Training [19]

1: Initialize: \( \theta_0 \).
2: for 1 \( \leq t \leq T \) do
3: \hspace{1em} Sample a mini-batch of size \( B \): \( \{x_{i1}, \ldots, x_{iB}\} \).
4: \hspace{1em} Set \( \delta_0 = 0 \), \( \hat{x}_j = x_{ij}, j = 1, \ldots, B \).
5: \hspace{1em} for 1 \( \leq k \leq K \) do
6: \hspace{2em} \( \delta_k = \Pi_{\Delta} (\delta_{k-1} + \eta_k \sum_{j=1}^{B} \nabla_{x} L(\theta_{t-1}, \hat{x}_j + \delta_{k-1})) \)
7: \hspace{1em} end for
8: \hspace{1em} \( \theta_t = \theta_{t-1} - \frac{\eta}{B} \sum_{j=1}^{B} \nabla_{\theta} L(\theta_{t-1}, \hat{x}_j + \delta_K) \)
9: end for.

Our approach is to approximate discrete-time adversarial training by a continuous-time dynamic, in terms of stochastic differential equation (SDE). To facilitate the continuous-time approximation, we consider a slight modification of the original min-max problem (2.1) of the following form:

\[
\min_{\theta \in \mathbb{R}^d} \max_{\delta_i \in [0, \epsilon]} \frac{1}{N} \sum_{i=1}^{N} L(\theta, x_i + \delta_i) - \lambda \cdot R(\delta_i), \quad (2.2)
\]

Here the function \( R: \mathbb{R}^d \rightarrow \mathbb{R} \) is the regularization term with \( \lambda \) a hyper-parameter. For instance, when the original constraint set \( \Delta \) is in the form \( \{ \delta \in \mathbb{R}^d : R(\delta) \leq 0 \} \), then the modified problem (2.2) is a Lagrange relaxation of the original problem (2.1). The main advantage to introduce (2.2) is to ensure that the perturbation in every inner iteration in the PGD Algorithm [1] can be captured by a continuous-time dynamic, as shown in the modified Algorithm [2] for the problem (2.2).

Moreover, to be consistent with the literature for adversarial training, \( R \) is assumed to be a convex function attaining the minimum at the origin, with \( \nabla_\delta R(0) = 0 \). The common \( l_p \) regularization satisfies this assumption.

To simplify the notation, throughout the paper, denote the objective function \( J \) as \( J(\theta, x, \delta) = L(\theta, x + \delta) - \lambda \cdot R(\delta) \).

In the next section, we will establish the continuous-time SDE approximation for Algorithm [2] with an analytical form for the approximation error bound. This SDE approximation enables us to establish analytically the robustness of adversarial training.

## 3 Continuous-time Approximation

To establish the continuous-time SDE dynamic for adversarial training, we will assume for ease of exposition and with little loss of generality the same learning rate \( \eta \) for both the inner and outer loops.

We can then focus on analyzing one step in Algorithm [2] to see how the parameter \( \theta \) is
updated from $t$ to $t+1$. Consider an inner loop starting with $\delta_0 = 0$, then

$$\delta_1 = \delta_0 + \frac{\eta}{B} \sum_{j=1}^{B} \nabla_\delta J(\theta_t, \hat{x}_j, 0) = \frac{\eta}{B} \sum_{j=1}^{B} \nabla_x L(\theta_t, \hat{x}_j),$$

$$\delta_2 = \delta_1 + \frac{\eta}{B} \sum_{j=1}^{B} (\nabla_x L(\theta_t, \hat{x}_j) + \delta_1) - \lambda \nabla_\delta R(\delta_1)
$$

$$= \frac{2\eta}{B} \sum_{j=1}^{B} \nabla_x L(\theta_t, \hat{x}_j) + O(\eta^2).$$

The second equality comes from Taylor’s expansion at $\delta = 0$. Continuing this calculation, we will see that any $K \geq 2$,

$$\delta_K = \frac{K\eta}{B} \sum_{j=1}^{B} \nabla_x L(\theta_t, \hat{x}_j) + O(\eta^2). \tag{3.3}$$

Since we only keep the first order terms, by the assumption on $R$, terms involving higher order derivatives of $R$ are negligible.

Given (3.3), the update on $\theta$ from the outer loop is given by

$$\theta_{t+1} = \theta_t - \frac{\eta}{B} \sum_{j=1}^{B} \nabla_\delta L \left( \theta_t, \hat{x}_j + \frac{K\eta}{B} \sum_{j=1}^{B} \nabla_x L(\theta_t, \hat{x}_j) + O(\eta^2) \right)
$$

$$= \theta_t - \frac{\eta}{B} \sum_{j=1}^{B} \nabla_\delta L(\theta_t, \hat{x}_j)
$$

$$- \frac{K\eta^2}{B^2} \sum_{i,j=1}^{B} \nabla_x L(\theta_t, \hat{x}_j) \nabla_x L(\theta_t, \hat{x}_i) + O(\eta^3). \tag{3.4}$$

Here $\nabla_\delta L$ is the matrix whose $i, j$-th entry is $\frac{\partial^2 L}{\partial \theta_i \partial \theta_j}$.

In order to find a continuous-time approximation for $\theta_t$, we first compute the first and second order moments $E[D]$ and $E[DD^T]$, with $D = \theta_t - \theta_0$ the one-step difference of $\theta$. The expectation here is taken over the randomness of the mini-batch samples $\{\hat{x}_j\}_{j=1}^{B}$. 

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**Algorithm 2 Adversarial Training with Modified Objective (2.2)**

1. **Input**: loss function $J(\theta, x, \delta) = L(\theta, x + \delta) - \lambda R(\delta)$, training set $\{x_i\}_{i=1}^{N}$, mini-batch size $B$, training step $T$, inner loop step $K$, learning rates for outer and inner loops $\eta_0, \eta_1$.
2. **Initialize**: $\theta_0$.
3. **for** $1 \leq t \leq T$ **do**
   4. Sample a mini-batch of size $B$: $\{x_{i_1}, \ldots, x_{i_B}\}$.
   5. Set $\delta_0 = 0$, $\hat{x}_j = x_{i_j}$, $j = 1, \ldots, B$.
6. **for** $1 \leq k \leq K$ **do**
   7. $\delta_k = \delta_{k-1} + \frac{\eta}{B} \sum_{j=1}^{B} \nabla_\delta J(\theta_{t-1}, \hat{x}_j, \delta_{k-1})$
8. **end for**
   9. $\theta_t = \theta_{t-1} - \frac{\eta_0}{B} \sum_{j=1}^{B} \nabla_\delta J(\theta_{t-1}, \hat{x}_j, \delta_K)$
10. **end for**
After some calculations (details to be shown in Appendix A), we see that
\[
E[D] = -\eta E[\nabla_\theta L(\theta_0, x)]
\]
\[
- K T \eta^2 E[\nabla_{\theta} L(\theta_0, x) | E[\nabla_\theta L(\theta_0, x)]]
\]
\[
- \frac{K T \eta^2}{B} \left[ E[E[\nabla_{\theta} L(\theta_0, x) | E[\nabla_\theta L(\theta_0, x)]]ight] + O(\eta^3).
\]

Next, we aim to find a stochastic process \{\Theta_t\}_{t \geq 0} with the following form
\[
d\Theta_t = (b_0(\Theta_t) + \eta b_1(\Theta_t))dt + \sigma(\Theta_t)dW_t.
\]

Here \{W_t\}_{t \geq 0} is a \(d_\theta\)-dimensional Brownian motion supported on a probability space \((\Omega, \mathcal{F}, \mathbb{P})\). The drift term \(b_0, b_1 : \mathbb{R}^{d_\theta} \to \mathbb{R}^{d_\theta}\) and the diffusion term \(\sigma : \mathbb{R}^{d_\theta} \to \mathbb{R}^{d_\theta}\) are Lipschitz continuous, and are chosen such that the first and second moments of the one-step difference \(\hat{D} = \Theta_t - \Theta_0\) match (3.5) and (3.6), respectively.

After some additional algebraic manipulations (detailed in Appendix A), we can show that one possible set of appropriate choices is given by
\[
b_0(\theta) = -\nabla_\theta G(\theta),
\]
\[
b_1(\theta) = -\frac{K}{2} \nabla_\theta (\|D(\theta)\|^2) - \frac{1}{4} \nabla_\theta (\|\nabla_\theta G(\theta)\|^2),
\]
\[
\sigma(\theta) = \sqrt{2\beta^{-1} (\text{Var}_x(\nabla_\theta L(\theta, x)))^{1/2}}.
\]

Here \(\beta = 2B/\eta\), the ratio between the batch size \(B\) and the learning rate \(\eta\), determines the scale of the diffusion, and
\[
G(\theta) := g(\theta) + K \beta^{-1} (E[\|\nabla_\theta L(\theta, x)\|^2] - \|D(\theta)\|^2)
\]
with
\[
g(\theta) := E[L(\theta, x)],
\]
\[
D(\theta) := E[\nabla_\theta L(\theta, x)].
\]

Indeed, under proper smoothness and boundedness conditions, we can prove \(E[D] = E[\hat{D}], E[DD^T] = E[\hat{D}\hat{D}^T]\). (See Appendix A)

Before we continue the analysis for the approximation error bound of this \(\theta\) by \(\Theta\), we pause here to compare this SDE approximation for adversarial training with that for the vanilla SGD.

