Batch Size Matters: A Diffusion Approximation Framework on Nonconvex Stochastic Gradient Descent

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Abstract

In this paper, we study the stochastic gradient descent method in analyzing nonconvex statistical optimization problems from a diffusion approximation point of view. Using the theory of large deviation of random dynamical system, we prove in the small stepsize regime and the presence of omnidirectional noise the following: starting from a local minimizer (resp. saddle point) the SGD iteration escapes in a number of iteration that is exponentially (resp. linearly) dependent on the inverse stepsize. We take the deep neural network as an example to study this phenomenon. Based on a new analysis of the mixing rate of multidimensional Ornstein-Uhlenbeck processes, our theory substantiate a very recent empirical results by Keskar et al. (2016), suggesting that large batch sizes in training deep learning for synchronous optimization leads to poor generalization error.

1 Introduction

First-order methods such as stochastic gradient descent (SGD) have enjoyed empirical success in many statistical learning tasks including maximum likelihood estimation, online learning, empirical risk minimization and deep neural networks due to its favorable computational and statistical efficiency (Bottou, 2010; Bubeck et al., 2015; Bottou et al., 2016). However, there is still lack of understanding in the theoretical properties of SGD. For instance, it remains largely unexplored why the algorithms often exhibit fast convergence towards local minimizers with desirable statistical performance. It is known that first-order algorithms only guarantee to converge to a stationary point Ghadimi & Lan (2013), and the problem of finding a global optimizer is in worst case NP-hard. In this paper, we aim at developing a new analytic framework of generic diffusion approximations, aiming at better understanding and analyzing the global dynamics of nonconvex SGD.

In nonconvex statistical optimization, a central issue for SGD to succeed is whether the iteration can escape from unstable stationary points including both saddle points and local maximizers. When

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the objective function has the **strict saddle property** that all unstable stationary points have a strictly negative eigenvalue, it is shown by Ge et al. (2015) that in both unconstrained and constrained cases, SGD with injected noises and appropriately chosen stepsizes converges to a local minimizer at a rate of $C \cdot d^\alpha \cdot T^{-1/4}$, where $d$ is the underlying dimension, $\alpha$ is at least 1 and constant $C$ absorbs a polylogarithmic factor of $T$. In this work, we only concentrate on why the iteration can escape from unstable stationary points when the randomness incorporated in the noisy gradients is sufficiently omnidirectional; that is, the noisy gradients are of large variances at every direction.

Another line of recent works characterize distributions of the SGD iterates via diffusion processes, which are solutions to some ordinary / stochastic differential equations (ODE / SDE). The method of diffusion approximation is advantageous in characterizing the randomness of updates by an Itô’s integral. It has hence been used to analyze variants of stochastic algorithms in (Li et al., 2015; Su et al., 2016; Li et al., 2016a,b; Krichene et al., 2015; Wibisono et al., 2016; Wilson et al., 2016). Among them, Li et al. (2016b) analyzes a projected SGD algorithm to solve the problem of independent component analysis (ICA). For the first time, their work introduces a novel local-global-local three-phase analysis based on the techniques of weak convergence to diffusions (Stroock & Varadhan, 1979; Ethier & Kurtz, 2005), implying an optimal $O(T^{-1/2})$-rate of convergence in $T$. In this paper, we extend the three-phase framework in Li et al. (2016b) and consider a broadly general unconstrained stochastic optimization problem. Our work provides a rigorous diffusion approximation characterization of the global dynamics of SGD initialized at some stationary point, which suggests the vital role of randomness in enabling the algorithm to fast escape from unstable stationary points, as well as efficient convergence to a stationary point.

Using our framework of the diffusion approximation for SGD algorithms which we refer to SGD diffusion, we theoretically prove the following results based on the large deviation theory of continuous dynamical system.

**Theorem 1.1** (Informal main results). (i) Let the stepsize $\eta$ be a sufficiently small constant. When the noises are omnidirectional, starting from an unstable stationary point (saddle point or local maximizer) the SGD diffusion escapes from such point in asymptotically $C \cdot \gamma^{-1} \eta^{-1} \log(\eta^{-1})$ time. Here $-\gamma < 0$ is the smallest eigenvalue of Hessian at an unstable stationary point.

(ii) When the stepsize $\eta$ is sufficiently small, starting from a stable stationary point (local minimizer) the SGD diffusion escapes from such point in asymptotically $\exp(C \eta^{-1})$ time.

The formal version of the above theorem are separately Theorems 3.2 and 3.3. In comparison, Ge et al. (2015) prove for discrete-time SGD with noise injection an escaping time of $C \cdot \eta^{-2}$, where $C$ absorbs a power of $d$ and polylogarithmic factor of $\eta^{-1}$, so our rate in Theorem 1.1(i) implies a much faster rate than Ge et al. (2015) for saddle points escaping. However the convergence rate result of Ge et al. (2015) is global and has no initialization assumption. In comparison, our theorem suggests a potentially much sharper convergence rate and has mild assumption of omnidirectional noises. We hope our work inspires more future works on SGD convergence rates along this line of research.
**More related works**  The SGD algorithms for nonconvex optimization problem is of central interest to a recent line of work. Pemantle (1990) proves from a gradient flow viewpoint the nonconvergence of the SGD algorithm with diminishing stepsizes to a nondegenerate unstable stationary point, provided that the difference between each SGD increment and its expectation (the *noise*) is sufficiently omnidirectional. Ghadimi & Lan (2013) proves that under some regularity conditions SGD converges to stationary points with an explicit rate of convergence; however, unlike in convex optimization, stationary points of nonconvex objective function may exhibit unfavorable statistical properties. For strict-saddle functions, Ge et al. (2015) shows that by adding unit spherical noise in each update, SGD converges to local minimizers but *not* saddle points, given that the objective function is strict-saddle. In addition when true gradients are available, Lee et al. (2016) proves that under uniformly randomized initialization, (noiseless) gradient descent method only converges to minimizers, and Jin et al. (2017) proves when adding ball-shaped noises periodically, the gradient descent method efficiently converges to a local minimizer at rate $O\left(polylog(d) \cdot T^{-1/2}\right)$.

**Application in Deep Learning**  In recent years, deep neural network has achieved state-of-the-art performance in a variety of applications including computer vision, natural language processing and reinforcement learning. Training a deep neural network frequently involves solving a nonconvex stochastic optimization problem using SGD algorithms and their variants, which has also raised many interesting theoretical questions. In this work, we establish a diffusion approximation framework to provide a new angle at this direction.

A number of recent works discuss the geometric properties of loss surfaces in deep neural networks. Dauphin et al. (2014) argues that for general multi-layer neural network, with high probability the loss function has a combinatorially large number of saddle points, and a majority of the saddle points possess many falling directions and errors at the points are much larger than the global minimizer. Choromanska et al. (2015) theoretically verifies that for geometry of local minimizers, loss surfaces for large neural nets have most local minimizers being essentially equivalent, yielding similar performance on a test set. They also conclude that the probability of finding a high-value *bad/poor* local minimizer decreases quickly with network size, and finding global minimizer on the training set is costly and may lead to overfitting. Keskar et al. (2016) empirically finds that the equivalent local minimizers with sharper curvatures have poor generalization error on testing data. Their analysis concludes that compared to small-batch methods, large-batch methods are almost invariably attracted to regions with unfavorable sharp minimizers and thus exhibit worse performance on testing data sets. Very recently, Kawaguchi (2016) proves that in deep linear neural network there are no *poor* local minimizers, and hence all local minimizers are global minimizers.