**SGD vs adversarial training.** Recall that the discrete-time dynamic for SGD is given by
\[
\theta^*_{t+1} = \theta^*_t - \frac{\eta}{B} \sum_{j=1}^{B} \nabla_\theta L(\theta^*_t, \bar{x}_j),
\]
for which the SDE approximation (see for example, [IS]) is given by:
\[
d\Theta^*_t = (b_0^*(\Theta^*_t) + \eta b_1^*(\Theta^*_t))dt + \sigma^*(\Theta^*_t)dW_t
\]
with
\[
b_0^*(\theta) = -\nabla_\theta g(\theta),
\]
\[
b_1^*(\theta) = -\frac{1}{4} \nabla_\theta (\|\nabla_\theta g(\theta)\|^2),
\]
\[
\sigma^*(\theta) = \sqrt{2\beta^{-1} (\text{Var}_x(\nabla_\theta L(\theta, x)))^{1/2}}.
\]
can be viewed as a special case of (3.7) by taking \( K = 0 \). The term \( b_0(\theta) \) in (3.8) differs from \( b_0^*(\theta) \) in (3.10) by an additional correction term \( K \beta^{-1}(E[\|\nabla_x L(\theta, x)\|^2] - \|D(\theta)\|^2) \), due to adversarial perturbations. Meanwhile, the term \( b_1(\theta) \) in (3.9) differs from \( b_1^*(\theta) \) in (3.16) by two additional terms, \( K \beta^{-1}(E[\|\nabla_x L(\theta, x)\|^2] - \|D(\theta)\|^2) \) and \( -\frac{K}{2} \nabla \theta(\|D(\theta)\|^2) \), also caused by adversarial perturbations.

Gradient flow and robustness of adversarial training. These differences between adversarial training and SGD enable us to explain analytically the robustness of adversarial training from a (new) gradient-flow viewpoint.

Indeed, if (3.7) is viewed (approximately) as the negative gradient flow with respect to the function \( G(\theta) \) and if (3.15) is viewed (approximately) as the negative gradient flow with respect to the expected loss function \( g(\theta) \), then the extra term \( E[\|\nabla_x L(\theta, x)\|^2] \) for adversarial training exactly reflects the sensitivity of the loss function \( L \) under the perturbation of data \( x \), contributing to the robustness of the trained model.

In other words, the continuous-time SDE approximation offers us a new perspective to explain why empirically using adversarial training results in more robust models than simply applying SGD: adversarial training chooses \( \theta \) to decrease the expected loss function \( g(\theta) \) while simultaneously improving the robustness according to the criterion \( E[\|\nabla_x L(\theta, x)\|^2] \), while SGD only focuses on decreasing the expected loss \( g(\theta) \).

This analytical explanation will be corroborated by a numerical experiment for a logistic regression problem in Section 6.3.

Approximation error bound. We now return to provide a rigorous justification that the SDE (3.7) is indeed the continuous-time approximation for Algorithm 2.

Theorem 3.1 Fix an arbitrary time horizon \( T > 0 \) and take the learning rate \( \eta \in (0, 1 \wedge T) \) and set the number of iterations \( N = \left\lfloor \frac{T}{\eta} \right\rfloor \). Under proper regularity assumptions on the loss function \( L \) and the test function \( f \), the approximation error of \( \theta_t \) in the discrete-time (3.4) by \( \Theta_{t\eta} \) in the continuous-time (3.7) is

\[
\max_{t=1,\ldots,N} |E[f(\theta_t)] - E[f(\Theta_{t\eta})]| \leq C\eta^2, \tag{3.19}
\]

for a constant \( C > 0 \).

Theorem 3.1 states that the approximation error between the continuous-time SDE dynamic (3.7) and the discrete-time training dynamic is in the order of \( O(\eta^2) \).

Note that the approximation is in the sense of distribution of trained parameters, meaning this result holds for a class of neural networks from this distribution.

Note also the particular order of error bound can vary depending on the specific form of continuous-time SDE dynamics, and may be further improved. See Appendix B for detailed technical assumptions and proofs. The SDE approximation further allows for the convergence analysis of adversarial training.

4 Convergence via Invariant Measure

The convergence of adversarial training is by studying the invariant measure of the SDE adopting methodologies from [25].

Recall the following definition of invariant measures [9].

Definition 4.1 A probability measure \( \mu^* \) is called an invariant measure for a stochastic process \( \{\Theta_t\}_{t \geq 0} \) if for any measurable bounded function \( f \) and any \( t \geq 0 \),

\[
\int E[f(\Theta_t)|\Theta_0 = \theta] \mu^*(d\theta) = \int f(\theta) \mu^*(d\theta).
\]
The main convergence result is the following.

**Theorem 4.2** Under proper regularity assumptions on the loss function \( L \), the SDE (3.7) admits a unique invariant measure \( \mu^* \) with an exponential convergence rate.

The proof of Theorem 4.2 as well as a complete list of technique assumptions, is deferred to Appendix C.

**Discussions on some technical assumptions.** It is worth pointing out that the existence of the invariant measure provides sufficient conditions for the convergence of adversarial training. In order to understand further the conditions that ensure this convergence, we highlight some assumptions in Theorem 4.2, which may provide insight for algorithm designs.

One assumption is the boundedness of \( b_0(\theta) + \eta b_1(\theta) \). This is an essential constraint on the gradient of the loss function with respect to model parameters. In particular, the boundedness assumption explains analytically some well-known practices in adversarial training, including the introduction of various forms of gradient penalties; see for example [27] and [11].

Another assumption requires that for \( \| \theta \|_2 \) sufficiently large, \( \theta^T (b_0(\theta) + \eta b_1(\theta)) \leq -r \| \theta \|_2 \), for some positive constant \( r \). It suggests that the training algorithm needs to be designed such that there exist strong gradient signals to keep \( \theta \) from being extremely large. In practice, this requirement can be satisfied by adding the \( l_2 \) regularization to \( \theta \). Hence, Theorem 4.2 justifies mathematically from a continuous-time viewpoint the widely-used \( l_2 \) regularization helps to stabilize the training process.

5 Optimal Learning Rate Analysis via SDE

Up to now we have shown that the continuous-time SDE approximation helps analyzing the robustness and convergence of adversarial training. The natural question is whether and how this theoretical analysis would help in algorithm designs.

In SGD and its variants, there are several important hyper-parameters in training, including choices of learning rates, choices of batch sizes, and choices of regularization functions. In this section, we formulate and analyze a stochastic control problem for learning rate tuning. This particular formulation illustrates how the SDE framework for adversarial training can be exploited for hyper-parameter tuning.

**Stochastic control formulation for adaptive learning rate.** To allow for adjustment of the learning rate, we slightly modify the gradient steps in Algorithm 2 with a multiplication factor \( u_t \) to the original constant learning rate: for the inner iteration \( k = 1, \cdots, K \),

\[
\delta_{k+1} = \delta_k + \frac{\eta u_t}{B} \sum_{j=1}^{B} \nabla \delta J(\theta_t, \hat{x}_j, \delta_k) \quad \text{and then} \quad \\
\theta_{t+1} = \theta_t - \frac{\eta u_t}{B} \sum_{j=1}^{B} \nabla \theta J(\theta_t, \hat{x}_j, \delta_K)).
\] (5.20)

Here the adjustment factor \( u_t \in [0, 1] \) and the constant \( \eta \) is the maximum allowed learning rate. The corresponding continuous-time SDE approximation for (5.20) takes the modified form of:

\[
d\Theta_t = (b_0(\Theta_t, u_t) + \eta b_1(\Theta_t, u_t))dt + \sigma(\Theta_t, u_t)dW_t.
\] (5.21)

(This modified form can be easily established using the methodology in Section 3 as detailed in Appendix D.) Here we slightly abuse the notations \( b_0, b_1, \sigma \) originally defined in (3.8)-(3.10).
and denote

\[
b_0(\theta, u) = -\nabla_\theta \left[ u g(\theta) + K \beta^{-1} u^2 \left( \mathbb{E}[\|\nabla_x L(\theta, x)\|^2] \right) \right] - \|D(\theta)\|^2 \right] ;
\]

\[
b_1(\theta, u) = -\frac{K}{2} u^2 \nabla_\theta (\|D(\theta)\|^2) - \frac{1}{4} \nabla_\theta (\|b_0(\theta, u)\|^2) ;
\]

\[
\sigma(\theta, u) = u \sqrt{2 \beta^{-1}} (\text{Var}_x(\nabla_\theta L(\theta, x)))^{1/2} .
\] (5.22)

Given the expected loss function \(g\) in (3.12), the problem of finding the optimal learning rate \(u_t\) can be formulated as the following stochastic optimal control problem

\[
\min_{u_t} \mathbb{E}[g(\Theta_T)] \text{ subject to Eqn. (5.21)}. \tag{5.23}
\]

Here \(u_t \in [0, 1]\) is the control of the learning rate chosen from an appropriate admissible control set. In general, this problem can be analyzed by considering the following Hamilton-Jacobi-Bellman equation [29]:

\[
-\partial_t V(\theta, t) = \min_{u \in [0, 1]} \left[ (b_0(\theta, u) + \eta b_1(\theta, u)) \cdot \nabla_\theta V(\theta, t) + u^2 \beta^{-1} \text{Tr}(\text{Var}_x(\nabla_\theta L(\theta, x)) \nabla_\theta ^2 V(\theta, t)) \right] ;
\]

\[
V(\theta, T) = g(\theta).
\] (5.24)

In other words, the SDE formulation translates the problem of tuning hyper-parameters into solving (analytically or numerically) a high-dimensional fully nonlinear PDEs. This alternative task is not easier especially when the dimension of parameter \(\theta\) is large. However, for some class of problems, it is possible to derive explicit solutions.