From a diffusion approximation theoretical perspective, the phenomenon observed by aforementioned works in deep learning can be explained as follows.

(i) Appropriate amount of omnidirectional noise enables rapid escaping from nondegenerate saddle points and hence consistently produce local minimizer with small errors. This explains the saddle-point escaping phenomenon exhibited in Dauphin et al. (2014); Keskar et al. (2016).

(ii) The variance of randomness in each iterate scales linearly with respect to the inverse batch
size, and therefore the randomness level of a small-batch method is higher than its large-batch counterpart. Also, our analysis shows that randomness accumulates faster at the basin of a sharp local minimizer, and hence the iteration needs fewer iterations to leave a sharp basin of attraction of a certain depth compared to a flat one. This is argued quantitatively in §4 under relatively weak additional assumptions, explaining the phenomenon of escaping from local minimizers observed in Keskar et al. (2016).

Our Contribution Based on theories of diffusion approximation and random dynamical system, we propose a new framework for characterizing the global dynamics of nonconvex statistical optimization. In the regime of small stepsize, we provide rigorous theoretical results on the local dynamics near unstable and stable stationary points, suggesting an exact asymptotic of the escaping time from stationary points. As an application, our work provides (to the best of the authors’ knowledge) a first theoretical explanation of the empirical evidence by Keskar et al. (2016). We hope our analysis can provide new perspectives on optimization theory to both optimization and machine learning communities.

2 Background

In this section we prepare for readers the basic settings of the SGD algorithm. For a generally nonconvex stochastic loss function \( f(x, \zeta) \) that is twice differentiable with respect to \( x \), our goal is to solve the following optimization problem

\[
\min_x \mathbb{E}[f(x, \zeta)],
\]

where \( \zeta \) is sampled from some distribution \( D \). At \( t \)th iteration, we evaluate the noisy gradient \( \nabla f(x^{(t-1)}, \zeta_t) \) and update the iteration according to

\[
x^{(t)} = x^{(t-1)} - \eta \nabla f(x^{(t-1)}, \zeta_t).
\]

(2.1)

Here \( \eta > 0 \) denotes the small constant stepsize, and the noisy gradient admits randomness that comes from both noise from stochastic gradient and possibly injected additive noise. It is straightforward to observe that the iteration \( \{x^{(t)}\} \) generated by (2.1) forms a discrete time, time-homogeneous Markov process. The advantages of stochastic gradient method are two folds: (i) it requires little memory and is hence scalable to the “big data” setting; (ii) it does not require the knowledge of the distribution \( \zeta_t \).

Throughout this paper, we focus on the case that the stochastic function \( f(x, \zeta) \) is twice-differentiable with respect to \( x \). We introduce the following definition.

**Definition 2.1 (Stationary Point).** Call \( x \in \mathbb{R}^d \) a stationary point if the gradient \( \nabla f(x) = 0 \). By investigating the Hessian matrix at point \( x \), we detail the definition in the following two cases:

(i) A stationary point \( x \) is **stable** if the Hessian matrix \( \nabla^2 f(x) \) is positive semidefinite, and the least eigenvalue is strictly positive;
(ii) A stationary point $x$ is \textit{unstable} if the least eigenvalue of Hessian matrix $\nabla^2 f(x)$ is strictly negative.

For local dynamics analysis, it is sufficient to analyze the second-order approximation of objective function, since by Taylor’s theorem we have

$$f(x) = f(x^*) + (\nabla f(x^*))^\top (x - x^*) + \frac{1}{2} (x - x^*)^\top \nabla^2 f(x^*)(x - x^*) + O(\|x - x^*\|^3)$$

$$= f(x^*) + \frac{1}{2} (x - x^*)^\top \nabla^2 f(x^*)(x - x^*) + O(\|x - x^*\|^3).$$

(2.2)

It is straightforward to observe that a stable stationary point is always a local minimizer, and an unstable stationary point can be either a local maximizer (when Hessian has only negative eigenvalues) or a saddle point (when Hessian has both negative and nonnegative eigenvalues). On a side notes, results in Dauphin et al. (2014) implies that nondegenerate stationary points are isolated and can hence be analyzed sequentially.

2.1 SGD Diffusion Process

In this subsection we introduce the concept of the SGD diffusion process analyzed throughout the entire paper, along with its local approximation by gradient flow and Ornstein-Uhlenbeck process. By calculating the infinitesimal mean and variance of (2.1), we conclude when $\text{var}(\nabla f(x, \zeta))$ has at least second moments such iteration can be \textit{approximated} by the solution to SDE

$$dX(t) = -\eta \nabla f(X(t)) \, dt + \eta S(X(t)) \, dB(t), \quad (2.3)$$

where for each $x \in \mathbb{R}^d$, $S(x) = [\text{var}(\nabla f(x, \zeta))]^{1/2}$ is a positive semidefinite matrix-valued function and $B(t)$ is a standard $d$-dimensional Brownian motion. We call the solution $X(t)$ to SDE (2.3) the \textit{SGD diffusion process} with respect to (2.1).

\textbf{Local Approximation} \quad \text{When } \|\nabla f(X(t))\| \geq \delta \text{ for some positive constant } \delta, X(t) \text{ is distant from a stationary point } x^* \text{ and hence in (2.3) the gradient dominates over noise and is approximate to the solution of ODE}

$$\frac{dX(t)}{dt} = -\eta \nabla f(X(t)). \quad (2.4)$$

\text{In contrast, when } \|\nabla f(X(t))\| < \delta \text{ we have } X(t) \text{ being close to a stationary point } x^* \text{ in which case the noise terms in (2.3) dominates the gradient and can be approximated by the solution to an SDE. To see this, we conduct the local linear approximation: since } \nabla f(x^*) = 0 \text{ we have by Taylor expansion}

$$\nabla f(x) \approx \nabla^2 f(x^*)(x - x^*) = H(x - x^*),$$

where $H \equiv \nabla^2 f(x^*)$ is the Hessian matrix of $f(x)$ at $x^*$. Let $S \equiv S(x^*)$, then for small $\eta$ the iteration $x^{(i)}$ is locally approximated by a local SDE:

$$dX(t) = -\eta H (X(t) - x^*) \, dt + \eta S \, dB(t). \quad (2.5)$$
The solution of SDE (2.5) is identified as a *multidimensional Ornstein-Uhlenbeck process* (Oksendal, 2003) which has the explicit form

\[
X(t) = x^* + \exp(-\eta \cdot tH)(X(0) - x^*) + \eta \int_0^t \exp(-\eta \cdot (t - s)H)S \, dB(s).
\]

In fact, with additional assumptions we can show that such approximation can be made solid via weak convergence of Markov processes (Stroock & Varadhan, 1979; Ethier & Kurtz, 2005). In the rest of this paper, we concentrate our analysis on the continuous process \(X(t)\) that solves (2.3), which gives us more insight about the original discrete-time SGD dynamics.

### 3 Limiting Behavior via Stochastic Analysis

Throughout this section, we introduce from stochastic analytical theory to study the limiting behavior of regime of small stepsize \(\eta \to 0^+\). For clarity purposes we add a \(\eta\) on the superscript of the SGD diffusion process \(X^\eta(t)\).

**Notations and Concepts** We denote by \(\|u\|\) as the Euclidean norm of a vector \(u \in \mathbb{R}^d\). For a real symmetric matrix \(H \in \mathbb{R}^{d \times d}\), let \(\lambda_{\text{min}}(H)\) be its least eigenvalue. Fixing a connected open set \(D \subset \mathbb{R}^d\), a function \(g : D \to \mathbb{R}\) is said to be continuously differentiable, denoted by \(C^1(D)\), if it has continuous first-order partial derivatives \(\partial g/\partial x_i\). Similarly, for any \(m \geq 2\), we say \(g\) is \(m\)th continuously differentiable, denoted by \(g \in C^m(D)\), if all the first order partial derivatives are \(C^{m-1}(D)\) functions. Let \(\nabla f(x)\) and \(\nabla^2 f(x)\) be the gradient vector and Hessian matrix at point \(x\) for a function \(f \in C^2(D)\). Finally, a matrix valued function \(S : D \to \mathbb{R}^{d \times d}\) is said to be \(C^m(D)\) if each entry of \(S\) is a \(C^m(D)\) function.

#### 3.1 Stable Stationary Points

In this subsection we aim at establishing the dynamics near local minimizers. In order to present the formal statement of our result, we introduce a condition that rigorously characterizes the omnidirectional noises. Recall that \(D\) is a bounded connected open set with smooth boundary \(\partial D\). We first define

**Definition 3.1.** We say a matrix valued function \(M(x) : D \to \mathbb{R}^{d \times d}\) is *uniformly positive definite* if \(M(x)\) is positive definite at every point \(x \in D\), and \(\inf_{x \in D} \lambda_{\text{min}}(M(x)) > 0\). In words, the smallest eigenvalue of \(M(x)\) is a positive and bounded away from 0.

Let the hitting time \(T^\eta\) of \(\partial D\) be

\[
T^\eta = \inf\{t > 0 : X^\eta(t) \in \partial D\}. \tag{3.1}
\]

Suppose that \(x^* = 0\) is a nondegenerate local minimizer. Also let \(E_x\) denote the conditional expectation operator on \(X^\eta(0) = x\). We conclude the following theorem.
**Theorem 3.2.** Consider the SDE (2.3). Suppose the matrix-valued function \( S(x) \in C^1 \), \( f(x) \in C^2 \) \( S(x)S(x)^\top \) is uniformly positive definite. Then for any sufficiently small \( \delta > 0 \) there exists an open ball \( B(0, \delta) \subset U \) such that for any convex open set \( D \) inside \( B(0, \delta) \) containing \( x = 0 \), there exists a constant \( \bar{V}_D \in (0, \infty) \) depending solely on \( D \) such that the expected hitting time \( T^\eta \) in (3.1) satisfies
\[
\lim_{\eta \to 0^+} \eta \log[\mathbb{E}_x T^\eta] = \bar{V}_D, \quad \forall x \in D.
\]

Further, we have uniform control of the mean exit time: there exist \( \delta_1 \in (0, \delta), C_1, C_2 > 0 \) and \( \eta_0 > 0 \) so that whenever \( \eta \leq \eta_0 \)
\[
C_1 \leq \inf_{x \in B(0, \delta_1)} \eta \log[\mathbb{E}_x T^\eta] \leq \sup_{x \in B(0, \delta_1)} \eta \log[\mathbb{E}_x T^\eta] \leq C_2.
\]

Proof of Theorem 3.2 is provided in §B in the Appendix, which utilizes large deviation theory developed in Dembo & Zeitouni (2010). Theorem 3.2 indicates that on average, the system will wander near the local minimizer for asymptotically \( \exp(C\gamma^{-1}) \) number of steps until an escaping event from local minimizer occurs.

**Remark.** \( \bar{V}_D \) is called the quasi-potential and is the cost for forcing the system to be at \( z \in \partial D \) starting from \( x = 0 \); see §B in the Appendix or Dembo & Zeitouni (2010) for more on this. Also, see Aldous (1989) for a Poisson clumping heuristics analysis for this process.

### 3.2 Unstable Stationary Points

For a generic nondegenerate saddle point (or local maximizer) \( x^* \) we are ready to present the following Theorem 3.3. For easiness of presentation, we continue to assume without loss of generality that \( x^* = 0 \). Also, since \( H \) is real symmetric, it has \( d \) real eigenvalues denoted by \( \lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_d \).

To be convenient, we introduce \( \gamma_i = -\lambda_{d-i} \), and hence \( \gamma_1 \geq \gamma_2 \geq \ldots \geq \gamma_d \) are the eigenvalues of \(-H\). Recall that \( x = 0 \) is a nondegenerate stationary point if \( \lambda_i \neq 0 \). For a nondegenerate minimizer, we clearly have \( \lambda_d > 0 \) or \( \gamma_1 < 0 \), and for a nondegenerate unstable point, \( \lambda_d < 0 \) or \( \gamma_1 > 0 \).

**Theorem 3.3.** Consider the SDE (2.3). Let \( D \subset \mathbb{R}^d \) be a bounded connected open set with smooth boundary containing the stationary point \( 0 \). Suppose \( S(x) : D \mapsto \mathbb{R}^{d \times d} \) is \( C^3 \) and \( S(x)S^\top(x) \) is uniformly positive definite, and \( f : D \mapsto \mathbb{R} \) is \( C^4 \). If \( x_0 = 0 \) is a nondegenerate unstable point that satisfies \( \gamma_i > 0 \), and \( \gamma_i \neq 0 \) for any \( 1 \leq i \leq d \), then the expected hitting time \( T^\eta \) in (3.1) conditional on \( X(0) = 0 \) satisfies
\[
\lim_{\eta \to 0} \frac{\mathbb{E}_0 T^\eta}{\eta^{-1} \log \eta^{-1}} = 0.5\gamma_1^{-1}.
\]

Furthermore for any \( x_0 \in D \), the expected hitting time \( T^\eta \) in (3.1) conditional on \( X(0) = x_0 \) satisfies
\[
\lim_{\eta \to 0} \frac{\mathbb{E}_{x_0} T^\eta}{\eta^{-1} \log \eta^{-1}} \leq 0.5\gamma_1^{-1}.
\]
Theorem 3.3 implies the same leading-order asymptotic behavior as in (A.7). Its proof is adapted from the classical dynamical system result in Kifer (1981) and detailed in §B in the Appendix. In addition, the analysis provided in Kifer (1981) suggests the following interesting phenomenon: if \( x_0 \) is a point such that the ODE (3.5) never hits \( \partial D \), then as \( \eta \to 0^+ \), \( X(T\eta) \) converges to a measure that concentrates on the intersection between \( \partial D \) and the trajectory of ODE initialized at a point \( x_0 \) that deviates tiny small from 0 at the eigendirection of Hessian corresponding to \( \gamma_1 \).