In particular, for a class of linear models, analysis of the control problem enables us to demonstrate the superior performance in terms of stability and convergence using adaptive learning rate over constant learning rate, as shown below.

**Example with explicit solutions.** To see this, let \(A \in \mathbb{R}^{d \times d_o}\) be a fixed-design matrix. Consider the loss function \(L\) and the data \(x\),

\[
L(\theta, x) = \|A \theta - x\|^2, \ x \sim \mathcal{N}(\mu, \Sigma).
\] (5.25)

In this case, by direct computation,

\[
b_0(\theta, u) = -2u(A^T A \theta - A^T \mu) ;
\]

\[
b_1(\theta, u) = -(u^2 \cdot A^T A + 4K u \cdot I)(A^T A \theta - A^T \mu) ;
\]

\[
\sigma(\theta, u) = u \sqrt{2 \beta^{-1}} (A^T \Sigma A)^{1/2}.
\]

Hence, the SDE dynamic (5.21) for adversarial training applied to model (5.25) becomes

\[
d\Theta_t = - (u_t(2 + 4K \eta) \cdot I + u^2_t \eta \cdot A^T A)A^T (A \Theta_t - \mu) dt + u_t \sqrt{2 \beta^{-1}} (A^T \Sigma A)^{1/2} dW_t.
\] (5.26)

Applying Itô’s formula to the expected loss function

\[
g(\theta) = \mathbb{E}_x[L(\theta, x)] = \theta^T A^T A \theta - 2 \mu^T A \theta + \mathbb{E}_x[x^T x]
\]

and then taking the expectation with respect to \(\Theta_t\), we will get

\[
\frac{d\mathbb{E}[g(\Theta_t)]}{dt} = \frac{8}{\beta} u_t^2 \cdot \text{Tr}(A^T \Sigma AA^T A) - 2(A^T A \Theta_t - A^T \mu)^T \cdot (u_t(2 + 4K \eta) \cdot I + u^2_t \eta \cdot A^T A)(A^T A \Theta_t - A^T \mu)
\]
For ease of exposition, consider a special case when $AA^T = \alpha I$ or $d_0 = 1, A^TA = \alpha \in \mathbb{R}$.

Then the above ODE can be further simplified to

$$\frac{ds_t}{dt} = -2s_t \cdot ((2 + 4K\eta)\alpha u_t + \eta\alpha^2 u_t^2) + \frac{8\alpha^2\sigma}{\beta} u_t^2.$$  \hspace{1cm} (5.27)

Here $\sigma := \text{Tr}(\Sigma)$ and $\mathbb{E}[g(\Theta_t)] = s_t$.

Solving the control problem (5.23) with respect to (5.27) yields the optimal control in a feedback form (see Appendix D for details):

$$u^*(s) = \begin{cases} \min \{1, \frac{(1+2K\eta)sB}{(2s-B)\alpha\eta}\} & \text{if } s < \frac{2\sigma}{B}, \\ 1 & \text{if } s \geq \frac{2\sigma}{B}. \end{cases} \hspace{1cm} (5.28)$$

According to the feedback policy in (5.28), for a given expected loss $s$, as the batch size $B$ goes up, $\frac{\sigma}{B}$ goes down, then choosing a large (and maximal) learning rate tends to be optimal. On the contrary, as the variance $\sigma$ goes up, so does $\frac{\sigma}{B}$, then the choice of a small learning rate is preferable.

## 6 Numerical Example

In this section, we present three numerical examples to test the theoretical results in Section 3 to Section 5, including explicit comparison of decay rates between adversarial training and SGD, the approximation error predicted in Theorem 3.1, the predicted robustness of adversarial training discussed in Section 3, and the advantage of adaptive learning rate over fixed rate in terms of convergence and stability from Section 5.

### 6.1 Decay Rates and Order of Approximation Error

In this experiment, we present a linear model for which the corresponding SDE can be explicitly solved, so that the dynamic of adversarial training can be explicitly compared with its SGD counterpart.

Let $H \in \mathbb{R}^{d \times d}$ be a symmetric positive definite matrix, with $0 < \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_d$ its eigenvalues. Consider the loss function

$$L(\theta, x) = \frac{1}{2}(\theta - x)^T H(\theta - x) - \text{Tr}(H),$$  \hspace{1cm} (6.29)

and the data $x \sim \mathcal{N}(0, I)$. In this case,

$$g(\theta) := \mathbb{E}_x[L(\theta, x)] = \frac{1}{2} \theta^T H \theta,$$

$$\nabla_x L(\theta, x) = -\nabla_\theta L(\theta, x) = H(x - \theta), \ \nabla_{x\theta} L(\theta, x) = H.$$  

Hence, the SDE approximation (3.7) for adversarial training applied to the model (6.29) is

$$d\Theta_t = -((H + (K + \frac{1}{2})\eta \cdot H^2)\Theta_t dt + \sqrt{2\beta^{-1}}H dW_t.$$  \hspace{1cm} (6.30)

The above linear SDE (6.30) is a multi-dimensional Ornstein-Uhlenbeck (OU) process and admits an explicit solution:

$$\Theta_t = e^{-\tilde{H} t} \Theta_0 + \sqrt{2\beta^{-1}} \int_0^t e^{-\tilde{H}(t-s)} dW_s,$$  \hspace{1cm} (6.31)

with $\tilde{H} := H + (K + \frac{1}{2})\eta \cdot H^2$.  

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By Itô’s isometry \[14\], we then deduce the dynamic of the objective function as
\[
\mathbb{E}[g(\Theta_t)] = \frac{1}{2} \Theta_0^T H e^{-2Ht} \Theta_0 + \frac{1}{\beta} \int_0^t \text{Tr}(H^3 e^{-2H(t-s)} ds + \frac{1}{\beta} \int_0^t \sum_{i=1}^d \lambda_i^2 e^{-(\theta, + (K+\frac{1}{2})\eta \lambda_i^2)} (t-s) ds
\]
\[
= \frac{1}{2} \Theta_0^T H e^{-2Ht} \Theta_0 + \frac{1}{\beta} \sum_{i=1}^d \lambda_i^2 \left( \frac{1 - e^{-(2\lambda_i + (2K+1)\eta \lambda_i^2)t}}{2 + (2K + 1)\eta \lambda_i} \right).
\]
(6.33)

**Decay rates.** From the above dynamic, adversarial training can be compared explicitly with its vanilla SGD counterpart.

Indeed, recall that the SDE approximation to the vanilla SGD for model (6.29) has the following dynamic \[18\]:
\[
d\Theta_t = -H\Theta_t dt + \sqrt{2\beta^{-1}H}dW_t,
\]
with \(\Theta_0 = \Theta_0\), and
\[
\mathbb{E}[g(\Theta_t)] = \frac{1}{2} \Theta_0^T H e^{-2Ht} \Theta_0 + \beta^{-1} \sum_{i=1}^d \lambda_i^2 \left( \frac{1 - e^{-2\lambda_i t}}{2 + (2K + 1)\eta \lambda_i} \right).
\]
(6.34)

As pointed out in \[18\], the first term in (6.34) decays exponentially with an asymptotic rate \(2\lambda_i\), and the second term is induced by noise with its asymptotic value proportional to the learning rate \(\eta\) as \(\beta^{-1} = \frac{\eta}{2H}\). This is the well-known two-phase behavior of SGD under constant learning rate: an initial descent phase induced by the deterministic gradient flow and an eventual fluctuation phase dominated by the variance of the stochastic gradients.

Now in adversarial training, the first term of the dynamic of the objective function (6.32) also decays exponentially, but with a faster asymptotic rate \(2\lambda_i + (2K + 1)\eta \lambda_i^2\). This is because the gradient descent direction with respect to \(\theta\) under this particular model (6.29) coincides with the gradient ascent direction with respect to \(x\), that is \(\nabla_x \mathcal{L}(\theta, x) = -\nabla_{\theta} \mathcal{L}(\theta, x)\). Hence, the inner loop is accelerating the convergence of \(\theta\). For the second term induced by the noise, its asymptotic value is also proportional to the learning rate \(\beta^{-1} = \frac{\eta}{2H}\) when \(\eta \to 0\).

Furthermore, the above calculation enables us to verify the second-order approximation result in Theorem 3.1 under the following experimental set-up.

**Order of approximation error.** Consider the model (6.29) with a randomly generated 10-by-10 positive definite matrix \(H\), and a random initial value \(\theta_0\). The regularization (penalty) term \(R(\delta)\) in (2.2) is set to be \(\|\delta\|_2^2\), along with other parameters choices of \(B = 20, K = 5, T = 20, \lambda = 20\).

As suggested by Theorem 3.1, we compute the error with the test function equal to the expected loss function: \(f(\theta) = \frac{1}{2} \theta^T H \theta\). The expectation of adversarial training dynamic \(\mathbb{E}[f(\Theta_T)]\) is averaged over 1e5 runs, while the expectation of continuous-time SDE dynamic \(\mathbb{E}[f(\Theta_T)]\) is computed via the explicit formula (6.32).