**Remark** Note that in (3.4), we have inequality. If the gradient flow ODE system

\[
\frac{dX(s)}{ds} = -\nabla f(X(s)), \quad X(0) = x_0, \tag{3.5}
\]

satisfies \( \theta(x_0) = \inf\{t : X(t) \in \partial D\} \in (0, \infty) \), then

\[
\lim_{\eta \to 0} \eta^{-1} E_{x_0} T^n = \theta(x_0).
\]

For such \( x_0 \) the limit in (3.4) implies \( E_{x_0} T^n/[\eta^{-1} \log \eta^{-1}] \) tends to 0 as \( \eta \to 0^+ \). Hence in the case of nondegenerate local maximum (3.4) gives the limit 0 for all points but 0. However in the case of saddle points, the limit is nonzero for all points on the so-called *stable manifold*.

## 4 Application in Deep Neural Networks

In deep learning, a generally nonconvex loss function is minimized to learn the weights of a deep neural network. To be concrete, our goal in training deep neural networks is to solve the following stochastic optimization problem

\[
\min_{x \in \mathbb{R}^d} f(x) = \frac{1}{M} \sum_{i=1}^{M} f_i(x),
\]

where each component \( f_i \) corresponds to the loss function for data point \( i \in \{1, \ldots, M\} \), \( x \) is the vector of weights being optimized. When we use mini-batch training and \( B \) is the size of minibatch uniformly sampled from \( \{1, \ldots, M\} \), the objective function can be further written as the expectation of a stochastic function

\[
\frac{1}{M} \sum_{i=1}^{M} f_i(x) = \mathbb{E}_B \left( \frac{1}{|B|} \sum_{i \in B} f_i(x) \right),
\]

Hence the SGD algorithm (2.1) for minimizing the objective function \( f(x) \) iteratively updates the algorithm as

\[
x^{(t)} = x^{(t-1)} - \eta \cdot \left( \frac{1}{|B_t|} \sum_{i \in B_t} \nabla f_i(x^{(t-1)}) \right),
\]

where \( \eta \) is the constant stepsize. This is the classical mini-batch version of the SGD. We first introduce a lemma that characterize the relation between the batch size and variance of the stochastic gradient.
Lemma 4.1. Suppose we draw a batch $B$ of $m$ data points uniformly from the entire data set $\{1, \ldots, M\}$ and estimate the gradient with the averaged sample gradients $(1/m) \sum_{i=1}^{M} \nabla f_i(x)1_{i \in B}$. The estimator is unbiased and the covariance is

$$\text{var} \left( \frac{1}{m} \sum_{i=1}^{M} \nabla f_i(x)1_{i \in B} \right) = \frac{1}{m} \left( 1 - \frac{m}{M} \right) (\bar{I}_1 - \bar{I}_2),$$

where

$$\bar{I}_1 = \frac{1}{M} \sum_{i=1}^{M} \nabla f_i(x) \nabla f_i(x)^\top, \quad \bar{I}_2 = \frac{1}{M(M-1)} \sum_{1 \leq i,j \leq M, i \neq j} \nabla f_i(x) \nabla f_j(x)^\top.$$

Proof of Lemma 4.1 is deferred to §B.3 in the Appendix. Lemma 4.1 implies that the covariance matrix of the stochastic gradient, corresponding to $S(x)^2$ in the approximating diffusion, scales as $O(1/m)$ when $m$ is large. If the data points are drawn with replacement we can obtain the same result using independence of samples.

Our goal in this section is to stand from a theoretical point of view and explain the recent deep learning theoretical works by Keskar et al. (2016), which studies the effect of batch size on the generalization performance of the learned model. The key empirical findings there are summarized as following:

(i) Large-batch method tends to converge to sharp minimizers of the training function. These minimizers are characterized by a significant number of large positive eigenvalues in $\nabla^2 f(x)$ and lead to poor generalization performances, since they are more sensitive to the weight variable $x$.

(ii) In contrast, small-batch methods are able to escape the basins of attraction of sharp minimizers and converge to flat minimizers characterized by admitting numerous small eigenvalues of $\nabla^2 f(x)$, while large-batch methods are unable to do so.

To quantify the sharpness of local minimizers, Keskar et al. (2016) introduce the $(C_\epsilon, A)$-sharpness of function $f$ at $x^*$ as

$$\phi_{x^*, f}(\epsilon, A) \equiv \frac{\max_{y \in C_\epsilon} f(x^* + Ay) - f(x^*)}{1 + f(x^*)} \times 100,$$

where $C_\epsilon$ is a cube region depending on $\epsilon$. Such metric describes the changing rate of function values in a small neighborhood of $x^*$. In the remaining, we will cast the problem into our framework and try to give more insight into this phenomenon.

4.1 Analysis

First, we claim for a general function $f(x)$, local dynamics around a minimizer can be analyzed with respect to a quadratic function. In fact, this is a result of Morse’s lemma (Milnor (2016)). The lemma says the function can be locally re-parameterized around a stationary point as

$$f(x^* + \Delta x) = f(x^*) + \frac{1}{2} \sum_{i=j}^{d} \lambda_j \Delta v_j^2,$$
where \( \lambda_j \) is the \( j \)th eigenvalues of the Hessian at \( x^* \), and \( \Delta v_j \)'s are the new parameters along eigenvectors \( u_i \) of Hessian at \( x^* \). This enables us to only consider the quadratic approximation 
\[
f(x) \approx f(x^*) + \frac{1}{2}(x - x^*)^\top H(x - x^*)
\]
of a general function \( f(x) \) to learn about the local dynamics around a minimizer \( x^* \).

We revisit the tools developed in previous sections and then discuss about its application in explaining the convergence to sharp/flat minimizers. Recall that for quadratic function with positive-definite Hessian, the dynamics of SGD \( x(t) \) around the minimizer \( x^* \) can be approximated by an OU-process \( X(t) \) defined in (2.5). In essence, Lemma 4.1 indicates that the variance of noise in the observed gradient for doing SGD is inverse proportional to the batch size. We will look at the effect of noise magnitude on the behavior near local minimizer. Without loss of generality, let us assume the local minimizer \( x^* = 0 \). Then in the neighborhood of \( x^* \), the function can be approximated by its second-order Taylor expansion
\[
f(x) \approx f(0) + \frac{1}{2} x^\top H x,
\]
where \( H \) is a positive definite matrix. Recall that
\[
X(t) = \exp (-\eta \cdot t H) x(0) + \eta \cdot \int_0^t \exp (\eta \cdot (s - t) H) \cdot S \cdot dB(s).
\]
Let \( Z(t) = H^{1/2} X(t) \). Then the function value
\[
f(X(t)) \approx f(0) + \frac{1}{2} \| Z(t) \|_2^2.
\]

To make our main points clear, we make two technical assumptions as follows:

**Assumption 4.2.** (i) the initial point \( x(0) = 0 \); (ii) \( H \) and \( S \) commute, i.e., \( HS = SH \).

We then obtain simplified \( X(t) \sim N \left( 0, (\eta/2) S^2 H^{-1} (I - e^{-2\eta t H}) \right) \), and thus
\[
Z(t) \sim N \left( 0, \frac{\eta}{2} S^2 (I - e^{-2\eta t H}) \right).
\]

For \( S \) and \( H \) to commute, it is sufficient for them to share the same set of eigenvectors. For illustration purpose here, we assume \( S = \text{diag}(\sigma_1, \ldots, \sigma_d) \) and \( H = \text{diag}(\lambda_1, \ldots, \lambda_d) \) are diagonal. Hence, the function value can be represented as a summation of independent random variables, i.e.
\[
f(X(t)) \approx f(0) + \frac{1}{2} \| Z(t) \|_2^2 = f(0) + \frac{1}{4} \sum_{j=1}^d \eta \sigma_j^2 (1 - e^{-2\eta \lambda_j}) \chi_j^2(1),
\]
where \( \{ \chi_j^2(1) \}_{j=1}^d \) is a sequence of i.i.d. \( \chi^2 \)-distributed random variables with 1 degree of freedom.

### 4.2 Insight and Interpretations

Why does this help to explain the phenomenon observed in Keskar et al. (2016)? Our argument follows two steps.
The stochastic process of function value $f(X(t))$ is \textit{almost} a deterministic process. It is known that deep neural network tends to be high dimensional in most applications. More than millions of parameters are learned simultaneously. In our context, that means $p$ is very large. Notice that the function value $f(X(t))$ is a summation of a large number of small independent random variables. The summation can thus be treated as almost deterministic, especially if there is a positive fraction of coordinates $\sum_{j=1}^{d} \sigma_j^2 (1 - \exp (-2\eta \lambda_j t))$ being bounded away from 0. In this sense, it suffices to study the expectation of the function value, i.e.
\[
\mathbb{E} f(X(t)) = f(0) + \frac{\eta}{4} \text{tr} \left( S^2 \left( I - \exp \left( -2\eta t H \right) \right) \right).
\]

The deterministic process has a natural interpretation regarding the effect of the noise magnitude on the convergence regime. We see that starting from the local minimizer, the gap between function value and the maximum level that can be achieved in the end decay exponentially, where the rate depends on the sharpness of the minimizer. The function value will converge to $\mathbb{E} f(X(\infty)) = f(0) + (\eta/4) \text{tr}(S^2)$, where $S$ depends on the batch size $m$. This implies that large batch with small $S^2$ cannot go far above the bottom of the valley, while small batch method with larger multiplier $S^2$ is more likely to escape the local minimizer.

We have also studied in previous sections that the higher noise in small batch method helps to escape from saddle points. Combined with the argument above, small batch method is more favorable in deep neural network training, which is consistent with the observations in Keskar et al. (2016).

### 5 Summary and Discussions

In this paper, we study the stochastic gradient descent method in analyzing nonconvex statistical optimization problems from a diffusion approximation point of view. Using the theory of large deviation of random dynamical system, we prove in the case of small stepsizes and the presence of omnidirectional noise the following: starting from an exact local minimizer (resp. saddle point) the SGD iteration escapes in a number of iteration that is exponentially (resp. linearly) dependent on the inverse stepsize. We take the deep neural network as an example to study this phenomenon. Based on a new analysis of the mixing rate of multidimensional Ornstein-Uhlenbeck processes, we provide theoretical support for the very recent empirical results by Keskar et al. (2016), suggesting that large batch sizes in training deep learning for synchronous optimization leads to poor generalization error.

Following the paper of Keskar et al. (2016) there has been recently an open debate in the deep learning community. For example, Dinh et al. (2017) questions the relation between sharpness of minimizers and its generalization ability using a specific deep networks with rectifier units, but does not address the convergence rates of convergence to such minimizers. We hope this theoretical work can provide useful insight for the aforementioned open debate, shedding light on the ability of stochastic gradient descent to escape from unfavorable stationary points.
References

Aldous, D. (1989). *Probability Approximations via the Poisson Clumping Heuristic*, volume 77. Springer.

Bottou, L. (2010). Large-scale machine learning with stochastic gradient descent. In *Proceedings of COMSTAT’2010* (pp. 177–186). Springer.

Bottou, L., Curtis, F. E., & Nocedal, J. (2016). Optimization methods for large-scale machine learning. *arXiv preprint arXiv:1606.04838*.

Bubeck, S. et al. (2015). Convex optimization: Algorithms and complexity. *Foundations and Trends® in Machine Learning*, 8(3-4), 231–357.

Choromanska, A., Henaff, M., Mathieu, M., Arous, G. B., & LeCun, Y. (2015). The loss surfaces of multilayer networks. In *AISTATS*.

Dauphin, Y. N., Pascanu, R., Gulcehre, C., Cho, K., Ganguli, S., & Bengio, Y. (2014). Identifying and attacking the saddle point problem in high-dimensional non-convex optimization. In *Advances in Neural Information Processing Systems* (pp. 2933–2941).

Dembo, A. & Zeitouni, O. (2010). *Large deviations techniques and applications*. Springer-Verlag, Berlin.

Devinatz, A., Ellis, R., & Friedman, A. (1974). The asymptotic behavior of the first real eigenvalue of second order elliptic operators with a small parameter in the highest derivatives. ii. *Indiana University Mathematics Journal*, 23, 991–1011.

Dinh, L., Pascanu, R., Bengio, S., & Bengio, Y. (2017). Sharp minima can generalize for deep nets. *arXiv preprint arXiv:1703.04933*.

Ethier, S. N. & Kurtz, T. G. (2005). *Markov Processes: Characterization and Convergence*, volume 282. John Wiley & Sons.

Ge, R., Huang, F., Jin, C., & Yuan, Y. (2015). Escaping from saddle points – online stochastic gradient for tensor decomposition. In *Proceedings of The 28th Conference on Learning Theory* (pp. 797–842).

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

Jin, C., Ge, R., Netrapalli, P., Kakade, S. M., & Jordan, M. I. (2017). How to escape saddle points efficiently. *arXiv preprint arXiv:1703.00887*.

Kawaguchi, K. (2016). Deep learning without poor local minima. *arXiv preprint arXiv:1605.07110*.


Keskar, N. S., Mudigere, D., Nocedal, J., Smelyanskiy, M., & Tang, P. T. P. (2016). On large-batch training for deep learning: Generalization gap and sharp minima. To appear in ICLR 2017, arXiv preprint arXiv:1609.04836.

Kifer, Y. (1981). The exit problem for small random perturbations of dynamical systems with a hyperbolic fixed point. Israel Journal of Mathematics, 40(1), 74–96.

Krichene, W., Bayen, A., & Bartlett, P. L. (2015). Accelerated mirror descent in continuous and discrete time. In Advances in Neural Information Processing Systems (pp. 2845–2853).

Lee, J. D., Simchowitz, M., Jordan, M. I., & Recht, B. (2016). Gradient descent only converges to minimizers. In Conference on Learning Theory (pp. 1246–1257).