Figure 1 shows the Log-log plot of \(\mathbb{E}[g(\Theta_T) - \mathbb{E}[g(\Theta_T)]\) under different \(\eta\). Theorem 3.1 suggests that the slope should be close to 2, which is consistent with the numerical result 2.081.

### 6.2 Linear Regression and Adaptive Optimal Learning Rate

The numerical experiment in this section is to demonstrate the effectiveness of the optimal learning rate, based on the linear regression model (5.25) presented in Section 5 and the explicit formula for the optimal learning rate in (5.28).
In the experiment shown in Figure 2, we randomly generated $A, \mu, \Sigma$ in (5.25) such that $\bar{A} \in \mathbb{R}^{20 \times 1}$. The regularization (penalty) term in (2.2) is chosen to be $R(\delta) = \|\delta\|_2^2$, along with other parameters choices of $B = 10, K = 5, T = 1.0, \lambda = 2.0, \eta = 0.01$.

**Results.** It is obvious from Figure 2 that the training curve from adversarial training (green) with the adaptive optimal learning rate given in (5.28) stays stable as the loss decreases to zero, while the training curves for both adversarial training and SGD with fixed learning rate fluctuate.

This phenomenon is repeated in Figure 3 for a high-dimension linear regression problem with $A, \mu, \Sigma$ in (5.25) randomly generated such that $\bar{A} \in \mathbb{R}^{20 \times 40}, AA^T = \alpha I. \eta = 0.005$ and the other parameters remains the same as in the previous case. Again, adversarial training with the optimal adaptive learning rate (green) outperforms others in terms of both the convergence and the stability properties.
6.3 Logistic Regression and Robustness

In this section a logistic regression model is adopted to illustrate the robustness in adversarial training discussed in Section 3.

We consider the randomly generated data \((x, y)\), where \(y \sim \text{Bernoulli}(p)\) and \(x|y = i \sim \mathcal{N}(\mu_i, \Sigma_i)\), i.e., given \(y\), \(x\) is sampled from a multivariate Gaussian distribution. We are to fit the data with a logistic regression model

\[
P(y = 1|x) = \frac{e^{b + \theta^T x}}{1 + e^{b + \theta^T x}}.
\]
with the cross-entropy loss function

\[ L(\theta, x, y) = \log(1 + e^{b + \theta^T x}) - y(b + \theta^T x). \]

Here \( p \in (0, 1), \mu_i \in \mathbb{R}^5, \Sigma_i \in \mathbb{R}^{5 \times 5} \) are randomly generated.

Meanwhile, we choose \( R \) in (2.2) to be the \( l_2 \) regularization, along with other parameters of \( B = 10, K = 5, T = 10.0, \lambda = 2.0, \eta = 0.005 \). For simplicity, we fix the bias \( b \) and only update \( \theta \).

In 50 randomly initialized experiments, SGD gets an average test accuracy around 0.84, while adversarial training gets a slightly lower average test accuracy around 0.78. This result is consistent with other empirical studies, for instance, [2] and [31] claiming that adversarial training may have a lower test accuracy on original samples as a trade-off for robustness.

The robustness of models, as suggested in Section 3 in terms of \( \mathbb{E}_x[\|\nabla_x L(\theta, x, y)\|^2] \), for both stochastic gradient descent and adversarial learning algorithm over the training iterations is plotted in Figure 4. Means and standard deviations are computed over 50 randomly initialized experiments.

![Figure 4: Robustness criterion \( \mathbb{E}_x[\|\nabla_x L(\theta, x, y)\|^2] \) of 2 algorithms over training iterations.](image)

**Results.** The model trained by adversarial training has a much lower and stable value \( \mathbb{E}_x[\|\nabla_x L(\theta, x, y)\|^2] \), indicating more robustness than the model trained by SGD. Meanwhile, \( \mathbb{E}_x[\|\nabla_x L(\theta, x, y)\|^2] \) first decreases then increases under SGD. In contrast, it keeps decreasing under adversarial training. This phenomenon is consistent with the the gradient-flow viewpoint discussed in Section 3: update in SGD leads to loss decreases only, while adversarial training leads to both improvements in robustness and reductions in loss.

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Appendix

Notations
The following notations will be used throughout the appendix.

- For $p \geq 1$, $\| \cdot \|_p$ denotes the $p$-norm over $\mathbb{R}^d$, i.e., $\|x\|_p = \left( \sum_{i=1}^{d} |x_i|^p \right)^{\frac{1}{p}}$ for any $x \in \mathbb{R}^d$.
- Let $M$ by a $n$-by-$m$ real-valued matrix with the $i, j$-th entry $m_{ij}$. $\|M\|_2 = \sqrt{\sum_{i,j} m_{ij}^2}$ denotes the Frobenius norm of $M$. $M^T$ denotes the transpose of $M$.
- Let $\mathcal{X}$ be an arbitrary nonempty subset of $\mathbb{R}^{d_1}$, and $f$ is a function from $\mathcal{X}$ to $\mathbb{R}^{d_2}$. We say $f$ is Lipschitz continuous if there exists some constant $L > 0$, such that for any $x, y \in \mathcal{X}$,
  \[ \|f(x) - f(y)\|_2 \leq L \|x - y\|_2. \]
- Let $\mathcal{X}$ be an arbitrary nonempty subset of $\mathbb{R}^d$, the set of $k$ continuously differentiable functions over some domain $\mathcal{X}$ is denoted by $C^k(\mathcal{X})$ for any nonnegative integer $k$. In particular when $k = 0, C^0(\mathcal{X}) = C(\mathcal{X})$ denotes the set of continuous functions.
- Let $J = (J_1, \ldots, J_d)$ be a $d$-tuple multi-index of order $|J| = \sum_{i=1}^{d} J_i$, where $J_i$ is a nonnegative integer for all $i = 1, \ldots, d$; then define the operator $\nabla^J = \left( \partial_1^{J_1}, \ldots, \partial_d^{J_d} \right)$.
- Fix an arbitrary $\alpha \in \mathbb{Z}^+$. $G^\alpha(\mathbb{R}^d)$ denotes a subspace of $C^\alpha(\mathbb{R}^d)$, where for any $g \in G^\alpha(\mathbb{R}^d)$ and any $d$-tuple multi-index $J$ with $|J| \leq \alpha$, there exist $k_1, k_2 \in \mathbb{N}$ such that
  \[ \nabla^J g(x) \leq k_1 \left( 1 + \|x\|_2^{2k_2} \right), \quad \forall x \in \mathbb{R}^d, \]
i.e. $g$’s partial derivatives up to and including order $\alpha$ have at most polynomial growth. In particular, $G$ denotes the space of continuous functions with at most polynomial growth.

A Preliminary Analysis
Let $\mathbb{P}_x$ be the probability distribution of data $x$ on $\mathbb{R}^d$. Let $L(\cdot, \cdot) : \mathbb{R}^{d_0} \times \mathbb{R}^d \rightarrow \mathbb{R}$ be the loss function depending on both model parameter $\theta \in \mathbb{R}^{d_0}$ and data $x \in \mathbb{R}^d$. The notation $d_0$ emphasizes the dimension of a given parameter space for $\theta$. Define $\nabla_x L$ and $\nabla_\theta L$ to be the gradients of $L$ with respect to $x$ and $\theta$, respectively. Define $\nabla_{x\theta} L$ to be the matrix whose $i, j$-th entry is $\frac{\partial^2 L}{\partial x_i \partial \theta_j}$. Throughout this paper, we assume the following facts about $L$.

Assumption A.1 The loss function $L$ satisfies
1. $L \in C^3(\mathbb{R}^{d_0+d})$;
2. for any $\theta \in \mathbb{R}^{d_0}$, $\mathbb{E}[\|L(\theta, x)\|] < \infty$ and $\mathbb{E}[\|\nabla_x L(\theta, x)\|_2^2] < \infty$;
3. for any $R > 0$, there exists $M_R > 0$ such that $\max_{\|\theta\|_2 \leq R} \|\nabla_x L(\theta, x)\|_2 \leq M_R$, $\max_{\|\theta\|_2 \leq R} \|\nabla_{x\theta} L(\theta, x)\|_2 \leq M_R$ and $\max_{\|\theta\|_2 \leq R} \|\nabla_{x\theta} L(\theta, x)\|_2 \leq M_R \mathbb{P}_x$-almost surely.

Note that in the empirical risk minimization case where the support of $\mathbb{P}_x$ is a finite set, the conditions above are often trivially satisfied. Assumption A.1 allows us to define the following functions

\[ g(\theta) := \mathbb{E}[L(\theta, x)], \quad D(\theta) := \mathbb{E}[\nabla_x L(\theta, x)], \quad H(\theta) := \mathbb{E}[\|\nabla_x L(\theta, x)\|_2^2], \]
\[ \Sigma(\theta) := \mathbb{E}[(\nabla_x L(\theta, x) - D(\theta))(\nabla_x L(\theta, x) - D(\theta))^T]. \]
Moreover, Assumption A.1.3 and the dominated convergence theorem allow us to change orders of taking expectations and taking derivatives, and justify the following computations.

\[
\nabla_{\theta} g(\theta) = \nabla_{\theta} \mathbb{E}[L(\theta, x)] = \mathbb{E}[\nabla_{\theta} L(\theta, x)],
\]

\[
\nabla_{\theta} D(\theta) = \nabla_{\theta} \mathbb{E}[\nabla_{x} L(\theta, x)] = (\mathbb{E}[\nabla_{x} L(\theta, x)])^T,
\]

\[
\nabla_{\theta} H(\theta) = \nabla_{\theta} \mathbb{E}[\|\nabla_{x} L(\theta, x)\|^2] = \mathbb{E}[\nabla_{\theta}(\|\nabla_{x} L(\theta, x)\|^2)] = 2\mathbb{E}[\nabla_{x} L(\theta, x)\nabla_{x} L(\theta, x)].
\]

Hence, under Assumption A.1, the functions \( g(\theta), D(\theta) \) and \( H(\theta) \) are differentiable.