Li, C. J., Wang, M., Liu, H., & Zhang, T. (2016a). Near-optimal stochastic approximation for online principal component estimation. arXiv preprint arXiv:1603.05305.

Li, C. J., Wang, Z., & Liu, H. (2016b). Online ICA: Understanding global dynamics of nonconvex optimization via diffusion processes. In Advances in Neural Information Processing Systems 29 (pp. 4967–4975).

Li, Q., Tai, C., & E, W. (2015). Dynamics of stochastic gradient algorithms. arXiv preprint arXiv:1511.06251.

Milnor, J. (2016). Morse Theory, volume 51. Princeton university press.

Oksendal, B. (2003). Stochastic Differential Equations. Springer.

Pemantle, R. (1990). Nonconvergence to unstable points in urn models and stochastic approximations. The Annals of Probability, (pp. 698–712).

Stroock, D. W. & Varadhan, S. S. (1979). Multidimensional Diffusion Processes, volume 233. Springer.

Su, W., Boyd, S., & Candes, E. J. (2016). A differential equation for modeling Nesterov’s accelerated gradient method: theory and insights. Journal of Machine Learning Research, 17(153), 1–43.

Wibisono, A., Wilson, A. C., & Jordan, M. I. (2016). A variational perspective on accelerated methods in optimization. Proceedings of the National Academy of Sciences, (pp. 201614734).

Wilson, A. C., Recht, B., & Jordan, M. I. (2016). A lyapunov analysis of momentum methods in optimization. arXiv preprint arXiv:1611.02635.
A Detailed Analysis for Quadratic Functions

A.1 Stable Stationarity

As we have seen in Theorem 3.2, when $\eta$ is sufficiently small it takes an exponentially number of steps in terms of $\eta^{-1}$ for the dynamics to escape from the local minimizer. As a result, the mass will be concentrated near $x = 0$ and there will be equilibrium distribution quickly. Applying again the Ito integral theory (Oksendal, 2003) we have $X(\eta t) \approx X(\infty)$ where $X(\infty)$ has the same distribution as $x^{(0)} + \eta^{0.5} \operatorname{tr}(S\eta^{-1/2})X$.

At large time $T_L = C\eta^{-1}\log \eta^{-1}$ for some constant $C > 0$ the process is close to an invariant distribution $X(\infty) = \eta \int_0^\infty \exp (-\eta \cdot tH) \cdot S \cdot dB(t)$.

In the case where $SH = HS$, $X(\infty)$ is a $N(0, (\eta/2)S^2H^{-1})$ random vector. Hence

$$E\|X(\infty)\|^2 = \eta \cdot \text{tr} (S(2H)^{-1}S) = \frac{\eta}{2} \cdot \text{tr} (S^2H^{-1}).$$

(A.1)

This means that the process tends to stationary distribution quickly and concentrated in a ball centered at $x^* = 0$ with radius of order $O(\eta^{1/2})$. This implies that escaping from the local minimizer is very hard (with exponential rare rate), for otherwise there will be no stationary distribution.

To get some intuition we turn to a simple case: when the noises generated from SGD is the unit noise, i.e., the uniform distribution on $d$-dimensional unit sphere $S^{d-1}$, in which case $S = \sigma d^{-1/2}I_d$, (A.1) has the following form

$$E\|X(T_L)\|^2 = \frac{\eta}{2} \cdot \text{tr} \left( \left( \sigma d^{-1/2}I_d \right)^2 H^{-1} \right) = \frac{\eta \sigma^2}{2d} \cdot \text{tr} (H^{-1}).$$

(A.2)

In §4 we analyze (A.2) in details via the example of deep neural network.

A.2 Unstable Stationarity

To study the dynamics near an unstable stationary point, let us first consider a simple problem that the initialization $x^{(0)}$ is at an unstable stationary point ($\gamma_1 > 0$), then the iteration $x^{(t)}$, as a stochastic process, can be approximated by $X(t)$ which is the solution to SDE (2.5), which is reminded here

$$dX(t) = -\eta HX(t) \, dt + \eta S \, dB(t)$$

(A.3)

Instead of solving (A.3), let us consider the direction specified by an eigenvector $v$ of $H$ corresponding to $-\gamma_1$, the smallest eigenvalue. Multiplying both sides by $v^\top$ in (A.3)

$$d[v^\top X(t)] = -\eta v^\top HX(t) \, dt + \eta v^\top S \, dB(t)$$

$$= \eta \gamma_1 [v^\top X(t)] \, dt + \eta v^\top S \, dB(t)$$

Let $\sigma = (v^\top S^2v)^{1/2}$ and $X(t) = v^\top X(t)$, then by linear transformation property of Brownian motion this reduces the problem to the following one-dimensional process:

$$dX(t) = \eta \gamma_1 X(t) \, dt + \eta \sigma \, dB(t)$$

(A.4)
Here $B(t)$ is a standard Brownian motion. Solving (A.4) we obtain an unstable Ornstein-Uhlenbeck process (Aldous, 1989) whose solution involves an Ito integral

$$v^T X(t) \approx X(t) = X(0) \exp(\eta \cdot \gamma_1 t) + \eta \sigma \int_0^t \exp(\eta \cdot \gamma_1 (t-s)) dB(s) \equiv V_{\eta t} \exp(\eta \cdot \gamma_1 t), \quad (A.5)$$

where

$$V_{\eta t} \equiv X(0) + \eta \sigma \int_0^t \exp(-\eta \cdot \gamma_1 s) dB(s).$$

For $t \geq C\eta^{-1} \log \eta^{-1}$ for some constant $C > 0$ we have from Ito integral theory (Oksendal, 2003) that $V_{\eta t} \approx V_\infty$ where $V_\infty$ has the same distribution as $x^{(0)} + \eta^{0.5} \left(\frac{\sigma^2}{2\gamma_1}\right)^{0.5} \chi$. For simplicity we do not distinguish identical variables and denote

$$V_\infty = x^{(0)} + \eta^{0.5} \left(\frac{\sigma^2}{2\gamma_1}\right)^{0.5} \chi, \quad (A.6)$$

where $\chi$ is a standard normal variable. Intuitively, in (A.6) one treats the iterates as a process that accumulates noises to generate a random initial start that is approximates to $V_\infty = O(\eta^{0.5})$ and, as (A.5) suggest, grows exponentially at rate $\gamma_1 \eta$.

Now using (A.5) and (A.6) we have by setting $f(X(t)) = (\gamma_1/2)|X(t)|^2 = L$ to conclude the number of iterates it takes escaping from $x^{(0)} = 0$ to $\pm (2L/\gamma_1)^{0.5} = O(1)$ is a random stopping time

$$N_L = (\gamma_1 \eta)^{-1} \log \left((2L/\gamma_1)^{0.5} |V_\infty|^{-1}\right)$$

$$= 0.5 \gamma_1^{-1} \eta^{-1} \left(\log \left(\eta^{-1}\right) + \log \left(2L\sigma^{-2}|\chi|^{-2}\right)\right),$$

which is asymptotically $0.5 \gamma_1^{-1} \eta^{-1} \log \left(\eta^{-1}\right)$ when $\eta$ is positively small.