Now as discussed in Section 3 given an initial model parameter \( \theta_0 \), and \( \{ \tilde{x}_j \}_{j=1}^B \) sampled independently from \( \mathbb{P}_x \), Algorithm 2 updates \( \theta_1 \) as

\[
\theta_1 = \theta_0 - \frac{\eta}{B} \sum_{j=1}^B \nabla_{\theta} L(\theta_0, \tilde{x}_j) + \frac{K\eta^2}{B} \sum_{j=1}^B \nabla_{x} L(\theta_0, \tilde{x}_j) + \mathcal{O}(\eta^2)
\]

\[
= \theta_0 - \frac{\eta}{B} \sum_{j=1}^B \nabla_{\theta} L(\theta_0, \tilde{x}_j) - \frac{K\eta^2}{B^2} \sum_{i,j=1}^B \nabla_{x\theta} L(\theta_0, \tilde{x}_j)\nabla_{x} L(\theta_0, \tilde{x}_i) + \mathcal{O}(\eta^3). \tag{A.35}
\]

This computation is justified by Assumption A.1.1 and third order Taylor’s expansion.

Define \( D := \theta_1 - \theta_0 \), and by direct computations

\[
\mathbb{E}[D] = -\frac{\eta}{B} \sum_{j=1}^B \mathbb{E}[\nabla_{\theta} L(\theta_0, \tilde{x}_j)] - \frac{K\eta^2}{B^2} \sum_{i,j=1}^B \mathbb{E}[\nabla_{x\theta} L(\theta_0, \tilde{x}_j)\nabla_{x} L(\theta_0, \tilde{x}_i)] + \mathcal{O}(\eta^3)
\]

\[
= -\eta \mathbb{E}[\nabla_{\theta} L(\theta_0, x)] - \frac{K\eta^2}{B^2} \sum_{i,j=1}^B \mathbb{E}[\nabla_{x\theta} L(\theta_0, \tilde{x}_j)\nabla_{x} L(\theta_0, \tilde{x}_i)] + \mathcal{O}(\eta^3)
\]

\[
= -\eta \mathbb{E}[\nabla_{\theta} L(\theta_0, x)] - \frac{K\eta^2}{B^2} \mathbb{E}[\nabla_{x\theta} L(\theta_0, x)\nabla_{x} L(\theta_0, x)] + \mathcal{O}(\eta^3)
\]

\[
= -\eta \nabla_{\theta} g(\theta_0) - \frac{K\eta^2}{2B} \nabla_{\theta} (\|D(\theta)\|^2) - \frac{K\eta^2}{2B} (\nabla_{\theta} H(\theta_0) - \nabla_{\theta} (\|D(\theta)\|^2)) + \mathcal{O}(\eta^3).
\]

\[
\mathbb{E}[DD^T] = \frac{\eta^2}{B^2} \sum_{i,j=1}^B \mathbb{E}[\nabla_{\theta} L(\theta_0, \tilde{x}_i)\nabla_{\theta} L(\theta_0, \tilde{x}_j)^T] + \mathcal{O}(\eta^3)
\]

\[
= \eta^2 \mathbb{E}[\nabla_{\theta} L(\theta_0, x)\nabla_{\theta} L(\theta_0, x)^T] + \mathcal{O}(\eta^3)
\]

\[
= \eta^2 \mathbb{E}[\nabla_{\theta} L(\theta_0, x)\nabla_{\theta} L(\theta_0, x)^T] + \frac{\eta^2}{B^2} \sum_{i=1}^B (\mathbb{E}[\nabla_{\theta} L(\theta_0, \tilde{x}_i)\nabla_{\theta} L(\theta_0, \tilde{x}_i)^T] - \mathbb{E}[\nabla_{\theta} L(\theta_0, \tilde{x}_i)\nabla_{\theta} L(\theta_0, \tilde{x}_i)^T]) + \mathcal{O}(\eta^3)
\]

\[
= \eta^2 \mathbb{E}[\nabla_{\theta} g(\theta_0)\nabla_{\theta} g(\theta_0)^T] + \frac{\eta^2}{B} \Sigma(\theta) + \mathcal{O}(\eta^3).
\]

The formal proof gives the following lemma.

**Lemma A.1** Assume Assumption A.1. Given an initial model parameter \( \theta_0 \), and \( \{ \tilde{x}_j \}_{j=1}^B \) sampled independently from \( \mathbb{P}_x \), let \( \theta_1 \) be the one-step update of Algorithm 2. The one-step difference \( D = \theta_1 - \theta_0 \) satisfies

\[
\mathbb{E}[D] = -\eta \nabla_{\theta} g(\theta_0) - \frac{K\eta^2}{2B} \nabla_{\theta} (\|D(\theta)\|^2) - \frac{K\eta^2}{2B} (\nabla_{\theta} H(\theta_0) - \nabla_{\theta} (\|D(\theta)\|^2)) + \mathcal{O}(\eta^3), \tag{A.36}
\]

\[
\mathbb{E}[DD^T] = \eta^2 \mathbb{E}[\nabla_{\theta} g(\theta_0)\nabla_{\theta} g(\theta_0)^T] + \frac{\eta^2}{B} \Sigma(\theta) + \mathcal{O}(\eta^3). \tag{A.37}
\]

and for any \( i, j, k \in \{1, \ldots, d_\theta\} \), \( \mathbb{E}[D_i D_j D_k] = \mathcal{O}(\eta^3) \), where \( D_i \) denotes the \( i^{th} \) coordinate of \( D \).
Next, we aim to find a stochastic process \( \{ \Theta_t \}_{t \geq 0} \) with the following form
\[
d\Theta_t = (b_0(\Theta_t) + \eta b_1(\Theta_t))dt + \sigma(\Theta_t)dW_t. \tag{A.38}
\]
Here \( \{ W_t \}_{t \geq 0} \) is a \( d_\theta \)-dimensional Brownian motion defined on a probability space \( (\Omega, \mathcal{F}, \mathbb{P}) \). The drift term \( b_0, b_1 : \mathbb{R}^{d_\theta} \to \mathbb{R}^{d_\theta} \) and the diffusion term \( \sigma : \mathbb{R}^{d_\theta} \to \mathbb{R}^{d_\theta} \) are Lipschitz continuous, and are chosen such that the first and second moments of the one-step difference \( \tilde{D} = \Theta_t - \Theta_0 \) match (A.36) and (A.37), respectively.

Define the following functions
\[
G(\theta) := g(\theta) + K\beta^{-1}(H(\theta) - \|D(\theta)\|^2_2), \tag{A.39}
\]
\[
b_0(\theta) := -\nabla_\theta G(\theta), \tag{A.40}
\]
\[
b_1(\theta) := -\frac{K}{2} \nabla_\theta (\|D(\theta)\|^2_2) - \frac{1}{4} \nabla_\theta (\|\nabla_\theta G(\theta)\|^2_2), \tag{A.41}
\]
\[
\sigma(\theta) := \sqrt{2\beta^{-1}\Sigma(\theta)^{1/2}}. \tag{A.42}
\]

Here \( \beta = 2B/\eta \), the ratio between the batch size \( B \) and the learning rate \( \eta \), determines the scale of the diffusion.

Note that \( G(\theta) \) in (A.39), \( b_0(\theta) \) in (A.40) and \( \sigma(\theta) \) in (A.42) are well-defined under Assumption A.1. But the definition of \( b_1(\theta) \) in (A.41) requires the second-order differentiability of \( G(\theta) \), which is in general not guaranteed by Assumption A.1. Hence, in order to justify the definitions and facilitate further analysis, we assume the following smoothness conditions on \( b_0(\theta) \), \( b_1(\theta) \) and \( \sigma(\theta) \).

**Assumption A.2** \( b_0, b_1 \) and \( \sigma \) defined in (A.40), (A.41) and (A.42) satisfy the following regularity conditions
\[
1. b_0, b_1 \text{ and } \sigma \text{ are Lipschitz continuous;}
\]
\[
2. b_0, b_1 \text{ and } \sigma \text{ are in } G^4(\mathbb{R}^{d_\theta}).
\]

Assumption A.2 is a standard assumption to guarantee that the SDE (A.38) has a unique (strong) solution. Meanwhile, Assumption A.2 helps to control the growth of the solution (and its partial derivatives) of (A.38), which is crucial to further analysis for approximation error. Assumption A.2 requires stronger regularity conditions than Assumption A.1. But in the empirical risk minimization case, a neural network with sufficiently smooth activation and loss functions often satisfies those conditions.

The following result, Lemma A.2, shows that, under Assumption A.2, the SDE dynamic (A.38) with \( b_0, b_1, \sigma \) defined in (A.40)-(A.42) indeed matches the first and second moments of the discrete-time adversarial training dynamic (A.35).

**Lemma A.2** Assume Assumption A.1 and Assumption A.2. The SDE dynamic (A.38) with \( \Theta_0 = \theta_0 \) admits a unique solution \( \{ \Theta_t \}_{t \geq 0} \). Moreover, \( \tilde{D} := \Theta_t - \Theta_0 \) satisfies
\[
E[\tilde{D}] = E[D], \quad E[\tilde{D} \tilde{D}^T] = E[DD^T],
\]
where \( E[D] \) and \( E[DD^T] \) are defined in (A.36) and (A.37), respectively. Moreover, for any \( i, j, k \in \{1, \cdots, d_\theta\} \), \( E[\tilde{D}_i \tilde{D}_j \tilde{D}_k] = O(\eta^3) \), where \( \tilde{D}_i \) denotes the \( i \)-th coordinate of \( \tilde{D} \).

**Proof.** The uniqueness of the solution to the SDE (A.38) is due to the Lipschitz condition in Assumption A.2 and a standard existence and uniqueness result for SDEs, see Theorem 5.2.9 in [14].

To provide the moment estimates, first define the following operators for any test function \( \psi \in G^4 \). Here \( G^4 \) denote the set of functions whose partial derivatives up to and including order
four have at most polynomial growth.

\[ \mathcal{L}_1 \psi(\theta) = b_0(\theta)^T \nabla \psi(\theta) \]
\[ \mathcal{L}_2 \psi(\theta) = b_1(\theta)^T \nabla \psi(\theta) + \frac{1}{2B} \text{Tr} \left( \Sigma(\theta) \nabla^2 \psi(\theta) \right) \]
\[ \mathcal{L}_3 \psi(\theta) = \frac{1}{\sqrt{B}} \Sigma(\theta)^{1/2} \nabla \psi(\theta) \]

Note that here \( \mathcal{L}_1 \psi(\theta) \) and \( \mathcal{L}_2 \psi(\theta) \) are real-valued functions on \( \mathbb{R}^{d_\psi} \), while \( \mathcal{L}_3 \psi(\theta) \) is a vector-valued function from \( \mathbb{R}^{d_\psi} \) to \( \mathbb{R}^{d_\psi} \). By Itô’s formula, for any test function \( \psi \in G^1 \),

\[ \psi(\Theta_t) = \psi(\Theta_0) + \int_0^t \mathcal{L}_1 \psi(\Theta_s) ds + \eta \int_0^t \mathcal{L}_2 \psi(\Theta_s) ds + \sqrt{\eta} \int_0^t \mathcal{L}_3 \psi(\Theta_s) dW_s. \]

By further application of the above formula to \( \mathcal{L}_1 \psi \) and \( \mathcal{L}_2 \psi \), we have

\[ \psi(\Theta_t) = \psi(\Theta_0) + \eta \mathcal{L}_1 \psi(\Theta_0) + \eta^2 \left( \frac{1}{2} \mathcal{L}_1^2 + \mathcal{L}_2 \right) \psi(\Theta_0) \]
\[ + \eta \int_0^t \int_0^s \left( \mathcal{L}_2 \mathcal{L}_1 + \mathcal{L}_1 \mathcal{L}_2 \right) \psi(\Theta_r) dvds + \int_0^t \int_0^s \int_0^r \mathcal{L}_3 \psi(\Theta_r) drdvds \]
\[ + \eta^2 \int_0^t \int_0^s \mathcal{L}_2^2 \psi(\Theta_r) dvds + \eta \int_0^t \int_0^s \int_0^r \mathcal{L}_2 \mathcal{L}_1 \psi(\Theta_r) drdvds \]
\[ + \sqrt{\eta} \int_0^t \int_0^s \mathcal{L}_3 \psi(\Theta_r) dW_s + \sqrt{\eta} \int_0^t \int_0^s \int_0^r \mathcal{L}_3 \mathcal{L}_1 \psi(\Theta_r) dW_r ds \]
\[ + \sqrt{\eta} \int_0^t \int_0^s \int_0^r \mathcal{L}_3 \mathcal{L}_2 \psi(\Theta_r) dW_r dvds + \eta^{3/2} \int_0^t \int_0^s \mathcal{L}_3 \mathcal{L}_2 \psi(\Theta_r) dW_r dvds. \]

Taking expectations on both sides, all terms in the integral are either equal to zero, or \( O(\eta^3) \).

Observe that all the integrands have at most third order derivatives in \( b_0, b_1, \sigma_0 \) and fourth order derivatives in \( \psi \), then from the assumption that \( b_0, b_1, \sigma_0 \in G^2 \) and \( \psi \in G^2 \), all the integrands belong to \( G^0 \). Thus, the expectation of each integrand is bounded by

\[ \kappa_1 \left( 1 + \sup_{t \in [0, \eta]} \mathbb{E} \left| X_t \right|^{2\kappa_2} \right) \]

for some \( \kappa_1, \kappa_2 \). By the Lipschitz condition in Assumption A.2 and standard moment estimates for SDEs, (see Theorem 5.2.9 [13]), (A.43) is finite.

Meanwhile, the last four stochastic integrals involving \( dW \) are martingales and their expectations are equal to zero. Therefore, the expectations of all the integrals are \( O(\eta^3) \), and

\[ \psi(\Theta_t) = \psi(\Theta_0) + \eta \mathcal{L}_1 \psi(\Theta_0) + \eta^2 \left( \frac{1}{2} \mathcal{L}_1^2 + \mathcal{L}_2 \right) \psi(\Theta_0) + O(\eta^3) \]  

(A.44)

Then Lemma A.2 follows from taking \( \psi(\Theta_t) = \tilde{D}_i, \tilde{D}_j, \) and \( \tilde{D}_i \tilde{D}_j \tilde{D}_k \) in (A.44), respectively.

Now by Lemma A.1 and Lemma A.2 we have checked that the one-step difference \( D \) for the discrete-time adversarial training dynamic (A.35) and \( \tilde{D} \) for the continuous-time SDE dynamic (A.38) share the same first and second moments up to \( O(\eta) \) error. In the next section, we will establish a connection between one-step approximation and approximation on a finite time interval.

### B Approximation Error Analysis

In this section, we will analyze the approximation error between the discrete-time adversarial training dynamic (A.35) and the continuous-time SDE dynamic (A.38). Since we are comparing
a discrete-time stochastic process \( \{ \theta_t \}_{t=0.1} \) with a continuous-time stochastic process \( \{ \Theta_t \}_{t \geq 0} \), we first need to define an appropriate notion of approximation.

Notice that the discrete-time process \( \{ \theta_t \}_{t=0.1, \ldots, N} \) is adapted to the filtration generated by \( \{ x_j \}_{j=1}^B \), which is the randomness in sampling the mini-batch, while the process \( \{ \Theta_t \}_{0 \leq t \leq T} \) is adapted to an independent Wiener filtration generated by \( \{ W_s \}_{0 \leq s \leq t} \). Hence, it is not appropriate to compare individual sample paths. Rather, following similar analogy in [13], we define below the notion of weak approximation by comparing the distributions of the two processes.

**Definition B.2** Let \( T > 0, \eta \in (0, 1 \land T) \), and \( \alpha \geq 1 \) be an integer. Set \( N = \lceil T/\eta \rceil \). We say that a continuous-time stochastic process \( \{ X_t : t \in [0, T] \} \) is an order \( \alpha \) weak approximation of a discrete stochastic process \( \{ x_t : t = 0, \ldots, N \} \), if for every \( g \in G^{\alpha+1} \), there exists a positive constant \( C \), independent of \( \eta \), such that

\[
\max_{t=0, \ldots, N} |\mathbb{E} g(x_t) - \mathbb{E} g(X_{t \eta})| \leq C \eta^\alpha.
\]

The weak approximation defined above is an approximation of the distribution of sample paths, instead of the sample paths themselves. It must be distinguished from the strong approximation, where one would require the actual sample-paths of the two processes to be close, for example,

\[
\max_{t=0, \ldots, N} \mathbb{E} |x_t - X_{t \eta}|^2 \leq C \eta^\alpha.
\]

In contrast, the weak approximation requires that the expectations of the two processes \( \{ X_t : t \in [0, T] \} \) and \( \{ x_t : t = 0, \ldots, N \} \) over a sufficiently large class of test functions to be close. The test function class \( G^{\alpha+1} \) is in fact quite large, and it includes all polynomials. In particular, it implies all moments of the two processes are close at the order of \( O(\eta^\alpha) \).

As pointed out in [13], one important advantage of the weak approximation is that a continuous-time process can in fact approximate a discrete-time stochastic process whose stepwise driving noise is not Gaussian, as long as appropriate moments are matched (see the following Lemma B.3). This additional flexibility is useful as it allows the treatment of more general classes of stochastic gradient iterations, for example, asynchronous stochastic gradient descent in [1] and GAN training in [4].

Now we introduce the following key lemma from [13], which builds the connection between one-step approximation and weak approximation on a finite time interval.

**Lemma B.3 (Li et al., 2019)** Let \( T > 0, \eta \in (0, 1 \land T) \) and \( N = \lceil T/\eta \rceil \). Let \( \alpha \geq 1 \) be an integer. Let \( \{ X_t : t \in [0, T] \} \) be a continuous-time stochastic process satisfying

\[
dX_t = b(X_t)dt + \sigma(X_t)dW_t.
\]

Here \( \{ W_t \}_{t \geq 0} \) is a \( d_0 \)-dimensional Brownian motion, and assume \( b(x) \), \( \theta(x) \) are both Lipschitz continuous. Let \( \{ x_t : t = 0, \ldots, N \} \) be a discrete-time stochastic process following

\[
x_{t+1} = x_t + \eta h(x_t, y_t, \eta),
\]

where \( h : \mathbb{R}^{d_1} \times \mathbb{R}^{d_2} \times \mathbb{R} \to \mathbb{R}^{d_1} \) and \( \{ y_t : t = 0, \ldots, N \} \subset \mathbb{R}^{d_2} \) is a set of independent samples from some distribution \( Y \), and \( \{ y_t : t = 0, \ldots, N \} \) is independent of \( \{ W_t \}_{t \geq 0} \).