Note in Ge et al. (2015), their Theorem 6 along with Lemma 9 implies the time complexity is $O(\eta^{-2})$. In comparison, our analysis above provides a tight estimate that, with probability $\geq 1 - C\varepsilon$

$$N_L \approx 0.5 \gamma_1^{-1} \eta^{-1} \log \left(\eta^{-1}\right). \quad (A.7)$$

In §3.2 we extend the above analysis to a broad general setting (A.7) in Theorem 3.3. This suggests that the magnitude of $0.5 \gamma_1^{-1} \eta^{-1} \log \left(\eta^{-1}\right)$ serves as a tight upper bound estimates for $N_L$, which implies a much sharper rate than Ge et al. (2015).

## B Missing Proofs

### B.1 Proof of Theorem 3.2

We now set $s = \eta t$. (As we have mentioned, the time $t$ corresponds to the iteration steps. If we understand the SGD as the discretized scheme for some SDE and $\eta$ is the time step, then $s$ is the true time for the system.) The SDE (Equation (2.3)) is now reduced to

$$dx = -\nabla f(x)ds + \sqrt{\eta}S(x)dB(s) \quad (B.1)$$
where \( B \) is a standard Brownian motion.

The hitting time for Equation (B.1), \( \tilde{T} \) then satisfies
\[
\tilde{T} \overset{d}{=} \eta T,
\]
where \( \overset{d}{=} \) means the two random variables have the same distribution. Hence, it suffices to study Equation (B.1) and \( \tilde{T} \).

**Proposition B.1.** Consider the SDE (B.1). Suppose \( S \in C^1, f \in C^2 \) and \( S(x)S(x)^\top \) is uniformly positive definite in some region containing 0. If \( x = 0 \) is a nondegenerate local minimum, then there exits a ball \( B(0, \delta) \subset U, \delta > 0 \) such that for any convex open set \( D \) inside \( B(0, \delta) \) containing \( x = 0 \), there exits \( \tilde{V}_D \in (0, \infty) \) such that the hitting time of \( \partial D \) satisfies
\[
\lim_{\eta \to 0^+} \eta \log [\mathbb{E}_x \tilde{T}] = \tilde{V}_D, \quad \forall x \in D.
\]

Further, we have uniform control of the mean exit time. In particular, there exist \( \delta_1 > 0, C_1 > 0, C_2 > 0 \) and \( \eta_0 > 0 \), so that
\[
C_1 \leq \inf_{x \in B(0, \delta_1)} \eta \log [\mathbb{E}_x \tilde{T}] \leq \sup_{x \in B(0, \delta_1)} \eta \log [\mathbb{E}_x \tilde{T}] \leq C_2.
\]
whenever \( \eta \leq \eta_0 \).

After we have shown Proposition B.1, Theorem 3.2 follows immediately since
\[
\eta \log \mathbb{E}_x \tilde{T} = \eta \log \eta + \eta \log \mathbb{E}_x T
\]

Proof of Proposition B.1. We will mainly use the Freidlin-Wentzell’s large deviation theory.

Since \( x = 0 \) is a nondegenerate local minimum, we are able to pick \( \delta > 0 \) such that \( \nabla f(x) \cdot x > \gamma |x|^2 \) for some \( \gamma > 0 \) whenever \( x \in B(0, \delta) \). Now, we fix \( D \subset B(0, \delta) \).

We first note that given any \( \sigma > 0 \) that is sufficiently small,
\[
\sup_{x \in D} \mathbb{E}_x \tilde{T} \leq T \exp((\tilde{V}_D + \sigma)/\eta)
\]
for some \( T > 0 \) when \( \eta \) is sufficiently small, by Equation (5.7.25) in Dembo & Zeitouni (2010).

We now prove the first claim. Applying (Dembo & Zeitouni, 2010, Theorem 5.7.11), we conclude that
\[
\lim_{\eta \to 0} \eta \log \mathbb{E}_x \tilde{T} = \tilde{V}_D < \infty, \quad \forall x \in D.
\]
We need to confirm that \( \tilde{V}_D > 0 \). Let \( \mu_1 \) be the principal eigenvalue of the operator
\[
\frac{\eta}{2} \sum_{ij} (S(x)S(x)^\top)_{ij} \frac{\partial^2}{\partial x_i \partial x_j} + \nabla f(x) \cdot \nabla
\]
over the domain with Dirichlet boundary condition. In Lemma B.3 below, we show
\[
\tilde{V}_D \geq \liminf_{\eta \to 0} \eta \log \left( \frac{1}{\mu_1} \right) > 0.
\]
We move onto inequality (B.4). The existence of $C_2 > 0$ follows directly from Equation (B.6). For the existence of $C_1 > 0$, we choose $\delta_1$ so that it satisfies the requirement on $\rho$ on Page 228 of Dembo & Zeitouni (2010). We apply the first inequality on Page 230 in Dembo & Zeitouni (2010),

$$P_x(\tilde{T} \leq e^{(\bar{V} - \sigma)/\eta}) \leq 4T_0^{-1}e^{-\sigma/2\eta}, \forall x \in B(0, \delta_1)$$

where we have used the fact that the first term in the inequality on Page 230 in Dembo & Zeitouni (2010) is zero since $X_0 = x \in B(0, \delta_1)$ and. As a result,

$$\mathbb{E}_x \tilde{T} \geq e^{(\bar{V} - \sigma)/\eta}(1 - P_x(\tilde{T} \leq e^{(\bar{V} - \sigma)/\eta})) > \exp\left(\frac{C_1}{\eta}\right)$$

(B.7)

uniformly for $x \in B(0, \delta_1)$.

We are left to show that $\bar{V}_D$ is strictly positive. We need to show that $\bar{V}_D$ is strictly positive. Denote

$$u(x) = \mathbb{E}_x \tilde{T}.$$ 

(B.8)

By Dembo & Zeitouni (2010, Corollary 5.7.4), $u(x)$ satisfies the following elliptic PDE with Dirichlet boundary condition

$$\begin{cases}
Lu = -1, & x \in D, \\
u = 0, & x \in \partial D
\end{cases}$$

(B.9)

where $L$ is the generator of the diffusion process given by

$$L = \frac{\eta}{2} \sum_{ij} \left(S(x)S(x)\right)_{ij} \frac{\partial^2}{\partial x_i \partial x_j} - \nabla f(x) \cdot \nabla$$

(B.10)

The following lemma is useful to us:

**Lemma B.2.** If there exist a function $\psi \in C^2(U) \cap C(\bar{U})$ with $\psi \geq 0$, $\|\psi\|_\infty > 0$, $\psi = 0$, $x \in \partial U$ for some $U \subset D$ and a positive number $\mu > 0$ such that $-L\psi \leq \mu \psi$, $x \in U$, then

$$u(x) \geq \frac{\psi}{\mu \|\psi\|_\infty}, \quad x \in U.$$ 

In particular, suppose $\mu_1$ is the principal eigenvalue of $-L$, then

$$\|u\|_\infty \geq \frac{1}{\mu_1}.$$ 

**Proof.** Consider

$$v = u - \frac{\psi}{\mu \|\psi\|_\infty}.$$ 

Then, $v \geq 0$, $x \in \partial U$. Also,

$$-Lv = 1 + \frac{L\psi}{\mu \|\psi\|_\infty} \geq 1 - \frac{\psi}{\|\psi\|_\infty} \geq 0.$$ 

Then, $v \geq 0$ for $x \in U$ by maximum principle.