Define \( \{ X^s_t : t \in [0, T], X^s_0 = s \} \) as the continuous-time stochastic process (B.45) starting from \( s \), and \( \{ x^s_t : t = 0, \ldots, N, x^s_0 = s \} \) as the discrete-time process (B.46) starting from \( s \). Define \( D(s) = x^s_1 - s \) and \( \tilde{D}(s) = X^s_\eta - s \). Suppose further that the following conditions hold:

1. There exists a function \( K_1 \in G^0 \) independent of \( \eta \) such that

\[
|\mathbb{E} \prod_{j=1}^k D(i_{j}) (s) - \mathbb{E} \prod_{j=1}^k \tilde{D}(i_{j}) (s)| \leq K_1(s) \eta^{\alpha+1}
\]
for \( k = 1, 2, \ldots, \alpha \) and
\[
\mathbb{E} \prod_{j=1}^{n+1} |D_{(i_j)}(s)| \leq K_1(s) \eta^{\alpha+1}
\]
for all \( i_j \in \{1, \cdots, d\} \).

2. For each integer \( m \geq 1 \), the \( 2m \)-moment of \( x_t \) is uniformly bounded with respect to \( t \) and \( \eta \), i.e. there exists a constant \( K_2 \in \mathbb{C}^0 \), independent of \( \eta, t \), such that
\[
\mathbb{E} \left[ \|x_t^\eta\|^{2m} \right] \leq K_2(s), \quad \text{for all } t = 0, \ldots, N.
\]

Then, for each \( g \in \mathbb{C}^{\alpha+1} \), there exists a constant \( C > 0 \) independent of \( \eta \) such that
\[
\max_{t=0, \ldots, N} |\mathbb{E} g(x_t) - \mathbb{E} g(X_{t\eta})| \leq C \eta^\alpha.
\]

Lemma B.3 allows us to prove the main approximation result in this paper. In particular, we will show that the SDE (A.38) is a second-order weak approximation for adversarial training dynamic (A.35). Note that the first condition in Lemma B.3 is about moment matching for one-step differences, which are studied in Lemma A.1 and Lemma A.2 under Assumptions A.1 and A.2. However, Assumptions A.1 and A.2 are in general not enough to guarantee the second condition in Lemma B.3 on the uniform moment bound for the discrete-time process. Hence, we further assume the following facts about the loss function \( L \).

**Assumption B.3** The loss function \( L \) and its derivatives satisfy the following linear growth conditions: there exist some function \( L \) sampled independently from \( \mathbb{R}^d \to \mathbb{R}^+ \), such that \( \mathbb{E}_{x \sim P_x} [L(x)^m] < \infty \) for any integer \( m > 1 \), and for any \( \theta \in \mathbb{R}^\theta \),
\[
\|\nabla_\theta L(\theta, x)\|_2 \leq L(x)(1 + \|\theta\|_2), \quad \|\nabla_{x\theta} L(\theta, x)\|_2 \nabla_\theta L(\theta, x)\|_2 \leq L(x)(1 + \|\theta\|_2).
\]

**Theorem B.3** Assume **Assumption A.1** **Assumption A.2** and **Assumption B.3**. Fix an arbitrary time horizon \( T > 0 \) and take the learning rate \( \eta \in (0, 1 \wedge T) \) and set the number of iterations \( N = \left\lfloor \frac{T}{\eta} \right\rfloor \). Let \( \{\theta_t\}_{t=0,1,\cdots,N} \) be the discrete-time adversarial training dynamic defined in (A.35), and let \( \{\Theta_t\}_{t \in [0,T]} \) be the continuous-time SDE dynamic defined in (A.38). Set \( \Theta_0 = \theta_0 \).

Then \( \{\Theta_t\}_{t \in [0,T]} \) is an order-2 weak approximation of \( \{\theta_t\}_{t=0,1,\cdots,N} \), i.e. for each \( g \in \mathbb{C}^{\alpha+1} \), there exists a constant \( C > 0 \) independent of \( \eta \) such that
\[
\max_{t=0, \ldots, N} |\mathbb{E} g(\theta_t) - \mathbb{E} g(\Theta_t\eta)| \leq C \eta^\alpha.
\]

**Proof.** It suffices to check the conditions in Lemma B.3 are satisfied by \( \{\theta_t\}_{t=0,1,\cdots,N} \) and \( \{\Theta_t\}_{t \in [0,T]} \) for \( \alpha = 2 \).

The first condition on one-step differences in Lemma B.3 holds by Assumption A.1 and Lemma A.2. It remains to check the second condition on bounded moments.

Recall that given \( \{\tilde{x}_j\}_{j=1}^B \) sampled independently from \( P_x \), the update in adversarial training is
\[
\theta_{t+1} = \theta_t - \frac{\eta}{B} \sum_{j=1}^B \nabla_\theta L(\theta_t, \tilde{x}_j) - \frac{K \eta^2}{B^2} \sum_{i,j=1}^B \nabla_{x\theta} L(\theta_t, \tilde{x}_j) \nabla_\theta L(\theta_t, \tilde{x}_i) + O(\eta^3) =: \theta_t + \eta h(\theta_t, \{\tilde{x}_i\}_{i=1}^B, \eta),
\]
where
\[
h(\theta_t, \{\tilde{x}_i\}_{i=1}^B, \eta) := -\frac{1}{B} \sum_{j=1}^B \nabla_\theta L(\theta_t, \tilde{x}_j) - \frac{K \eta}{B^2} \sum_{i,j=1}^B \nabla_{x\theta} L(\theta_t, \tilde{x}_j) \nabla_\theta L(\theta_t, \tilde{x}_i) + O(\eta^2).
\]
By Assumption [B.3]

\[
\| h(\theta_t, \{\tilde{x}_i\}_{i=1}^B, \eta) \|_2 \leq \frac{1}{B} \sum_{j=1}^B \| \nabla \theta L(\theta_t, \tilde{x}_j) \|_2 + \frac{K\eta}{B^2} \sum_{i,j=1}^B \| \nabla_{\theta \theta} L(\theta_t, \tilde{x}_j) \|_2 \| \nabla_x L(\theta_t, \tilde{x}_i) \|_2 + O(\eta^2)
\]  

(B.47)

\[
\leq \frac{1}{B} \sum_{j=1}^B L(\tilde{x}_j) (1 + \| \theta_t \|_2) + \frac{K\eta}{B^2} \sum_{i,j=1}^B L(\tilde{x}_j) (1 + \| \theta_t \|_2) + O(\eta^2)
\]  

(B.48)

\[
\leq \left( \frac{1}{B} \sum_{j=1}^B L(\tilde{x}_j) + \frac{K\eta}{B^2} \sum_{i,j=1}^B L(\tilde{x}_j) \right) (1 + \| \theta_t \|_2).
\]  

(B.49)

Define the random variable

\[ L_t := \frac{1}{B} \sum_{j=1}^B L(\tilde{x}_j) + \frac{K\eta}{B^2} \sum_{i,j=1}^B L(\tilde{x}_j) + 1. \]

By the independence of \( \{ \tilde{x}_j \}_{j=1}^B \) and the finite moment condition in Assumption [B.3], we can conclude that \( \mathbb{E}[L_t^m] < \infty \) for any \( m > 1 \).

To simplify the notation, we use \( h_t \) to denote \( h(\theta_t, \{\tilde{x}_i\}_{i=1}^B, \eta) \) in the remaining proof.

Now for any integer \( m > 1 \) and \( t \geq 0 \), we have

\[
\| \theta_{t+1} \|_2^m \leq \| \theta_t \|_2^m + \sum_{l=1}^m \binom{m}{l} \| \theta_t \|_2^{m-l} \eta^l \| h_t \|_2^l.
\]

Now, for \( 1 \leq l \leq m \), using Assumption [B.3] and the fact that \( h_t \) is independent of \( \theta_t \),

\[
\mathbb{E} \left[ \| \theta_t \|_2^{m-l} \| h_t \|_2^l \right] = \mathbb{E} \left[ \| \theta_t \|_2^{m-l} \mathbb{E} \left[ \| h_t \|_2^l | \theta_t \right] \right]
\]

\[
\leq \mathbb{E} \left[ \| \theta_t \|_2^{m-l} \mathbb{E} \left[ L_t^l (1 + \| \theta_t \|_2)^l | \theta_t \right] \right]
\]

\[
= \mathbb{E} \left[ \| \theta_t \|_2^{m-l} (1 + \| \theta_t \|_2)^l \mathbb{E} \left[ L_t^l | \theta_t \right] \right]
\]

\[
= \mathbb{E} \left[ \| \theta_t \|_2^{m-l} (1 + \| \theta_t \|_2)^l \right]
\]

\[
= \mathbb{E} \left[ L_t^l \right] \mathbb{E} \left[ \| \theta_t \|_2^{m-l} (1 + \| \theta_t \|_2)^l \right]
\]

\[
\leq ME \left[ L_t^l \right] \left( 1 + E \left[ \| \theta_t \|_2^m \right] \right).
\]

In the last line, the constant \( M \) is independent of \( \eta \) and \( t \), but may depend on the uniform \( r^{th} \)-moment bound for \( l < m \), the existence of which can be justified by induction on \( m \). Hence, if we let \( a_t := \mathbb{E} \| \theta_t \|_2^m \), we have

\[
a_{t+1} \leq (1 + C\eta)a_t + C'\eta
\]

where \( C, C' > 0 \) are independent of \( \eta \) and \( t \), which immediately implies

\[
a_t \leq (a_0 + C'/C)(1 + C\eta)^t - C'/C
\]

\[
\leq (a_0 + C'/C)e^{(T/n)\log(1+C\eta)} - C'/C
\]

\[
\leq (a_0 + C'/C)e^{C'T} - C'/C.
\]

Therefore, the second condition on bounded moments in Lemma [B.3] holds and the weak approximation result follows. \( \square \)
C Convergence Analysis

In this section, we will establish the convergence result for adversarial training via studies of the invariant measure of the SDE (A.38). The following assumptions are needed to formally state the convergence result.

Assumption C.4 \( b_0, b_1 \) and \( \sigma \) defined in (A.40), (A.41) and (A.42) satisfy the following regularity conditions

1. \( b_0, b_1 \) and \( \sigma \) are Lipschitz continuous;
2. there exist some positive real numbers \( r \) and \( R \), independent of \( \eta \), such that for any \( \theta \in \mathbb{R}^{d_\theta} \) with \( \|\theta\|_2 \geq R \),
   \[ \theta^T (b_1(\theta) + \eta b_2(\theta)) \leq -r\|\theta\|_2. \]
3. there exists a constant \( l > 0 \) such that for any \( \theta \in \mathbb{R}^{d_\theta} \),
   \[ \theta^T \Sigma(\theta) \theta \geq l\|\theta\|_2^2. \]

Assumption C.4.1 is a standard assumption to guarantee that the existence of a unique (strong) solution to the SDE (A.38). Assumption C.4.2 requires that the drift term points inward when \( \theta \) sufficiently large, and it is closely related to the recurrence property of the process \[3\]. Assumption C.4.3 requires \( \Sigma(\theta) \) to be uniformly elliptic, i.e. the eigenvalues of \( \Sigma(\theta) \) are uniformly lower bounded by a positive number \( l \). It is also known as the non-degenerate condition \[14\]. Both Assumption C.4.2 and Assumption C.4.3 are common in the literature studying invariant measure and ergodicity of SDEs, see for example \[25\], \[15\] and \[13\].

Theorem C.4 Assume Assumption A.1 and Assumption C.4. The stochastic process \( \{\Theta_t\}_{t \geq 0} \) satisfies the SDE (A.38) admits a unique invariant measure \( \mu^* \), with an exponential convergence rate. More specifically, there exists a unique probability measure \( \mu^* \) such that for any measurable bounded function \( f \) and any \( t \geq 0 \),

\[
\int \mathbb{E}[f(\Theta_t)|\Theta_0 = \theta] \mu^*(d\theta) = \int f(\theta) \mu^*(d\theta).
\]

Moreover, there exist a constant \( \rho > 0 \) and a positive function \( C : \mathbb{R}^{d_\theta} \to \mathbb{R}_+ \), such that for any measurable set \( A \subset \mathbb{R}^{d_\theta} \),

\[
|\mathbb{P} [\Theta_t \in A|\Theta_0 = \theta] - \mathbb{P}_\mu(A)| \leq C(\theta)e^{-\rho t}.
\]

Proof. The uniqueness and existence follow from Corollary 3.15 in \[3\], while the exponential convergence rate is a direct consequence of \[25\]. \( \square \)

D Adaptive Learning Rate

In this section, we will provide rigorous justifications and more explicit computations for the results in Section 5. In particular, we will derive the SDE approximation for the learning rate adjustment problem, and derive the optimal learning rate for a class of linear models.

D.1 SDE Approximation for Adaptive Learning Rate

Recall in Section 5 to allow for adjustment of the learning rate, we modify the gradient steps in Algorithm 2 by a multiplication factor \( u_t \) to the original constant learning rate: for the inner
iteration \( k = 1, \cdots, K, \)
\[
\delta_{k+1} = \delta_k + \frac{\eta u_t}{B} \sum_{j=1}^B \nabla J(\theta_t, x_j, \delta_k) \text{ and then}
\]
\[
\theta_{t+1} = \theta_t - \frac{\eta u_t}{B} \sum_{j=1}^B \nabla J(\theta_t, x_j, \delta_K)).
\]

(D.50)

Here the adjustment factor \( u_t \in [0, 1] \) and the constant \( \eta \) is the maximum allowed learning rate.

It suffices to notice that the current iteration (D.50) is equivalent to applying Algorithm 2 to the scaled loss function \( u_t J \). Hence, by properly scaling all the functions \( g(\theta), D(\theta), H(\theta), \Sigma(\theta) \), we can conclude by Theorem [B.3] that the corresponding second order weak approximation to (D.50) takes the following modified form of:
\[
d\Theta_t = (b_0(\Theta_t, u_t) + \eta b_1(\Theta_t, u_t))dt + \sigma(\Theta_t, u_t)dW_t.
\]

(D.51)

Here we slightly abuse the notations \( b_0, b_1, \sigma \) originally defined in (A.40)-(A.42) and denote
\[
b_0(\theta, u) = -\nabla_\theta \left[u g(\theta) + K \beta^{-1} u^2 \left(H(\theta) - \|D(\theta)\|^2\right)\right];
\]
\[
b_1(\theta, u) = -\frac{K}{2} u^2 \nabla_\theta(\|D(\theta)\|^2) - \frac{1}{4} \nabla_\theta(\|b_0(\theta, u)\|^2);
\]
\[
\sigma(\theta, u) = u \sqrt{2\beta^{-1} (\Sigma(\theta))^{1/2}}.
\]

(D.52)

### D.2 Adaptive Learning Rate for Linear Models

Recall the linear model (5.25) considered in Section 5. The calculations in Section 5 imply that finding the optimal learning rate for the model (5.25) is equivalent to solving the following optimal control problem:
\[
\min_{u:[0,T] \rightarrow [0,1]} s_T \text{ subject to } \frac{ds_t}{dt} = -2s_t \cdot \left((2 + 4K\eta)\alpha u_t + \eta \alpha^2 u_t^2\right) + \frac{8\alpha^2 \sigma}{\beta} u_t^2.
\]

(D.53)

Here \( s_t \) is the expected loss at time \( t \). A standard way to solve (D.53) is through the dynamic programming principle [29]. For \( t \in [0, T] \) and \( s \in \mathbb{R} \), we define the value function
\[
V(s, t) := \min_{u:[t,T] \rightarrow [0,1]} \left\{ s_T \mid \frac{ds_r}{dr} = -2s_r \cdot \left((2 + 4K\eta)\alpha u_r + \eta \alpha^2 u_r^2\right) + \frac{8\alpha^2 \sigma}{\beta} u_r^2, \text{ and } s_t = s \right\},
\]

(D.54)

which is the optimal value of the problem (D.53) when the trajectory starts in position \( s \) at time \( t \).

The dynamic programming principle allows us to derive the following partial differential equation satisfied by the value function \( V \) (D.54), which is known as the Hamilton-Jacobi-Bellman equation.
\[
-\partial_t V(s, t) = \min_{u \in [0,1]} \left( -2s \cdot \left((2 + 4K\eta)\alpha u + \eta \alpha^2 u^2\right) + \frac{8\alpha^2 \sigma}{\beta} u^2 \right) \cdot \partial_s V(s, t); \quad V(s, T) = s.
\]

(D.55)

After solving (D.55), the corresponding optimal learning rate factor \( u^* \) is in the feedback form as a function of \( t \) and \( s \), and is given by the formula
\[
u^*(s, t) = \arg \min_{u \in [0,1]} \left( -2s \cdot \left((2 + 4K\eta)\alpha u + \eta \alpha^2 u^2\right) + \frac{8\alpha^2 \sigma}{\beta} u^2 \right) \cdot \partial_s V(s, t),
\]

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i.e. at time $t$, with the expected loss $s$, it is optimal to choose the learning rate factor $u = u^*(s, t)$.

In this particular problem (D.53), in fact, we do not need to solve (D.55) for $V (D.54)$ first. It is not hard to see that $\partial_s V(s, t) \geq 0$ for all $s \in \mathbb{R}$ and $t \in [0, T]$. This is because, the lower the $s$ is, the closer we are to the optimum and hence the minimum cost achievable in the same time interval $[t, T]$ should be less. Therefore, the optimal learning rate factor is in the feedback form as a function of the expected loss $s$, and is given by

$$u^*(s) = \arg \min_{u \in [0, 1]} \left( -2s \cdot ((2 + 4K\eta)\alpha u + \eta\alpha^2 u^2) + \frac{8\alpha^2 \sigma^2}{\beta} u^2 \right)$$

$$= \begin{cases} 
\min \left\{ 1, \frac{(1 + 2K\eta)sB}{(2\sigma - sB)\alpha\eta} \right\} & \text{if } s < \frac{2\sigma}{B}, \\
1 & \text{if } s \geq \frac{2\sigma}{B}.
\end{cases}$$