Picking $\mu = \mu_1$ and $\psi$ to be the principal eigenfunction, we obtain the second claim. \qed
We now show the claim we want:

**Lemma B.3.** \( \bar{V}_D \geq \lim_{\eta \to 0} \eta \log(1/\mu_1) > 0. \)

**Proof.** By (Devinatz et al., 1974, Theorem 4.4),

\[
\lim_{\eta \to 0^+} \eta \log(1/\mu_1) > 0.
\]

Then, by Equation (B.6), Lemma B.2, we have

\[
\bar{V}_D + \sigma \geq \lim_{\eta \to 0} \eta \sup_{x \in D} \log \mathbb{E}_x \tilde{T} \geq \lim_{\eta \to 0} \eta \log \left( \frac{1}{\mu_1} \right) > 0.
\]

(B.11)

Since \( \sigma \) can be arbitrarily small, the claim follows. \( \square \)

**Remark B.4.** We now give the expression for the quasi-potential \( \bar{V}_D \). Introduce the set of functions (Dembo & Zeitouni, 2010, Chap. 5)

\[
V_s(z) = \left\{ u \in L^2(0, s) : \exists \phi \in C[0, s], \phi(s) = z, \forall 0 \leq \tau \leq s, \phi(\tau) = \int_0^\tau (-\nabla f(\phi(\xi)))d\xi + \int_0^\tau S(\phi(\xi))u(\xi)d\xi \right\},
\]

where \( L^2(0, s) \) means square integrable functions on the interval \([0, s]\). Then, the quasi-potential is given by

\[
\bar{V}_D = \inf_{z \in \partial D} \inf_{s > 0} \inf_{u \in V_s(z)} \frac{1}{2} \int_0^s |u(\tau)|^2d\tau.
\]

This quasi-potential clearly depends on how one choose \( S \) (for example, one may multiply a constant on \( S \) and redefine \( \eta \)). However, Equation B.3 is always true.

**B.2 Proofs of Theorem 3.3**

Since \( D \) is bounded, we can modify the values of \( S \) and \( f \) outside \( D \) so that they and their derivatives are bounded in the whole space, which clearly does not change the hitting time.

For Theorem 3.3, we again study the equivalent SDE (B.1) and stopping time \( \tilde{T} \).

\[
\eta \mathbb{E}_x \tilde{T} = \mathbb{E}_x \tilde{T}.
\]

(B.12)

Recall that \( x = 0 \) is a nondegenerate saddle point or a nondegenerate local maximum point. Consider the dynamics system given by

\[
\frac{d}{ds} x(s) = -\nabla f(x(s)), \ x(0) = x
\]

Let

\[
\mathcal{W}^S = \{ x \in D : \lim_{s \to \infty} x(s) = 0, x(0) = x \neq 0 \},
\]

(B.13)
which is called the stable manifold of the dynamics system and define
\[ \theta(x) = \inf\{s > 0 : x(s) \in \partial D\}. \tag{B.14} \]

In (Kifer, 1981, Theorem 2.2), the following asymptotics for the mean exit time were proved, which applies to local maximum point as well:

**Proposition B.5.** If \( x \in \mathcal{W}^S \cup \{0\} \), then
\[
\lim_{\eta \to 0} \frac{1}{\eta} \log \eta \mathbb{E}_x \bar{T} = \frac{1}{2\gamma_1}.
\]
If \( x \in D \setminus (\mathcal{W}^S \cup \{0\}) \), then
\[
\lim_{\eta \to 0} \mathbb{E}_x \bar{T} = \theta(x).
\]

Switching back to \( t \) and \( T \), we obtain what we want.

**Remark B.6.** The escaping time (3.3) from the unstable critical point can be understood intuitively as following: in the ball \( B(0, \eta^{0.5}) \), the Brownian motion dominates and the time that the process arrives at the boundary is \( s = \mathcal{O}(1) \). From \( \partial B(0, \eta^{0.5}) \) to \( \partial B(0, 1) \), the convection term dominates and it is essentially \( X' = \gamma_1 X \) and hence time spent for the second stage is \( s \sim \log(\eta^{-1}) \).

**B.3 Proof of Lemma 4.1**

**Proof.** First we compute
\[
\text{var}(1_{i \in B}) = \mathbb{E}(1_{i \in B})^2 - (\mathbb{E}1_{i \in B})^2 = \mathbb{P}(i \in B) - \mathbb{P}(i \in B)^2 = \frac{m}{M} - \frac{m^2}{M^2},
\]
and similarly
\[
\text{cov}(1_{i \in B}, 1_{j \in B}) = \mathbb{P}(i \in B, j \in B) - \mathbb{P}(i \in B)\mathbb{P}(j \in B) = \frac{m(m - 1)}{M(M - 1)} - \frac{m^2}{M^2} = -\frac{m(M - m)}{M^2(M - 1)}.
\]
Using these results, we have

\[
\text{var} \left( \frac{1}{m} \sum_{i=1}^{M} \nabla f_i(x) 1_{i \in B} \right) = \frac{1}{m^2} \text{var} \left( \sum_{i=1}^{M} \nabla f_i(x) 1_{i \in B} \right) \\
= \frac{1}{m^2} \sum_{i=1}^{M} \text{var} \left( \nabla f_i(x) 1_{i \in B} \right) \\
+ \frac{1}{m^2} \sum_{1 \leq i,j \leq M, i \neq j} \text{cov} \left( \nabla f_i(x) 1_{i \in B}, \nabla f_j(x) 1_{j \in B} \right) \\
= \frac{1}{m^2} \sum_{i=1}^{M} \nabla f_i(x) \nabla f_i(x)^\top \text{var} \left( 1_{i \in B} \right) \\
+ \frac{1}{m^2} \sum_{1 \leq i,j \leq M, i \neq j} \nabla f_i(x) \nabla f_j(x)^\top \text{cov} \left( 1_{i \in B}, 1_{j \in B} \right) \\
= \frac{1}{m^2} \sum_{i=1}^{M} \nabla f_i(x) \nabla f_i(x)^\top \left( \frac{m}{M} - \frac{m^2}{M^2} \right) \\
+ \frac{1}{m^2} \sum_{1 \leq i,j \leq M, i \neq j} \nabla f_i(x) \nabla f_j(x)^\top \left( -\frac{m(M-m)}{M^2(M-1)} \right) \\
= \frac{1}{m} \left( 1 - \frac{m}{M} \right) (\bar{I}_1 - \bar{I}_2),
\]

where

\[
\bar{I}_1 = \frac{1}{M} \sum_{i=1}^{M} \nabla f_i(x) \nabla f_i(x)^\top, \quad \bar{I}_2 = \frac{1}{M(M-1)} \sum_{1 \leq i,j \leq M, i \neq j} \nabla f_i(x) \nabla f_j(x)^\top.
\]

This completes our proof. \(\square\)